Supporting Information

Rh-Catalyzed Alkoxycarbonylation of Unactivated Alkyl Chlorides

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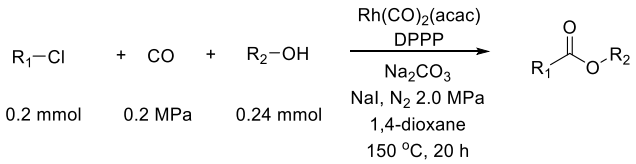
Table of Contents

Supplement to the experiments

1.1 Reagents and analysis

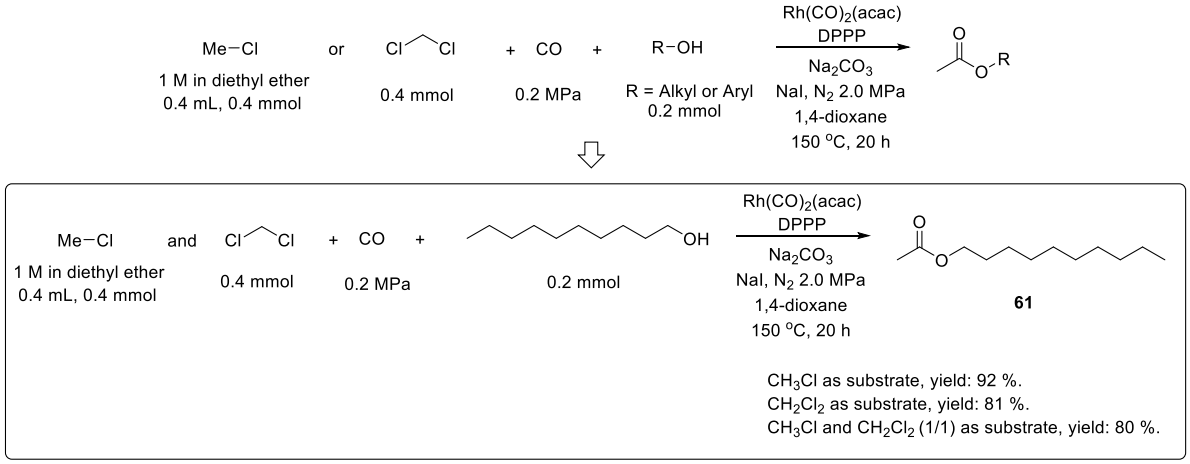
The chemical reagents were purchased from ABCR Chemicals, TCI Chemicals, FlouroChem, Merck Chemicals and were used as received. The ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker 300 spectrometer. Chemical shifts δ (ppm) are given relative to solvent: references for $CDCl_3$ are 7.26 ppm (^{1}H NMR) and 77.16 ppm (^{13}C NMR), references for *d*-DMSO are 2.50 ppm (^{1}H NMR) and 39.50 ppm (^{13}C NMR). references for CD_3OH are 3.31 ppm (^{1}H NMR) and 49.00 ppm (^{13}C NMR). Multiplets are assigned as s (singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublet), m (multiplet). Conversion and selectivity are determined by Agilent 6890N Gas chromatography (GC) and Agilent 5973 Network GC-MS, using splitless injection and FID detector (column: HP-5 (30 m × 320 μm × 0.25 μm); inlet temperature: 250 ºC; starting oven temperature: 50 ºC; rate: 8 ºC/min; final temperature: 260 ºC, carrier gas: N_2 25 mL/min).

1.2 General procedures for alkoxycarbonylation of alkyl chlorides



In a typical experiment, 2-chloroethyl)benzene or other unactivated alkyl chlorides (0.2 mmol), $Rh(acac)(CO)_2$ (0.01 mmol), phosphine ligand (0.06 mmol in case of monophosphine ligand or 0.03 mmol in case of bisphosphine ligand), NaI (0.20 mmol), the respective alcohol or phenol (0.2 mmol) and Na_2CO_3 (0.24 mmol) were dissolved sequentially in 1,4-dioxane (0.5 mL) in a 50 mL stainless steel autoclave. The obtained mixture was purged with CO (0.2 MPa) for three times and pressured to 0.2 MPa; then, N_2 was flushed into the reactor (2.0 MPa). In order to prevent the solvent from being ejected from the reaction system, 2.0 MPa N_2 is needed. The reaction mixture was stirred at the appointed temperature for 20 h. Upon completion, the autoclave was cooled down to room temperature and depressurized carefully. The reaction solution was analyzed by GC and GC-MS to determine the conversion and the chemical selectivity (*n*-dodecane (C12) as internal standard). The purified product was obtained after column chromatography and ^{1}H NMR and ^{13}C NMR spectroscopy were used to identify the structure of the products.

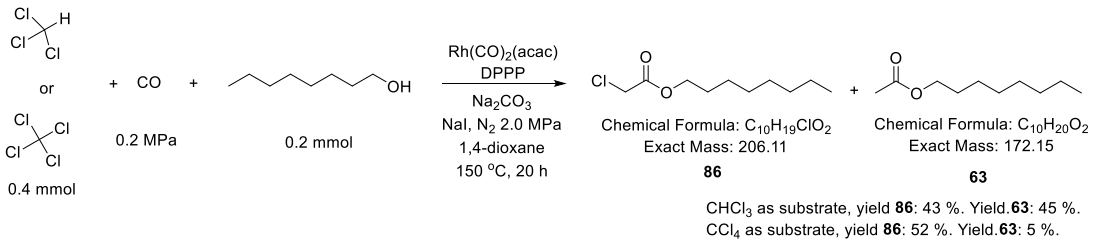
1.3 General procedure for alkoxycarbonylation of chloromethane and dichloromethane



In a typical experiment chloromethane or dichloromethane (0.4 mmol), $Rh(acac)(CO)_2$ (0.01 mmol), DPPP (0.03 mmol), NaI (0.20 mmol), the respective alcohol or phenol (0.2 mmol) and Na_2CO_3 (0.24 mmol) were dissolved sequentially in 1,4-dioxane (0.5 mL) in a 50 mL stainless steel autoclave. The obtained mixture was purged with CO (0.2 MPa) for three times and pressured to 0.2 MPa; then, N_2 was flushed into the reactor (2.0 MPa). In order to prevent the solvent from being ejected from the reaction system, 2.0 MPa N_2 is needed. The reaction mixture was stirred at 150 °C for 20 h. Upon completion of the reaction, the autoclave was cooled down to room temperature and depressurized carefully. The reaction solution was analyzed by GC and GC-MS to determine the conversion and the chemical selectivity (*n*-dodecane as internal standard). The product yield was determined after column chromatography and ^1H NMR and ^{13}C NMR spectroscopy were used to identify the structure of the products. Because CH_3Cl and CH_2Cl_2 are highly volatile and have low boiling points, an excess amount of them is needed and the yield is based on the respective alcohol or phenol.

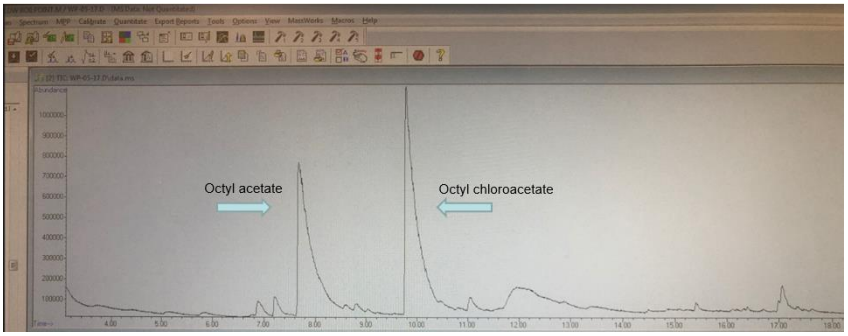
For the mixture of chloromethane and dichloromethane, the experimental procedure is as follows: chloromethane and dichloromethane (1/1 ratio, 0.4 mmol in total), $Rh(acac)(CO)_2$ (0.01 mmol), DPPP (0.03 mmol), NaI (0.20 mmol), 1-decanol (0.2 mmol) and Na_2CO_3 (0.24 mmol) were dissolved in 1,4-dioxane (0.5 mL) in a 50 mL stainless steel autoclave. The obtained mixture was purged with CO (0.2 MPa) for three times and pressured to 0.2 MPa. Then, N_2 was flushed into the reactor (2.0 MPa). The reaction mixture was stirred at 150 °C for 20 h. Upon completion, the autoclave was cooled down to room temperature and depressurized carefully. The products were separated by column chromatography and ^1H NMR and ^{13}C NMR were used to identify the structure of **61** (see below).

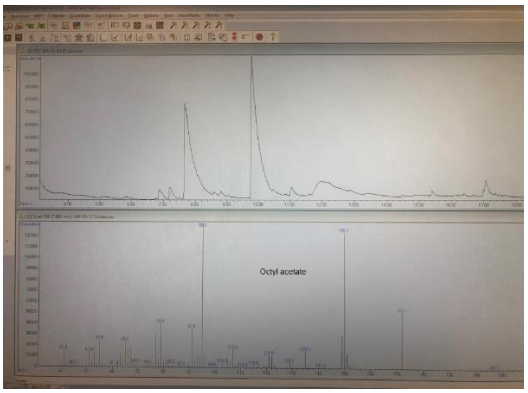
1.4 General procedure for alkoxycarbonylation of chloroform and tetrachloromethane

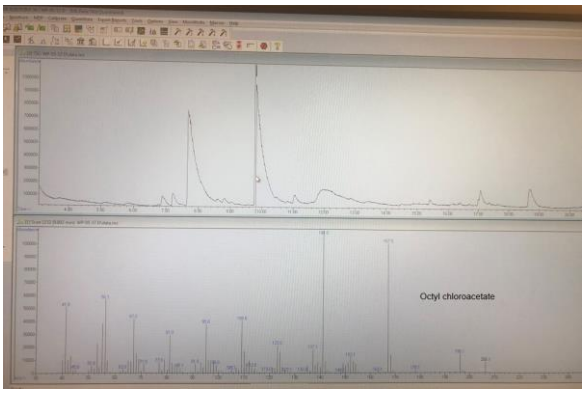


In a typical experiment, chloroform or tetrachloromethane (0.4 mmol), $Rh(acac)(CO)_2$ (0.01 mmol), DPPP (0.03 mmol), NaI (0.20 mmol), 1-octanol (0.2 mmol) and Na_2CO_3 (0.24 mmol) were dissolved sequentially in 1,4-dioxane (0.5 mL) in a 50 mL stainless steel autoclave. The obtained mixture was purged with CO (0.2 MPa) for three times and pressured to 0.2 MPa; then, N_2 was flushed into the reactor (2.0 MPa). In order to prevent the solvent from being ejected from the reaction system, 2.0 MPa N_2 is needed. The reaction mixture was stirred at 150 °C for 20 h. Upon completion of the reaction, the autoclave was cooled down to room temperature and depressurized carefully. The crude reaction solution was analyzed by GC and GC-MS (for **63** see below). Apart from other products octyl acetate and octyl chloroacetate were detected (*n*-dodecane as internal standard).

GC-MS spectra of the crude reaction mixture of the alkoxycarbonylation of chloroform:

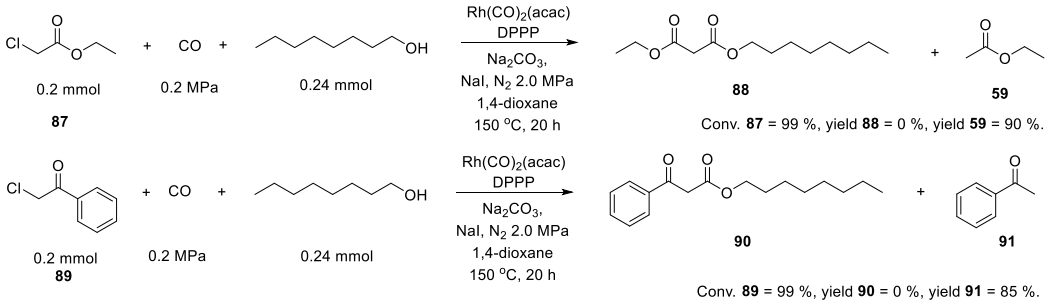






Agilent 5973 Network GC-MS, using splitless injection and FID detector (column: HP-5 (30 m × 250 μm × 0.25 μm); inlet temperature: 250 ºC; starting oven temperature: 50 ºC; rate: 10 ºC/min; final temperature: 300 ºC, carrier gas: He 1.2 mL/min).

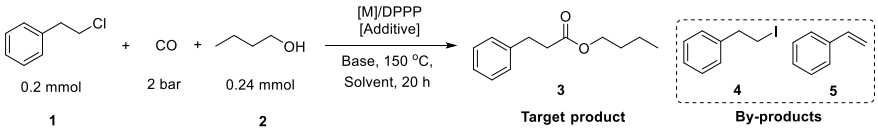
Control experiments:



1.5 Supplement to Alkoxycarbonylation of Alkyl Chlorides

All metal precursors, additives and solvents which were used are commercially available.

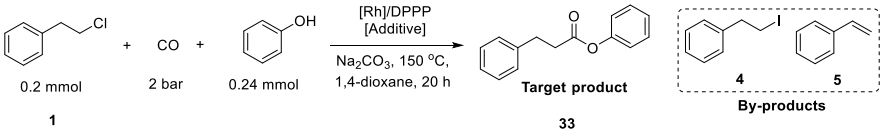
Table S1. Alkoxycarbonylation of (2-chloroethyl)benzene with different metal precursors, additives, bases and solvents [a]



Entry	Rh-precursor	Base (1.2 e.q.)	Additive (1.0 e.q.)	Solvent (0.5 mL)	Conv. (%) [b]	Sel.$_3$ (%) [b]
1	$Rh(acac)(CO)_2$	Na_2CO_3	NaI	1,4-dioxane	99	91
2	$[Rh(cod)Cl]_2$	Na_2CO_3	NaI	1,4-dioxane	99	80
3	$Pd(OAc)_2$	Na_2CO_3	NaI	1,4-dioxane	99	6
4	$Ru_3(CO)_{12}$	Na_2CO_3	NaI	1,4-dioxane	99	12
5	$Pd_2(dba)_3$	Na_2CO_3	NaI	1,4-dioxane	99	3
6	$Rh(acac)(CO)_2$	Na_2CO_3	NaCl	1,4-dioxane	99	0
7	$Rh(acac)(CO)_2$	Na_2CO_3	NaBr	1,4-dioxane	99	3
8	$Rh(acac)(CO)_2$	Na_2CO_3	KI	1,4-dioxane	99	62
9	$Rh(acac)(CO)_2$	Na_2CO_3	*n*-Bu_4NBr	1,4-dioxane	99	2
10	$Rh(acac)(CO)_2$	Na_2CO_3	*n*-Bu_4NCl	1,4-dioxane	99	0
11	$Rh(acac)(CO)_2$	Na_2CO_3	KOAc	1,4-dioxane	99	0
12	$Rh(acac)(CO)_2$	K_2CO_3	NaI	1,4-dioxane	99	73
13	$Rh(acac)(CO)_2$	*t*BuOK	NaI	1,4-dioxane	99	6
14	$Rh(acac)(CO)_2$	Et_3N	NaI	1,4-dioxane	99	16
15	$Rh(acac)(CO)_2$	Bu_3N	NaI	1,4-dioxane	99	14
16	$Rh(acac)(CO)_2$	TBEA	NaI	1,4-dioxane	99	5
17	$Rh(acac)(CO)_2$	TMEDA	NaI	1,4-dioxane	99	0
18	$Rh(acac)(CO)_2$	Na_2CO_3	NaI	Cyclohexane	99	24
19	$Rh(acac)(CO)_2$	Na_2CO_3	NaI	THF	99	65
20	$Rh(acac)(CO)_2$	Na_2CO_3	NaI	Toluene	72	11
21	$Rh(acac)(CO)_2$	Na_2CO_3	NaI	DMSO	99	0
22	$Rh(acac)(CO)_2$	Na_2CO_3	NaI	DMF	97	0
23	$Rh(acac)(CO)_2$	Na_2CO_3	NaI	DMAc	99	0
24	$Rh(acac)(CO)_2$	Na_2CO_3	NaI	CH_3CN	99	47

[a] (2-Chloroethyl)benzene (0.2 mmol), *n*-butanol 0.24 mmol (1.2 e.q.), [M] 5 mol%, S/Rh mol ratio = 20, DPPP 15 mol%, [Rh]/P-ligand molar ratio = 1/6, Base 0.24 mmol (1.2 e.q.), additive 0.20 mmol (1.0 e.q.), CO = 2 bar, N_2 20 bar; 150 °C, Solvent 0.5 mL, time 20 h. [b] Determined by GC and GC-MS, dodecane (C_{12}) as internal standard.

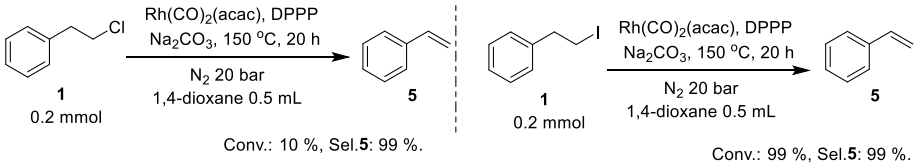
Table S2. Alkoxycarbonylation of (2-chloroethyl)benzene with phenol using different metal precursors and additives [a]



Entry	Rh-precursor	Base (1.0 e.q.)	Additive (1.0 e.q.)	Solvent (0.5 mL)	Conv. (%) [b]	Sel.$_{33}$ (%) [b]
1 [c]	$Rh(acac)(CO)_2$	Na_2CO_3	NaI	1,4-dioxane	99	94
2	$[Rh(cod)Cl]_2$	Na_2CO_3	NaI	1,4-dioxane	99	91
3	$Pd(OAc)_2$	Na_2CO_3	NaI	1,4-dioxane	99	13
4	$Ru_3(CO)_{12}$	Na_2CO_3	NaI	1,4-dioxane	99	15
5	$Pd_2(dba)_3$	Na_2CO_3	NaI	1,4-dioxane	99	4
11 [d]	$Rh(acac)(CO)_2$	Na_2CO_3	NaI	1,4-dioxane	99	75
12 [e]	$Rh(acac)(CO)_2$	Na_2CO_3	NaI	1,4-dioxane	99	29
13	$Rh(acac)(CO)_2$	Na_2CO_3	NaCl	1,4-dioxane	99	0
14	$Rh(acac)(CO)_2$	Na_2CO_3	NaBr	1,4-dioxane	99	14
15	$Rh(acac)(CO)_2$	Na_2CO_3	TBAB	1,4-dioxane	99	0
16	$Rh(acac)(CO)_2$	Na_2CO_3	TBACl	1,4-dioxane	99	0
17	$Rh(acac)(CO)_2$	Na_2CO_3	KOAc	1,4-dioxane	99	0

[a] (2-Chloroethyl)benzene (0.2 mmol), phenol 0.24 mmol (1.2 e.q.), [Rh] 5 mol%, S/Rh mol ratio = 20, DPPP 15 mol%, [Rh]/P-ligand molar ratio = 1/6, Na_2CO_3 0.24 mmol (1.2 e.q.), additive 0.20 mmol (1.0 e.q.), CO = 2 bar, N_2 20 bar; 150 °C, 1,4-dioxane 0.5 mL, time 20 h. [b] Determined by GC and GC-MS, dodecane (C_{12}) as internal standard. [c] Isolated yield is 87 % for entry 1. [d] [Rh] 2.5 % mmol, S/Rh mol ratio = 40, P-ligand 7.5 mol%, [Rh]/P-ligand molar ratio = 1/6. [e] [Rh] 1 mol%, S/Rh mol ratio = 100, P-ligand 3 mol%, [Rh]/P-ligand molar ratio = 1/6.

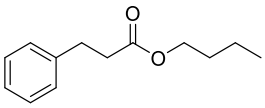
Scheme S1. *β*-Elimination of HX (X = Cl, I) from (2-chloroethyl)benzene and 1-iodo-2-phenylethane.



NMR data of the main products

Column chromatography for product separation were performed according to references [1-9].

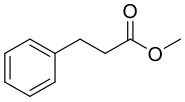
Butyl 3-phenylpropanoate (**3**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36-7.17 (m, 5H), 4.10 (t, *J* = 6.7 Hz, 2H), 3.02-2.92 (m, 2H), 2.71-2.60 (m, 2H), 1.64-1.55 (m, 2H), 1.44-1.31 (m, 2H), 0.94 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 173.04, 140.59, 128.48, 128.29, 126.23, 64.36, 35.95, 31.02, 30.67, 19.11, 13.70.

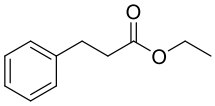
Methyl 3-phenylpropanoate (**6**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40-7.19 (m, 5H), 3.71 (s, 3H), 3.01 (t, *J* = 7.8 Hz, 2H), 2.74-2.63 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 173.34, 140.56, 128.55, 128.32, 126.31, 51.62, 35.73, 30.98.

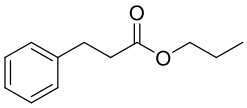
Ethyl 3-phenylpropanoate (**7**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39-7.20 (m, 5H), 4.17 (q, *J* = 7.1 Hz, 2H), 3.00 (t, *J* = 7.8 Hz, 2H), 2.73-2.62 (m, 2H), 1.28 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.91, 140.63, 128.51, 128.34, 126.27, 60.42, 35.98, 31.02, 14.24.

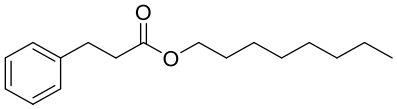
Propyl 3-phenylpropanoate (**8**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.22-7.08 (m, 5H), 3.96 (t, *J* = 6.7 Hz, 2H), 2.89 (t, *J* = 7.8 Hz, 2H), 2.60-2.51 (m, 2H), 1.63-1.47 (m, 4H), 0.84 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 173.05, 140.59, 128.49, 128.30, 126.24, 66.10, 35.95, 31.02, 21.97, 10.37.

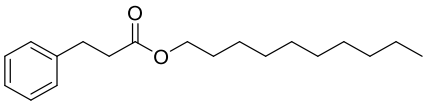
Octyl 3-phenylpropanoate (**9**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.26-7.08 (m, 5H), 3.99 (t, *J* = 6.7 Hz, 2H), 2.88 (dd, *J* = 8.5, 7.1 Hz, 2H), 2.61-2.49 (m, 2H), 1.56-1.49 (m, 2H), 1.26-1.10 (m, 10H), 0.87-0.77 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 173.05, 140.60, 128.49, 128.30, 126.24, 64.69, 35.96, 31.79, 31.02, 29.22, 29.19, 28.62, 25.91, 22.66, 14.11.

Decyl 3-phenylpropanoate (**10**)

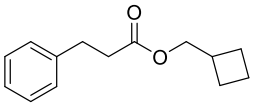


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38-7.16 (m, 5H), 4.09 (t, *J* = 6.7 Hz, 2H), 2.98 (t, *J* = 7.8 Hz, 2H), 2.71-2.60 (m, 2H), 1.66-1.57 (m, 2H), 1.31 (d, *J* = 6.5 Hz, 14H), 0.96-0.86 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 173.04, 140.60, 128.49, 128.30, 126.24, 64.68, 35.96, 31.91, 31.03, 29.55, 29.53, 29.33, 29.27, 28.63, 25.92, 22.70,

14.14.

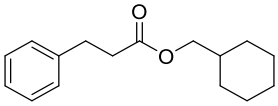
Cyclobutylmethyl 3-phenylpropanoate (**11**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36–7.19 (m, 5H), 4.07 (d, *J* = 6.8 Hz, 2H), 3.03–2.95 (m, 2H), 2.73–2.55 (m, 3H), 2.06–1.66 (m, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 173.13, 140.59, 128.48, 128.29, 126.24, 68.32, 35.91, 34.07, 31.04, 24.73, 18.40.

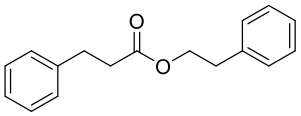
Cyclohexylmethyl 3-phenylpropanoate (**12**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.26-7.06 (m, 5H), 3.81 (d, *J* = 6.5 Hz, 2H), 2.88 (t, *J* = 7.8 Hz, 2H), 2.60-2.52 (m, 2H), 1.74-1.42 (m, 7H), 1.19-1.09 (m, 2H), 0.93-0.77 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 173.07, 140.58, 128.49, 128.30, 126.23, 69.67, 37.08, 35.95, 31.06, 29.64, 26.36, 25.68.

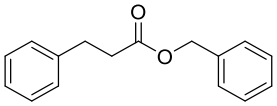
Phenethyl 3-phenylpropanoate (**13**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28-7.06 (m, 10H), 4.22 (t, *J* = 7.0 Hz, 2H), 2.91-2.79 (m, 4H), 2.58-2.49 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.85, 140.50, 137.82, 128.92, 128.51, 128.30, 126.57, 126.27, 64.96, 35.91, 35.10, 30.93.

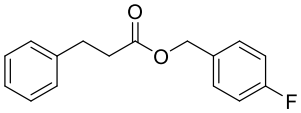
Benzyl 3-phenylpropanoate (**14**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41–7.22 (m, 10H), 5.16 (s, 2H), 3.06–2.97 (m, 2H), 2.77–2.66 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.76, 140.42, 135.92, 128.57, 128.52, 128.32, 128.29, 128.23, 126.29, 66.31, 35.92, 30.96.

4-Fluorobenzyl 3-phenylpropanoate (**15**)

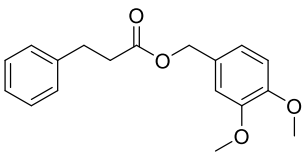


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34–7.28 (m, 4H), 7.24–7.20 (m, 3H), 7.06 (t, *J* = 8.7 Hz, 2H), 5.10 (d, *J* = 0.7 Hz, 2H), 3.00 (t, *J* = 7.7 Hz, 2H), 2.76–2.67 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.68, 140.33, 130.28, 130.17, 128.92, 128.53, 128.51, 128.31, 126.31, 115.61, 115.33, 65.56, 35.87, 30.94.

^{19}F NMR (282 MHz, CDCl3) δ -113.72.

3,4-Dimethoxybenzyl 3-phenylpropanoate (**16**)

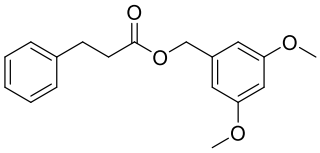


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31–7.18 (m, 5H), 6.95–6.83 (m, 3H), 5.07 (d, *J* = 0.6 Hz, 2H), 3.90 (d, *J* = 4.3 Hz, 6H), 2.99 (dd, *J* = 8.3, 7.2 Hz, 2H), 2.75–2.65 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.81, 149.12, 148.98, 140.44, 128.49, 128.44, 128.31, 126.27, 121.32, 111.81, 111.00, 66.43, 55.94, 55.89, 35.94,

30.95.

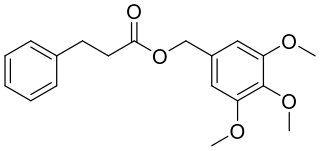
3,5-Dimethoxybenzyl 3-phenylpropanoate (**17**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34–7.18 (m, 5H), 6.51–6.41 (m, 3H), 5.07 (d, *J* = 0.6 Hz, 2H), 3.81 (s, 6H), 3.01 (dd, *J* = 8.5, 7.1 Hz, 2H), 2.76–2.68 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.68, 160.93, 140.42, 138.15, 128.52, 128.31, 126.30, 105.98, 100.17, 66.23, 55.38, 35.90, 30.94.

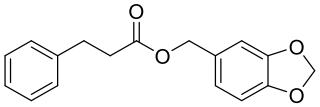
3,4,5-Trimethoxybenzyl 3-phenylpropanoate (**18**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.24-7.09 (m, 5H), 6.47 (s, 2H), 4.96 (s, 2H), 3.77 (d, *J* = 1.2 Hz, 9H), 2.91 (t, *J* = 7.7 Hz, 2H), 2.66-2.57 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.74, 153.31, 140.38, 137.95, 131.47, 128.51, 128.31, 126.31, 105.54, 66.59, 60.85, 56.14, 35.89, 30.93.

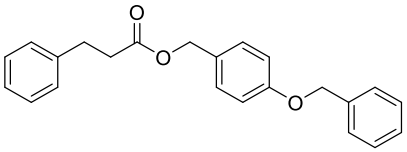
Benzo[d][1,3]dioxol-5-ylmethyl 3-phenylpropanoate (**19**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35-7.16 (m, 5H), 6.85-6.77 (m, 3H), 5.99 (s, 2H), 5.03 (s, 2H), 2.99 (dd, *J* = 8.5, 7.1 Hz, 2H), 2.73-2.64 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.75, 147.79, 147.63, 140.40, 129.68, 128.52, 128.31, 126.29, 122.30, 109.06, 108.24, 101.17, 66.29, 35.93, 30.95.

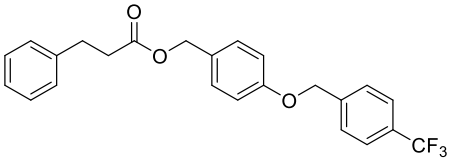
4-(Benzyloxy)benzyl 3-phenylpropanoate (**20**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51–7.16 (m, 13H), 7.04–6.94 (m, 2H), 5.09 (d, *J* = 8.0 Hz, 4H), 2.99 (t, *J* = 7.8 Hz, 2H), 2.75–2.63 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.82, 158.83, 140.47, 136.87, 130.10, 128.64, 128.51, 128.36, 128.32, 128.04, 127.46, 126.26, 114.89, 70.05, 66.10, 35.96, 30.97.

4-((4-(Trifluoromethyl)benzyl)oxy)benzyl 3-phenylpropanoate (**21**)

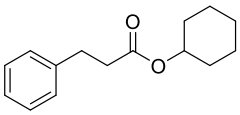


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.68 (dq, *J* = 8.0, 1.0 Hz, 2H), 7.58 (ddt, *J* = 8.1, 1.5, 0.7 Hz, 2H), 7.33–7.19 (m, 7H), 7.02–6.92 (m, 2H), 5.16 (d, *J* = 1.1 Hz, 2H), 5.08 (s, 2H), 2.99 (t, *J* = 7.8 Hz, 2H), 2.73–2.63 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.80, 158.40, 140.96, 140.44, 131.14, 130.41, 130.16, 129.98, 129.50, 128.80, 128.51, 128.32, 127.36, 126.27, 125.67, 125.62, 125.57, 125.52, 122.28, 114.84, 69.15, 65.99, 35.94, 30.96.

^{19}F NMR (282 MHz, $CDCl_3$) δ -62.56.

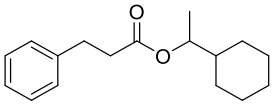
Cyclohexyl 3-phenylpropanoate (**22**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.25-7.08 (m, 5H), 4.68 (dq, *J* = 9.0, 4.3 Hz, 1H), 2.88 (t, *J* = 7.8 Hz, 2H), 2.60-2.49 (m, 2H), 1.79-1.44 (m, 6H), 1.31-1.18 (m, 4H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.42, 140.65, 128.44, 128.33, 126.19, 72.69, 36.29, 31.62, 31.10, 25.39, 23.75.

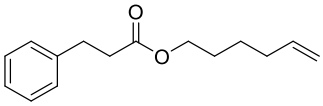
1-Cyclohexylethyl 3-phenylpropanoate (**23**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31-7.20 (m, 5H), 4.75 (p, *J* = 6.4 Hz, 1H), 2.98 (t, *J* = 7.8 Hz, 2H), 2.70-2.59 (m, 2H), 1.73-1.59 (m, 5H), 1.47-1.21 (m, 4H), 1.15 (d, *J* = 6.4 Hz, 3H), 1.01-0.87 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.62, 140.61, 128.44, 128.32, 126.19, 74.71, 42.52, 36.22, 31.11, 28.48, 28.42, 26.38, 26.05, 26.00, 17.06.

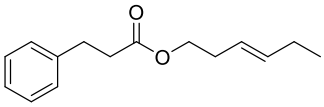
Hex-5-en-1-yl 3-phenylpropanoate (**24**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34–7.19 (m, 5H), 5.81 (ddt, *J* = 16.9, 10.2, 6.7 Hz, 1H), 5.09–4.93 (m, 2H), 4.10 (t, *J* = 6.6 Hz, 2H), 2.98 (t, *J* = 7.8 Hz, 2H), 2.69–2.61 (m, 2H), 2.14–2.03 (m, 2H), 1.66–1.58 (m, 2H), 1.50–1.39 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 173.01, 140.56, 138.36, 128.49, 128.30, 126.25, 114.83, 64.42, 35.93, 33.28, 31.01, 28.05, 25.17.

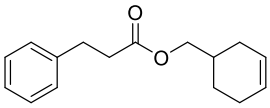
(E)-Hex-3-en-1-yl 3-phenylpropanoate (**25**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34–7.19 (m, 5H), 5.62–5.50 (m, 1H), 5.43–5.30 (m, 1H), 4.10 (t, *J* = 6.9 Hz, 2H), 2.98 (dd, *J* = 8.5, 7.1 Hz, 2H), 2.69–2.60 (m, 2H), 2.32 (dddd, *J* = 8.0, 6.8, 5.7, 1.2 Hz, 2H), 2.03 (dddd, *J* = 8.6, 7.4, 6.2, 5.0 Hz, 2H), 0.99 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.91, 140.59, 135.09, 128.49, 128.30, 126.25, 124.04, 64.16, 35.94, 31.94, 31.00, 25.63, 13.75.

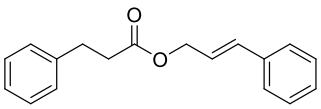
Cyclohex-3-en-1-ylmethyl 3-phenylpropanoate (**26**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34–7.17 (m, 5H), 5.75–5.61 (m, 2H), 4.00 (d, *J* = 6.6 Hz, 2H), 2.99 (t, *J* = 7.8 Hz, 2H), 2.71–2.63 (m, 2H), 2.11–2.04 (m, 3H), 1.99–1.88 (m, 1H), 1.79–1.65 (m, 2H), 1.40–1.17 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 173.05, 140.53, 128.50, 128.29, 127.04, 126.26, 125.51, 68.78, 35.93, 33.01, 31.05, 28.13, 25.26, 24.41.

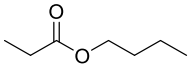
Cinnamyl 3-phenylpropanoate (**27**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41–7.23 (m, 10H), 6.66 (d, *J* = 15.9 Hz, 1H), 6.29 (dt, *J* = 15.9, 6.4 Hz, 1H), 4.77 (dd, *J* = 6.4, 1.3 Hz, 2H), 3.06–2.98 (m, 2H), 2.75–2.68 (m, 2H).

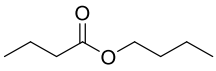
^{13}C NMR (75 MHz, $CDCl_3$) δ 172.69, 140.48, 136.23, 134.23, 128.63, 128.54, 128.35, 128.10, 126.65, 126.31, 123.19, 65.09, 35.94, 31.00.

Butyl propionate (**28**)



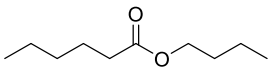
^{1}H NMR (300 MHz, $CDCl_3$) δ 4.04 (t, *J* = 6.7 Hz, 2H), 2.28 (q, *J* = 7.6 Hz, 2H), 1.64–1.52 (m, 2H), 1.42–1.28 (m, 2H), 1.10 (t, *J* = 7.6 Hz, 3H), 0.94–0.85 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.46, 64.07, 30.66, 27.52, 19.08, 13.60, 9.05.

Butyl butyrate (**29**)



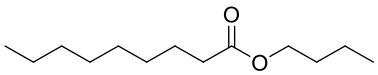
^{1}H NMR (300 MHz, $CDCl_3$) δ 4.02 (t, *J* = 6.7 Hz, 2H), 2.22 (dd, *J* = 7.7, 7.1 Hz, 2H), 1.67–1.49 (m, 4H), 1.40–1.26 (m, 2H), 0.94–0.84 (m, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 173.57, 63.91, 36.14, 30.65, 19.06, 18.39, 13.56, 13.52.

Butyl hexanoate (**30**)



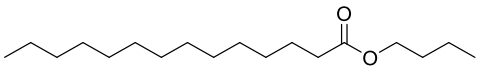
^{1}H NMR (300 MHz, $CDCl_3$) δ 4.06–3.94 (m, 2H), 2.27–2.15 (m, 2H), 1.55 (dd, *J* = 7.1, 2.3 Hz, 4H), 1.27–1.23 (m, 6H), 0.84 (dt, *J* = 7.0, 4.2 Hz, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 173.88, 64.01, 34.31, 31.30, 30.69, 24.67, 22.28, 19.11, 13.83, 13.63.

Butyl nonanoate (**31**)



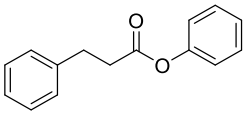
^{1}H NMR (300 MHz, $CDCl_3$) δ 4.00 (t, *J* = 6.7 Hz, 2H), 2.26-2.17 (m, 2H), 1.57-1.52 (m, 2H), 1.39-1.11 (m, 14H), 0.89-0.77 (m, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.07, 64.12, 34.43, 31.82, 30.72, 29.24, 29.17, 29.14, 25.04, 22.65, 19.16, 14.10, 13.73.

Butyl tetradecanoate (**32**)



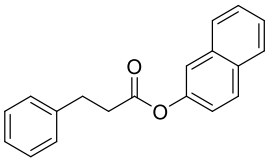
^{1}H NMR (300 MHz, $CDCl_3$) δ 4.06 (t, *J* = 6.7 Hz, 2H), 2.27 (t, *J* = 7.5 Hz, 2H), 1.66–1.53 (m, 4H), 1.42–1.19 (m, 22H), 0.96–0.82 (m, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 173.86, 64.00, 34.34, 31.91, 30.70, 29.66, 29.63, 29.58, 29.45, 29.34, 29.25, 29.14, 24.99, 22.66, 19.12, 14.04, 13.64.

Phenyl 3-phenylpropanoate (**33**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.29-7.12 (m, 8H), 6.98-6.88 (m, 2H), 3.01 (dd, *J* = 8.2, 7.0 Hz, 2H), 2.81 (ddd, *J* = 8.1, 7.2, 0.9 Hz, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.42, 150.68, 140.15, 129.42, 128.61, 128.43, 126.47, 125.82, 121.55, 36.02, 30.99.

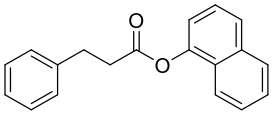
Naphthalen-2-yl 3-phenylpropanoate (**34**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80-7.64 (m, 3H), 7.45-7.33 (m, 3H), 7.30-7.14 (m, 5H), 7.07 (dd, *J* = 8.9, 2.3 Hz, 1H), 3.04 (dd, *J* = 8.0, 6.7 Hz, 2H), 2.87 (ddd, *J* = 8.3, 7.2, 1.0 Hz, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.62, 148.31, 140.16, 133.76, 131.47, 129.41, 128.66, 128.48, 127.79, 127.66, 126.57, 126.52, 125.72, 121.12,

118.53, 36.10, 31.03.

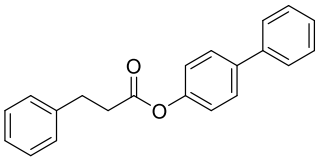
Naphthalen-1-yl 3-phenylpropanoate (**35**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92–7.85 (m, 1H), 7.76 (dt, *J* = 8.3, 1.1 Hz, 1H), 7.68–7.59 (m, 1H), 7.53–7.31 (m, 8H), 7.21 (dd, *J* = 7.5, 1.1 Hz, 1H), 3.27–3.17 (m, 2H), 3.15–3.07 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.53, 146.58, 140.12, 134.65, 128.73, 128.56, 127.99, 126.75, 126.58, 126.45, 126.42, 126.05, 125.85, 125.39, 121.17, 118.04, 36.02, 31.12.

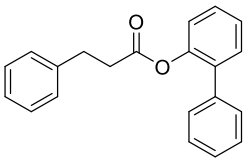
[1,1'-biphenyl]-4-yl 3-Phenylpropanoate (**36**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.68-7.55 (m, 4H), 7.52-7.43 (m, 2H), 7.42-7.23 (m, 6H), 7.23-7.09 (m, 2H), 3.20-3.08 (m, 2H), 2.95 (ddd, *J* = 8.2, 7.2, 1.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.52, 150.08, 140.40, 140.14, 139.01, 128.82, 128.65, 128.47, 128.19, 127.37, 127.15, 126.51, 121.84, 36.06, 31.01.

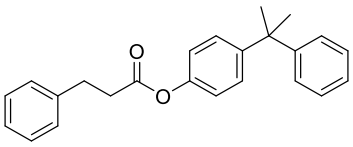
[1,1'-Biphenyl]-2-yl 3-phenylpropanoate (**37**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46–7.11 (m, 14H), 2.88 (d, *J* = 8.2 Hz, 2H), 2.72 (ddd, *J* = 8.3, 7.2, 1.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.35, 147.79, 140.22, 137.59, 134.96, 130.91, 129.00, 128.57, 128.55, 128.32, 128.29, 127.52, 126.38, 122.85, 35.80, 30.67.

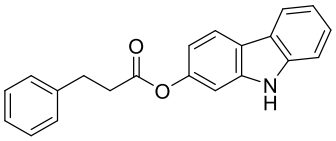
4-(2-Phenylpropan-2-yl)phenyl 3-phenylpropanoate (**38**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38–7.21 (m, 12H), 7.00–6.92 (m, 2H), 3.12 (t, *J* = 7.6 Hz, 2H), 2.92 (ddd, *J* = 8.2, 7.3, 0.9 Hz, 2H), 1.72 (d, *J* = 0.7 Hz, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.57, 150.37, 148.49, 148.24, 140.19, 128.63, 128.46, 128.09, 127.86, 126.82, 126.48, 125.77, 120.87, 42.75, 36.05, 31.02, 30.96, 30.87.

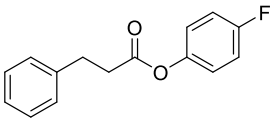
9H-Carbazol-2-yl 3-phenylpropanoate (**39**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 (s, 1H), 8.01 (ddt, *J* = 8.4, 7.6, 0.7 Hz, 2H), 7.42–7.25 (m, 8H), 7.09 (dd, *J* = 2.0, 0.5 Hz, 1H), 6.89 (dd, *J* = 8.4, 2.0 Hz, 1H), 3.16 (dd, *J* = 8.0, 6.8 Hz, 2H), 2.98 (ddd, *J* = 8.2, 7.2, 1.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.94, 140.21, 128.65, 128.48, 126.49, 125.70, 122.91, 121.31, 120.78, 120.15, 119.73, 113.28, 110.63, 103.79, 36.13, 31.06.

4-Fluorophenyl 3-phenylpropanoate (**40**)

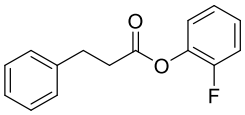


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28–7.10 (m, 5H), 7.00–6.83 (m, 4H), 2.98 (t, *J* = 7.8 Hz, 2H), 2.79 (ddd, *J* = 8.2, 7.2, 1.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.46, 161.85, 158.61, 146.49, 146.45, 140.03, 128.64, 128.42, 126.53, 123.00, 122.88, 116.22, 115.91, 35.91, 30.95.

^{19}F NMR (282 MHz, $CDCl_3$) δ -117.04.

2-Fluorophenyl 3-phenylpropanoate (**41**)

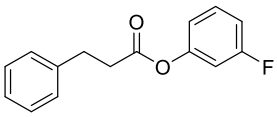


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36–6.83 (m, 9H), 3.02 (ddd, *J* = 8.3, 7.3, 1.1 Hz, 2H), 2.85 (ddd, *J* = 8.3, 7.1, 1.1 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.39, 155.76, 152.46, 140.01, 138.19, 138.02, 128.61, 128.38, 127.13, 127.03, 126.48, 124.47, 124.42, 123.74, 116.82, 116.58, 35.53, 30.90.

^{19}F NMR (282 MHz, $CDCl_3$) δ -128.42-128.50 (m).

3-Fluorophenyl 3-phenylpropanoate (**42**)

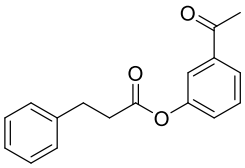


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33–7.12 (m, 6H), 6.92–6.80 (m, 1H), 6.79–6.64 (m, 2H), 3.07–2.93 (m, 2H), 2.81 (ddd, *J* = 8.2, 7.2, 1.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.98, 164.49, 161.21, 151.53, 151.38, 139.94, 130.21, 130.08, 128.64, 128.40, 126.54, 117.38, 117.34, 113.00, 112.73, 109.86, 109.53, 35.94, 30.90.

^{19}F NMR (282 MHz, $CDCl_3$) δ -111.08-111.14 (m).

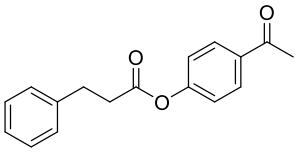
3-Acetylphenyl 3-phenylpropanoate (**43**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (ddd, *J* = 7.8, 1.6, 1.0 Hz, 1H), 7.61–7.45 (m, 3H), 7.39–7.28 (m, 5H), 3.13 (d, *J* = 7.5 Hz, 2H), 2.99–2.89 (m, 2H), 2.61 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 196.97, 171.24, 150.85, 139.93, 138.51, 129.64, 128.65, 128.42, 126.55, 126.42, 125.75, 121.44, 35.93, 30.93, 26.70.

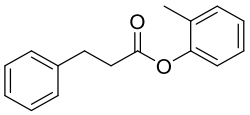
4-Acetylphenyl 3-phenylpropanoate (**44**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.94 (s, 2H), 7.38–7.29 (m, 3H), 7.12 (d, *J* = 0.4 Hz, 1H), 6.94 (s, 2H), 3.18–3.05 (m, 2H), 3.00–2.90 (m, 2H), 2.59 (s, 3H).

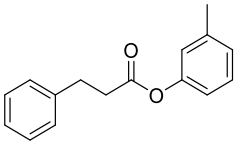
^{13}C NMR (75 MHz, $CDCl_3$) δ 197.39, 170.96, 154.42, 139.85, 134.67, 131.03, 130.01, 128.67, 128.40, 126.59, 121.79, 115.38, 36.01, 30.87, 26.35.

o-Tolyl 3-phenylpropanoate (**45**)



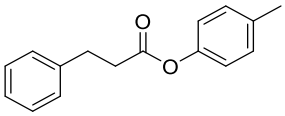
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45–7.11 (m, 9H), 7.03–6.92 (m, 1H), 3.15 (dd, *J* = 8.0, 6.8 Hz, 2H), 3.02–2.92 (m, 2H), 2.13 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.16, 149.34, 140.18, 131.15, 130.12, 128.63, 128.46, 126.93, 126.50, 126.05, 121.87, 35.80, 31.04, 16.11.

m-Tolyl 3-phenylpropanoate (**46**)



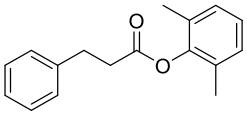
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28–7.09 (m, 6H), 6.99–6.88 (m, 1H), 6.78–6.66 (m, 2H), 2.99 (t, *J* = 7.8 Hz, 2H), 2.78 (ddd, *J* = 8.1, 7.2, 0.9 Hz, 2H), 2.25 (t, *J* = 0.7 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.55, 150.63, 140.21, 139.62, 129.15, 128.62, 128.46, 126.65, 126.47, 122.17, 118.50, 36.05, 31.02, 21.33.

p-Tolyl 3-phenylpropanoate (**47**)



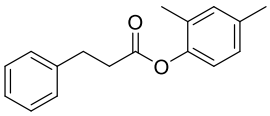
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38–7.24 (m, 5H), 7.22–7.15 (m, 2H), 6.96–6.88 (m, 2H), 3.11 (t, *J* = 7.7 Hz, 2H), 2.95–2.86 (m, 2H), 2.36 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.64, 148.43, 140.21, 135.45, 129.93, 128.60, 128.44, 126.44, 121.21, 36.03, 31.02, 20.88.

2,6-Dimethylphenyl 3-phenylpropanoate (**48**)



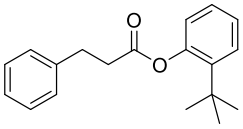
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45–7.22 (m, 5H), 7.14–7.02 (m, 3H), 3.22–3.11 (m, 2H), 3.05–2.93 (m, 2H), 2.10 (t, *J* = 0.8 Hz, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 170.67, 148.20, 140.21, 130.12, 128.62, 128.59, 128.46, 126.49, 125.86, 35.51, 31.02, 16.26.

2,4-Dimethylphenyl 3-phenylpropanoate (**49**)



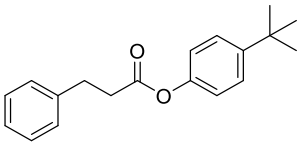
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41–7.20 (m, 5H), 7.08–6.97 (m, 2H), 6.85 (d, *J* = 8.0 Hz, 1H), 3.18–3.06 (m, 2H), 2.95 (ddd, *J* = 8.2, 7.2, 1.0 Hz, 2H), 2.34 (s, 3H), 2.08 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.37, 147.08, 140.23, 135.60, 131.77, 129.65, 128.61, 128.45, 127.46, 126.46, 121.50, 35.81, 31.07, 20.84, 16.03.

2-*tert*-Butylphenyl 3-phenylpropanoate (**50**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45–7.17 (m, 8H), 6.96 (ddd, *J* = 7.6, 1.7, 0.7 Hz, 1H), 3.20–3.12 (m, 2H), 3.02–2.94 (m, 2H), 1.37 (d, *J* = 0.7 Hz, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.49, 149.22, 140.99, 140.20, 128.65, 128.54, 128.50, 127.24, 126.91, 126.51, 125.76, 123.99, 36.63, 34.48, 30.81, 30.23.

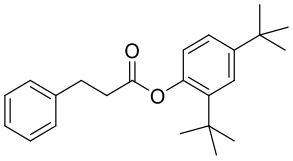
4-*tert*-Butylphenyl 3-phenylpropanoate (**51**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33-7.11 (m, 7H), 6.88-6.81 (m, 2H), 3.00 (dd, *J* = 8.4, 7.2 Hz, 2H), 2.80 (ddd, *J* = 8.1, 7.2, 0.9 Hz, 2H), 1.23 (s, 9H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.63, 148.62, 148.30, 140.21, 128.60, 128.45, 126.44, 126.32, 120.83, 36.04, 34.48, 31.42, 31.02.

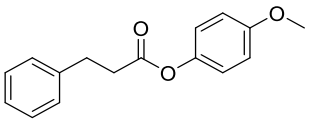
2,4-di-*tert*-Butylphenyl 3-phenylpropanoate (**52**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46–7.21 (m, 7H), 6.87 (dd, *J* = 8.5, 1.0 Hz, 1H), 3.15 (t, *J* = 7.7 Hz, 2H), 3.01–2.92 (m, 2H), 1.40–1.29 (m, 18H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.62, 148.09, 146.79, 140.25, 139.89, 128.61, 128.49, 126.46, 124.13, 123.78, 123.16, 36.64, 34.69, 34.64, 31.52, 30.83, 30.28.

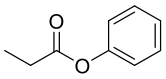
4-Methoxyphenyl 3-phenylpropanoate (**53**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40–7.24 (m, 5H), 6.97–6.88 (m, 3H), 6.84–6.75 (m, 1H), 3.82 (s, 3H), 3.10 (t, *J* = 7.8 Hz, 2H), 2.90 (ddd, *J* = 8.1, 7.3, 0.9 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.85, 157.24, 144.15, 140.19, 128.60, 128.43, 126.45, 122.29, 114.45, 55.60, 35.97, 31.01.

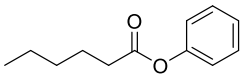
Phenyl propionate (**54**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47–7.37 (m, 2H), 7.33–7.23 (m, 1H), 7.21–7.10 (m, 2H), 2.63 (q, *J* = 7.6 Hz, 2H), 1.32 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.92, 150.89, 129.43, 125.73, 121.62, 27.76, 9.10.

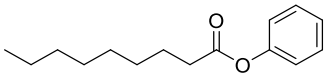
Phenyl hexanoate (**55**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46–7.35 (m, 2H), 7.31–7.20 (m, 1H), 7.17–7.04 (m, 2H), 2.58 (t, *J* = 7.5 Hz, 2H), 1.86–1.72 (m, 2H), 1.50–1.35 (m, 4H), 1.00–0.92 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.36, 150.79, 129.40, 125.71, 121.60, 77.24, 34.40, 31.29, 24.66, 22.35, 13.94.

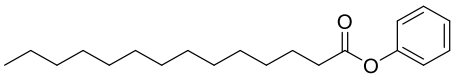
Phenyl nonanoate (**56**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34-7.24 (m, 2H), 7.19-7.09 (m, 1H), 7.04-6.84 (m, 2H), 2.52-2.43 (m, 2H), 1.76-1.60 (m, 2H), 1.36-1.18 (m, 10H), 0.85-0.78 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 172.37, 150.79, 129.40, 125.71, 121.61, 34.44, 31.83, 29.25, 29.15, 29.14, 24.98, 22.67, 14.12.

Phenyl tetradecanoate (**57**)

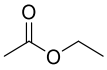


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45–7.36 (m, 2H), 7.31–7.21 (m, 1H), 7.15–7.06 (m, 2H), 2.62–2.53 (m, 2H), 1.84–1.71 (m, 2H), 1.29 (s, 20H), 0.95–0.89 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 172.35, 150.79, 129.40, 125.71, 121.60, 34.44, 31.95, 29.72, 29.70, 29.68, 29.62, 29.49, 29.39, 29.29, 29.14, 24.99, 22.72, 14.14.

Methyl acetate (**58**)

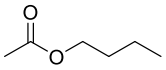
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.54 (d, *J* = 1.2 Hz, 3H), 1.93 (d, *J* = 1.2 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.19, 51.28, 20.34.

Ethyl acetate (**59**)



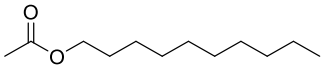
^{1}H NMR (300 MHz, $CDCl_3$) δ 4.11 (q, *J* = 7.1 Hz, 2H), 2.03 (s, 3H), 1.24 (t, *J* = 7.1 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.05, 60.33, 20.97, 14.14.

Butyl acetate (**60**)



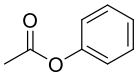
^{1}H NMR (300 MHz, $CDCl_3$) δ 4.05 – 3.95 (m, 2H), 2.05 – 1.89 (m, 3H), 1.61 – 1.48 (m, 2H), 1.40 – 1.24 (m, 2H), 0.94 – 0.81 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.01, 170.99, 64.19, 30.58, 20.80, 19.03, 13.56.

Decyl acetate (**61**)



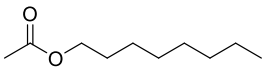
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.98 (t, *J* = 6.7 Hz, 2H), 1.98 (s, 3H), 1.55 (t, *J* = 7.2 Hz, 2H), 1.22 (d, *J* = 11.4 Hz, 14H), 0.83 – 0.78 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.26, 64.68, 31.89, 29.53, 29.31, 29.26, 28.61, 25.92, 22.68, 21.03, 14.11.

Phenyl acetate (**62**)



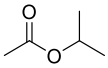
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 – 7.38 (m, 2H), 7.32 – 7.23 (m, 1H), 7.19 – 7.10 (m, 2H), 2.33 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 169.49, 150.77, 129.47, 125.86, 121.63, 21.13.

Octyl acetate (**63**)



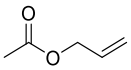
^{1}H NMR (300 MHz, $CDCl_3$) δ 4.04 (t, *J* = 6.8 Hz, 2H), 2.03 (s, 3H), 1.59 (dt, *J* = 8.0, 6.3 Hz, 2H), 1.37 – 1.19 (m, 10H), 0.96 – 0.79 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.12, 64.59, 31.75, 29.19, 29.15, 28.58, 25.89, 22.60, 20.92, 14.02.

Isopropyl acetate (**64**)



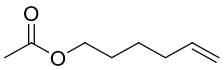
^{1}H NMR (300 MHz, $CDCl_3$) δ 5.06 – 4.86 (m, 1H), 1.99 (dd, *J* = 1.6, 0.8 Hz, 3H), 1.22 – 1.16 (m, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 170.55, 67.54, 21.75, 21.34.

Allyl acetate (**65**)



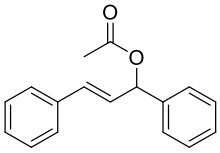
^{1}H NMR (300 MHz, $CDCl_3$) δ 5.95 – 5.77 (m, 1H), 5.33 – 5.14 (m, 2H), 4.52 (dt, *J* = 5.8, 1.5 Hz, 2H), 2.05 – 1.99 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 170.51, 132.18, 118.03, 65.02, 20.75.

Hex-5-en-1-yl acetate (**66**)



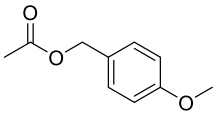
^{1}H NMR (300 MHz, $CDCl_3$) δ 5.77 (ddt, *J* = 16.9, 10.2, 6.6 Hz, 1H), 5.04 – 4.91 (m, 2H), 4.04 (t, *J* = 6.6 Hz, 2H), 2.11 – 2.00 (m, 5H), 1.69 – 1.56 (m, 2H), 1.50 – 1.38 (m, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.09, 138.27, 114.77, 64.33, 33.25, 28.00, 25.14, 20.91.

(E)-1,3-Diphenylallyl acetate (**67**)



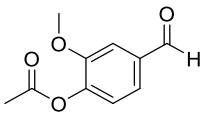
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 – 7.37 (m, 10H), 6.74 (dd, *J* = 15.8, 3.5 Hz, 1H), 6.61 – 6.39 (m, 2H), 2.21 (dd, *J* = 1.9, 0.8 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 170.13, 139.36, 136.27, 132.70, 128.74, 128.69, 128.28, 128.18, 127.61, 127.16, 126.81, 76.27, 21.41.

4-Methoxybenzyl acetate (**68**)



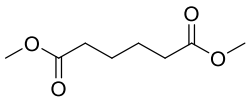
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 – 7.28 (m, 2H), 6.95 – 6.86 (m, 2H), 5.06 (s, 2H), 3.81 (d, *J* = 0.7 Hz, 3H), 2.09 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 170.92, 159.68, 130.14, 128.11, 113.96, 66.10, 55.24, 21.04.

4-Formyl-2-methoxyphenyl acetate (**69**)



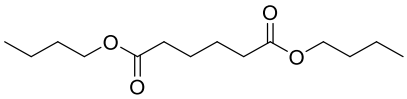
^{1}H NMR (300 MHz, $CDCl_3$) δ 9.90 – 9.81 (m, 1H), 7.39 (dt, *J* = 9.6, 1.6 Hz, 2H), 7.13 (dd, *J* = 7.9, 1.4 Hz, 1H), 3.85 – 3.78 (m, 3H), 2.30 – 2.23 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 191.04, 168.33, 151.97, 144.93, 135.23, 124.69, 123.42, 110.85, 56.08, 20.62.

Dimethyl adipate (**70**)



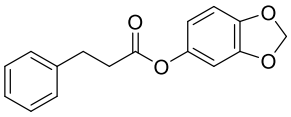
^{1}H NMR (300 MHz, CDCl3) δ 3.63–3.56 (m, 6H), 2.28 (tq, J = 4.5, 2.0 Hz, 4H), 1.65–1.53 (m, 4H).
^{13}C NMR (75 MHz, CDCl3) δ 173.62, 51.41, 33.56, 24.29.

Dibutyl adipate (**71**)



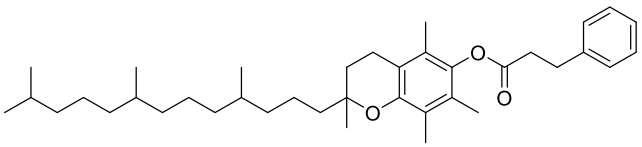
^{1}H NMR (300 MHz, $CDCl_3$) δ 4.03 (t, *J* = 6.7 Hz, 4H), 2.33 – 2.20 (m, 4H), 1.68 – 1.50 (m, 8H), 1.40 – 1.26 (m, 4H), 0.89 (t, *J* = 7.4 Hz, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 173.31, 64.13, 33.88, 30.63, 24.39, 19.08, 13.62.

Benzo[d][1,3]dioxol-5-yl 3-phenylpropanoate (**72**)



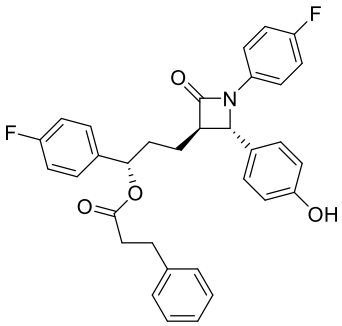
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38–7.25 (m, 5H), 6.78 (dd, *J* = 8.3, 0.3 Hz, 1H), 6.56–6.53 (m, 1H), 6.47 (ddd, *J* = 8.3, 2.4, 0.3 Hz, 1H), 5.99 (s, 2H), 3.09 (t, *J* = 7.6 Hz, 2H), 2.88 (ddd, *J* = 8.1, 7.3, 0.9 Hz, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.77, 147.98, 145.36, 144.95, 140.09, 128.62, 128.43, 126.50, 113.90, 107.97, 103.72, 101.70, 35.92, 30.98.

2,5,7,8-Tetramethyl-2-(4,8,12-trimethyltridecyl)chroman-6-yl 3-phenylpropanoate (**73**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 – 7.22 (m, 5H), 3.15 (dd, *J* = 8.1, 6.8 Hz, 2H), 2.98 (ddd, *J* = 8.3, 7.2, 1.1 Hz, 2H), 2.61 (t, *J* = 6.8 Hz, 2H), 2.12 (s, 3H), 2.00 – 1.94 (m, 3H), 1.91 (s, 3H), 1.81 (dt, *J* = 9.4, 6.8 Hz, 2H), 1.65 – 1.24 (m, 19H), 1.22 – 1.09 (m, 6H), 0.93 – 0.87 (m, 12H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.53, 149.42, 140.48, 140.38, 128.57, 128.49, 126.67, 126.40, 124.90, 123.03, 117.36, 75.06, 39.42, 37.58, 37.50, 37.43, 37.33, 35.63, 32.82, 32.73, 31.07, 28.02, 24.86, 24.49, 22.77, 22.68, 21.07, 20.63, 19.80, 19.73, 19.70, 19.67, 19.64, 12.89, 12.04, 11.86.
HRMS (ESI-TOF): calcd. for $[C_{38}H_{58}O_3+Na]^+$ 585.4278, found 585.4294.

(S)-1-(4-Fluorophenyl)-3-((2S,3R)-1-(4-fluorophenyl)-2-(4-hydroxyphenyl)-4-oxoazetidin-3-yl)propyl 3-phenylpropanoate (**74**)



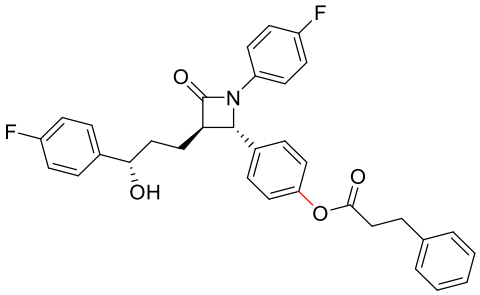
^{1}H NMR (300 MHz, CD_3OH) δ 7.49 – 7.42 (m, 4H), 7.30 – 7.27 (m, 4H), 7.21 (d, *J* = 3.3 Hz, 2H), 7.07 (td, *J* = 8.9, 2.6 Hz, 3H), 7.00 – 6.94 (m, 4H), 6.75 (d, *J* = 8.6 Hz, 1H), 4.77 (d, *J* = 9.8 Hz, 1H), 4.66 (s, 1H), 3.05 – 3.00 (m, 1H), 2.93 – 2.85 (m, 2H), 2.73 – 2.61 (m, 2H), 2.30 – 2.16 (m, 2H), 2.09 – 2.00 (m, 1H), 1.78 – 1.64 (m, 1H).

^{13}C NMR (75 MHz, CD_3OH) δ 172.54, 171.72, 150.41, 140.25, 138.35, 133.81, 131.58, 128.16, 128.08, 128.00, 127.90, 127.64, 127.39, 127.28, 126.02, 122.63, 122.52, 122.27, 122.16, 121.11, 114.88, 114.58, 114.33, 81.34, 79.12, 51.59, 35.39, 32.52, 30.52, 27.74.

^{19}F NMR (282 MHz, CD_3OH) δ -117.46 – -117.65 (m), -120.07 (tt, *J* = 9.1, 4.9 Hz).

HRMS (ESI-TOF): calcd. for $[C_{38}H_{29}F_2NO_4+Na]^+$ 564.1957, found 564.1965.

4-((2S,3R)-1-(4-Fluorophenyl)-3-((S)-3-(4-fluorophenyl)-3-hydroxypropyl)-4-oxoazetidin-2-yl)phenyl 3-phenylpropanoate (**75**)



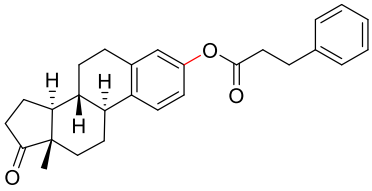
^{1}H NMR (300 MHz, CD_3OH) δ 7.47 – 7.44 (m, 2H), 7.32 – 7.27 (m, 7H), 7.08 – 6.97 (m, 6H), 6.73 (s, 2H), 4.67 (d, *J* = 3.9 Hz, 2H), 2.75 – 2.65 (m, 2H), 2.32 – 2.16 (m, 4H), 2.09 – 1.97 (m, 2H), 1.81 – 1.61 (m, 2H).

^{13}C NMR (75 MHz, CD_3OH) δ 172.89, 163.72, 160.99, 160.49, 157.79, 156.87, 138.88, 138.84, 134.07, 131.57, 127.99, 127.44, 127.33, 122.28, 122.17, 114.86, 114.57, 114.30, 81.78, 79.23, 51.42, 47.06, 46.77, 32.63, 27.85.

^{19}F NMR (282 MHz, CD_3OH) δ -117.59 (ddd, *J* = 14.0, 9.0, 5.3 Hz), -120.23 (tt, *J* = 8.5, 4.7 Hz).

HRMS (ESI-TOF): calcd. for $[C_{38}H_{29}F_2NO_4+Na]^+$ 564.1957, found 564.1970.

(8R,9S,13S,14S)-13-Methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl 3-phenylpropanoate (**76**)

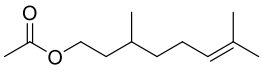


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 – 7.28 (m, 5H), 6.84 – 6.75 (m, 2H), 6.68 – 6.60 (m, 1H), 3.10 (dd, *J* = 8.3, 7.0 Hz, 2H), 2.92 – 2.86 (m, 3H), 2.59 – 2.40 (m, 2H), 2.21 – 1.97 (m, 4H), 1.72 – 1.40 (m, 8H), 0.93 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 220.90, 171.74, 148.54, 140.19, 138.00, 137.38, 128.60, 128.45, 126.45, 126.40, 121.56, 118.73, 50.44, 47.98, 44.16, 38.01, 36.03, 35.88, 31.56, 31.02, 29.40, 26.35, 25.76, 21.61, 13.85.

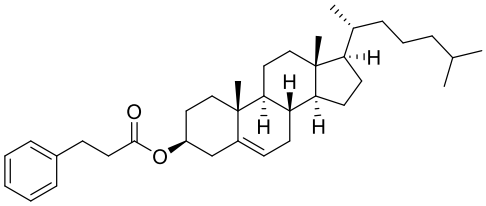
HRMS (ESI-TOF): calcd. for $[C_{27}H_{30}O_3+Na]^+$ 425.2087, found 425.2099.

Citronellyl acetate (**77**)



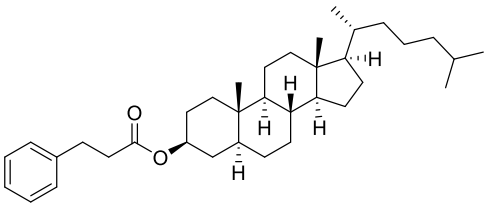
^{1}H NMR (300 MHz, $CDCl_3$) δ 5.07 (ddt, *J* = 7.1, 5.7, 1.5 Hz, 1H), 4.15 – 4.02 (m, 2H), 2.07 – 1.88 (m, 5H), 1.71 – 1.27 (m, 10H), 1.24 – 1.10 (m, 1H), 0.90 (d, *J* = 6.5 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.09, 131.23, 124.54, 62.95, 36.94, 35.39, 29.43, 25.65, 25.34, 20.94, 19.36, 17.58.

(3S,8S,9S,10R,13R,14S,17R)-10,13-Dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 3-phenylpropanoate (**78**)



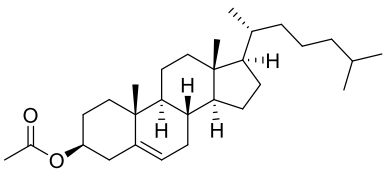
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 – 7.17 (m, 5H), 5.43 – 5.35 (m, 1H), 4.69 – 4.57 (m, 1H), 2.97 (t, *J* = 7.8 Hz, 2H), 2.63 (dd, *J* = 8.5, 7.1 Hz, 2H), 2.30 (d, *J* = 8.2 Hz, 2H), 2.04 – 1.81 (m, 5H), 1.64 – 1.10 (m, 21H), 1.05 – 1.02 (m, 3H), 0.94 (d, *J* = 6.5 Hz, 3H), 0.89 (dd, *J* = 6.6, 1.4 Hz, 6H), 0.70 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 172.35, 140.62, 139.67, 128.46, 128.34, 126.21, 122.66, 74.03, 56.70, 56.15, 50.03, 42.33, 39.74, 39.53, 38.10, 37.00, 36.60, 36.26, 36.20, 35.81, 31.91, 31.87, 31.07, 28.25, 28.03, 27.76, 24.30, 23.84, 22.84, 22.58, 21.04, 19.33, 18.73, 11.87.
HRMS (ESI-TOF): calcd. for $[C_{36}H_{54}O_2+Na]^+$ 541.4020, found 541.4033.

(3S,5S,8R,9S,10S,13R,14S,17R)-10,13-Dimethyl-17-((R)-6-methylheptan-2-yl)hexadecahydro-1H-cyclopenta[a]phenanthren-3-yl 3-phenylpropanoate (**79**)



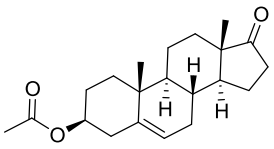
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.25 – 7.08 (m, 5H), 4.62 (ddd, *J* = 11.2, 6.4, 4.8 Hz, 1H), 2.86 (t, *J* = 7.8 Hz, 2H), 2.52 (dd, *J* = 8.5, 7.1 Hz, 2H), 1.89 (d, *J* = 12.3 Hz, 1H), 1.75 – 1.34 (m, 10H), 1.28 – 0.91 (m, 20H), 0.83 (d, *J* = 6.5 Hz, 3H), 0.81 – 0.79 (m, 3H), 0.79 – 0.77 (m, 3H), 0.74 (d, *J* = 2.6 Hz, 3H), 0.57 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 172.53, 140.66, 128.44, 128.34, 126.19, 73.84, 56.43, 56.28, 54.22, 44.66, 42.60, 39.99, 39.53, 36.76, 36.31, 36.18, 35.81, 35.49, 35.47, 34.02, 32.00, 31.09, 28.62, 28.25, 28.03, 27.46, 24.22, 23.85, 22.83, 22.57, 21.21, 18.68, 12.23, 12.08.
HRMS (ESI-TOF): calcd. for $[C_{36}H_{56}O_2+Na]^+$ 543.4177, found 543.4189.

(3S,8S,9S,10R,13R,14S,17R)-10,13-Dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl acetate (**80**)



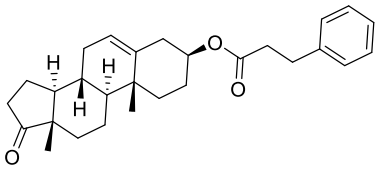
^{1}H NMR (300 MHz, $CDCl_3$) δ 5.30 (d, *J* = 5.0 Hz, 1H), 4.60 – 4.46 (m, 1H), 2.25 (d, *J* = 6.8 Hz, 2H), 1.95 (s, 3H), 1.82 – 1.73 (m, 3H), 1.57 – 0.98 (m, 22H), 0.95 (s, 3H), 0.87 – 0.76 (m, 10H), 0.61 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 170.40, 139.61, 122.63, 73.93, 56.69, 56.16, 50.04, 42.31, 39.74, 39.53, 38.13, 37.01, 36.58, 36.21, 35.82, 31.90, 31.86, 28.25, 28.01, 27.78, 24.29, 23.86, 22.84, 22.59, 21.41, 21.05, 19.31, 18.73, 11.86.

(3S,8R,9S,10R,13S,14S)-10,13-Dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl acetate (**81**)



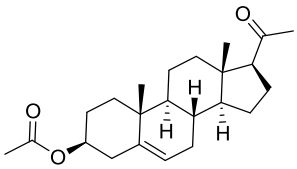
^{1}H NMR (300 MHz, $CDCl_3$) δ 5.43 – 5.35 (m, 1H), 4.67 – 4.52 (m, 1H), 2.51 – 2.41 (m, 1H), 2.37 – 2.29 (m, 2H), 2.15 – 2.05 (m, 2H), 2.03 (s, 3H), 1.97 – 1.46 (m, 12H), 1.34 – 1.24 (m, 2H), 1.04 (s, 3H), 0.88 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 220.96, 170.47, 139.91, 121.86, 73.69, 51.68, 50.13, 47.50, 38.07, 36.93, 36.72, 35.83, 31.45, 31.40, 30.76, 27.69, 21.87, 21.41, 20.31, 19.33, 13.54.

(3S,8R,9S,10R,13S,14S)-10,13-Dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 3-phenylpropanoate (**82**)



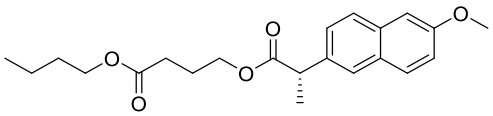
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 – 7.18 (m, 5H), 5.42 (d, *J* = 5.0 Hz, 1H), 4.63 (td, *J* = 11.2, 5.4 Hz, 1H), 2.97 (t, *J* = 7.8 Hz, 2H), 2.69 – 2.59 (m, 2H), 2.54 – 2.43 (m, 1H), 2.40 – 2.28 (m, 2H), 2.18 – 2.04 (m, 2H), 2.03 – 1.80 (m, 4H), 1.74 – 1.50 (m, 6H), 1.32 (ddd, *J* = 12.4, 8.3, 4.5 Hz, 3H), 1.22 – 1.10 (m, 1H), 1.07 (d, *J* = 3.0 Hz, 3H), 0.91 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 221.07, 172.34, 140.58, 139.94, 128.47, 128.34, 126.23, 121.88, 73.77, 50.15, 47.54, 38.09, 38.06, 36.94, 36.74, 36.22, 35.86, 31.48, 31.42, 31.05, 30.79, 27.69, 21.89, 20.33, 19.36, 13.56.
HRMS (ESI-TOF): calcd. for $[C_{28}H_{36}O_3+Na]^+$ 443.2556, found 433.2571.

Pregnanolone acetate (**83**)



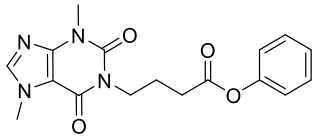
^{1}H NMR (300 MHz, $CDCl_3$) δ 5.38 (dt, *J* = 5.3, 1.5 Hz, 1H), 4.61 (dtt, *J* = 10.5, 5.5, 2.4 Hz, 1H), 2.54 (t, *J* = 8.7 Hz, 1H), 2.39 – 2.28 (m, 2H), 2.24 – 2.11 (m, 4H), 2.08 – 1.95 (m, 5H), 1.92 – 1.81 (m, 2H), 1.72 – 1.39 (m, 8H), 1.26 – 1.09 (m, 3H), 1.02 (d, *J* = 1.2 Hz, 4H), 0.63 (d, *J* = 1.3 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 209.48, 170.51, 139.65, 122.32, 73.81, 63.66, 56.82, 49.88, 43.97, 38.78, 38.06, 37.00, 36.59, 31.81, 31.75, 31.55, 27.72, 24.48, 22.81, 21.43, 21.03, 19.30, 13.22.

Butyl (S)-4-((2-(6-methoxynaphthalen-2-yl)propanoyl)oxy)butanoate (**84**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.66 – 7.56 (m, 3H), 7.32 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.10 – 7.01 (m, 2H), 4.10 – 3.92 (m, 4H), 3.84 (s, 4H), 2.23 – 2.14 (m, 2H), 1.91 – 1.76 (m, 2H), 1.54 – 1.43 (m, 5H), 1.32 – 1.21 (m, 2H), 0.84 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.59, 172.90, 157.65, 135.66, 133.70, 129.28, 128.94, 127.16, 126.21, 125.92, 118.99, 105.58, 64.39, 63.72, 55.32, 45.46, 30.63, 24.03, 19.12, 18.49, 13.71.
HRMS (ESI-TOF): calcd. for $[C_{22}H_{28}O_5+Na]^+$ 395.1829, found 395.1834.

Phenyl 4-(3,7-dimethyl-2,6-dioxo-2,3,6,7-tetrahydro-1H-purin-1-yl)butanoate (**85**)



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (t, *J* = 1.1 Hz, 1H), 7.42 – 7.34 (m, 2H), 7.26 – 7.19 (m, 1H), 7.16 – 7.05 (m, 2H), 4.19 (t, *J* = 6.9 Hz, 2H), 4.01 – 4.00 (m, 3H), 3.60 (d, *J* = 1.2 Hz, 3H), 2.67 (t, *J* = 7.5 Hz, 2H), 2.19 – 2.13 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.43, 155.32, 151.57, 150.76, 148.88, 141.51, 129.37, 125.72, 121.59, 107.63, 40.42, 33.61, 31.86, 29.74, 23.35.

HRMS (ESI-TOF): calcd. for $[C_{17}H_{18}N_4O_4+H]^+$ 343.1406, found 343.1402.

References

[1] Han-Jun Ai, Hai Wang, Chong-Liang Li, Xiao-Feng Wu, *ACS Catal*., **2020**, 10, 5147-5152.
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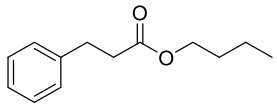
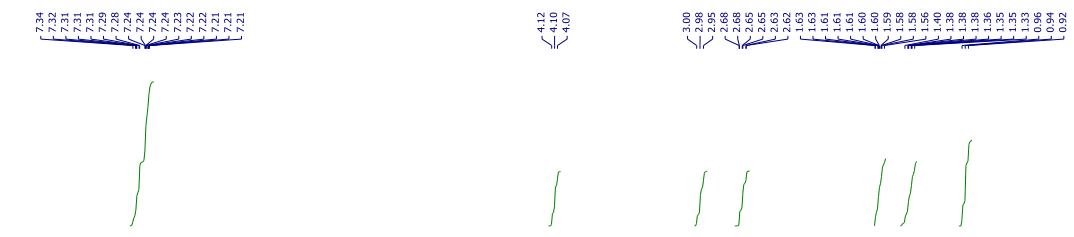
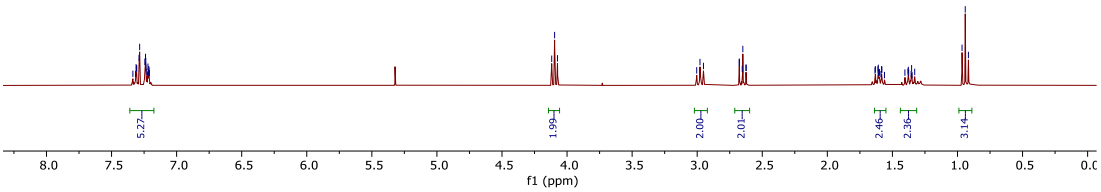
[9] Ya-Hui Li, Xiao-Feng Wu, *Commun. Chem.*, **2018**, 1, 39.

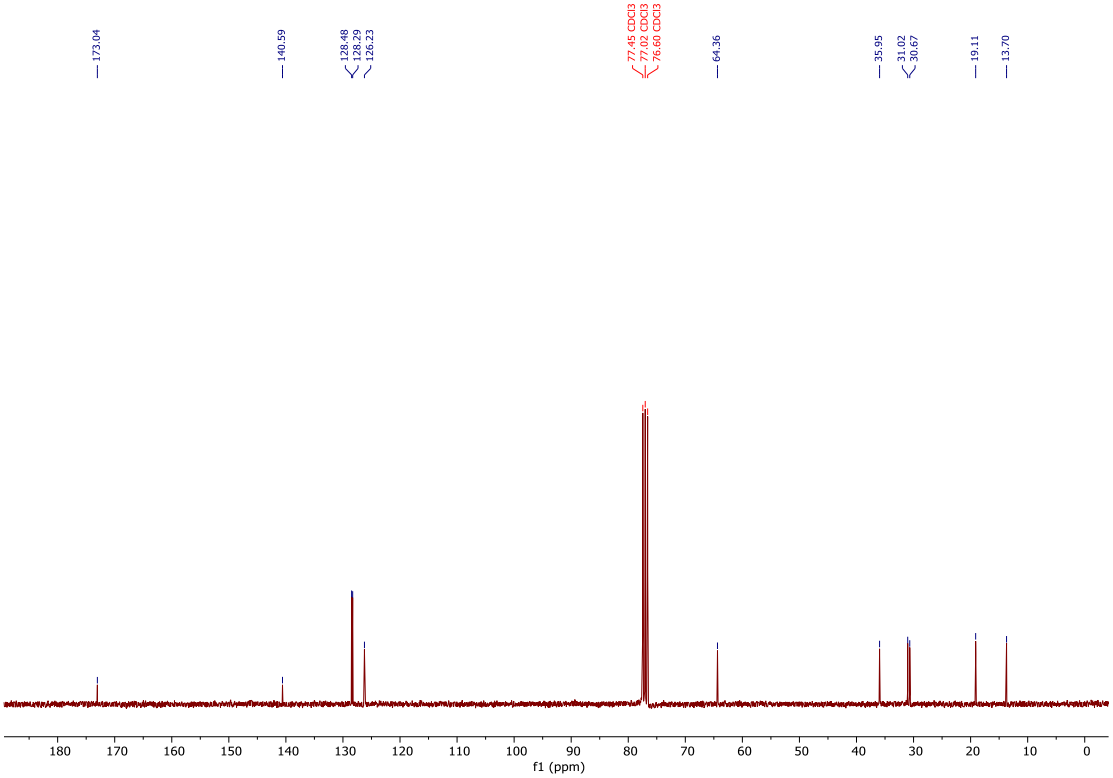
NMR Spectra

Butyl 3-phenylpropanoate (**3**)

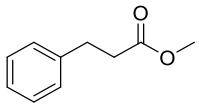


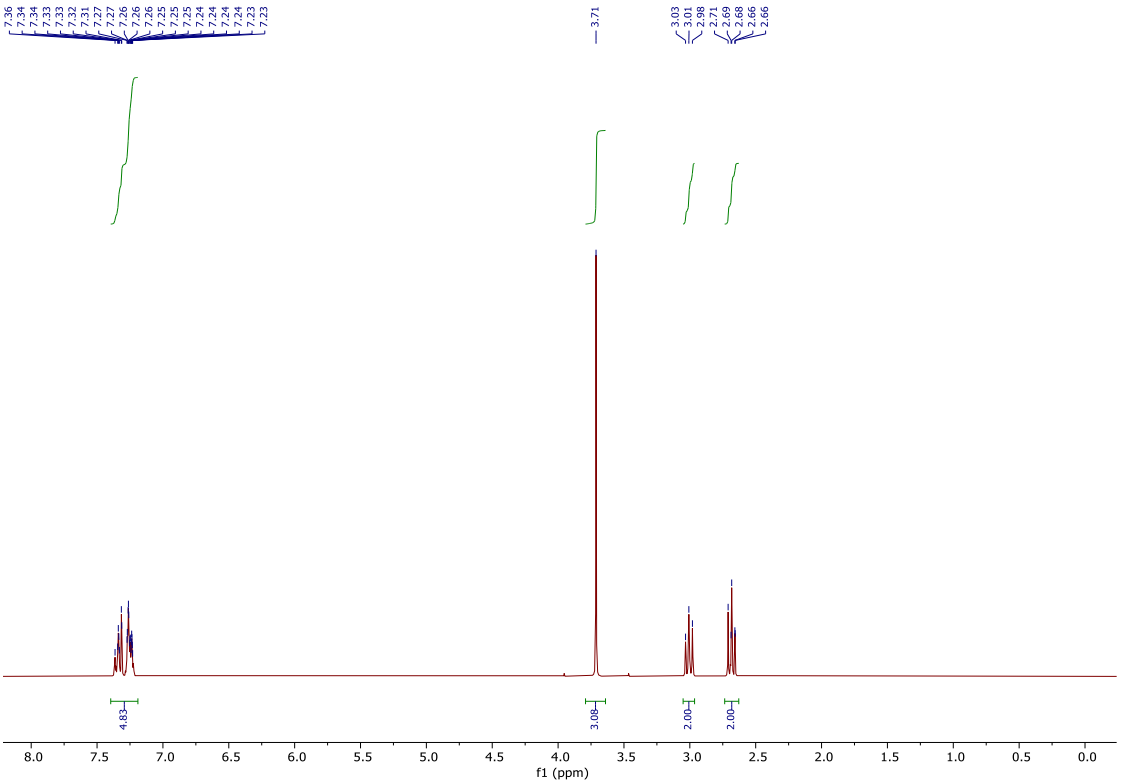


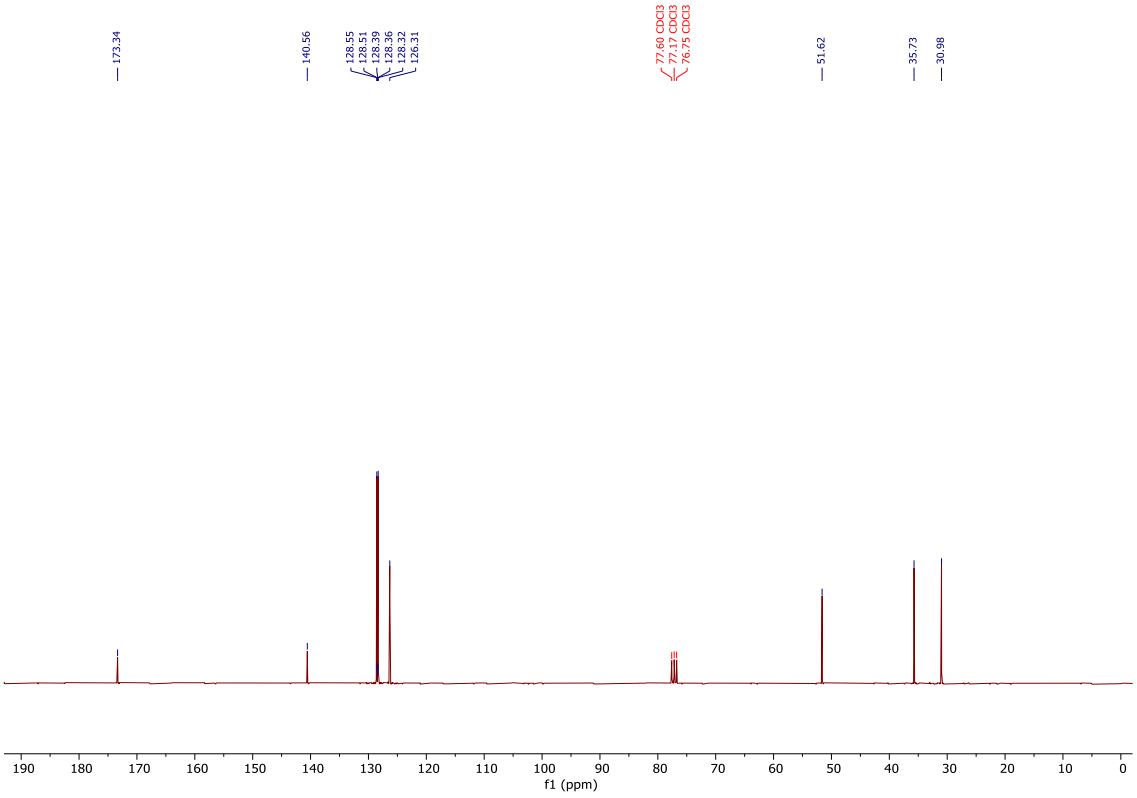




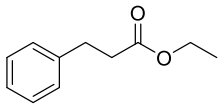
Methyl 3-phenylpropanoate (**6**)

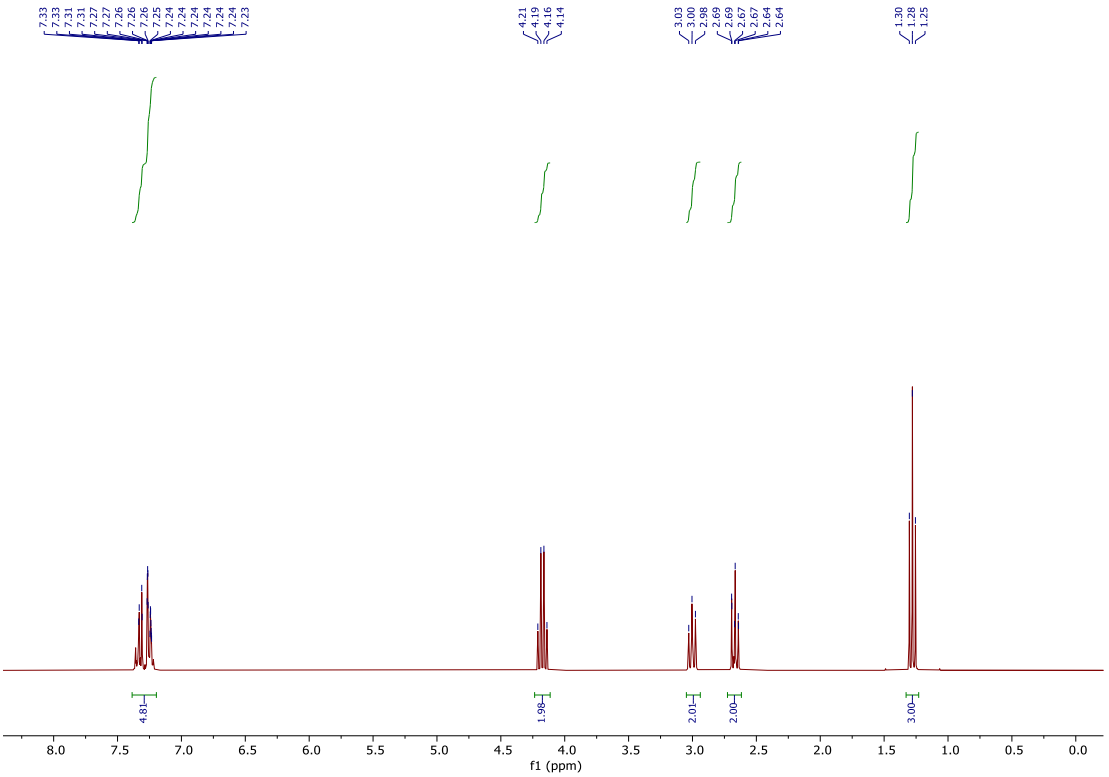


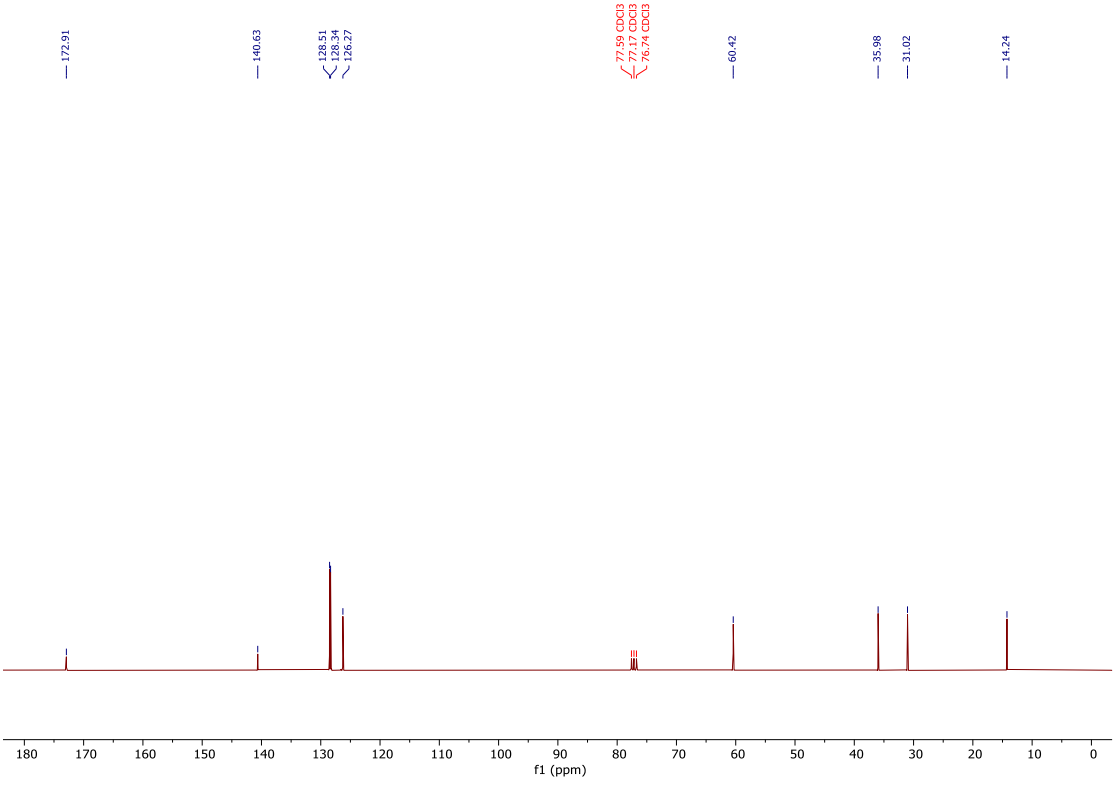




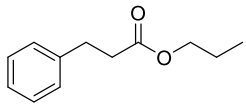
Ethyl 3-phenylpropanoate (**7**)

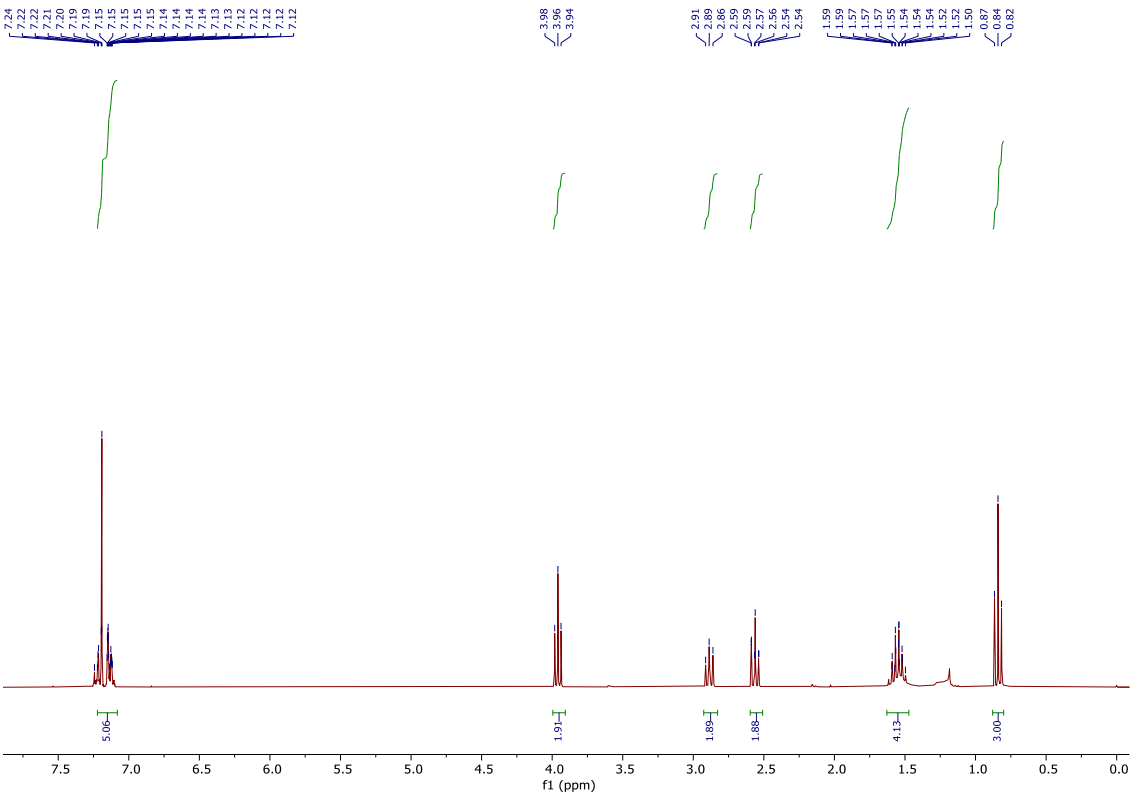


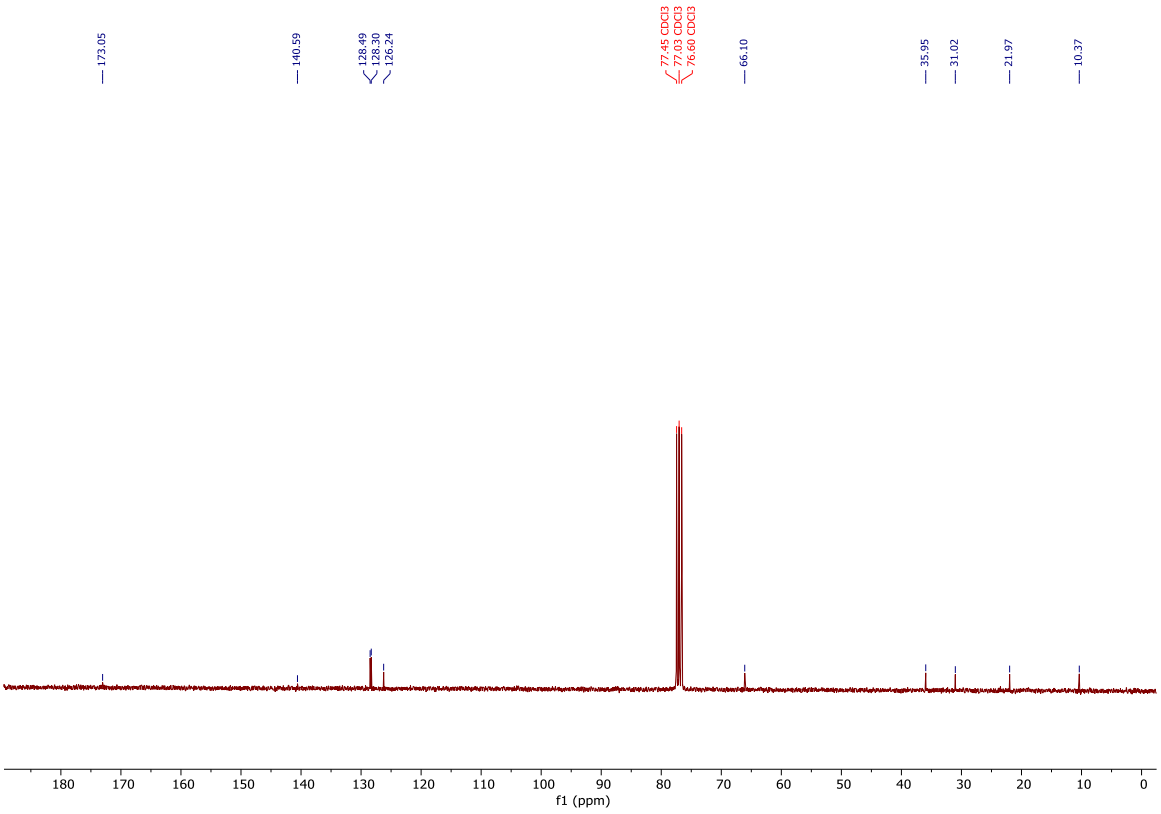




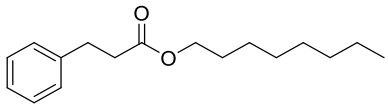
Propyl 3-phenylpropanoate (**8**)

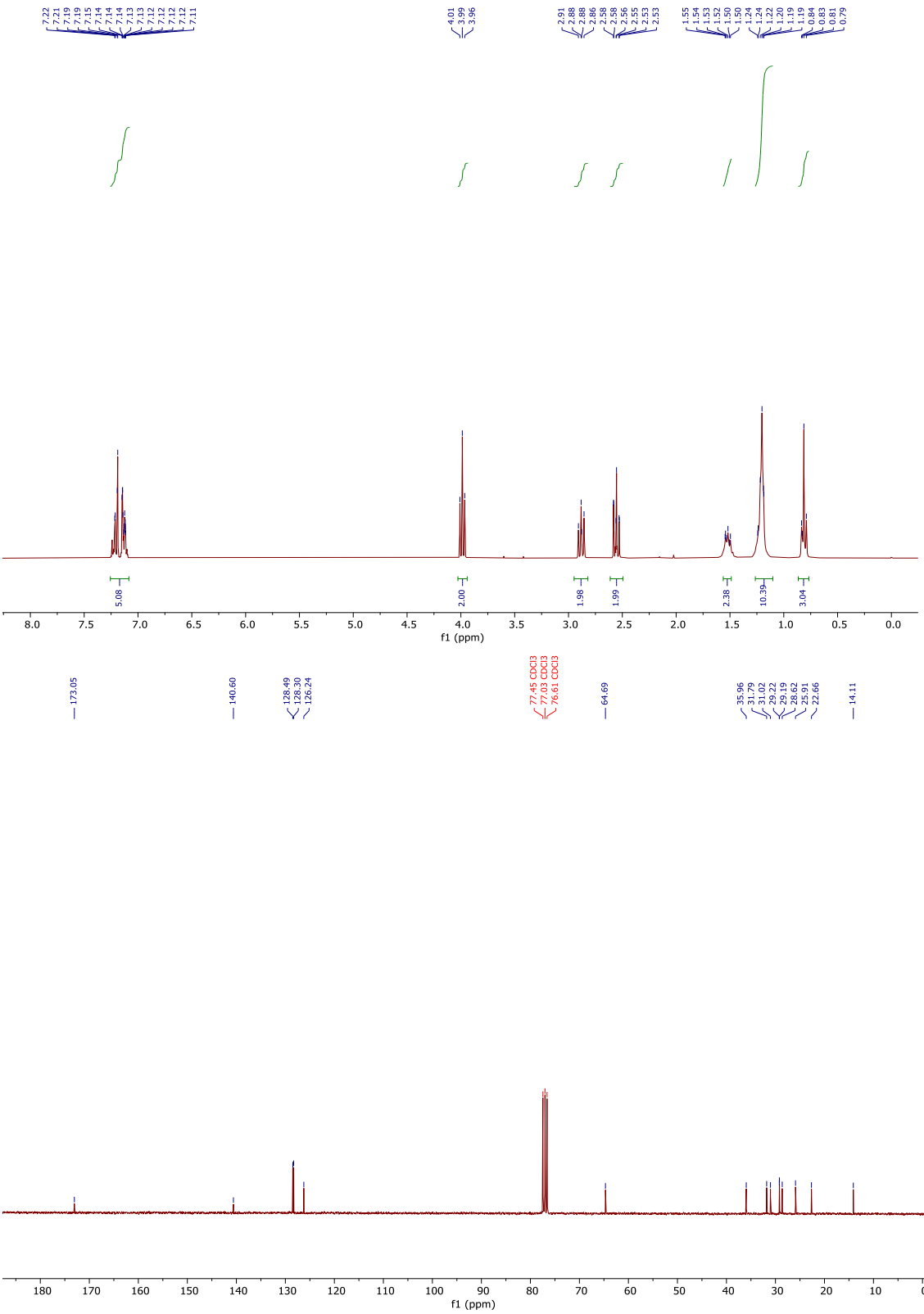




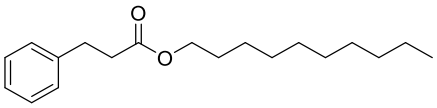


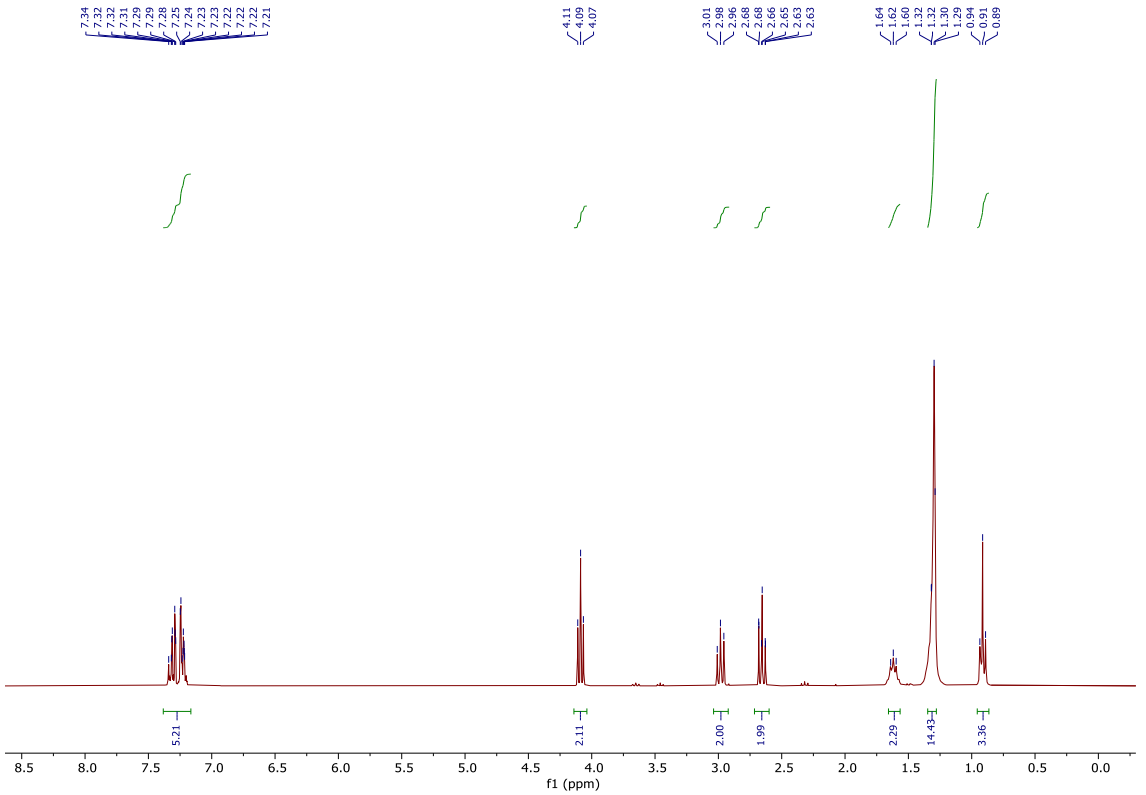
Octyl 3-phenylpropanoate (**9**)

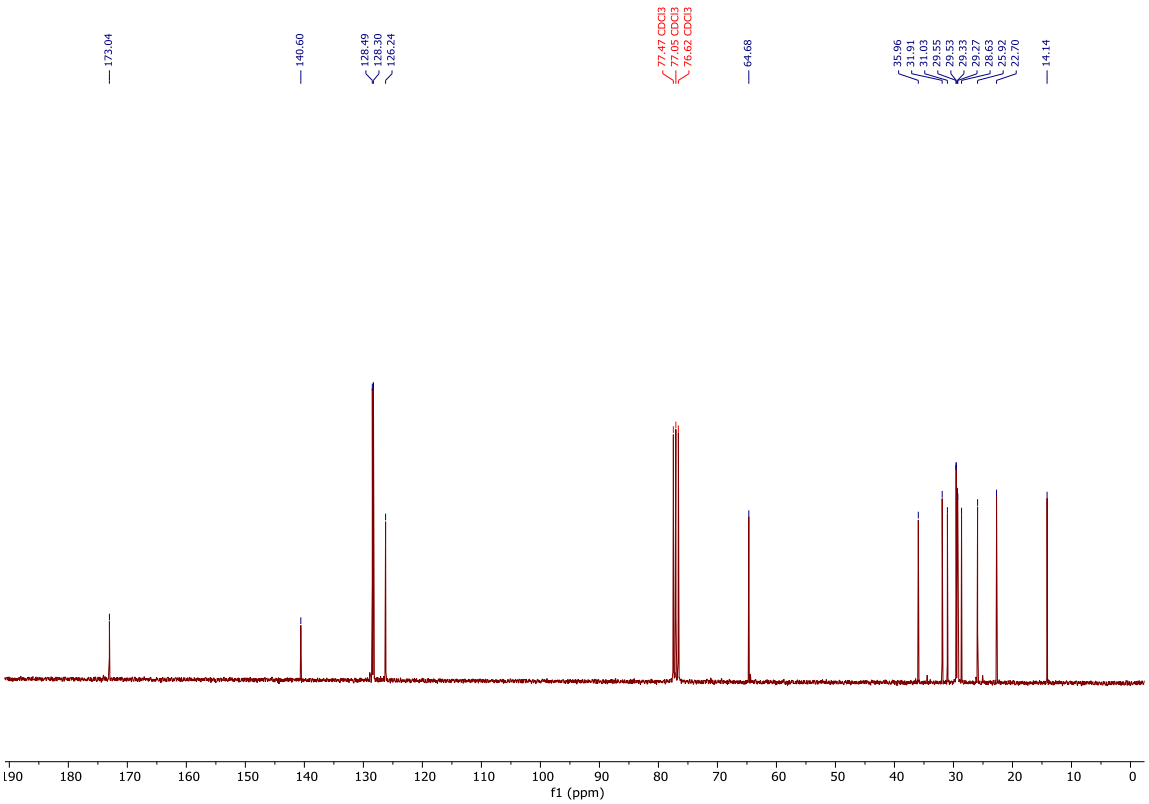




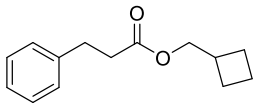
Decyl 3-phenylpropanoate (**10**)

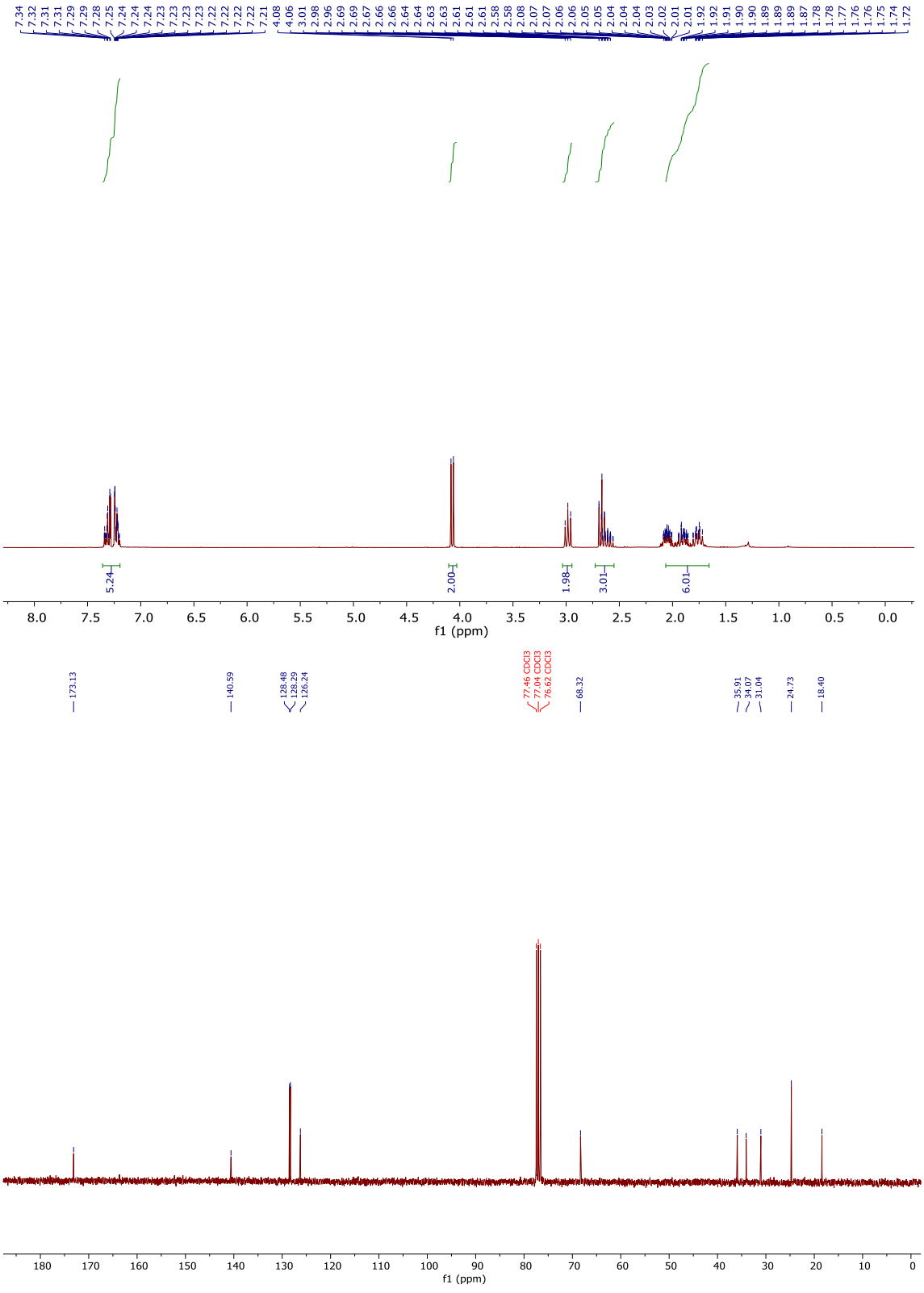




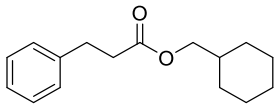


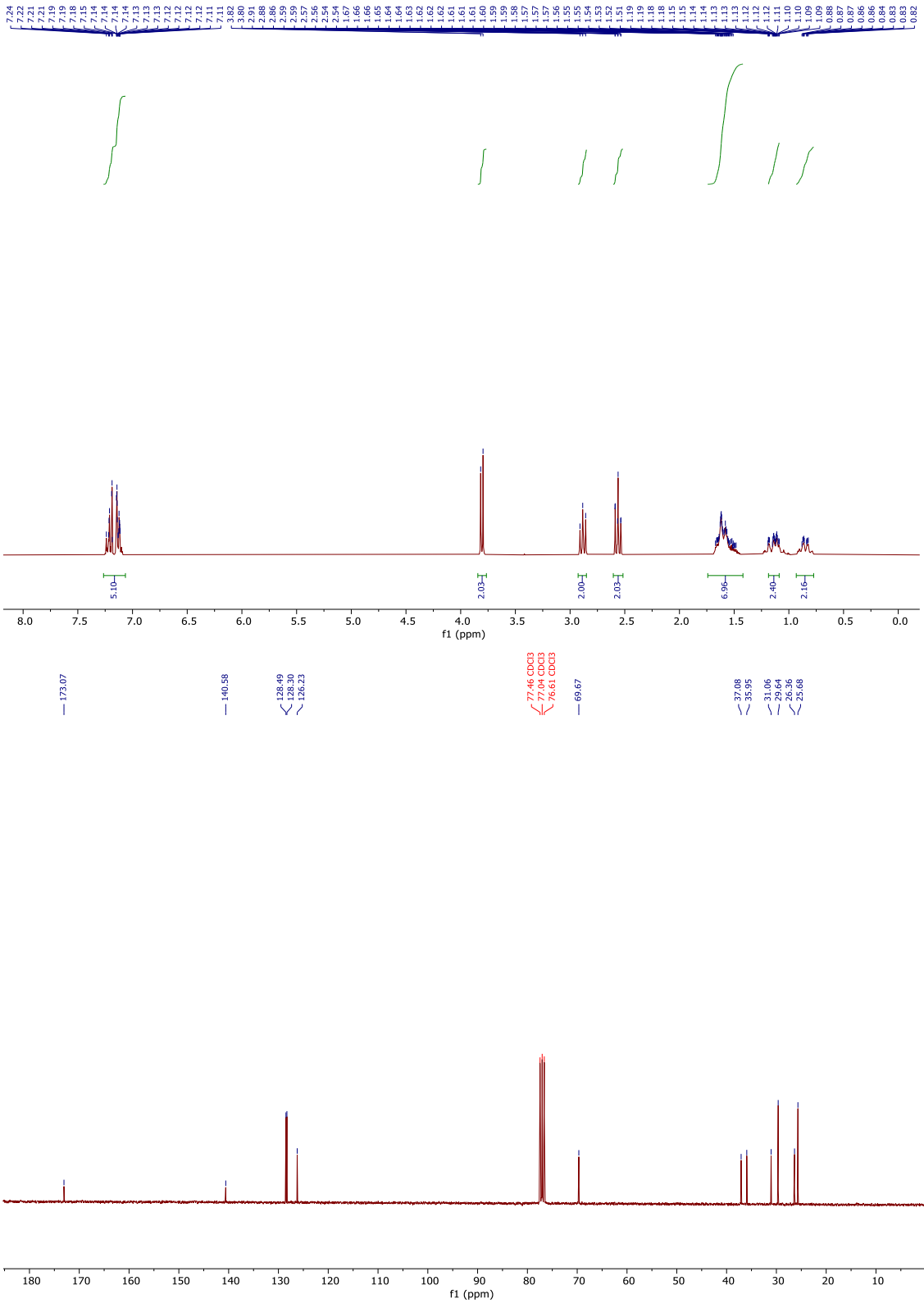
Cyclobutylmethyl 3-phenylpropanoate (**11**)



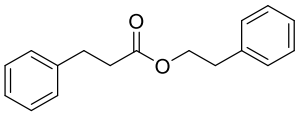


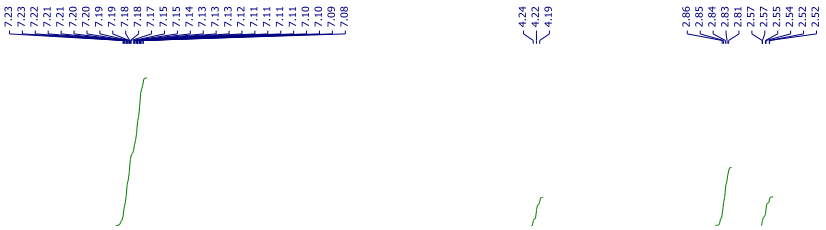
Cyclohexylmethyl 3-phenylpropanoate (**12**)

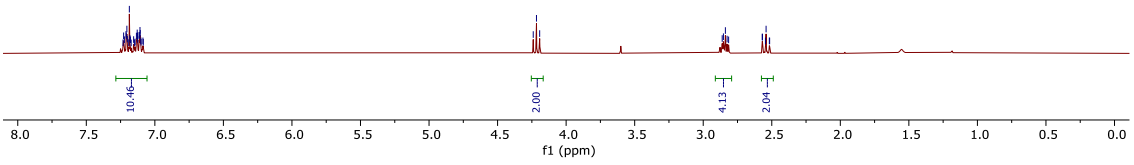


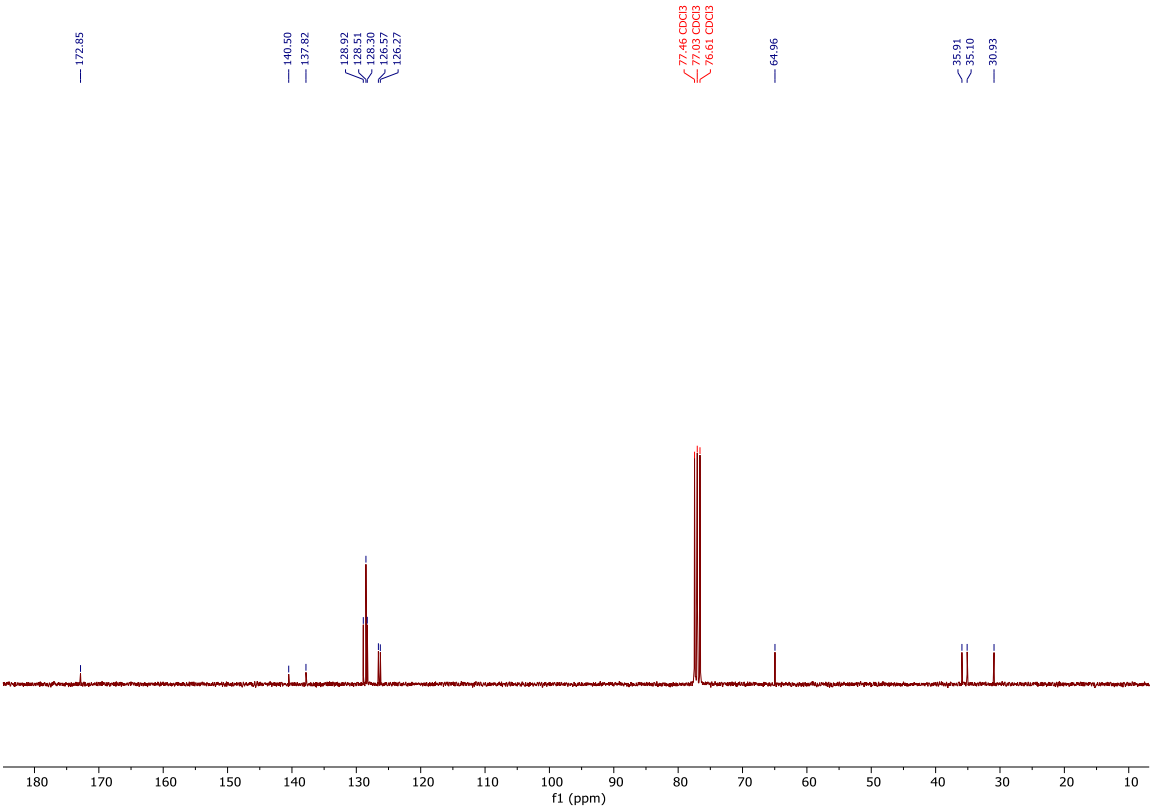


Phenethyl 3-phenylpropanoate (**13**)

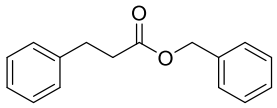


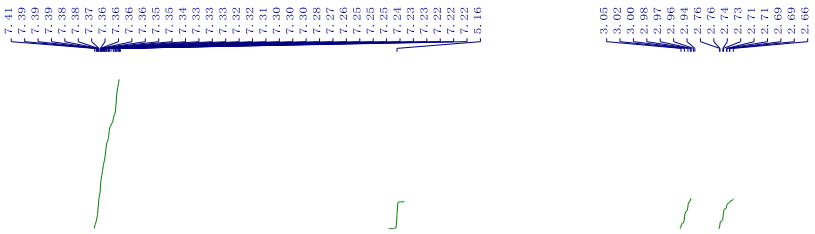


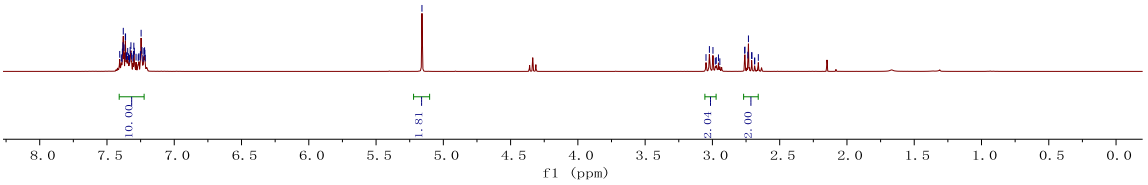


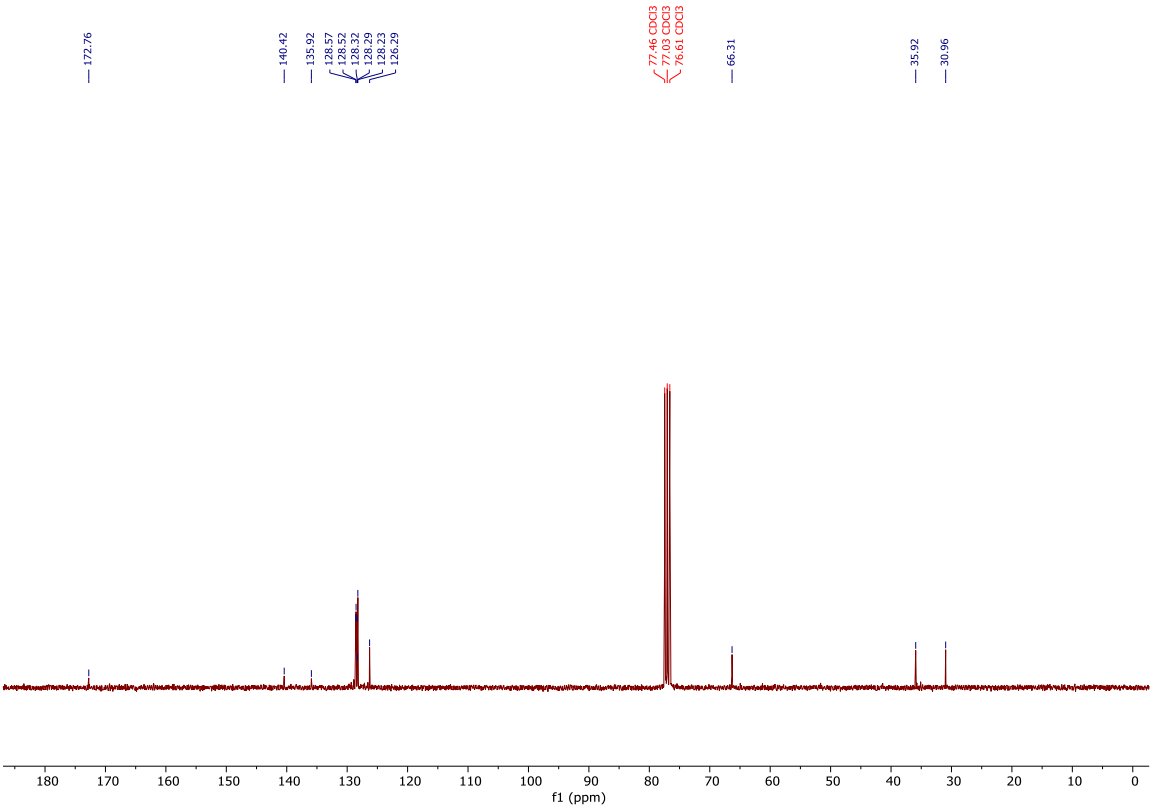


Benzyl 3-phenylpropanoate (**14**)

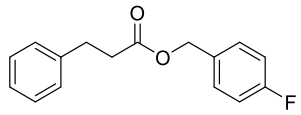


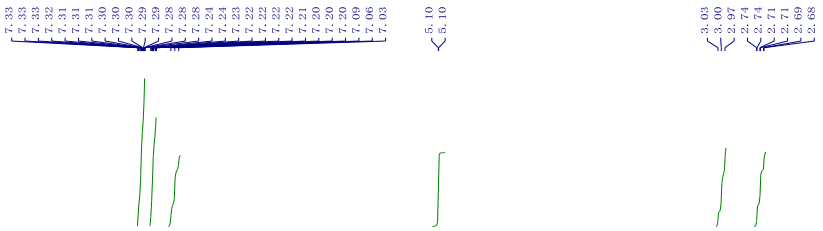


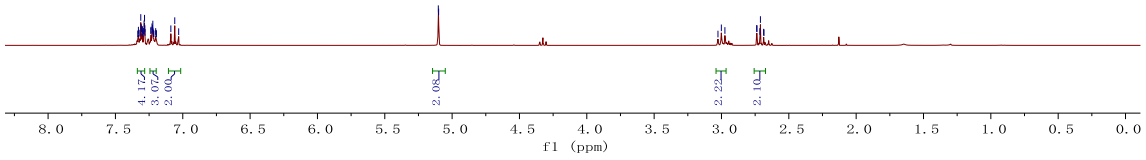


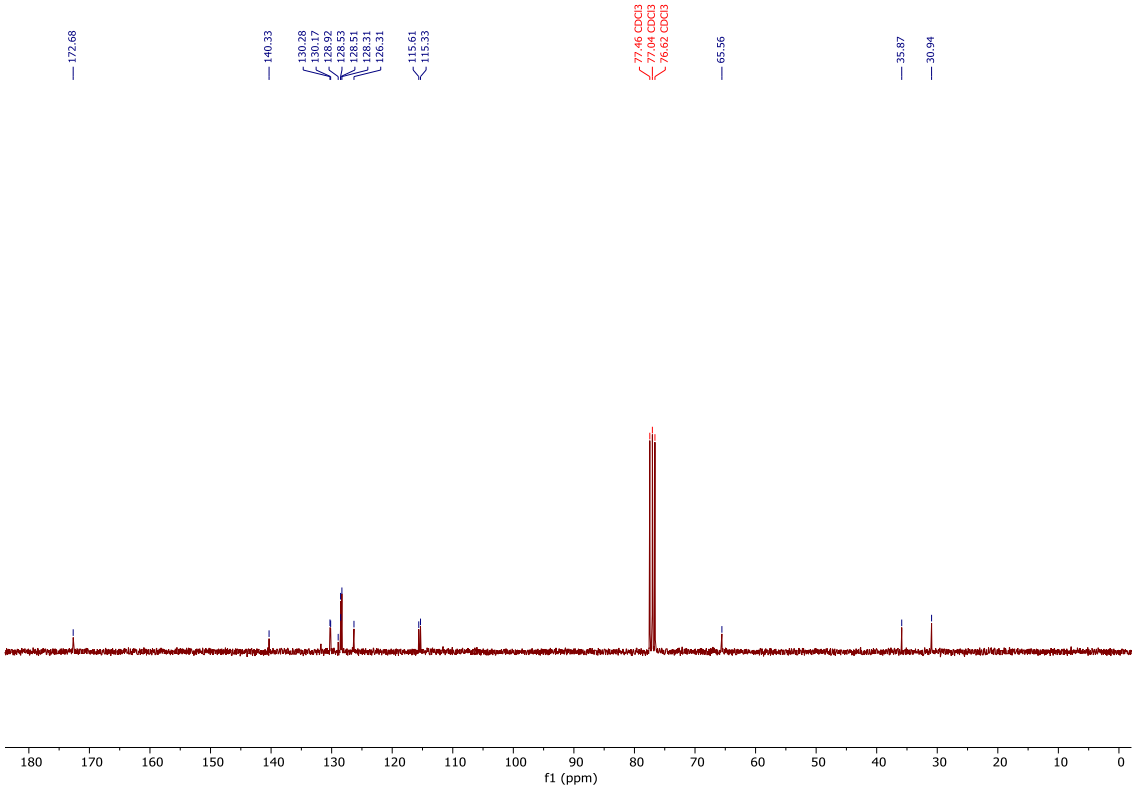


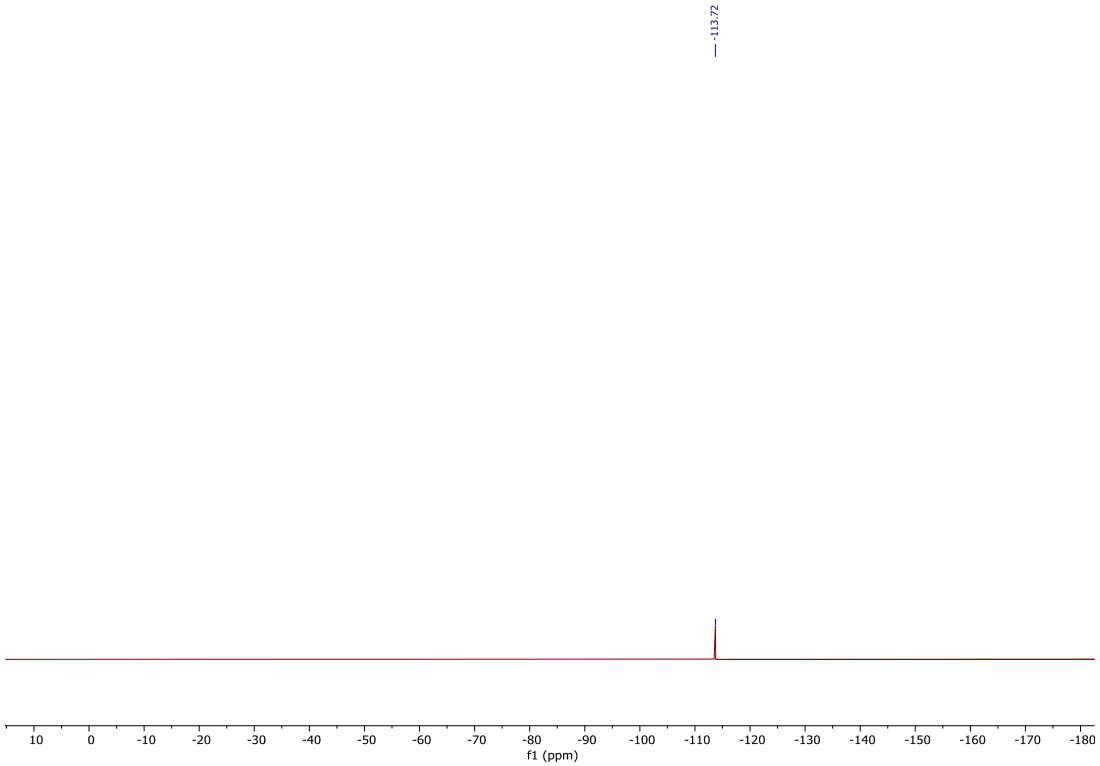
4-Fluorobenzyl 3-phenylpropanoate (**15**)







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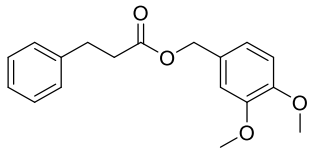
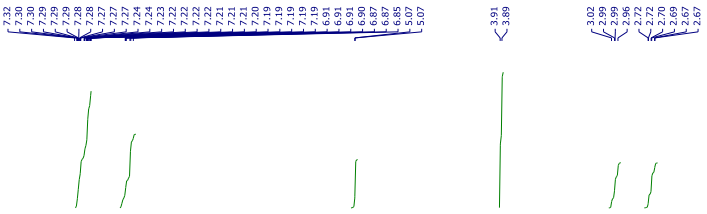
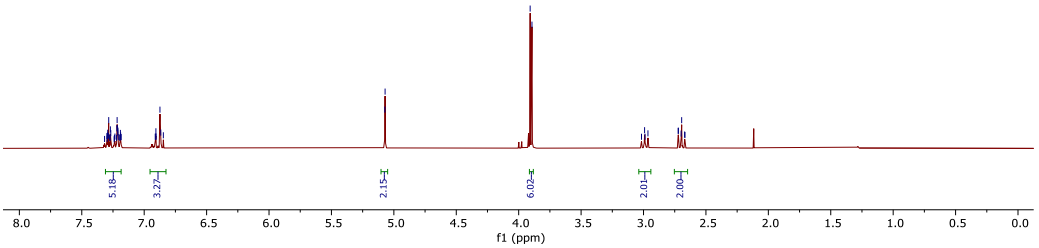
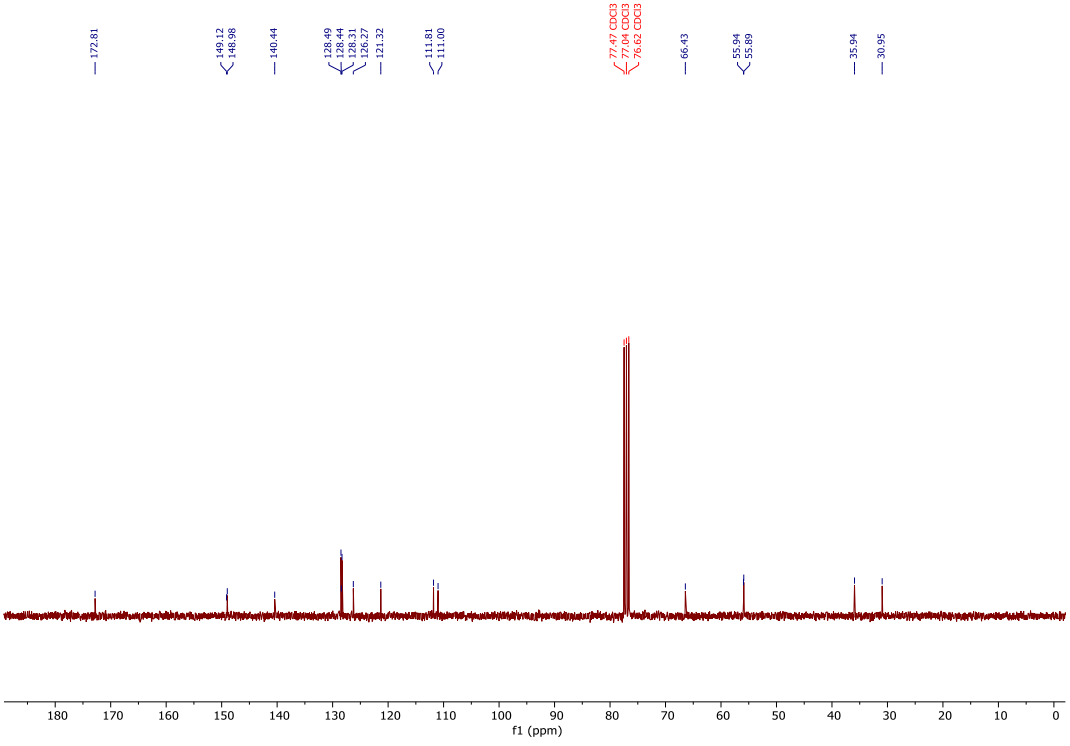
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
f1 (ppm)

3,4-Dimethoxybenzyl 3-phenylpropanoate (**16**)

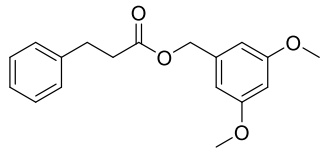


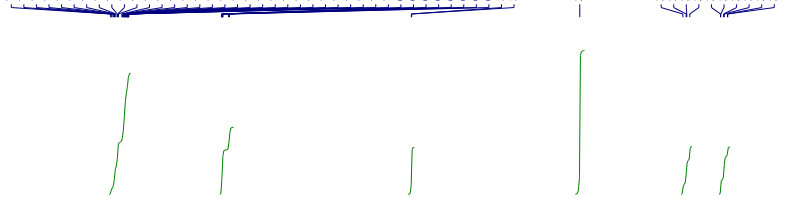


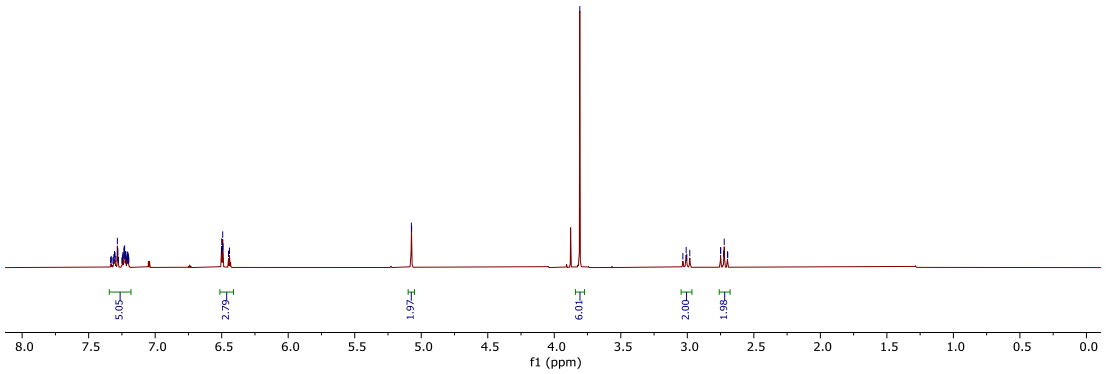


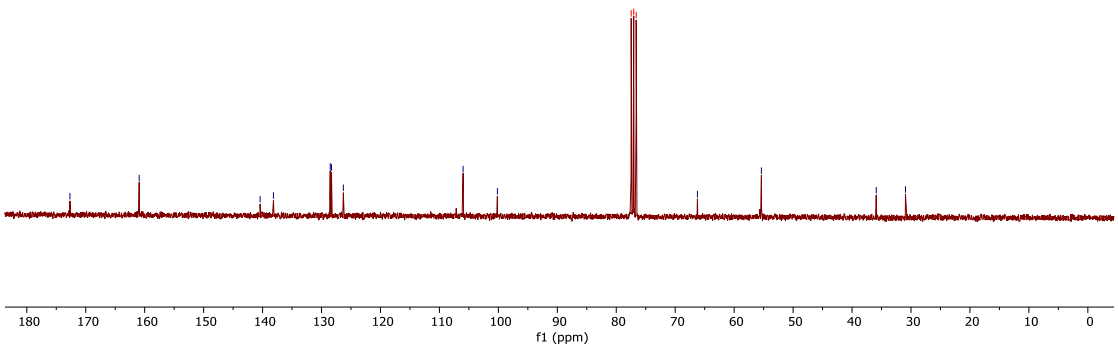


3,5-Dimethoxybenzyl 3-phenylpropanoate (**17**)

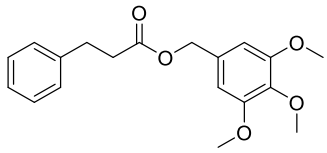


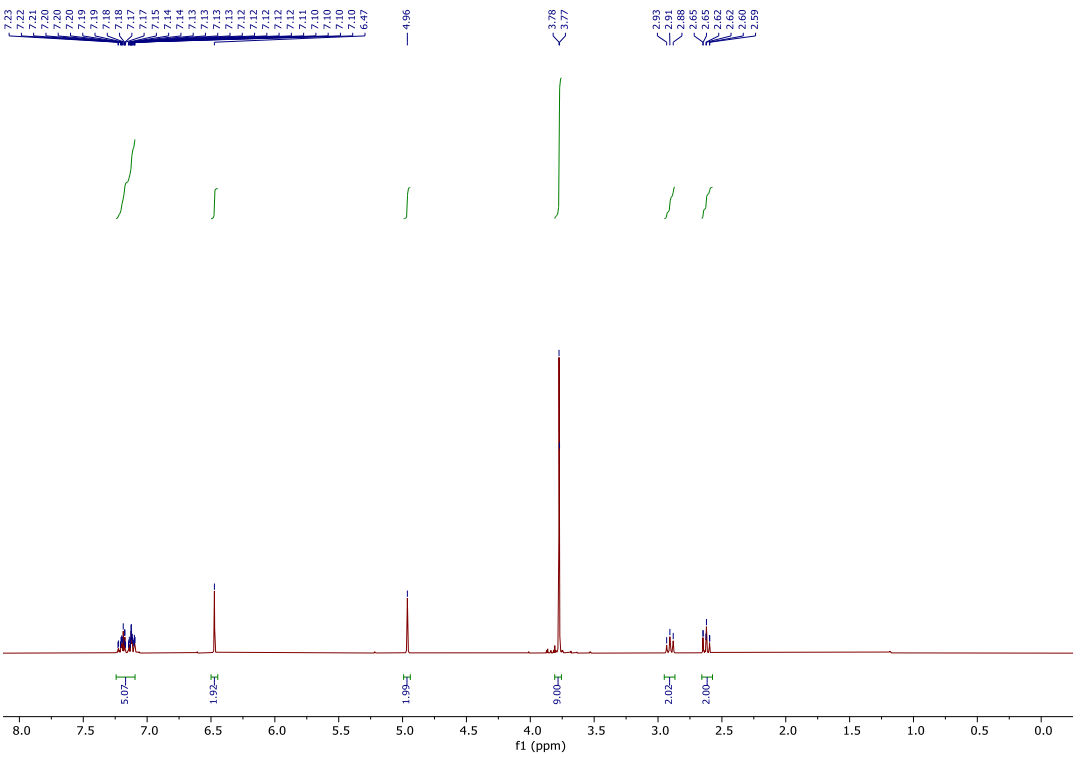


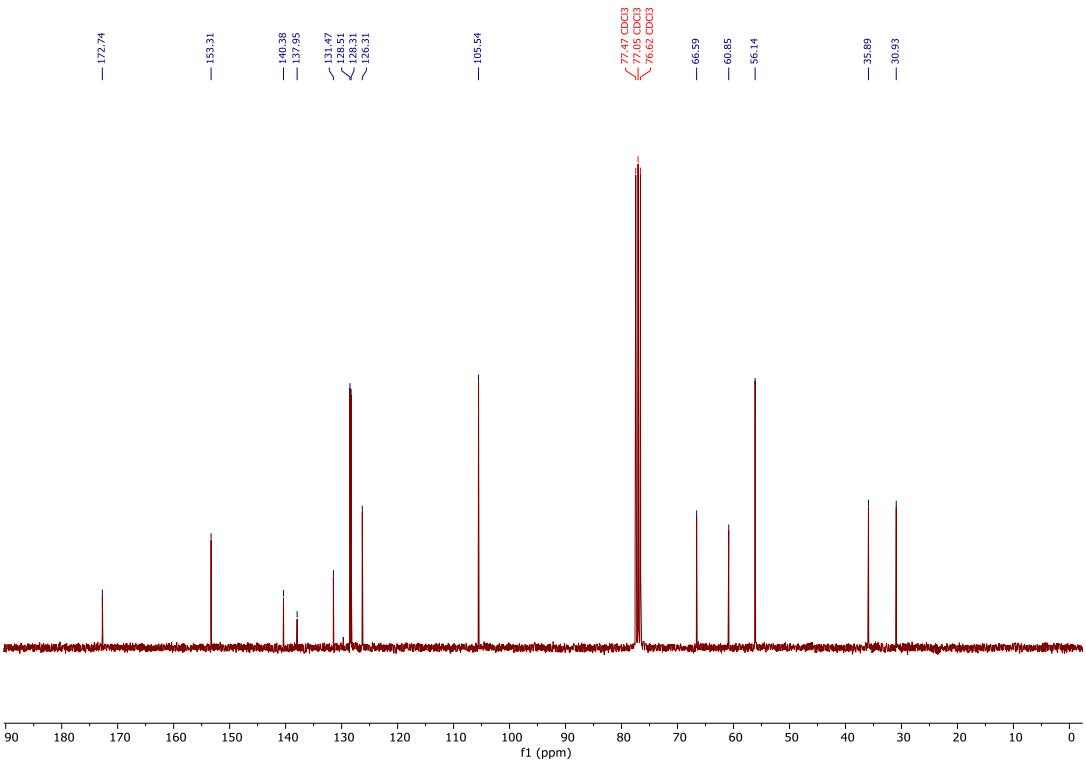




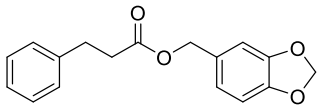
3,4,5-Trimethoxybenzyl 3-phenylpropanoate (**18**)

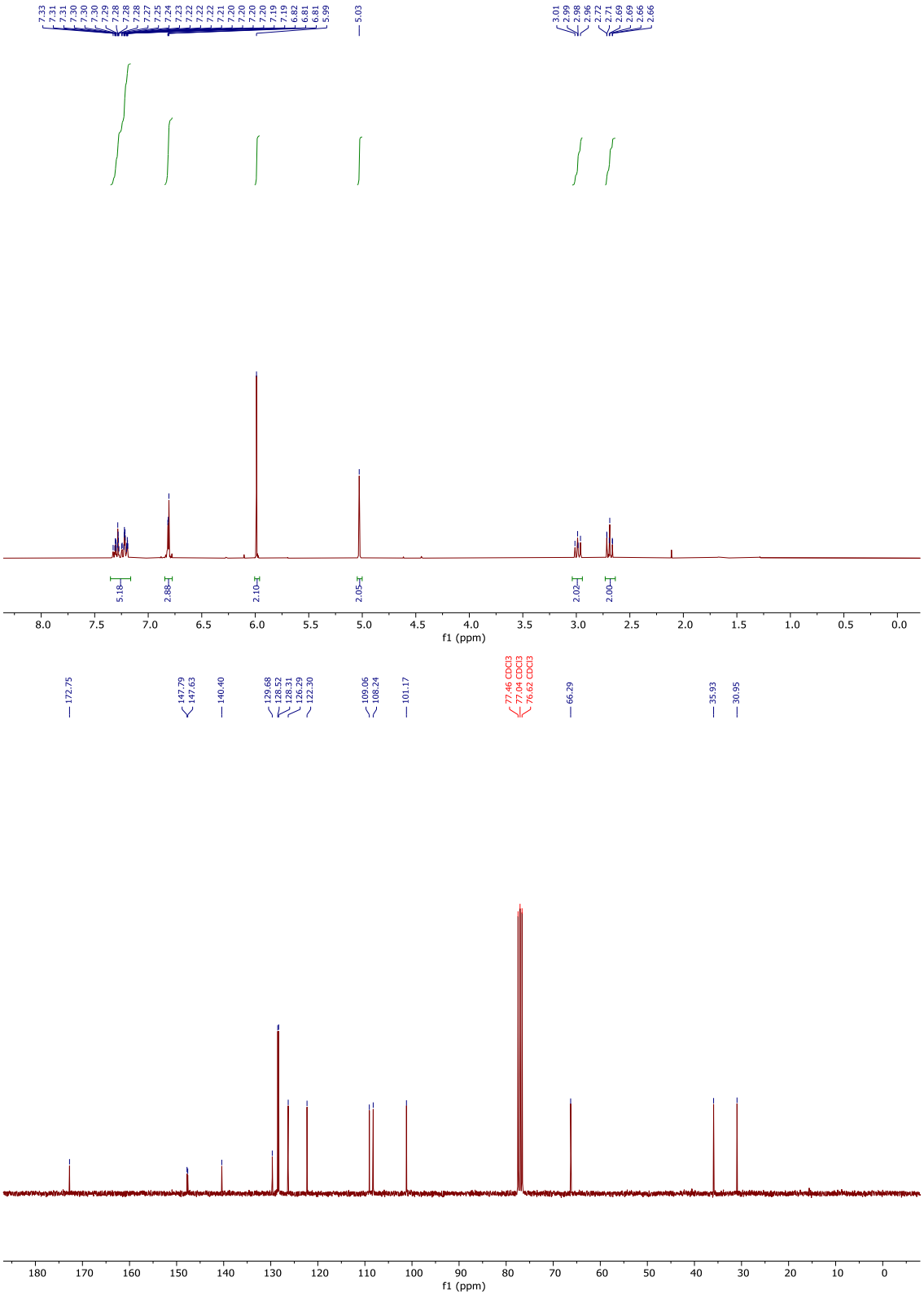




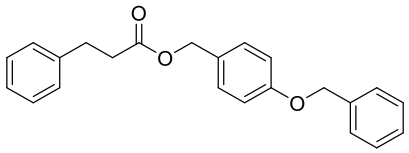


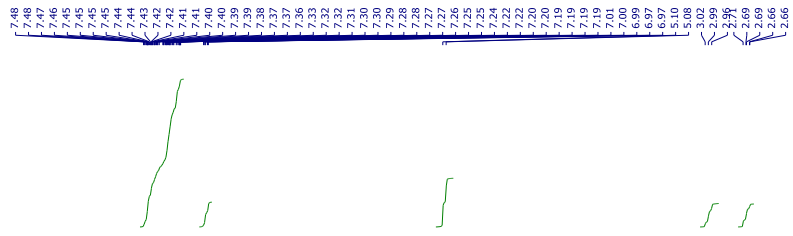
Benzo[d][1,3]dioxol-5-ylmethyl 3-phenylpropanoate (**19**)

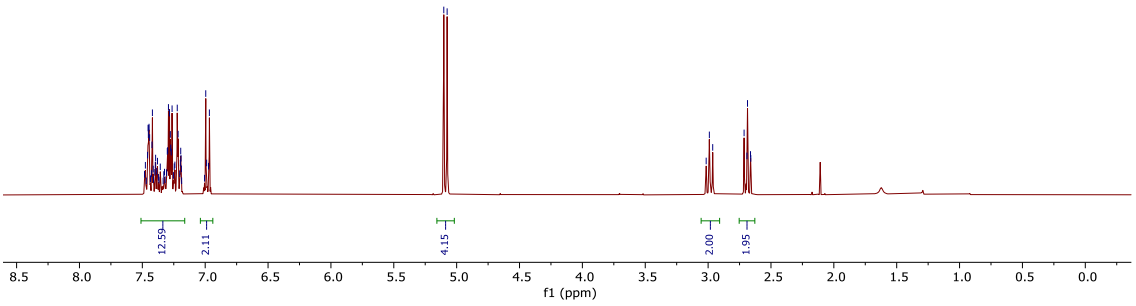


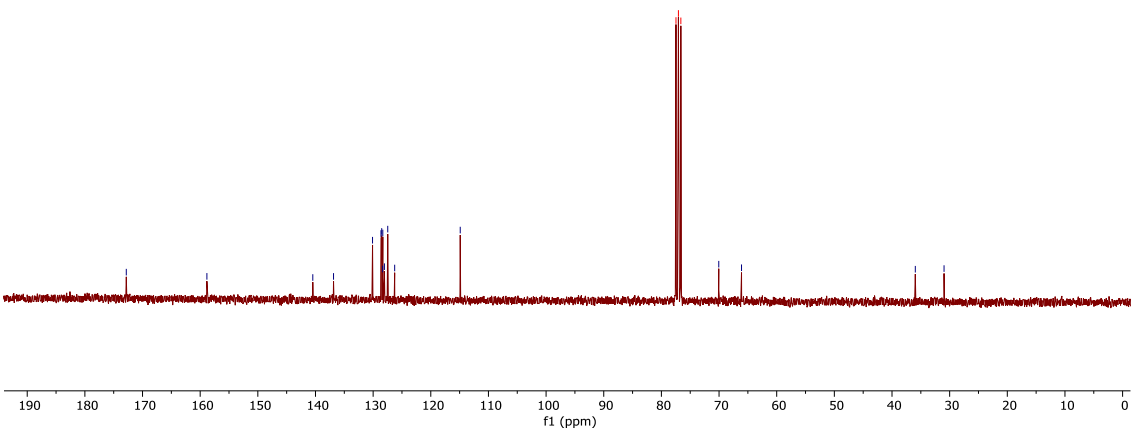


4-(Benzyloxy)benzyl 3-phenylpropanoate (**20**)

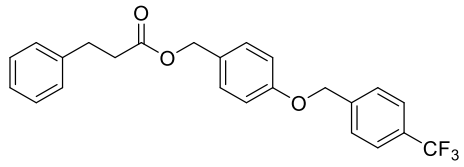


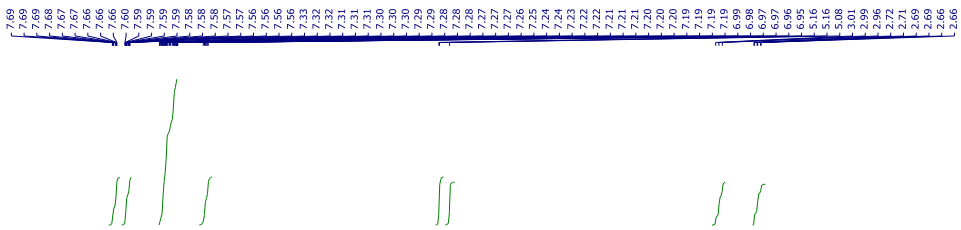


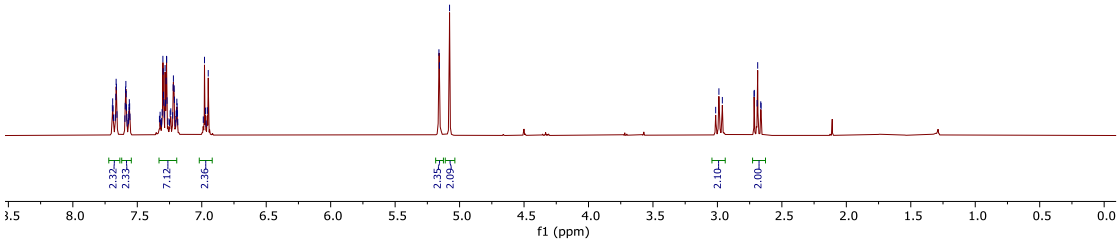


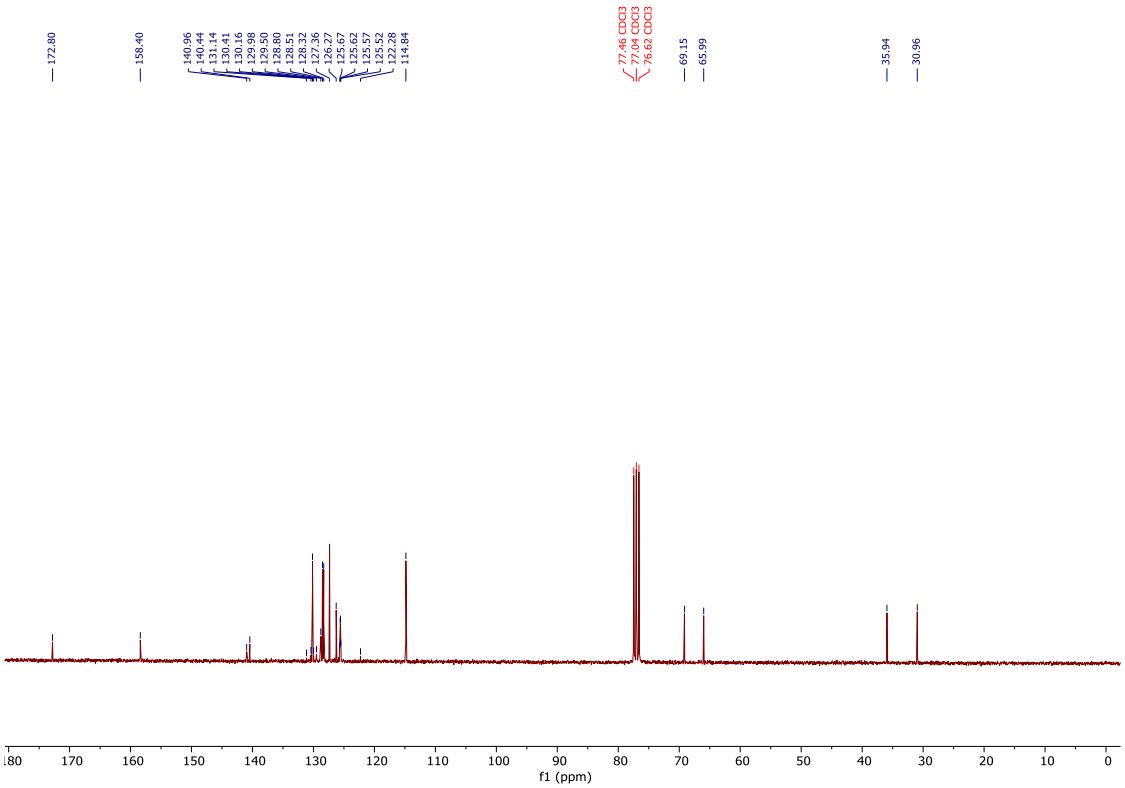


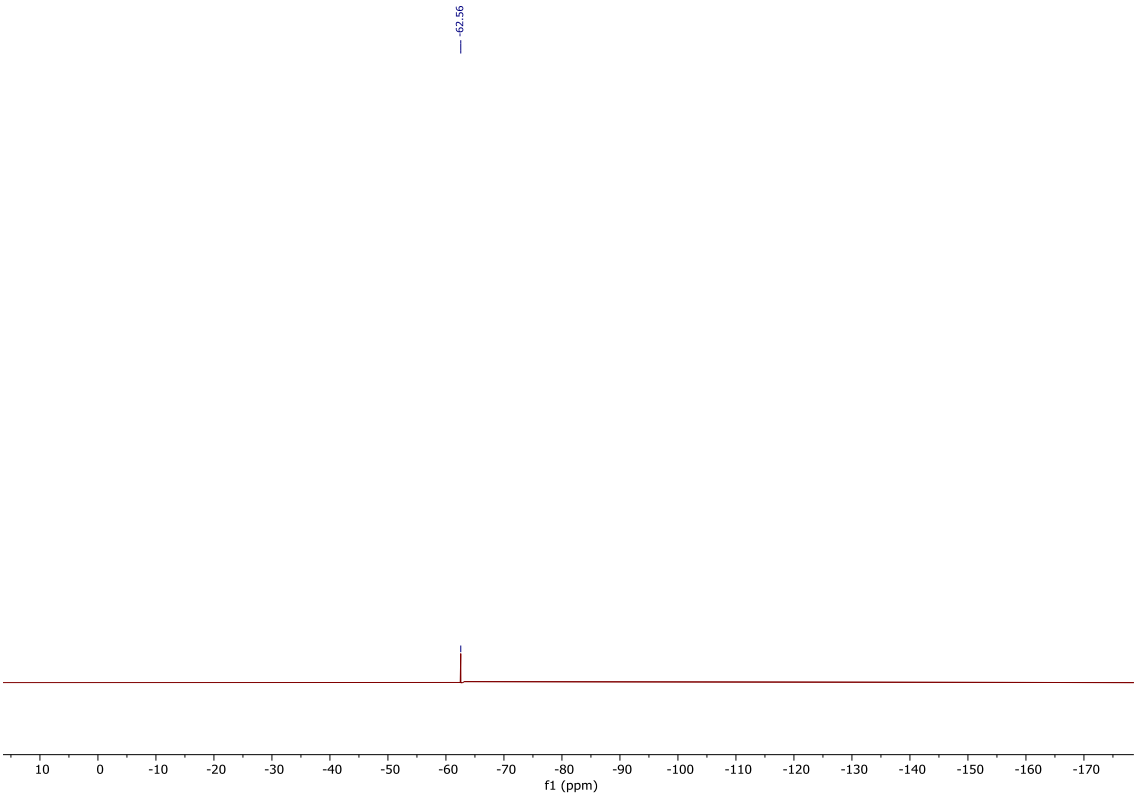
4-((4-(Trifluoromethyl)benzyl)oxy)benzyl 3-phenylpropanoate (**21**)



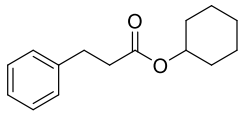


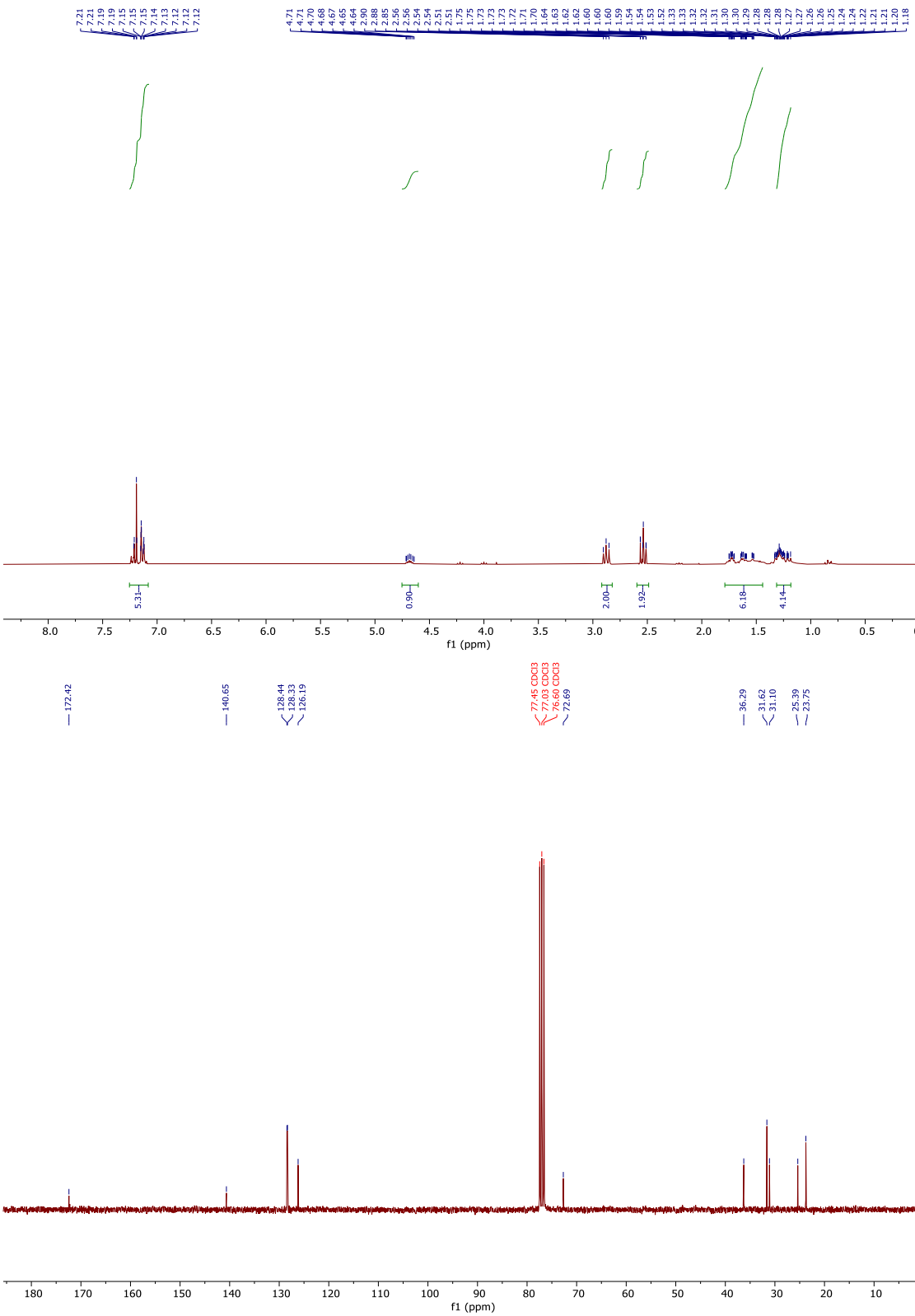




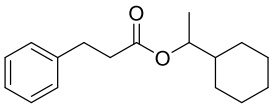

-62.56
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
f1 (ppm)

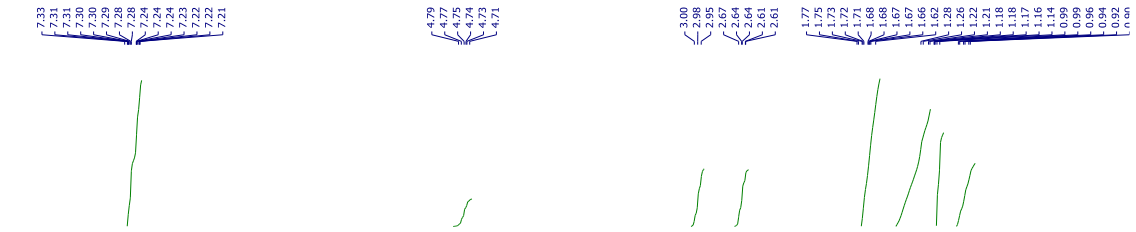
Cyclohexyl 3-phenylpropanoate (**22**)

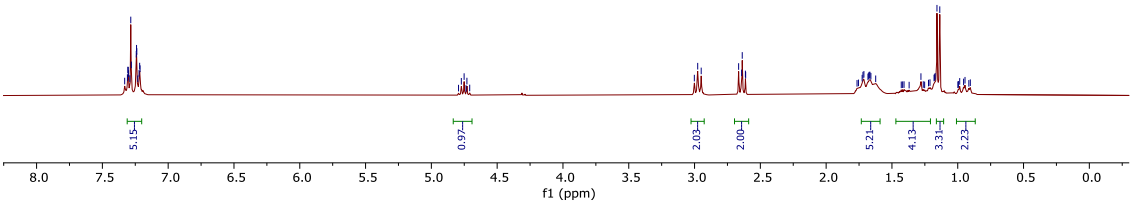


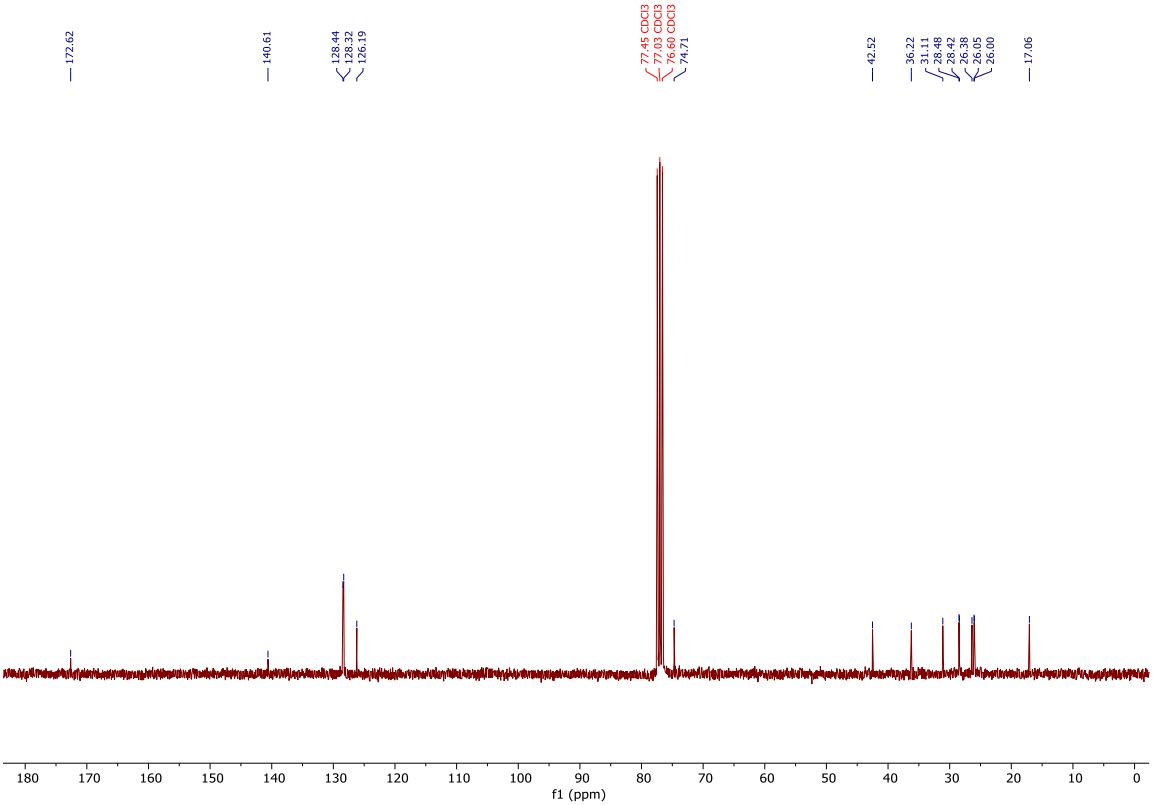


1-Cyclohexylethyl 3-phenylpropanoate (**23**)

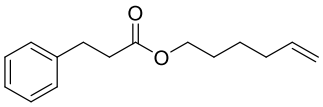


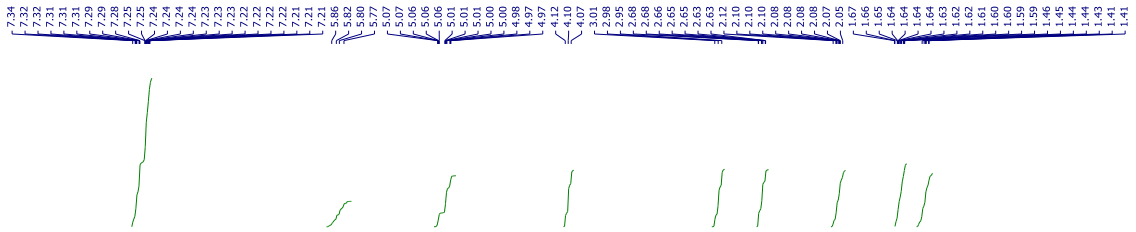


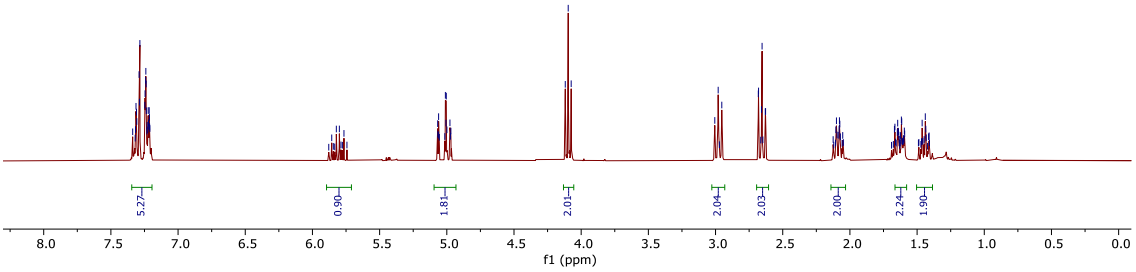


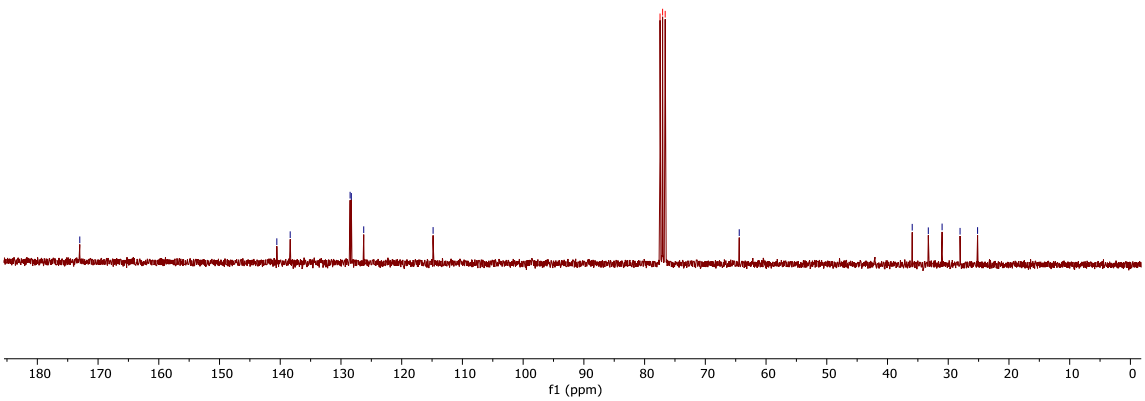


Hex-5-en-1-yl 3-phenylpropanoate (**24**)

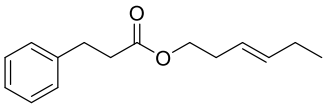


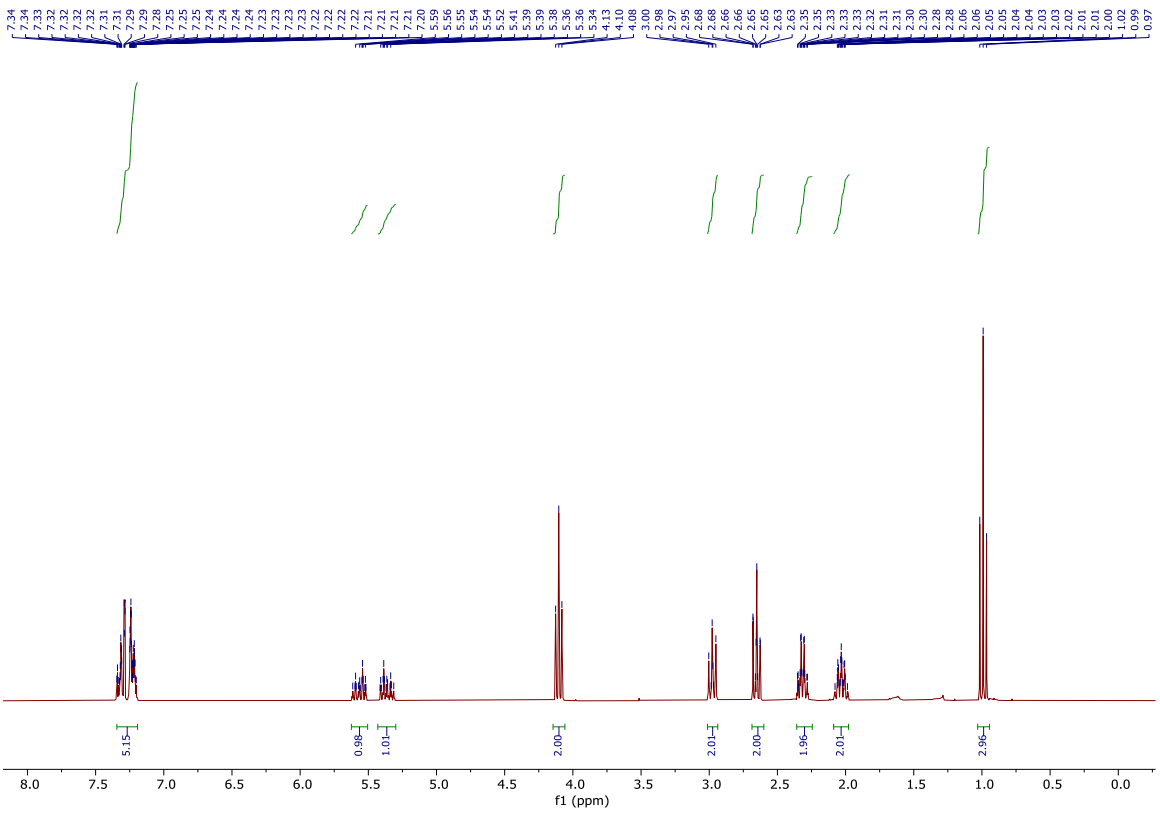


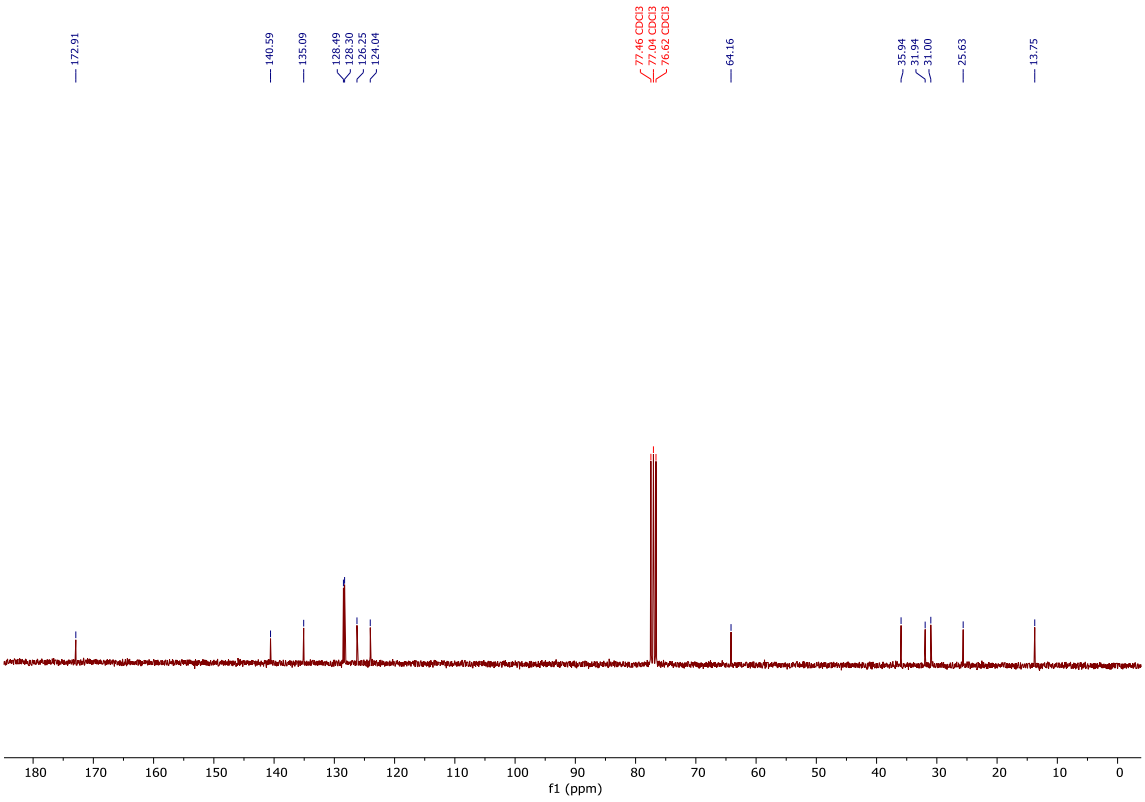




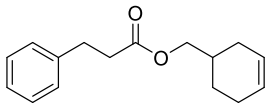
(E)-Hex-3-en-1-yl 3-phenylpropanoate (**25**)

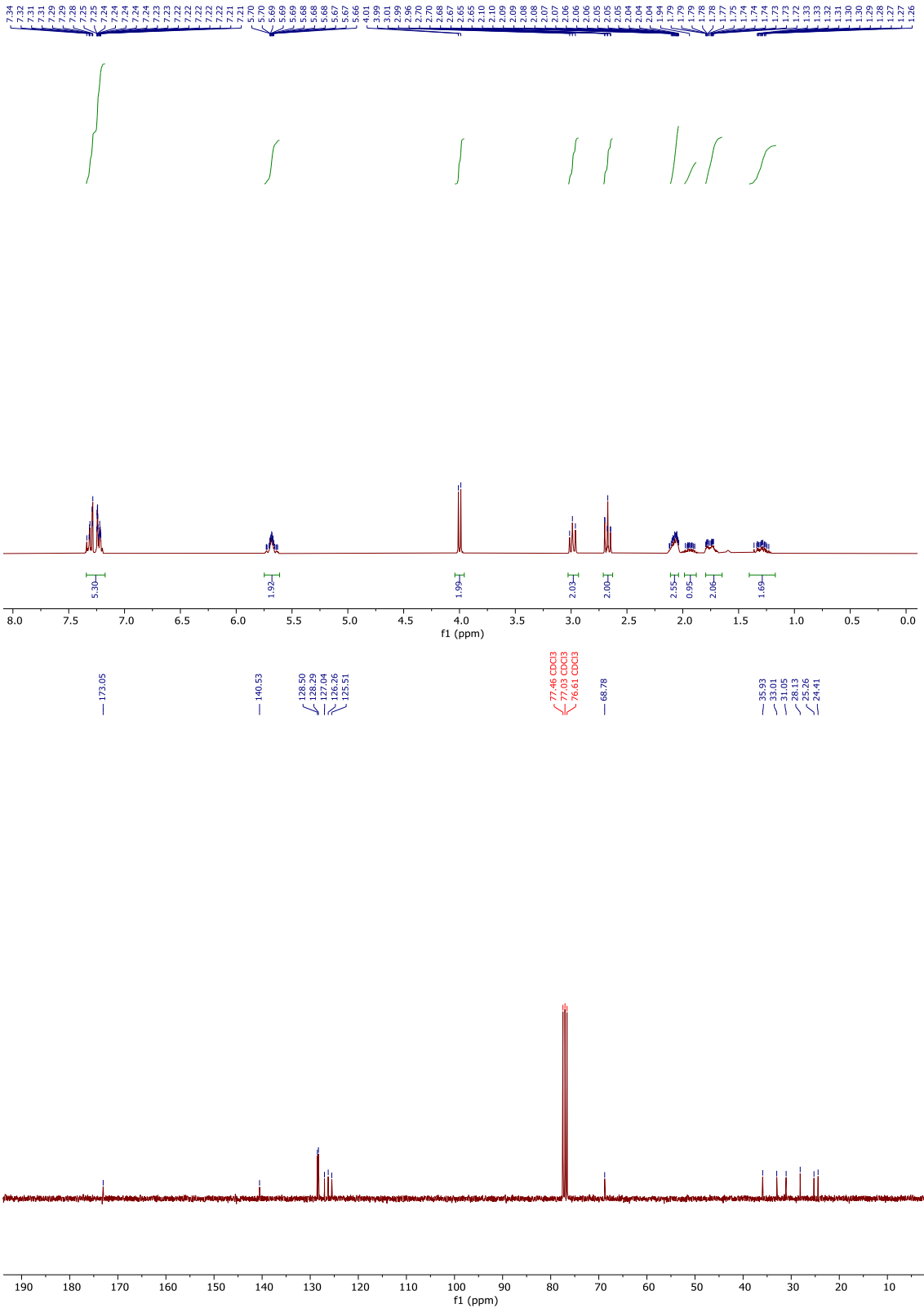




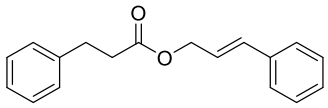


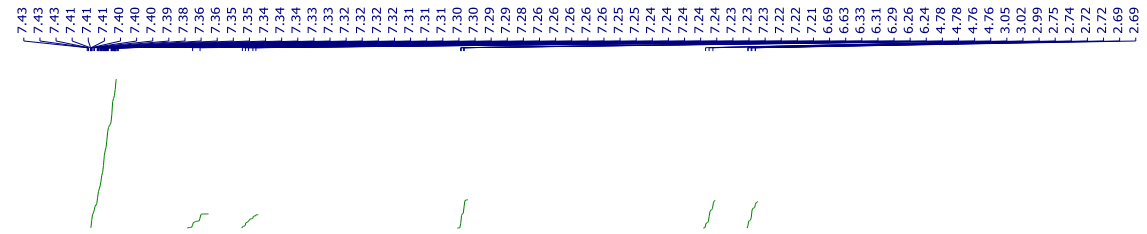
Cyclohex-3-en-1-ylmethyl 3-phenylpropanoate (**26**)

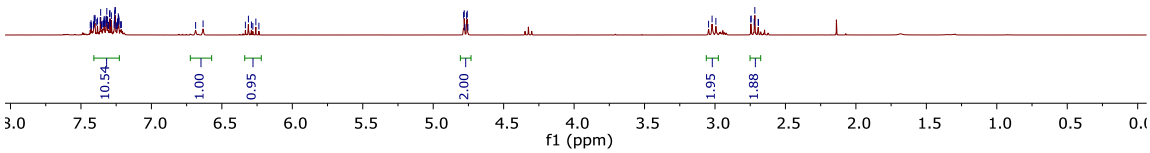


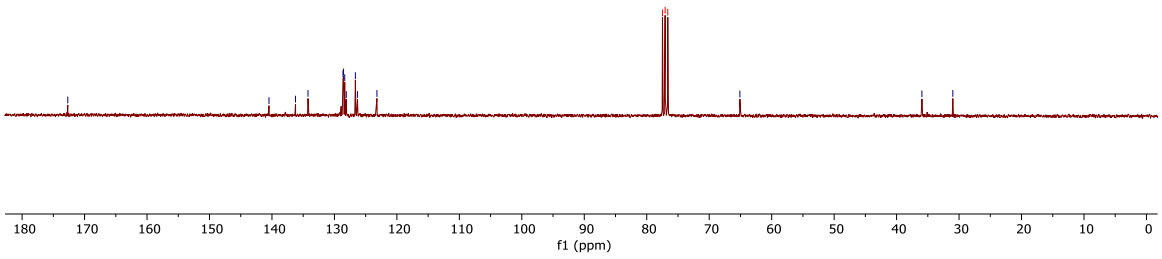


Cinnamyl 3-phenylpropanoate (**27**)

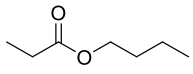


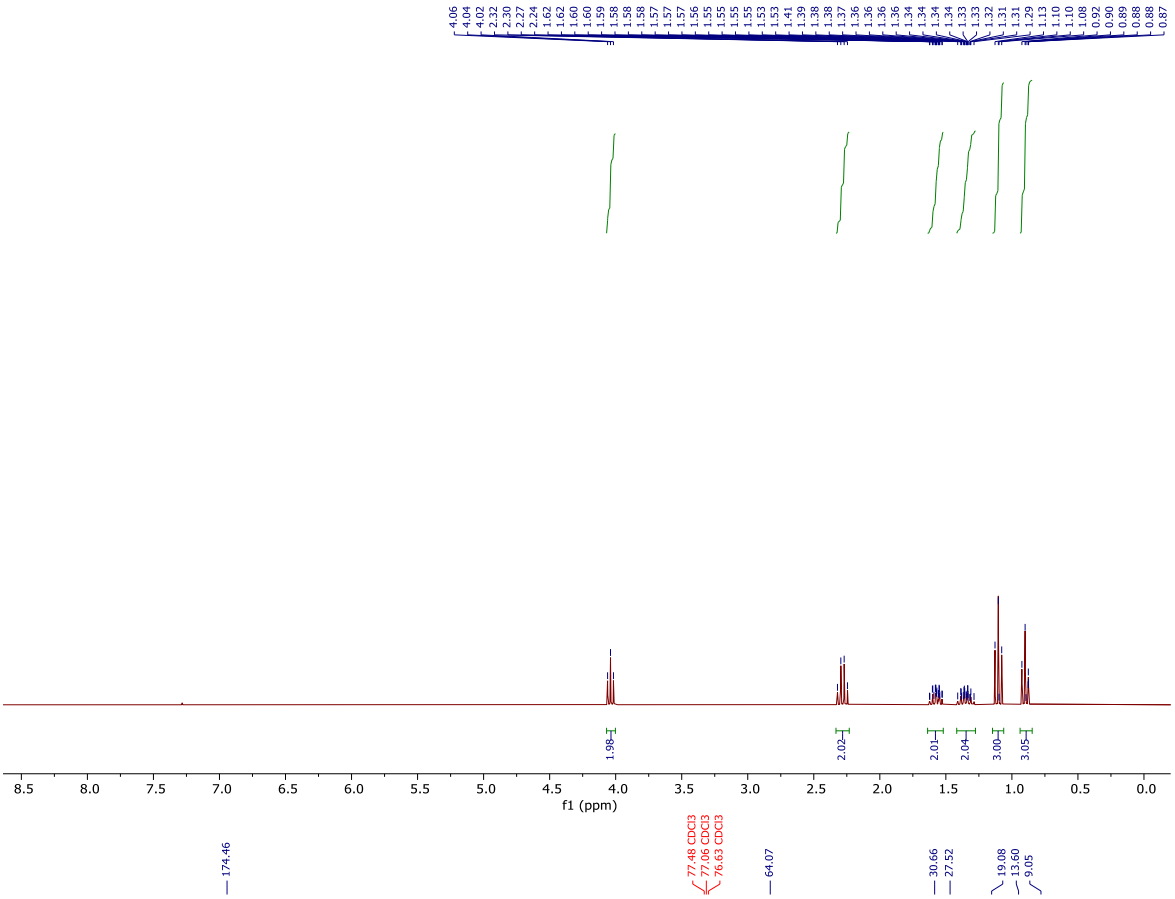


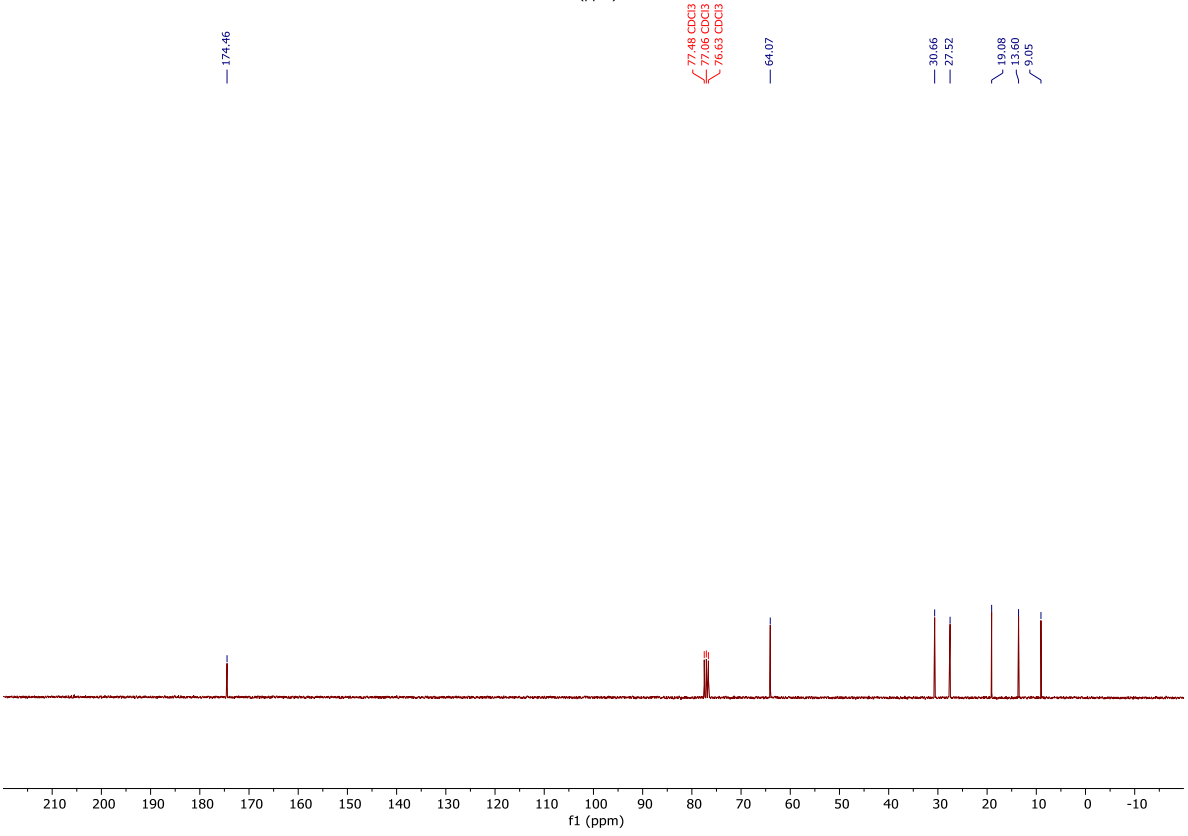




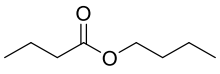
Butyl propionate (**28**)

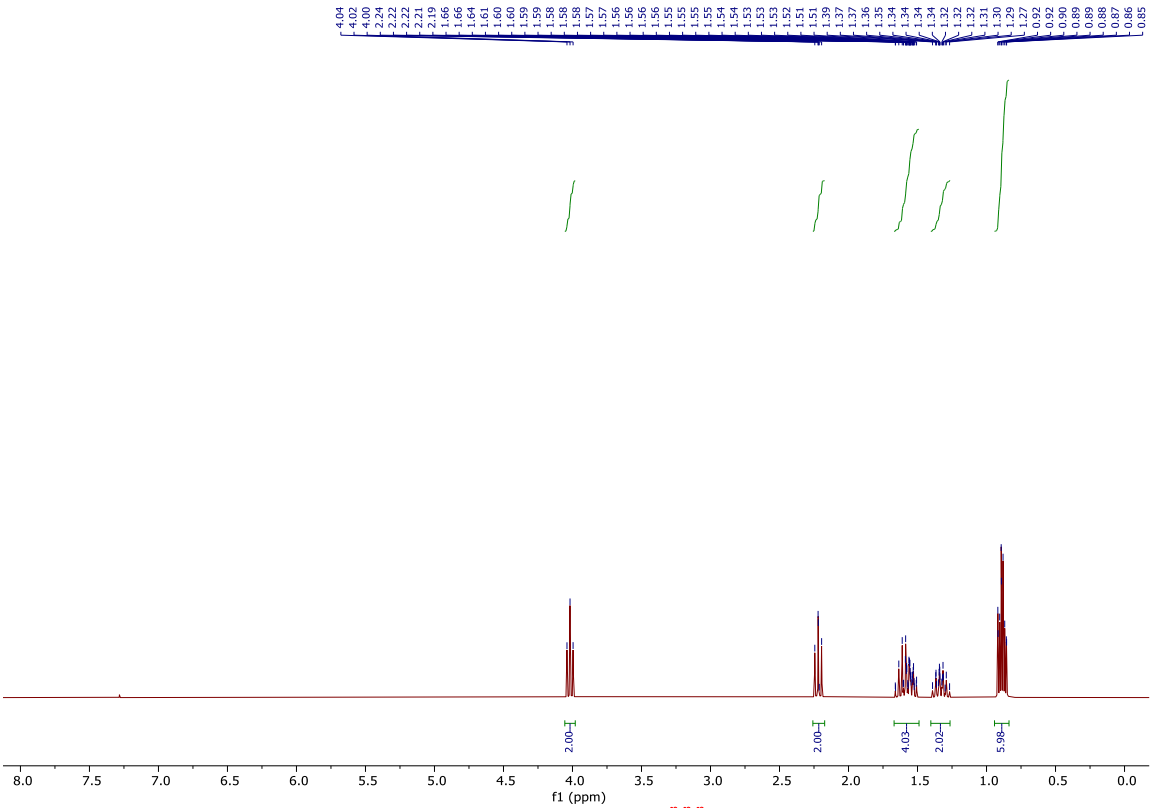


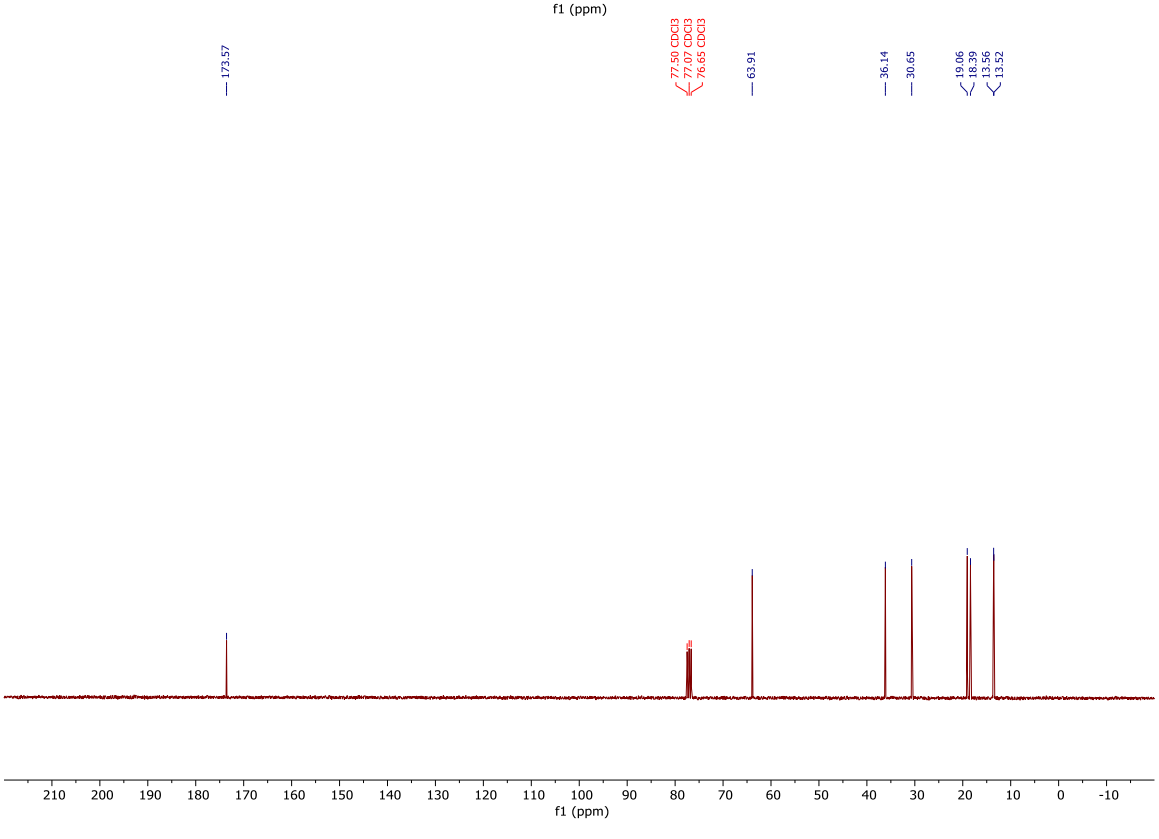




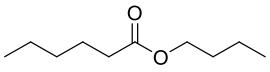
Butyl butyrate (**29**)

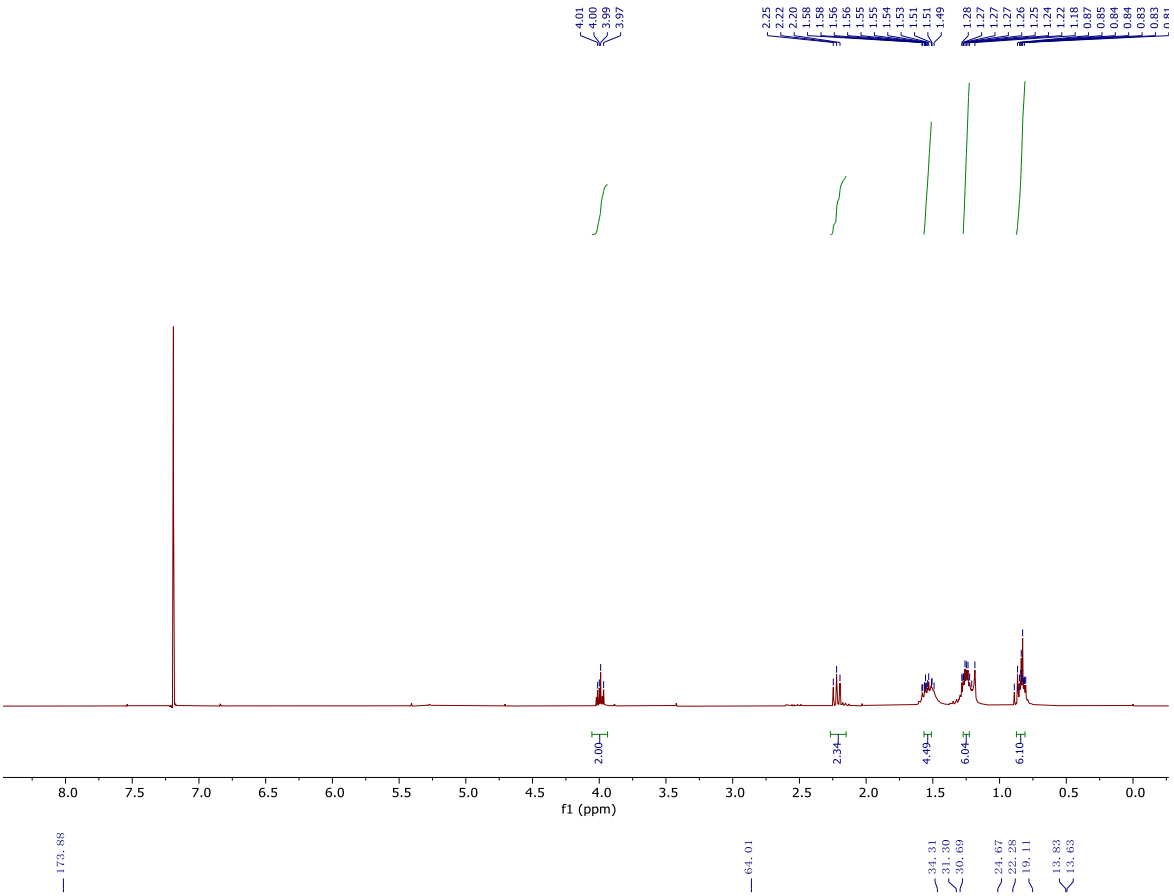


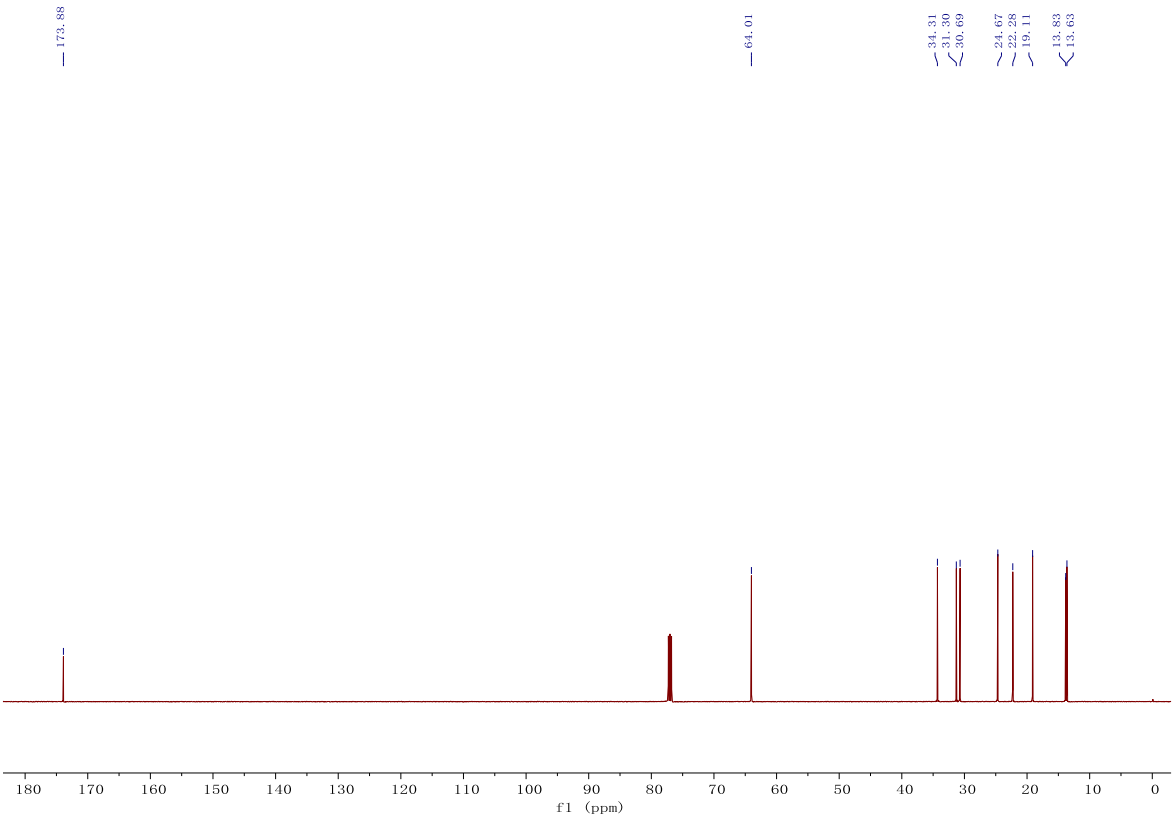




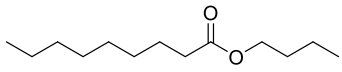
Butyl hexanoate (**30**)

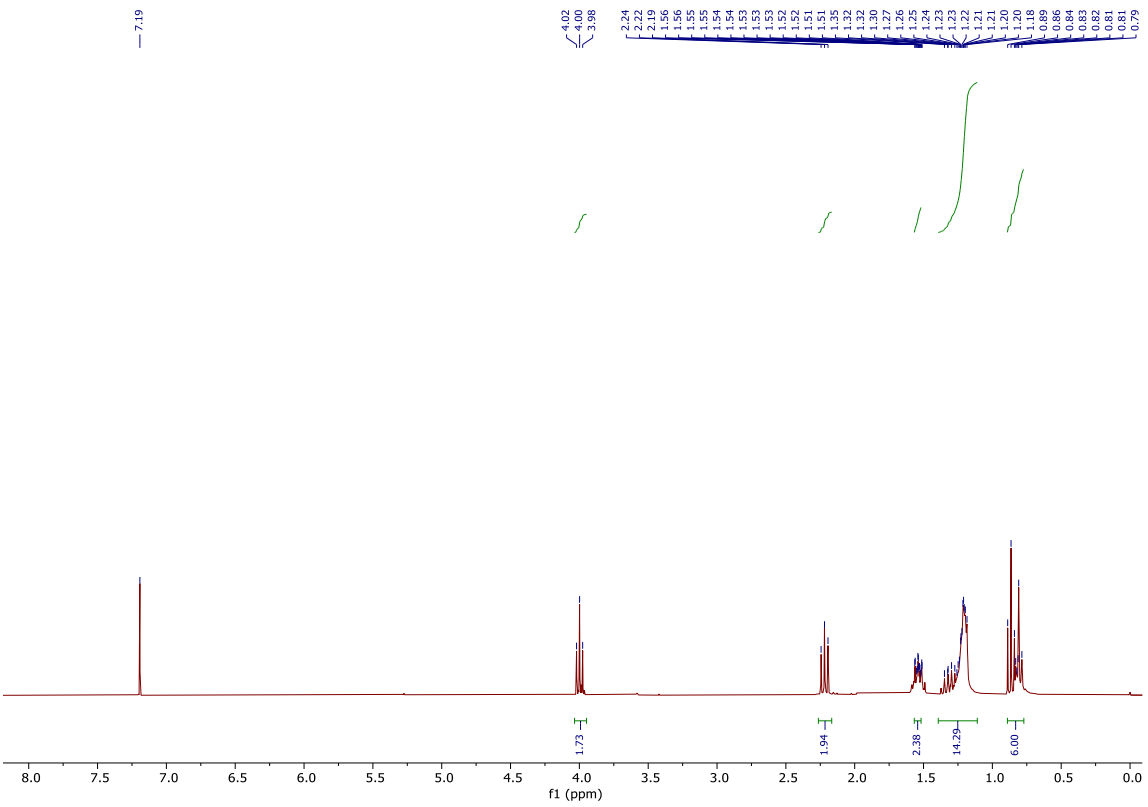


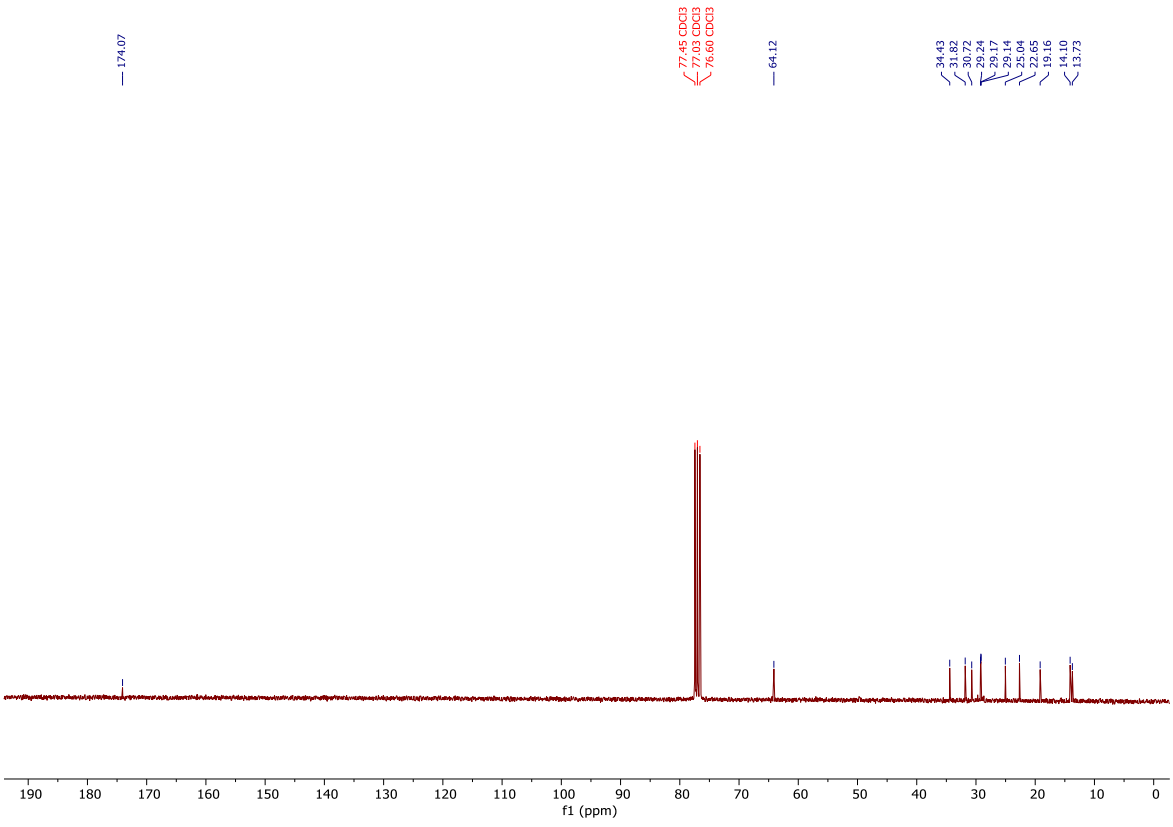




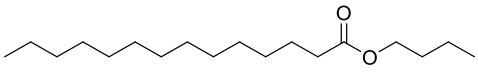
Butyl nonanoate (**31**)

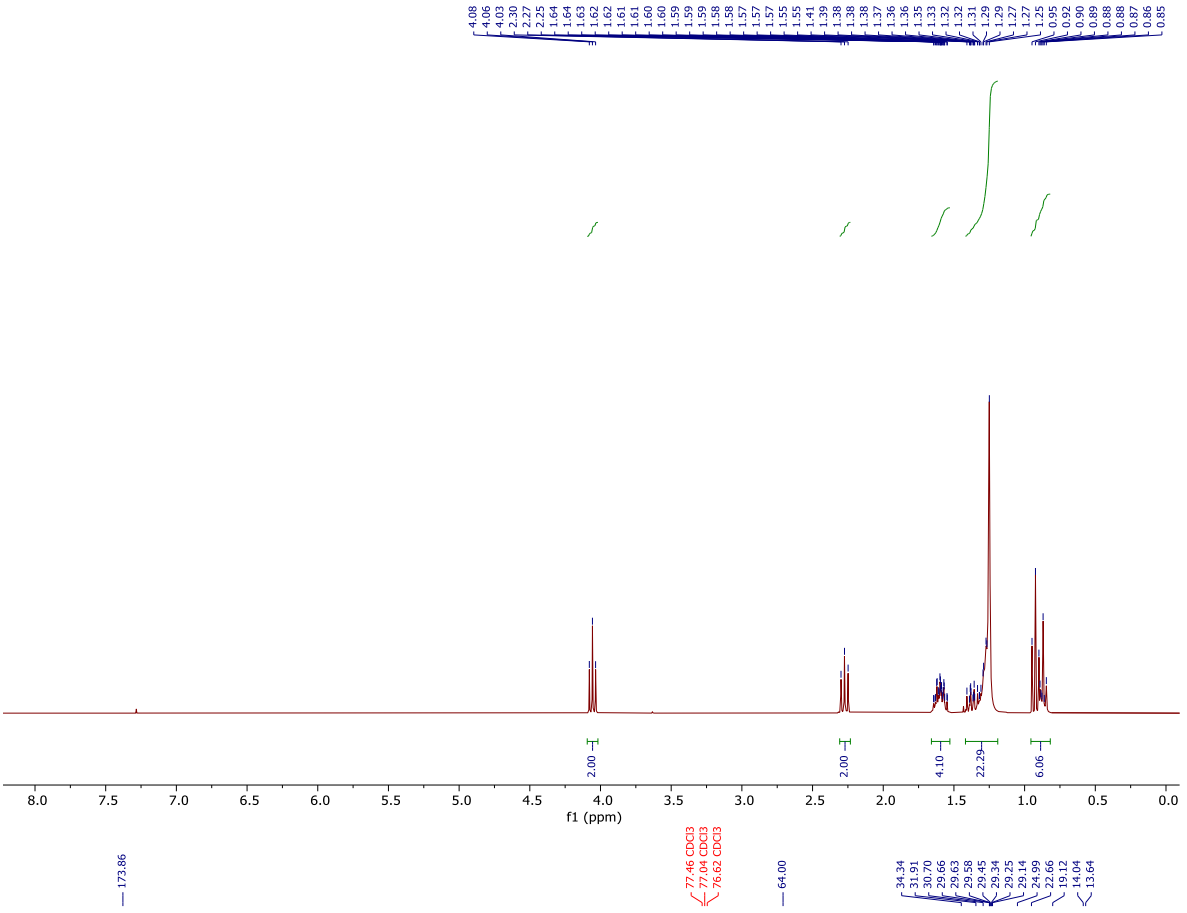


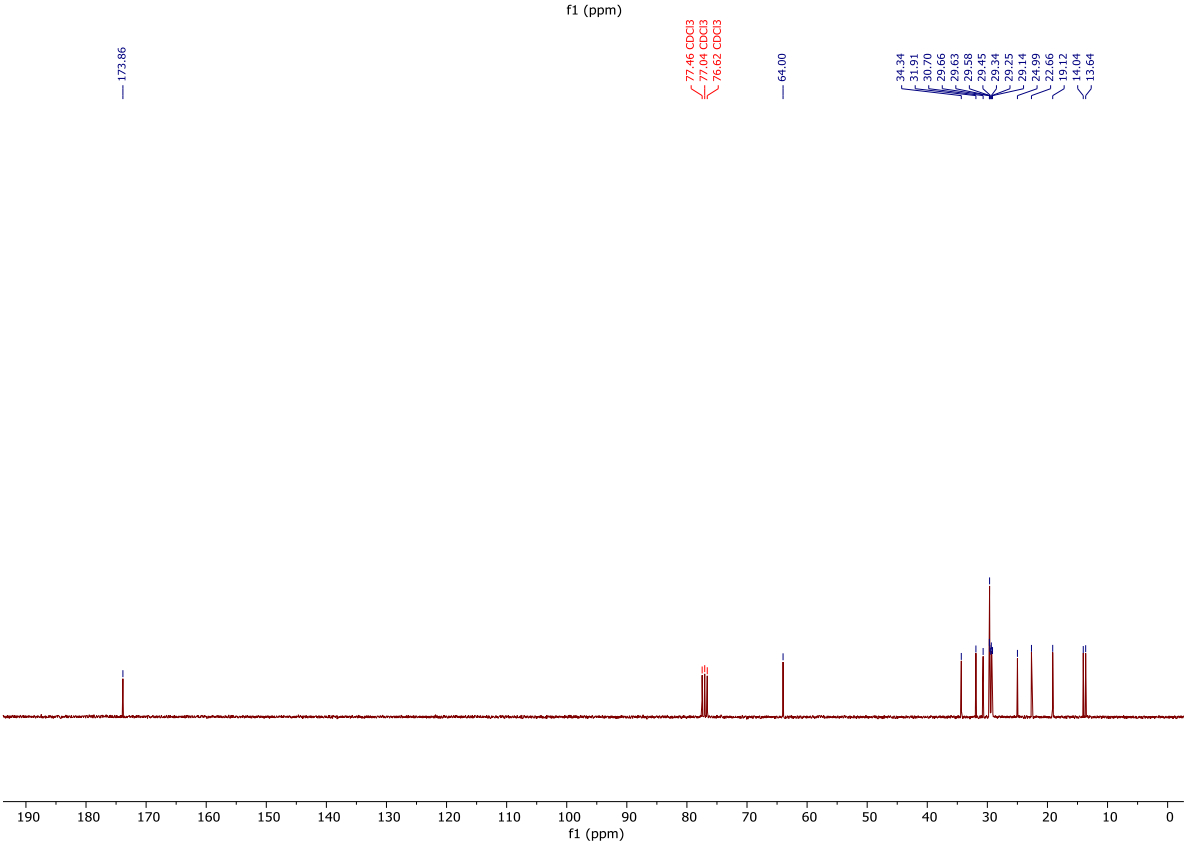




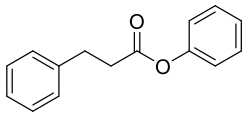
Butyl tetradecanoate (**32**)

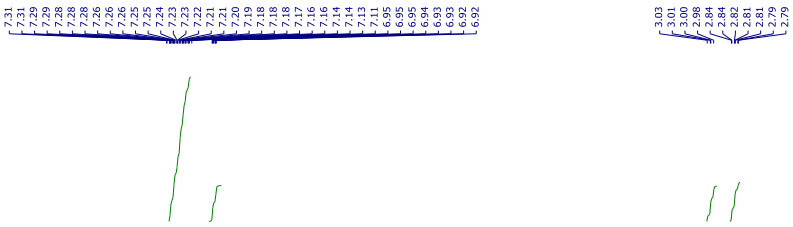


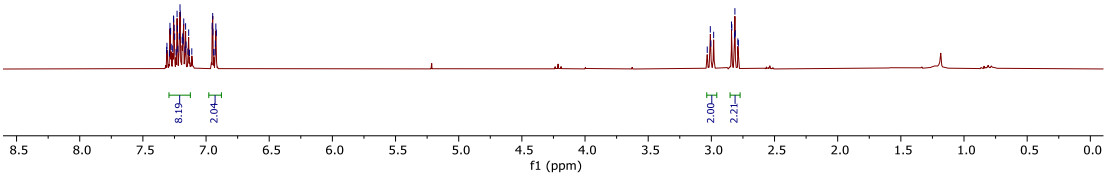


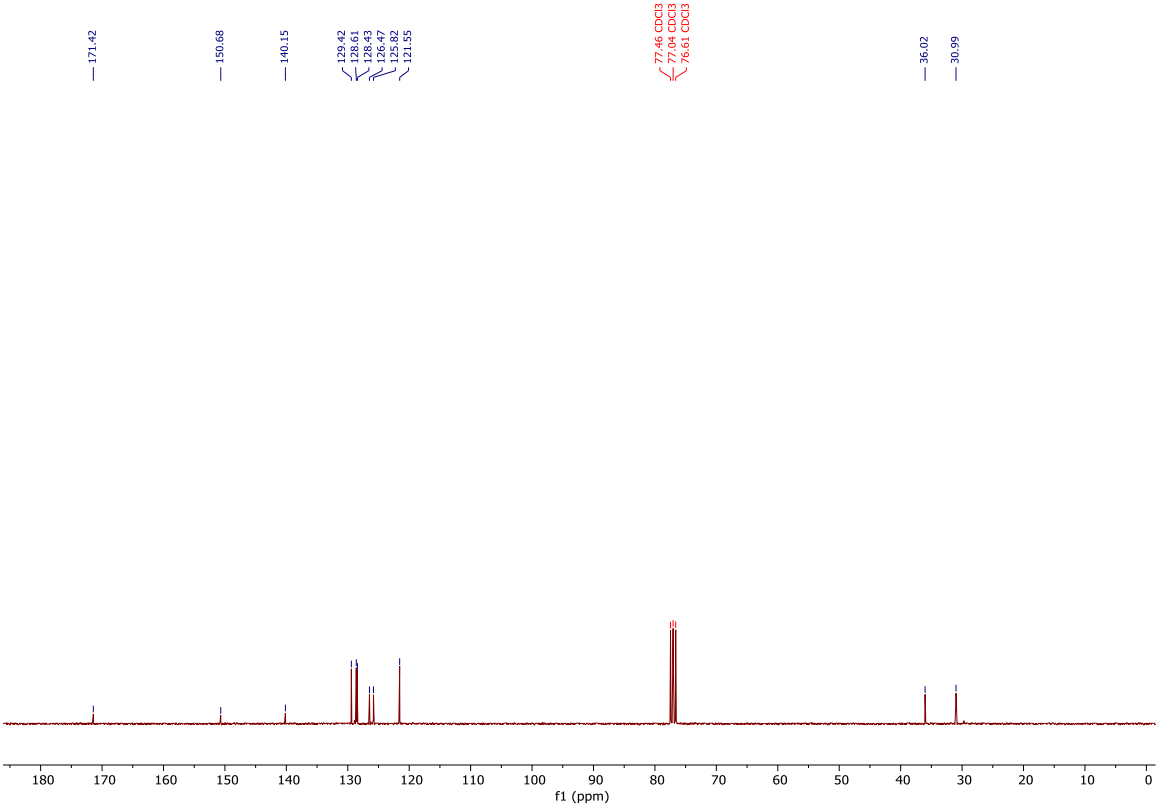


Phenyl 3-phenylpropanoate (**33**)

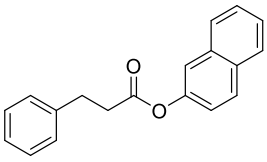


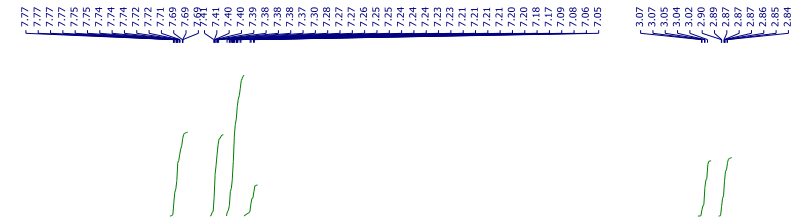


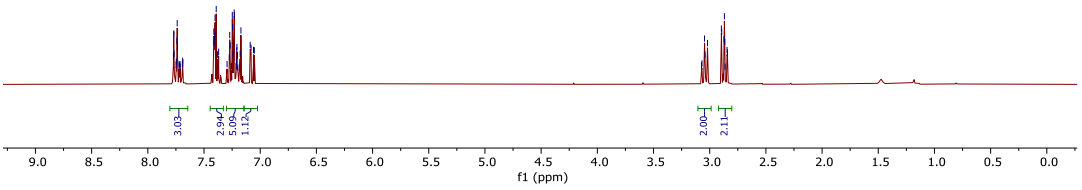


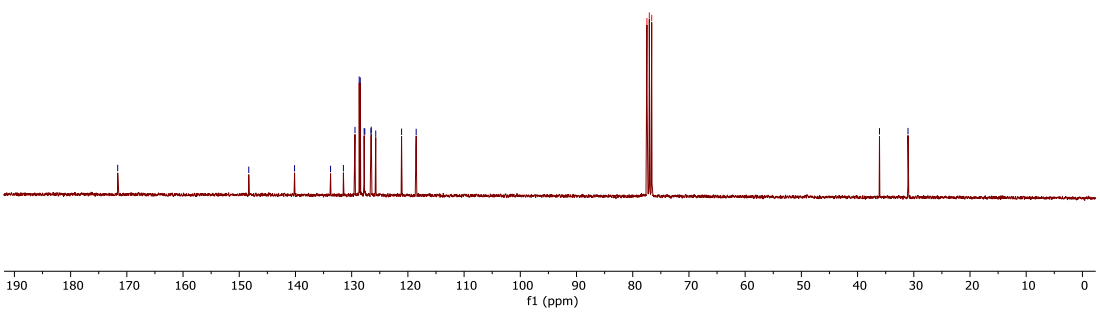


Naphthalen-2-yl 3-phenylpropanoate (**34**)

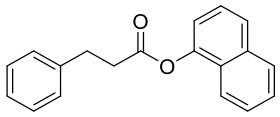


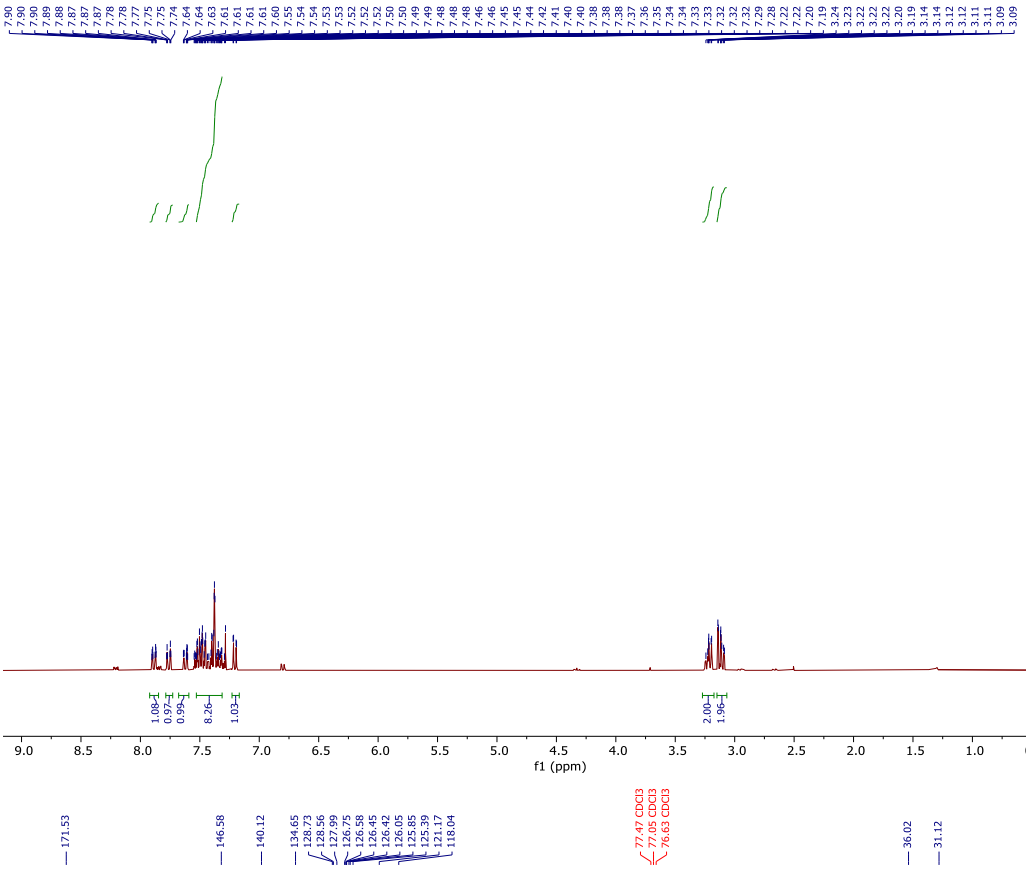


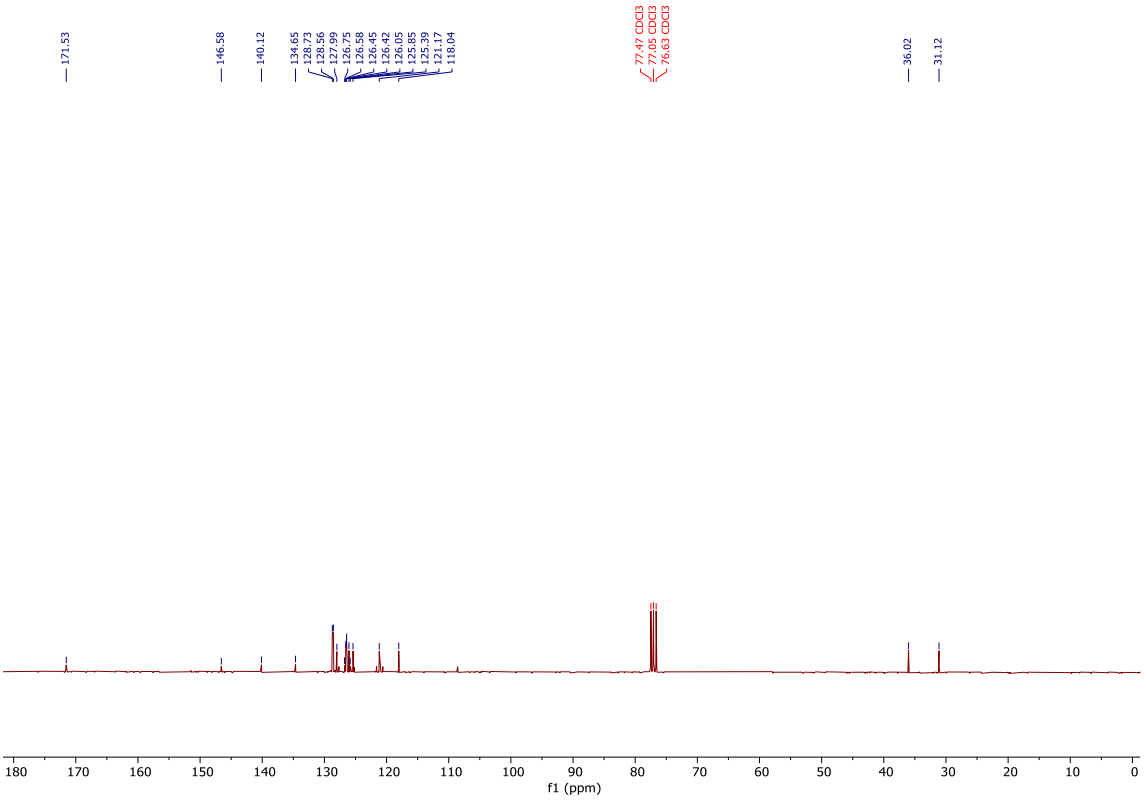




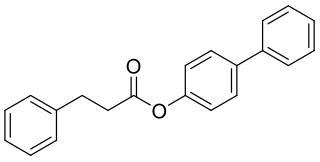
Naphthalen-1-yl 3-phenylpropanoate (**35**)

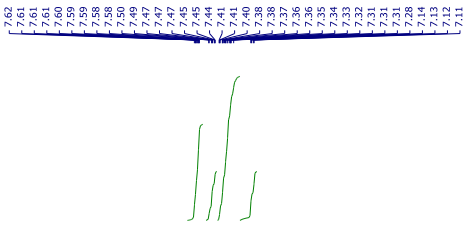


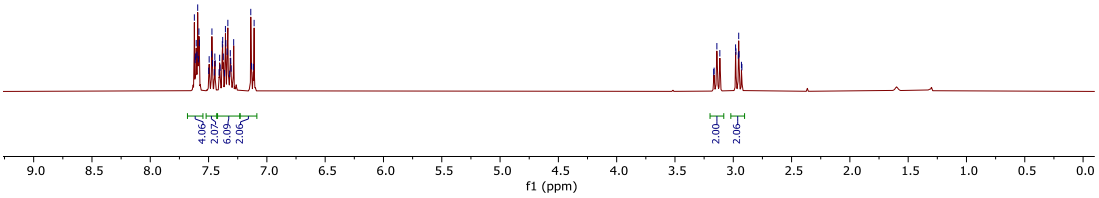


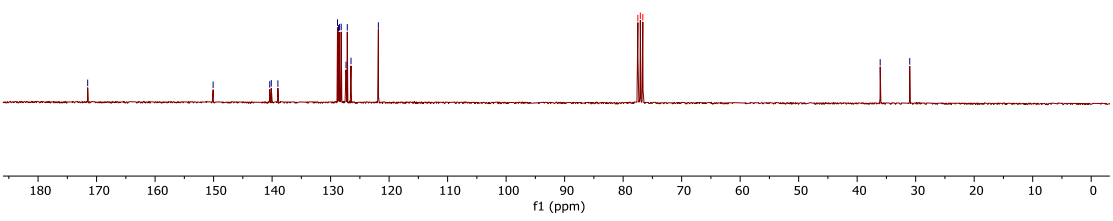


[1,1'-Biphenyl]-4-yl 3-phenylpropanoate (**36**)

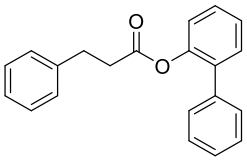


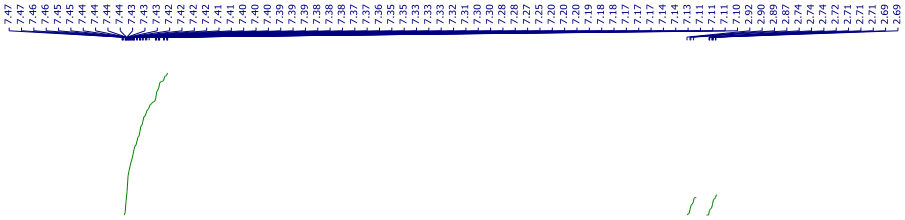


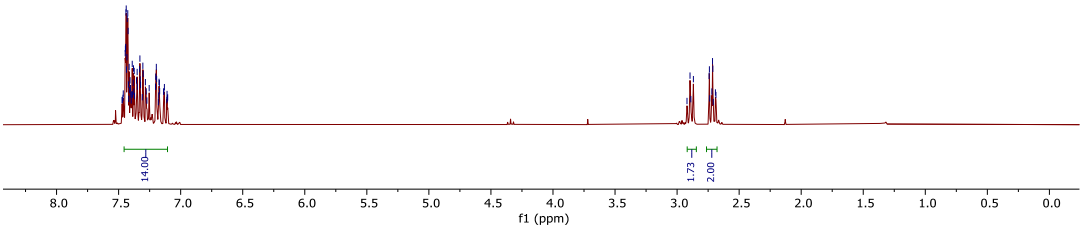


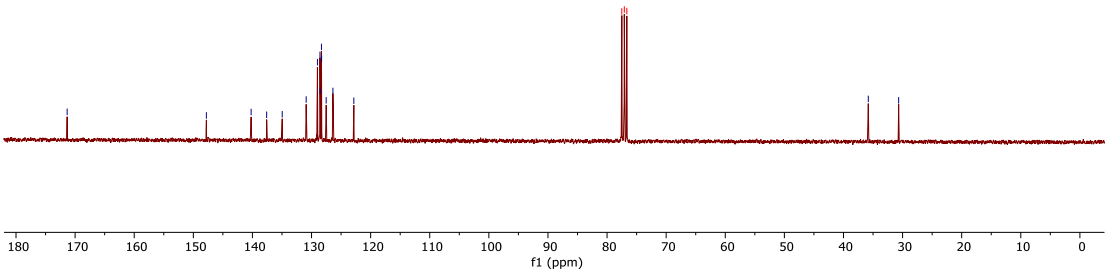


[1,1'-Biphenyl]-2-yl 3-phenylpropanoate (**37**)

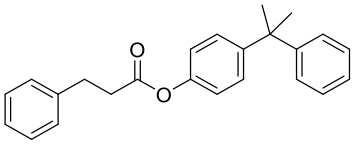


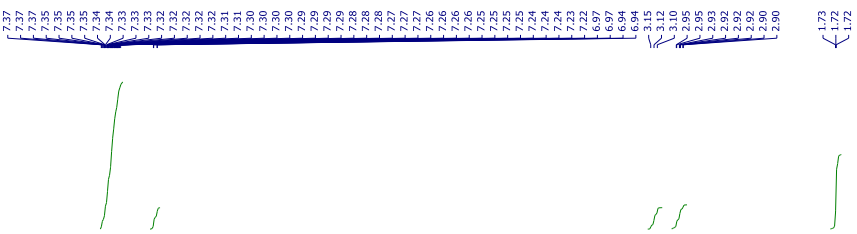


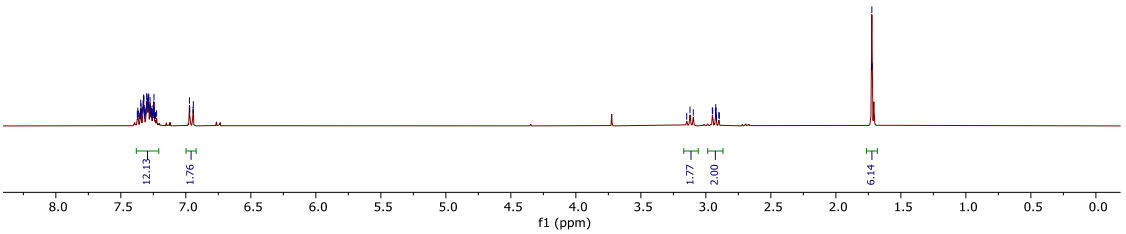


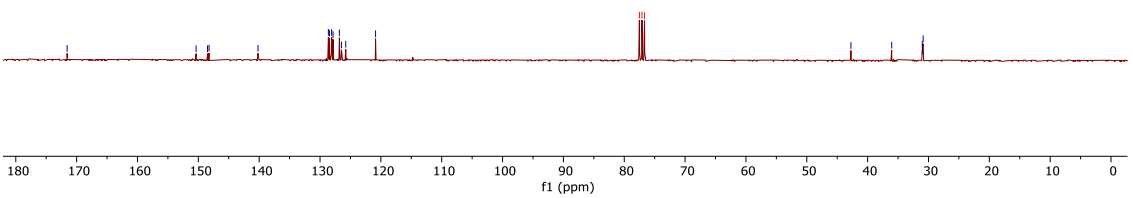


4-(2-Phenylpropan-2-yl)phenyl 3-phenylpropanoate (**38**)

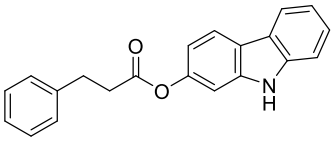


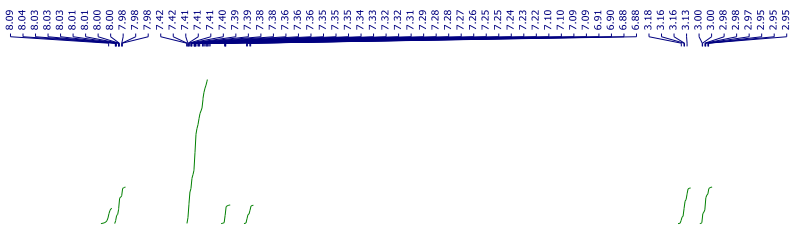


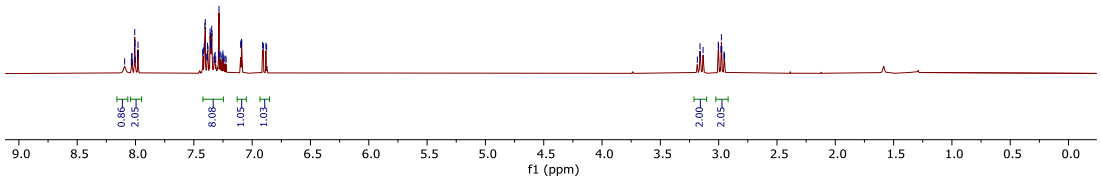


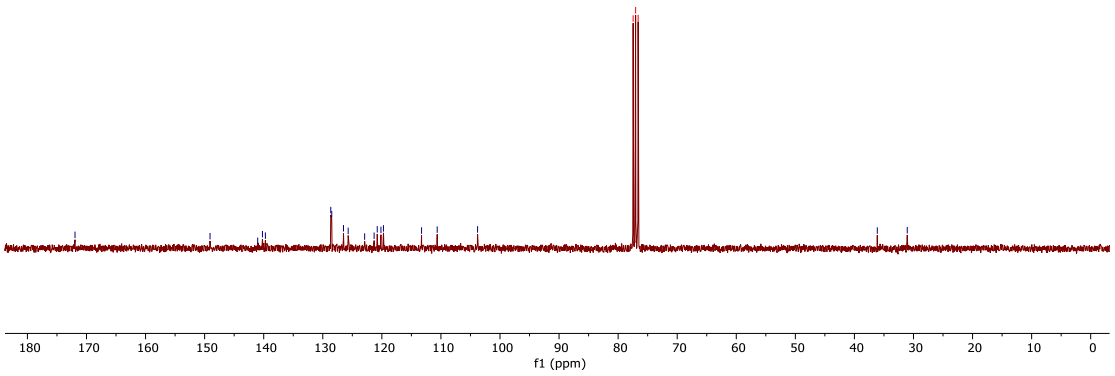


9H-Carbazol-2-yl 3-phenylpropanoate (**39**)

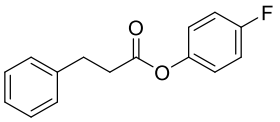


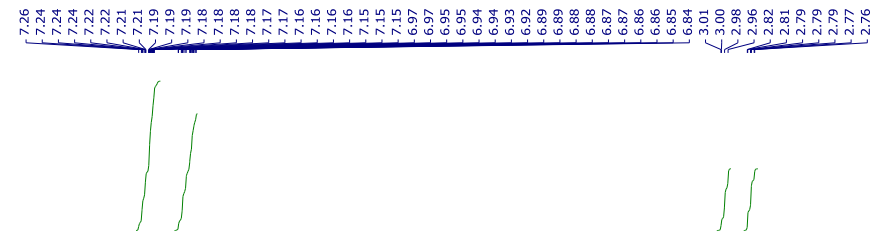


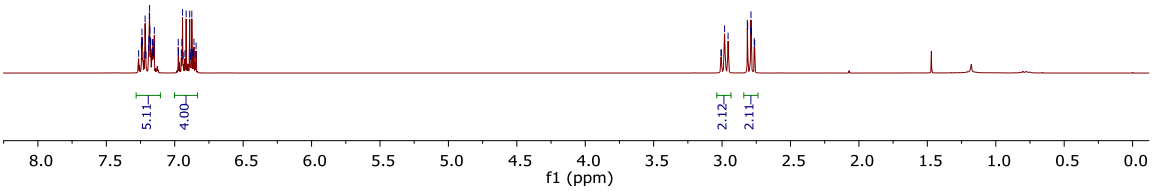


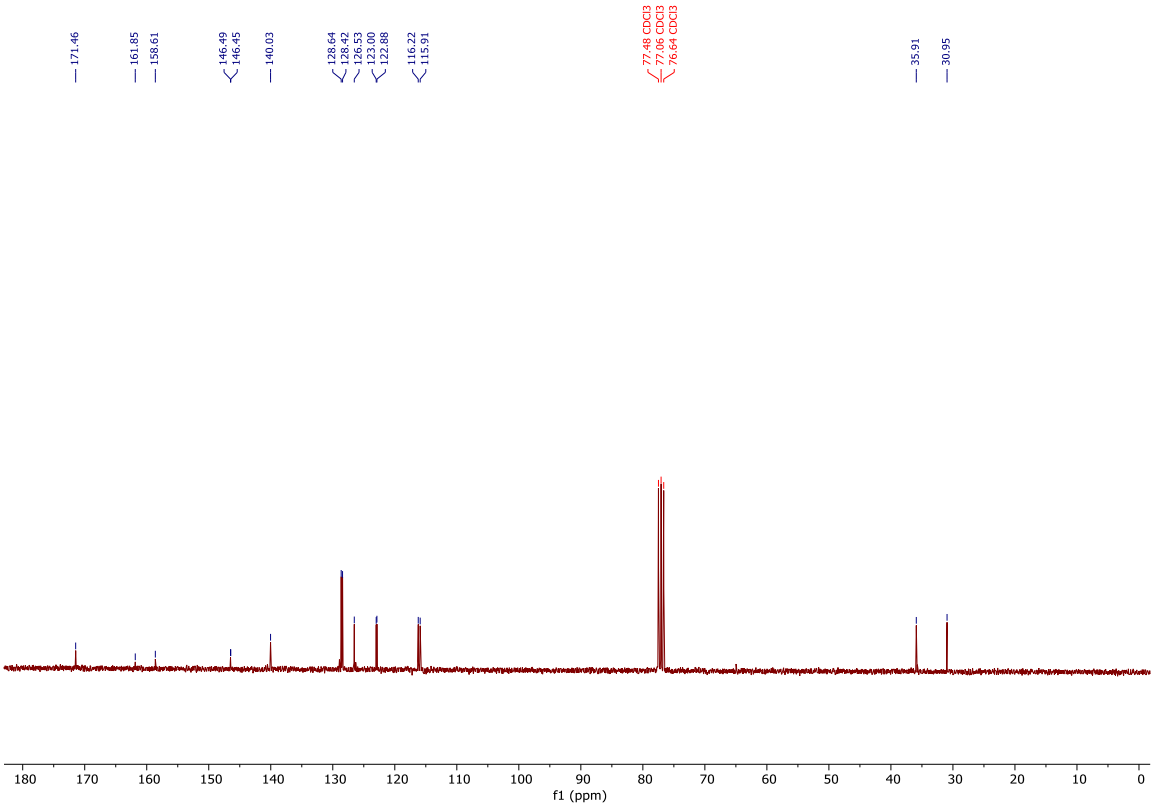


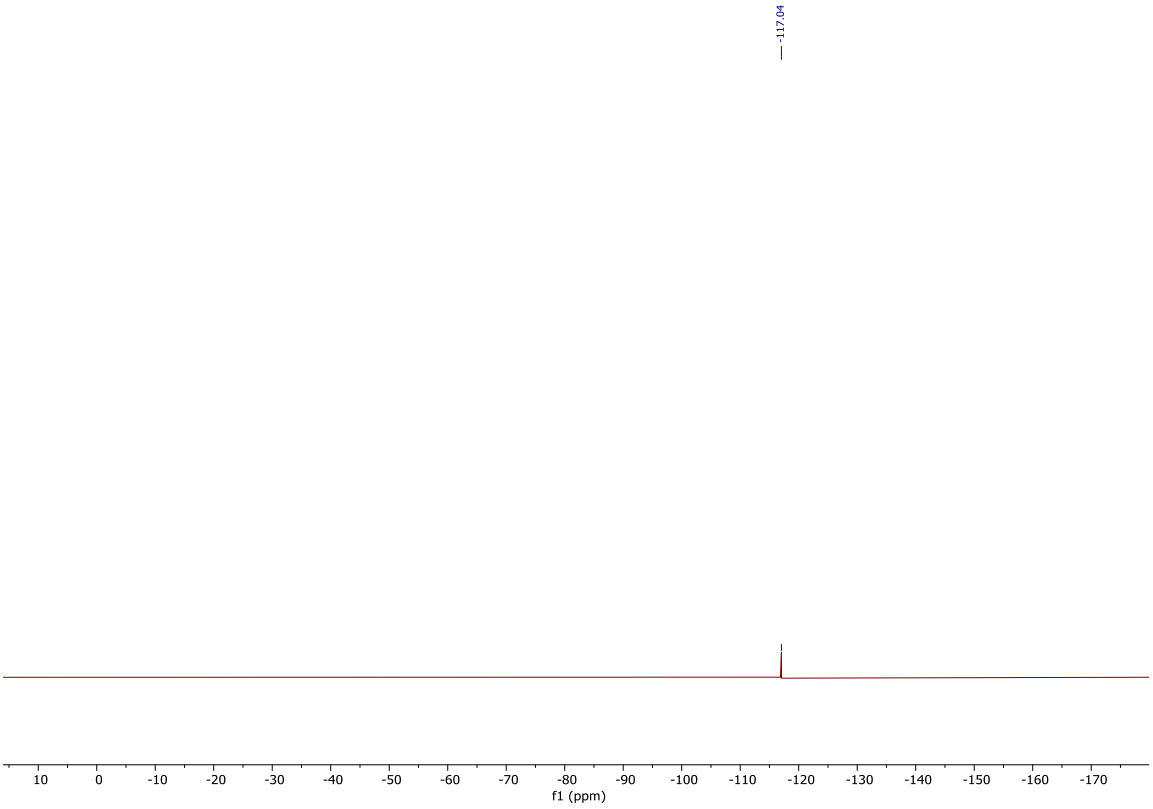
4-Fluorophenyl 3-phenylpropanoate (**40**)



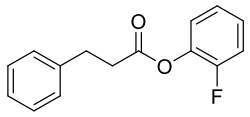


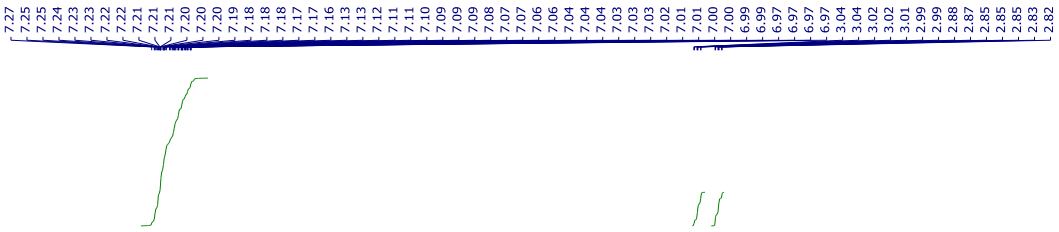


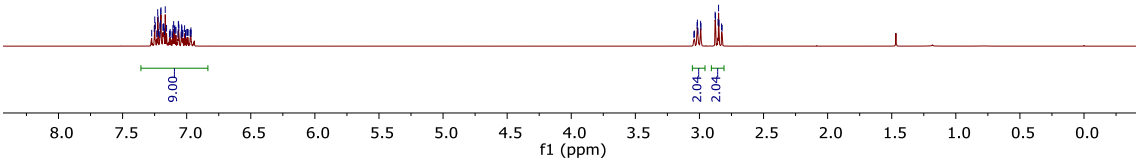


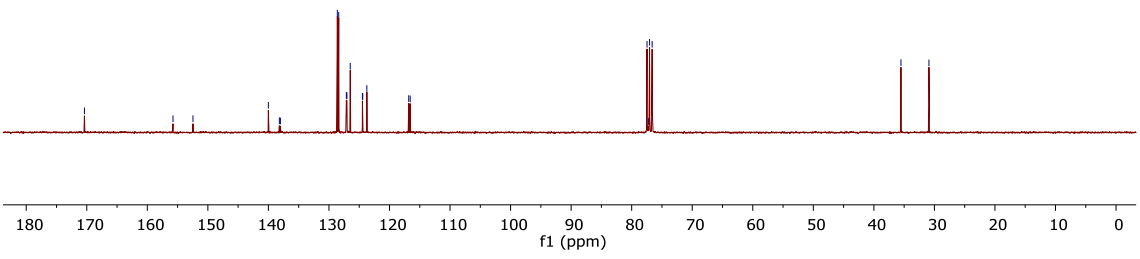

-117.04
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
f1 (ppm)

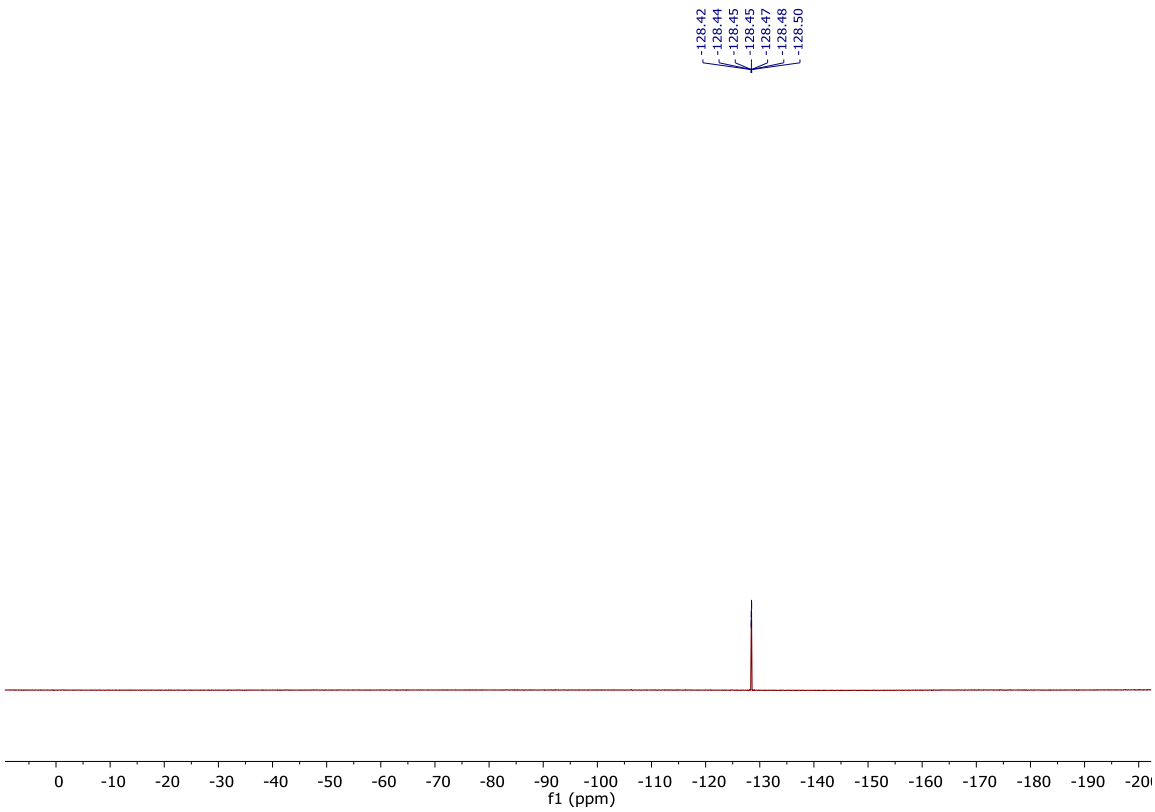
2-Fluorophenyl 3-phenylpropanoate (**41**)



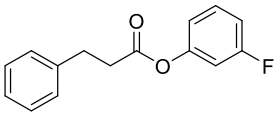


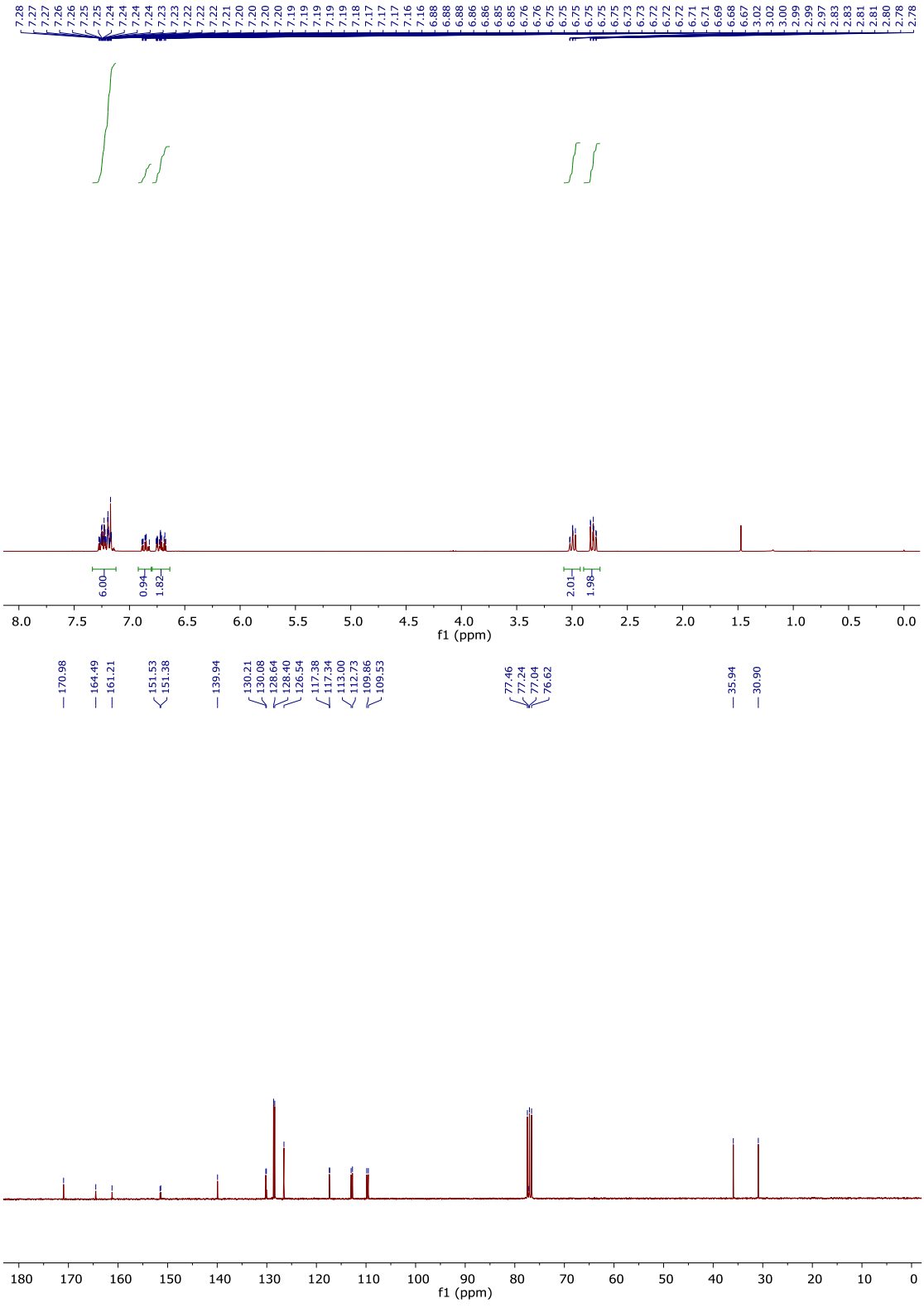


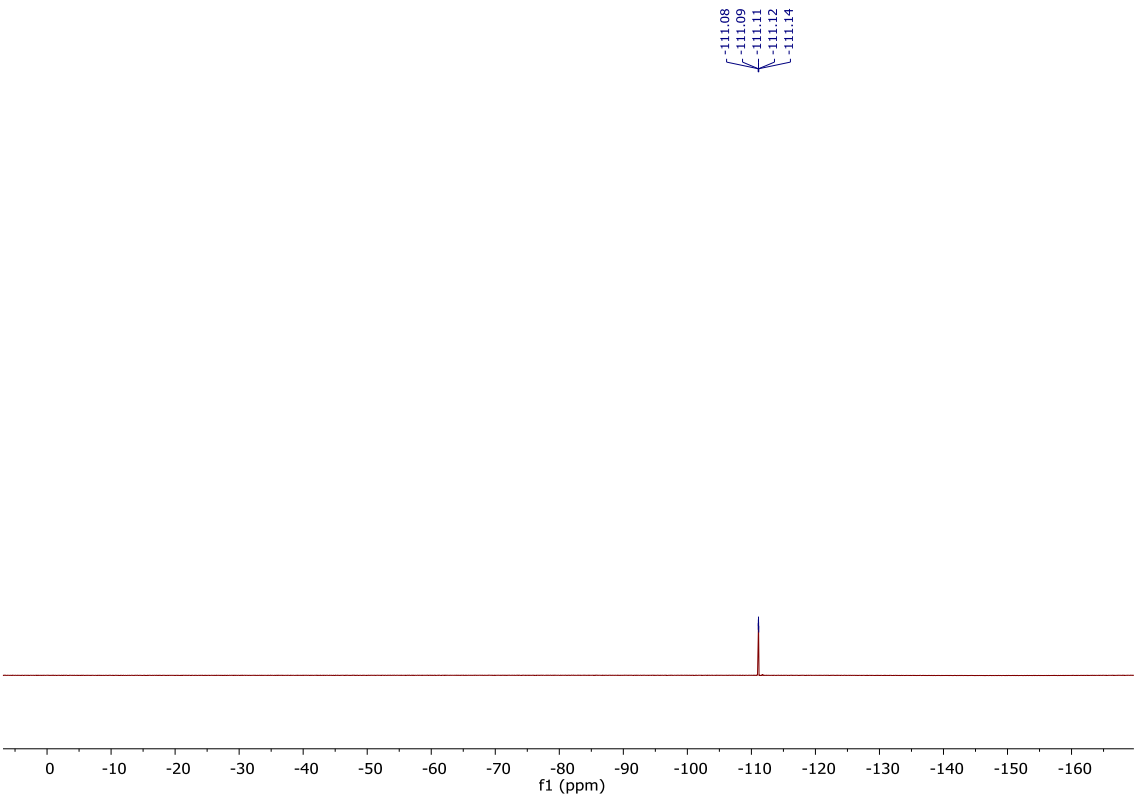



-128.42
-128.44
-128.45
-128.45
-128.47
-128.48
-128.50
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

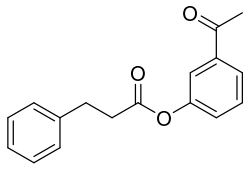
3-Fluorophenyl 3-phenylpropanoate (**42**)

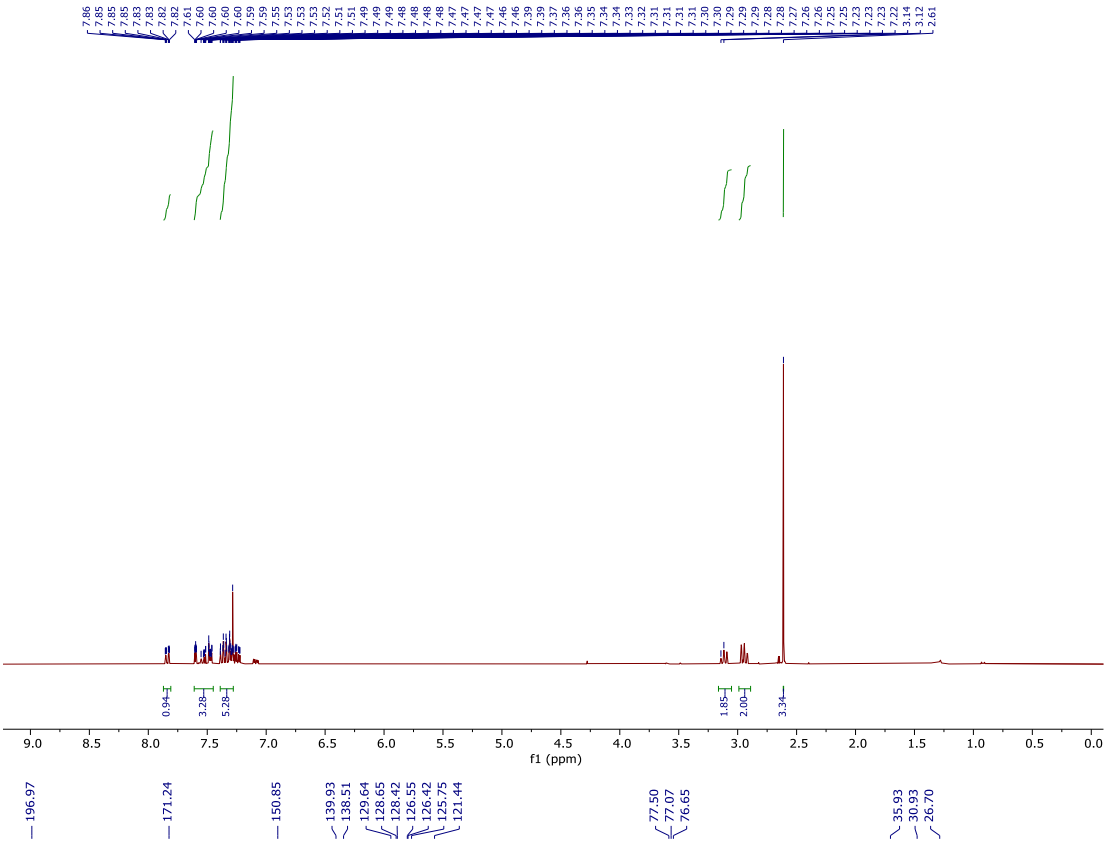


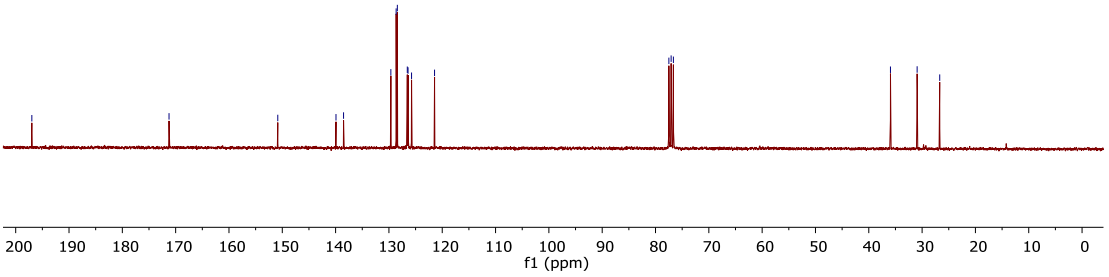



-111.08
-111.09
-111.11
-111.12
-111.14
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
f1 (ppm)

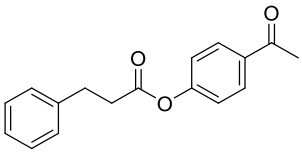
3-Acetylphenyl 3-phenylpropanoate (**43**)

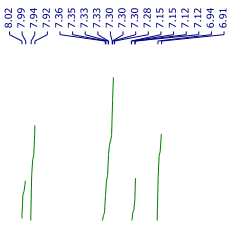


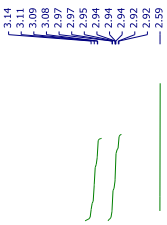


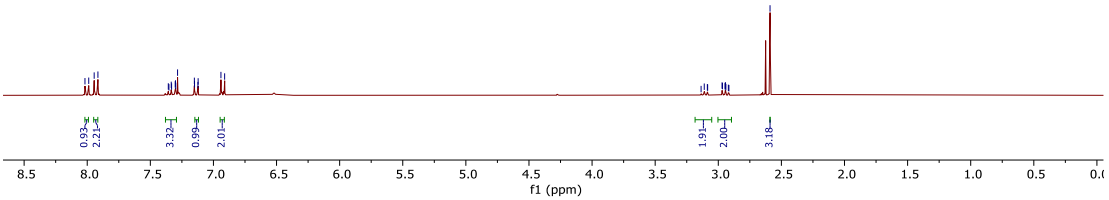


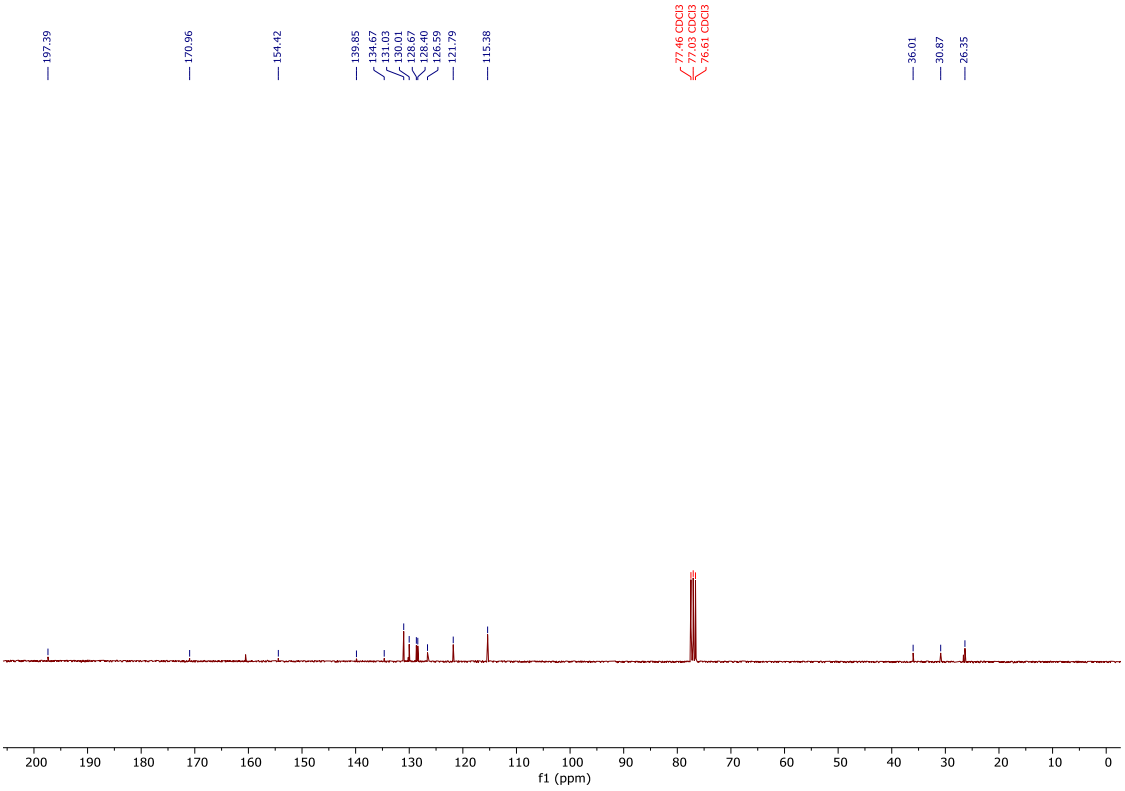
4-Acetylphenyl 3-phenylpropanoate (**44**)



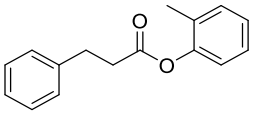


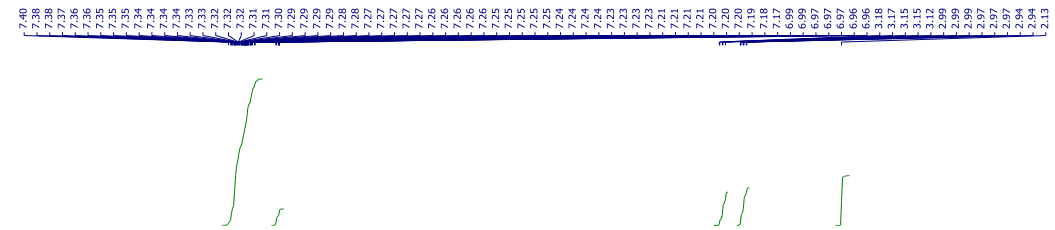


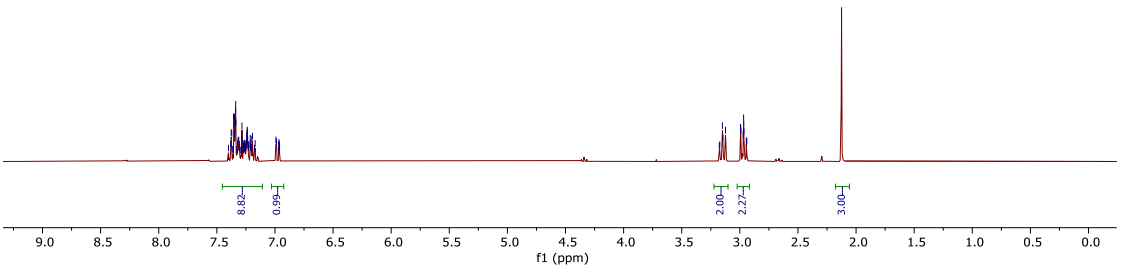


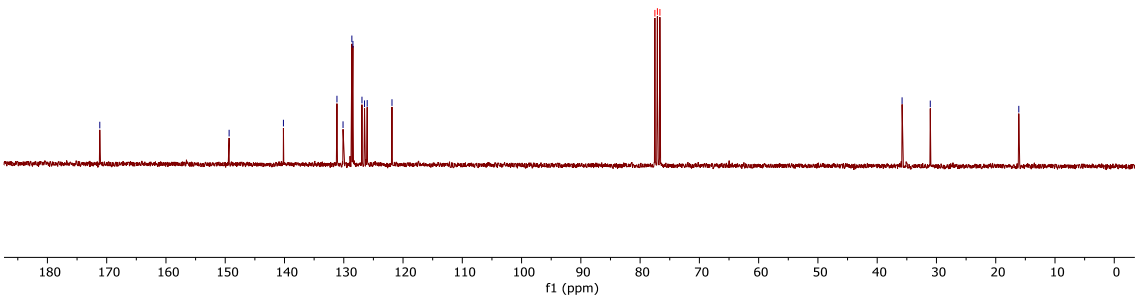


o-Tolyl 3-phenylpropanoate (**45**)

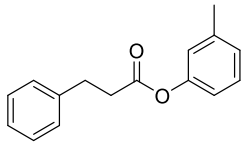


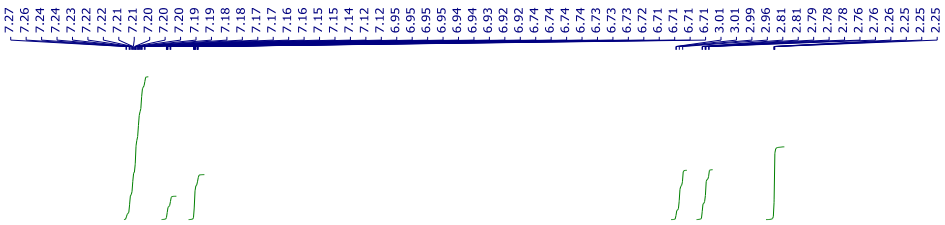


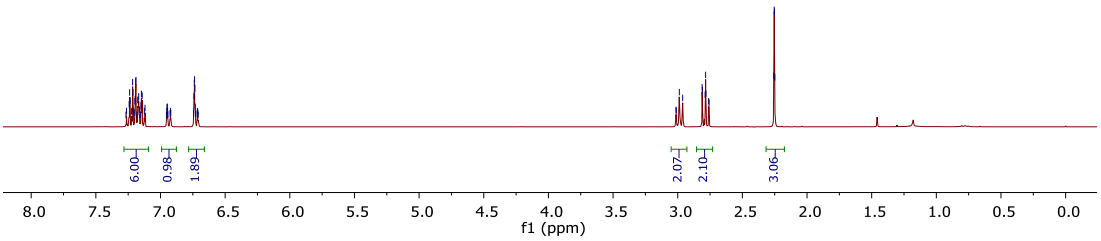


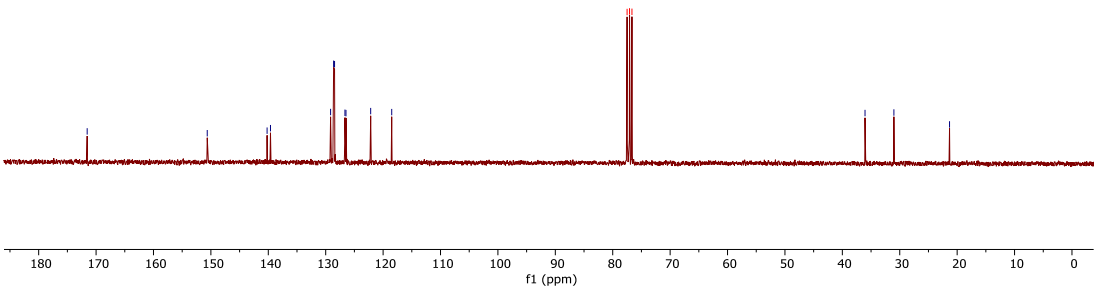


m-Tolyl 3-phenylpropanoate (**46**)

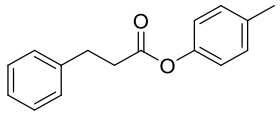


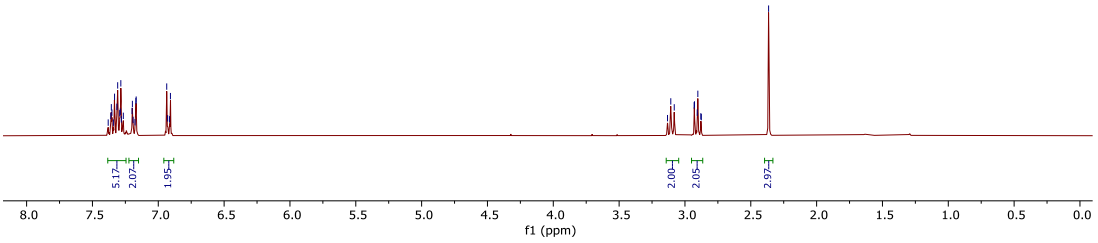


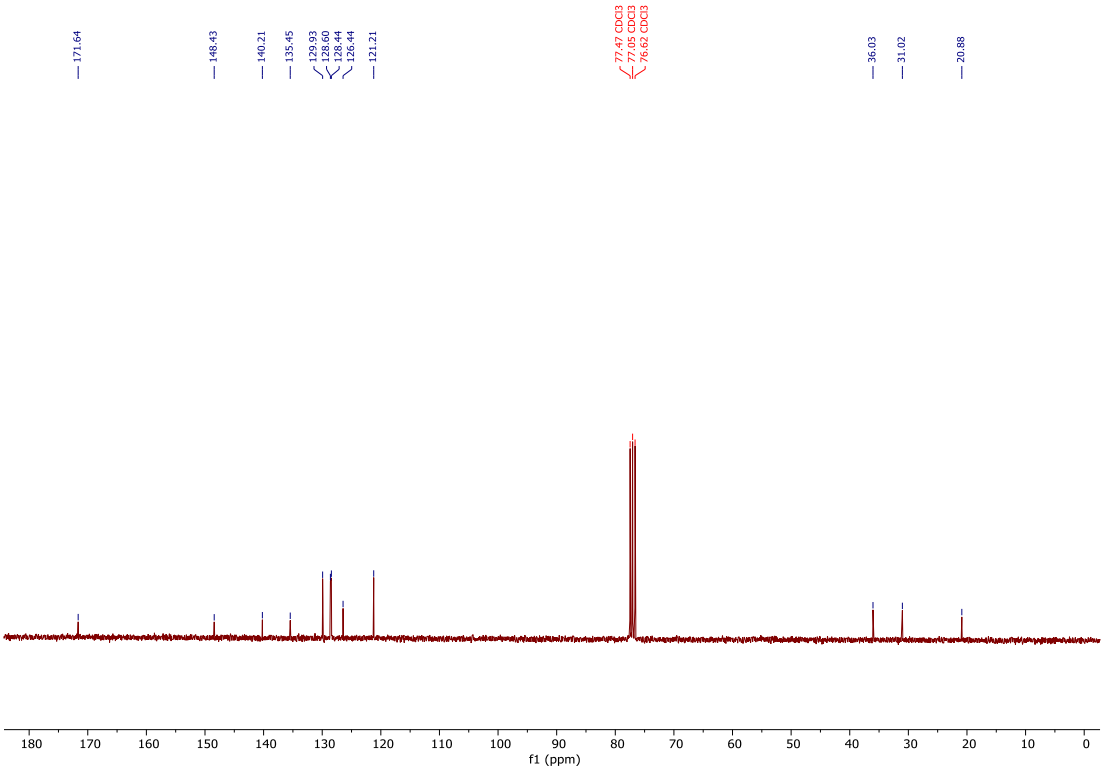




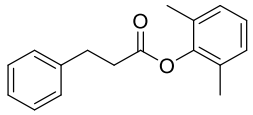
p-Tolyl 3-phenylpropanoate (**47**)

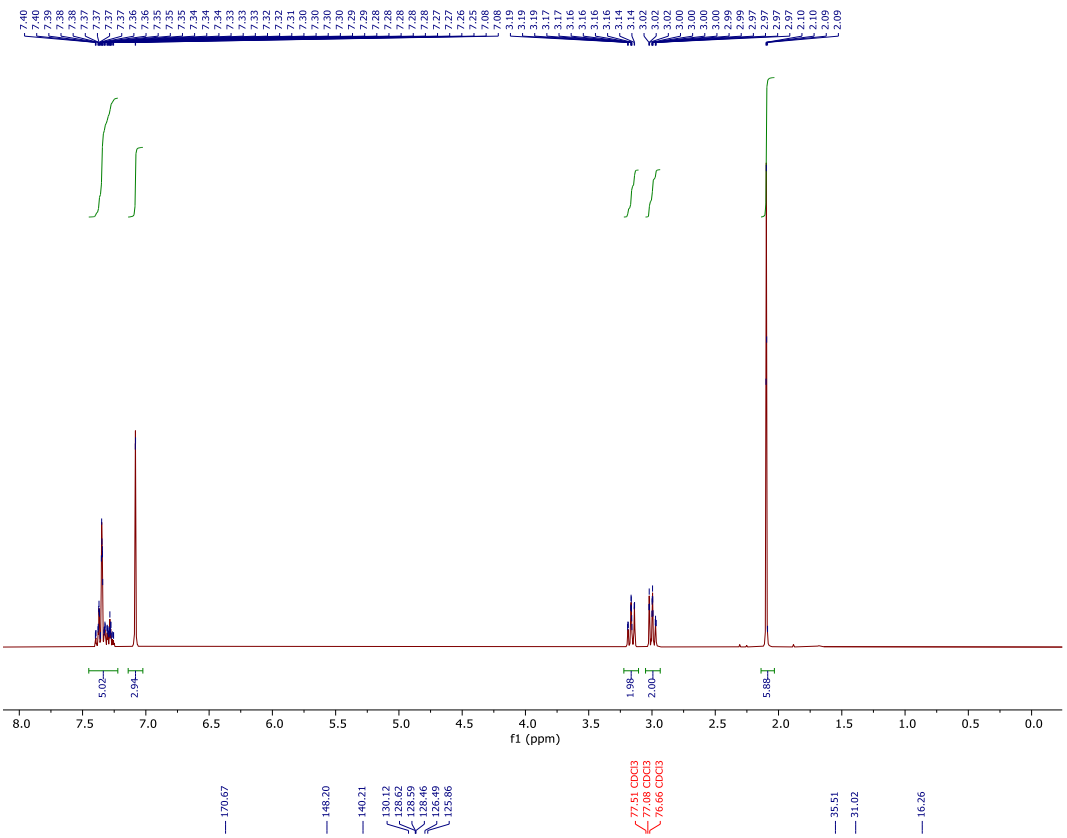


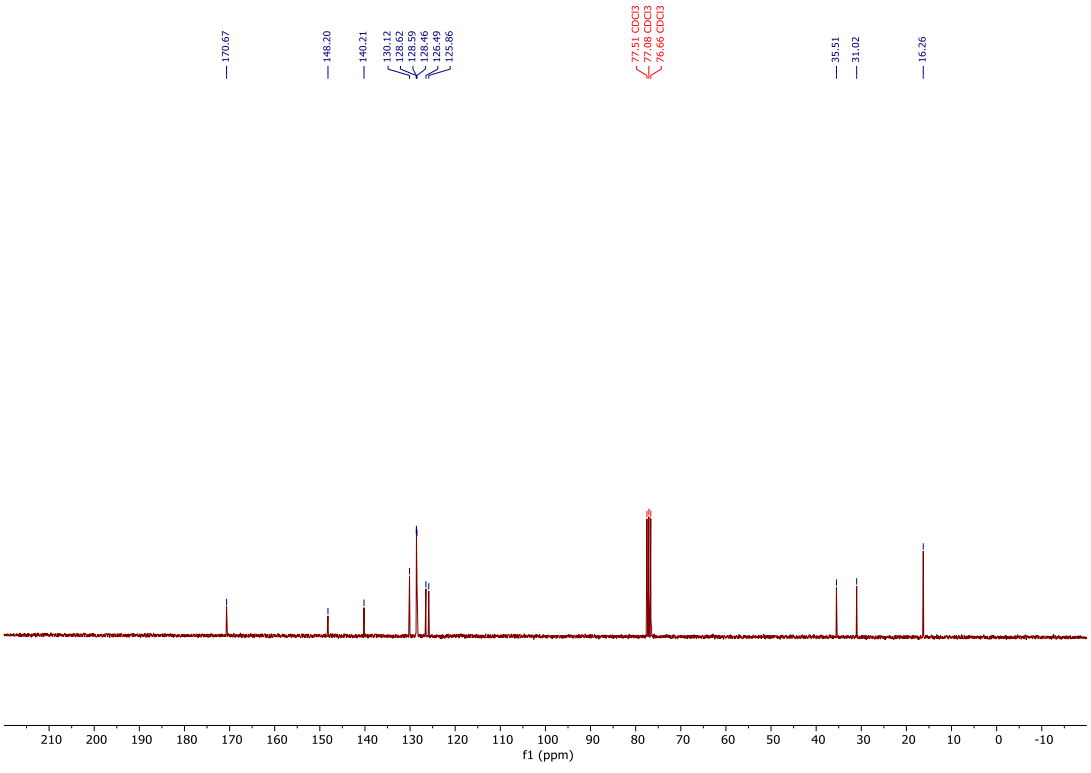




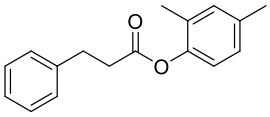
2,6-Dimethylphenyl 3-phenylpropanoate (**48**)

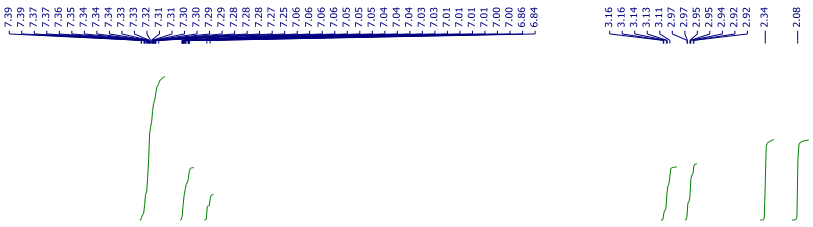


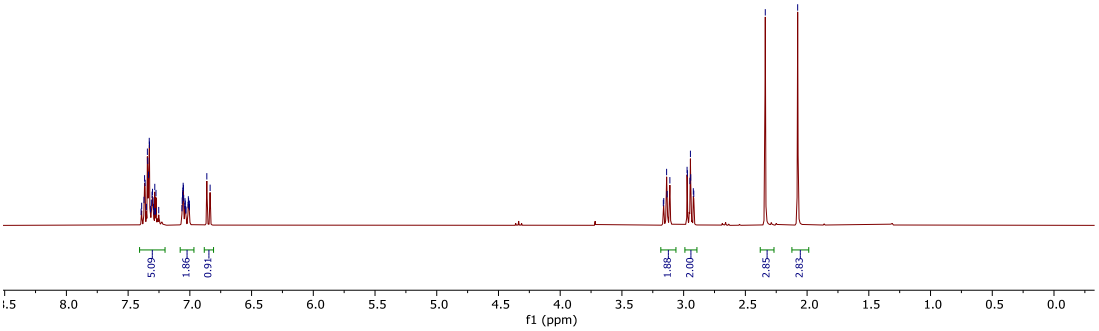


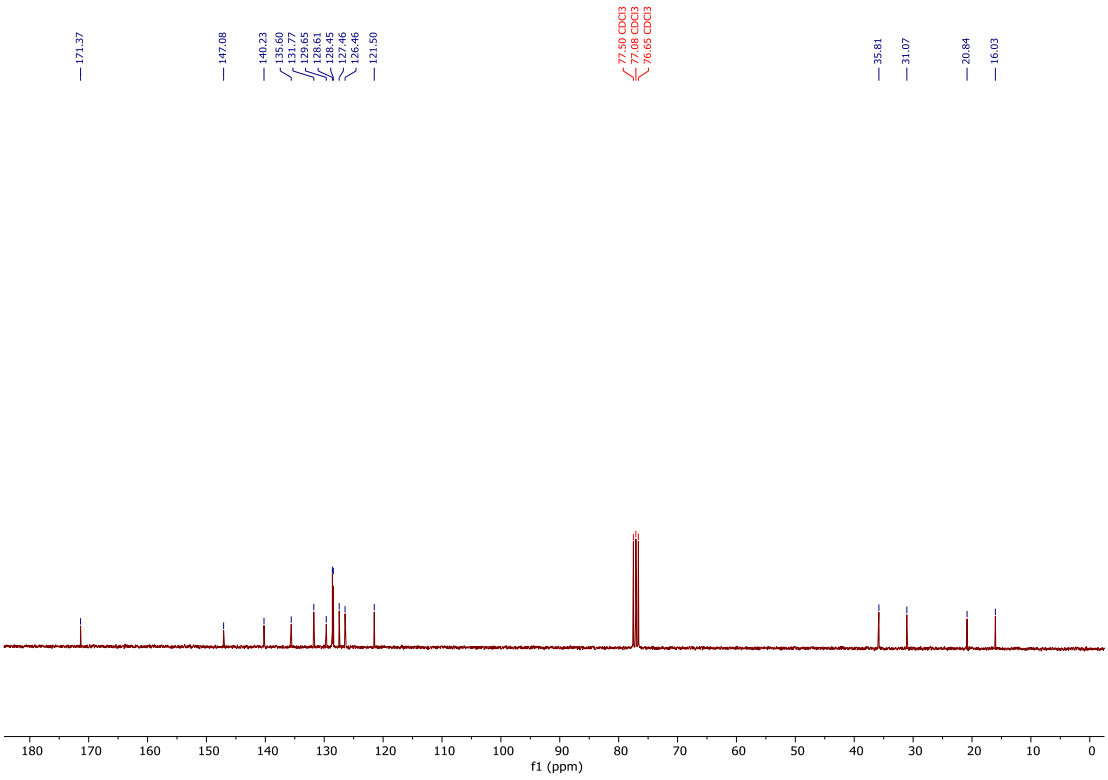


2,4-Dimethylphenyl 3-phenylpropanoate (**49**)

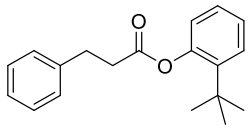


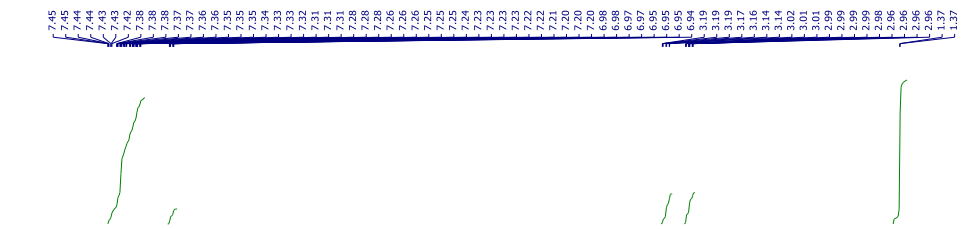


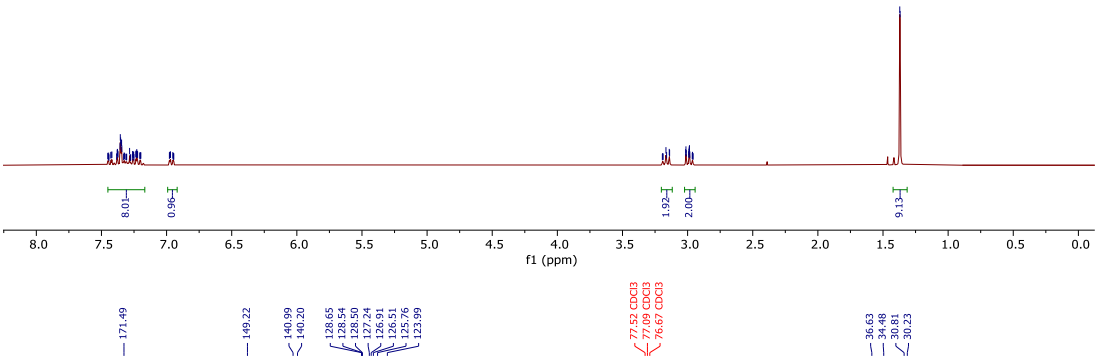


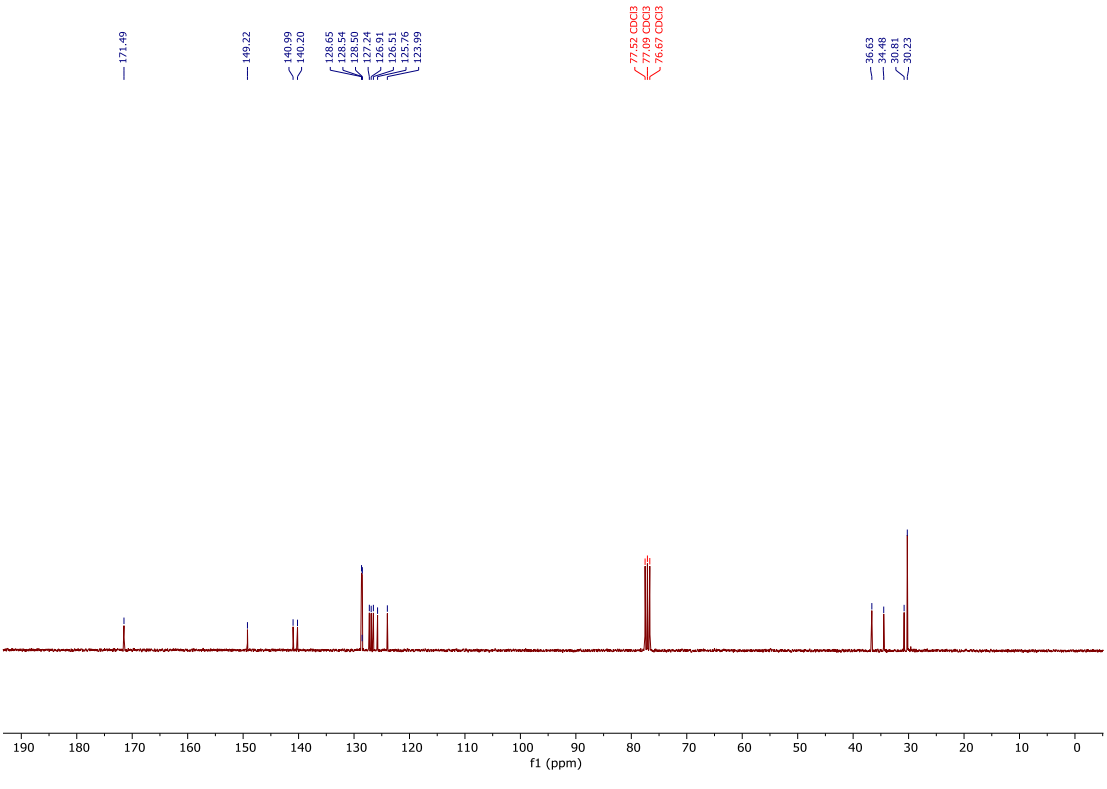


2-*tert*-Butylphenyl 3-phenylpropanoate (**50**)

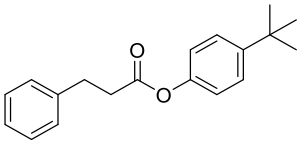


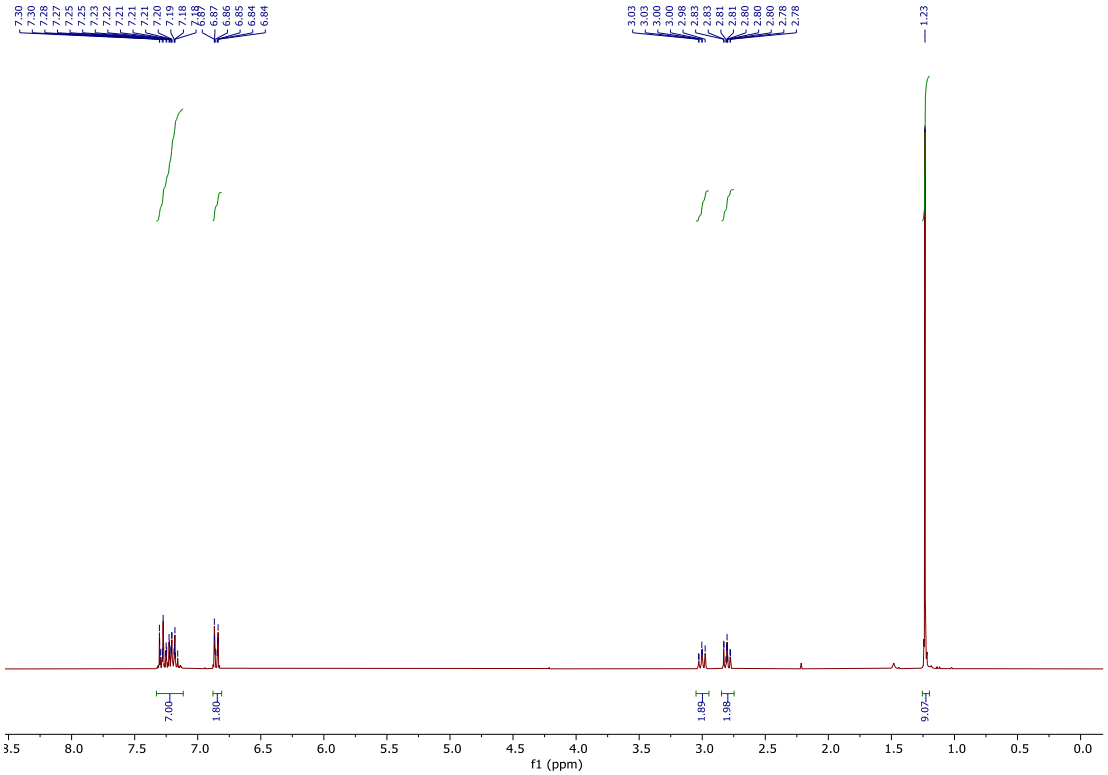


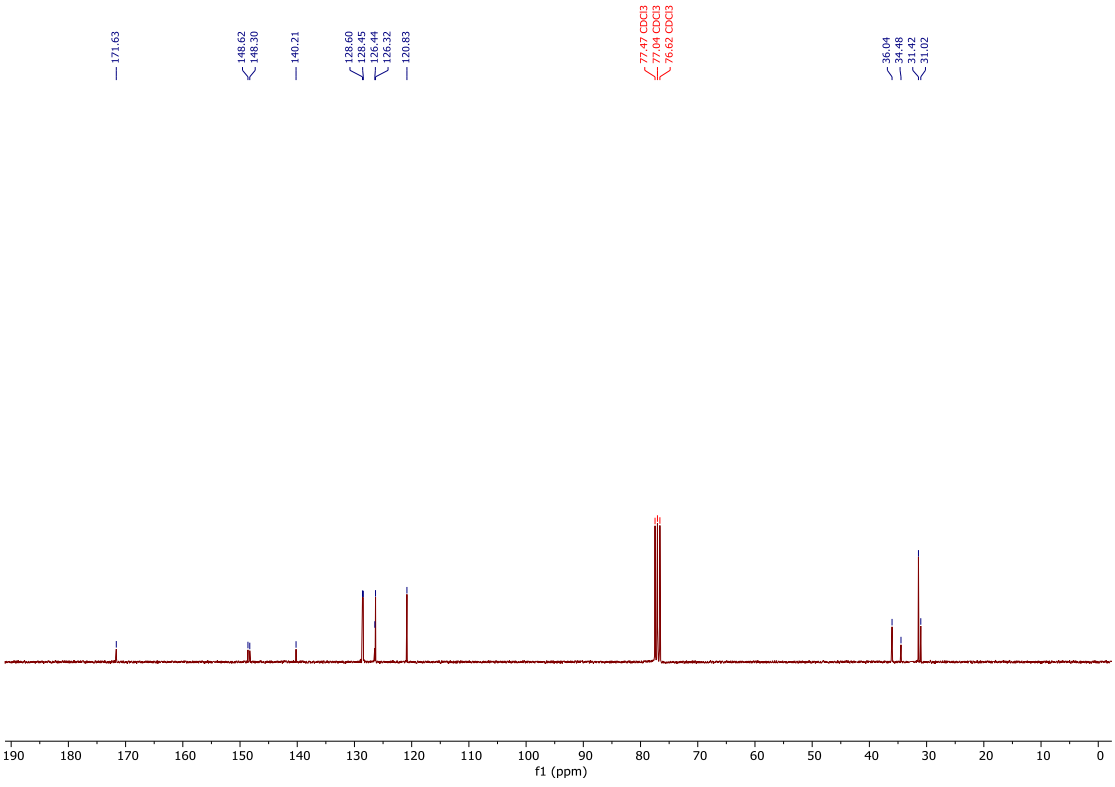




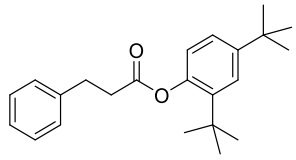
4-*tert*-Butylphenyl 3-phenylpropanoate (**51**)

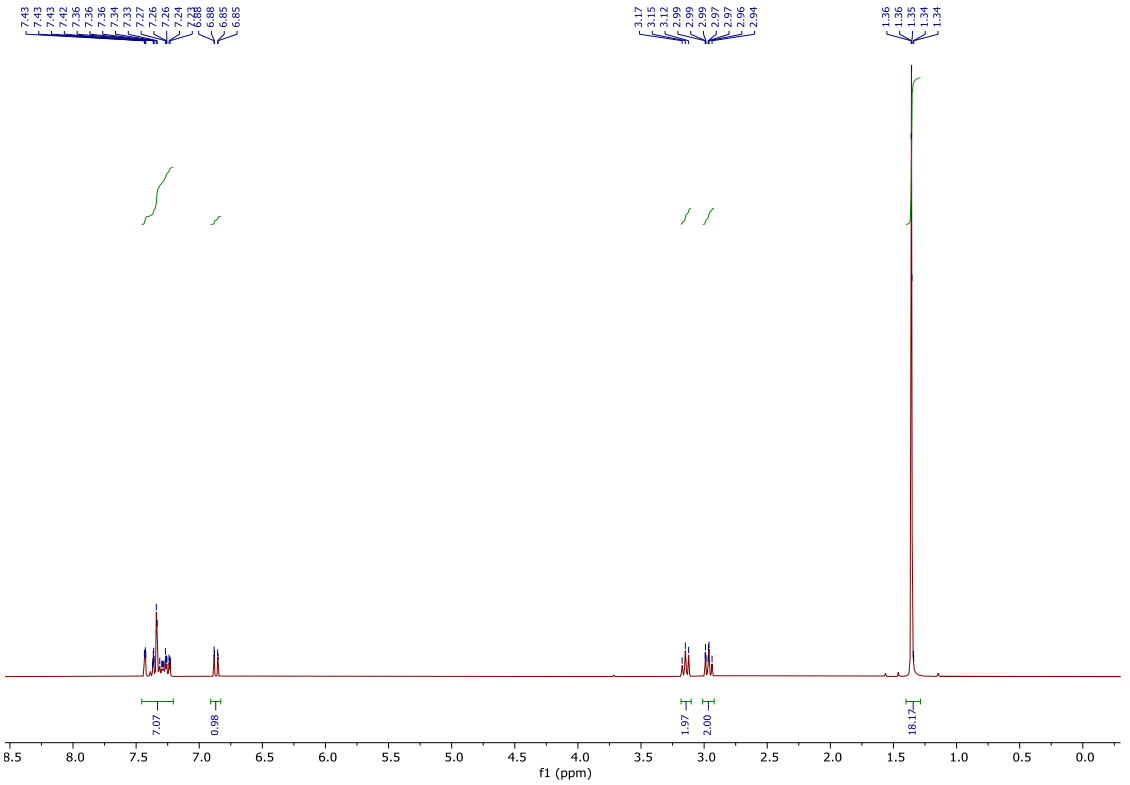


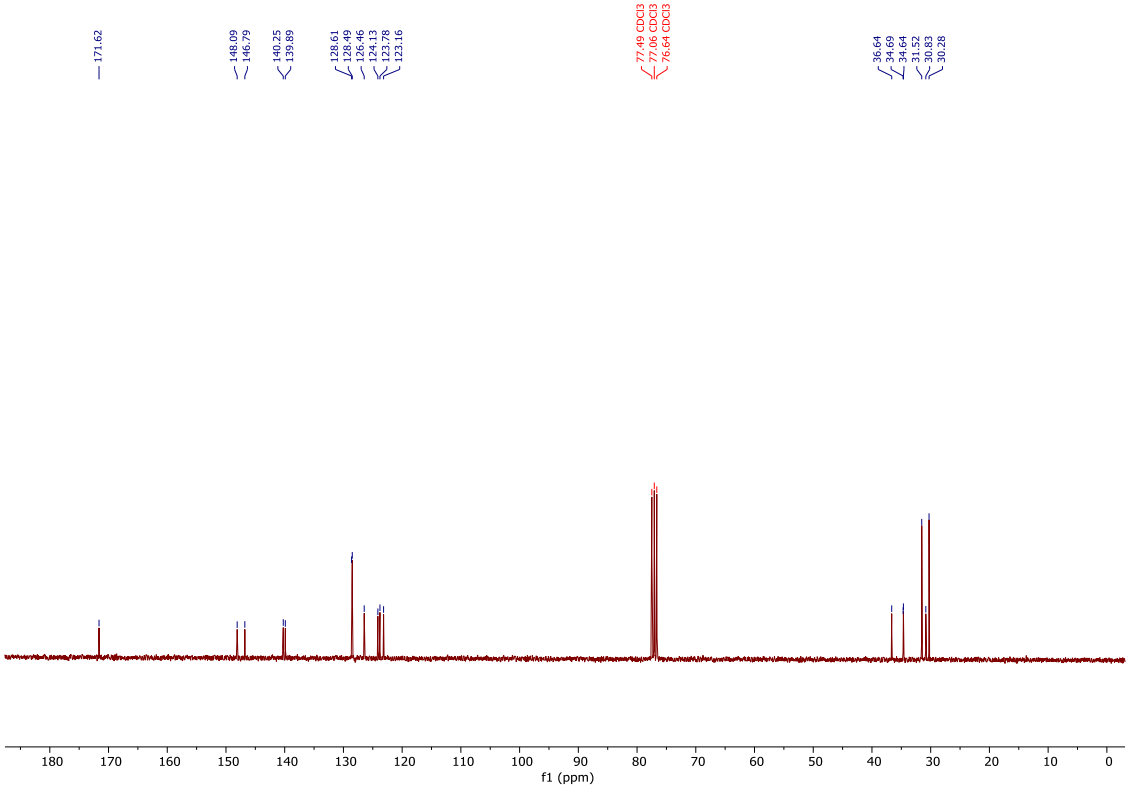




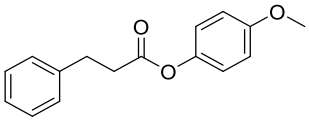
2,4-di-*tert*-Butylphenyl 3-phenylpropanoate (**52**)

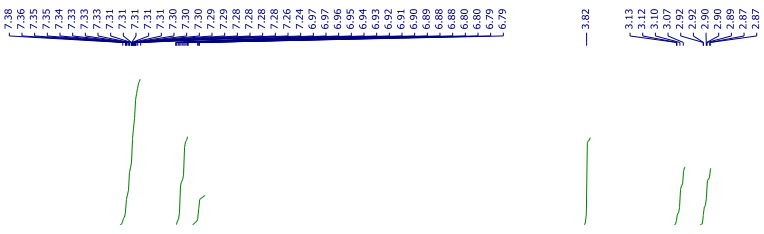


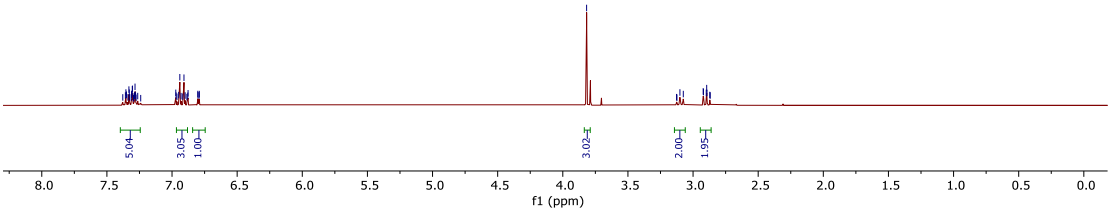


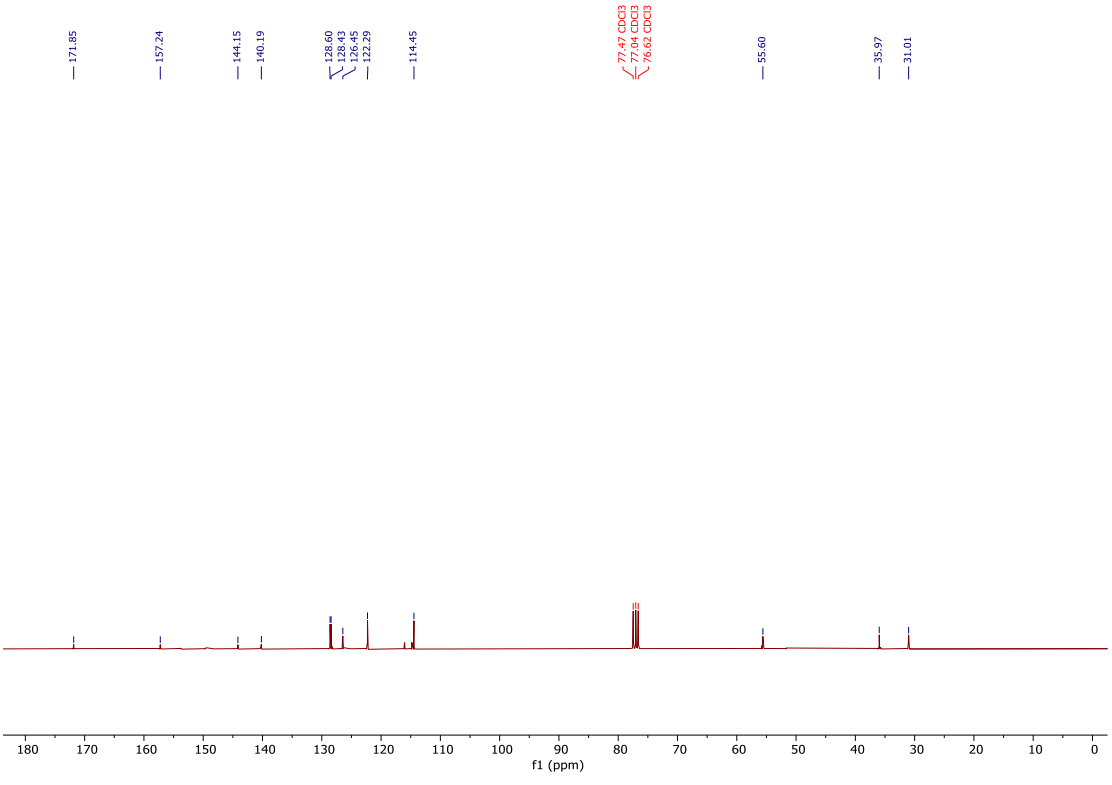


4-Methoxyphenyl 3-phenylpropanoate (**53**)

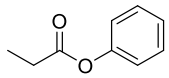


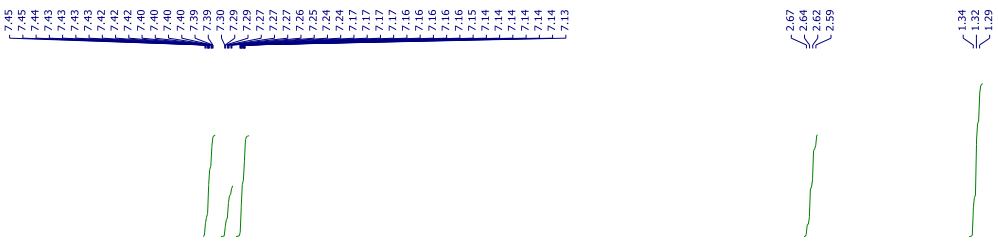


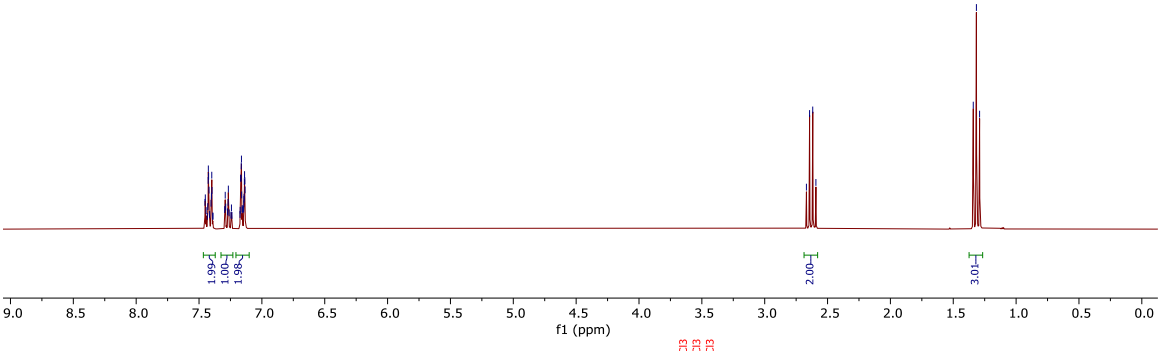


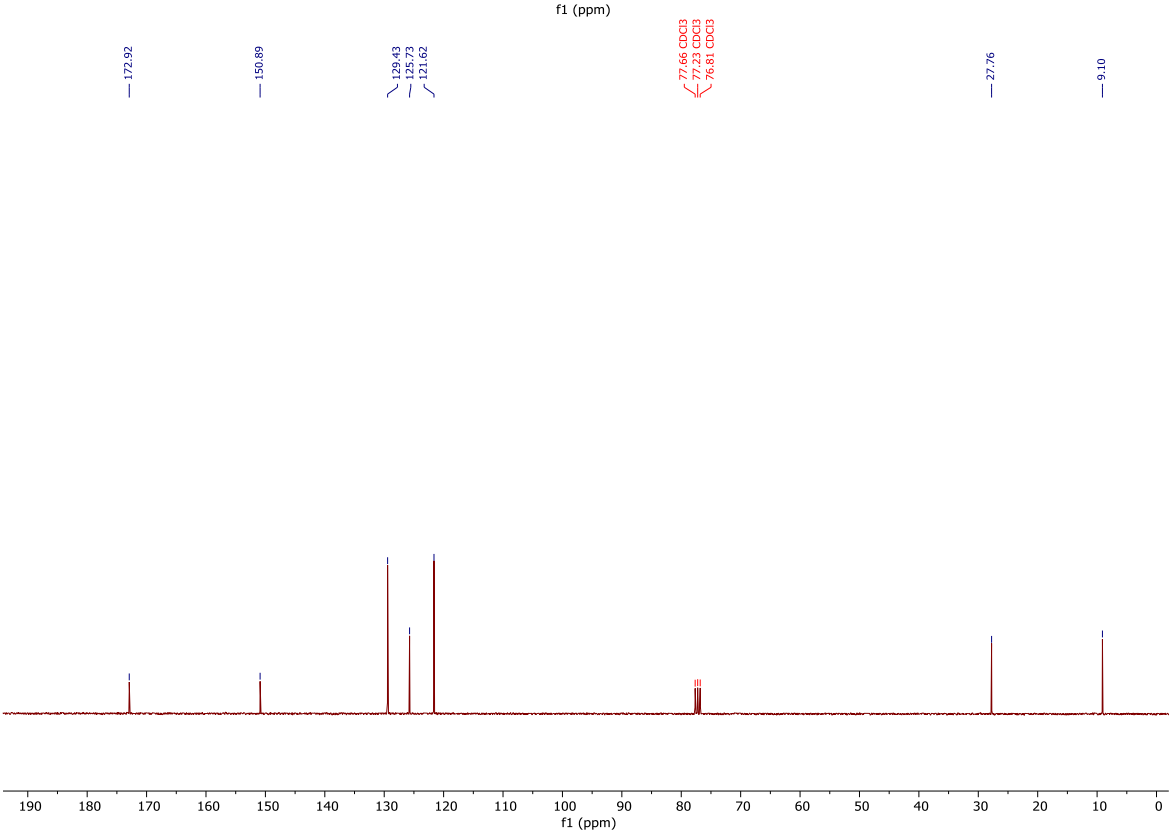


Phenyl butyrate (**54**)

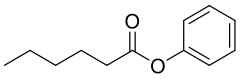


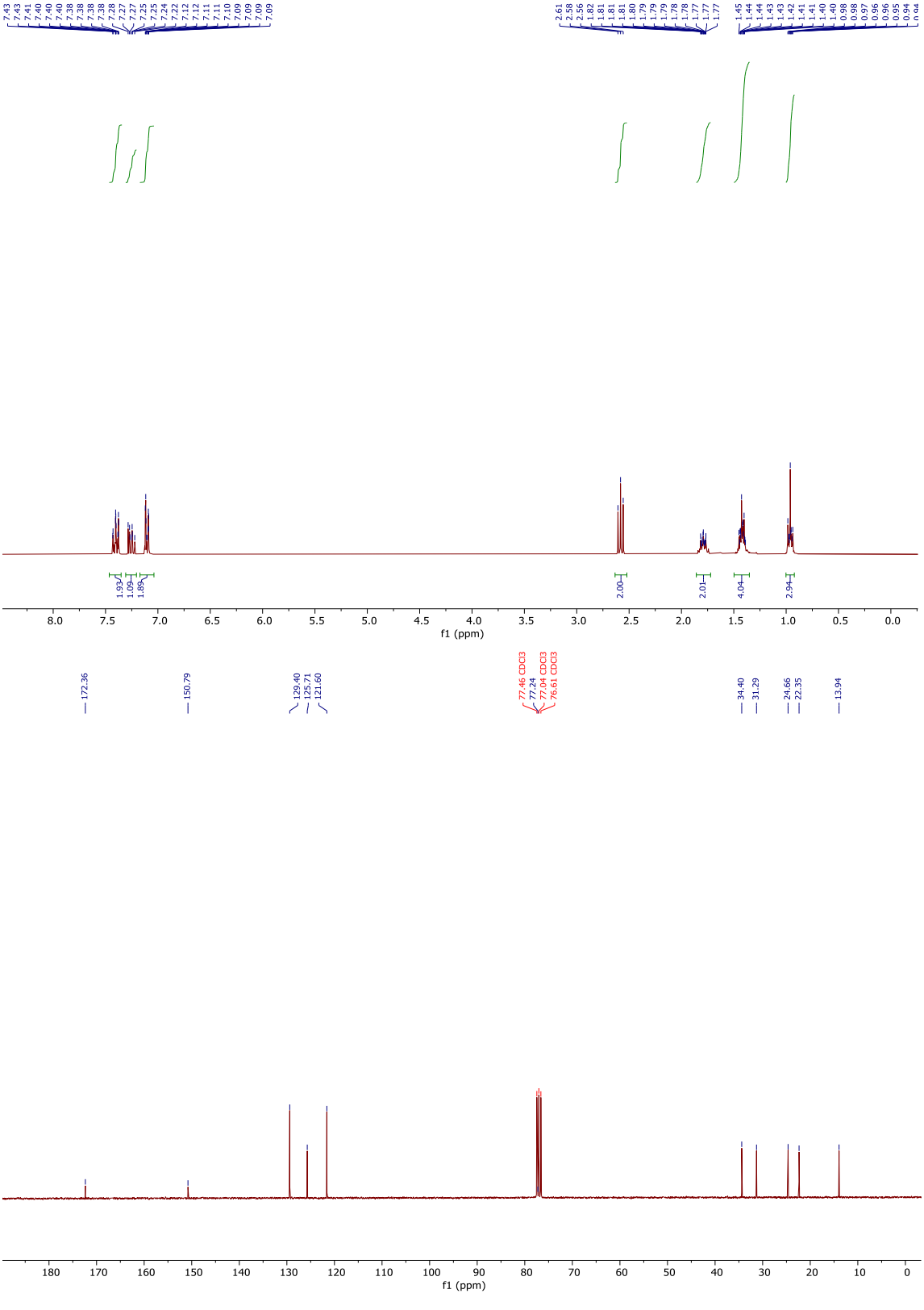




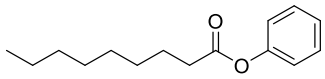


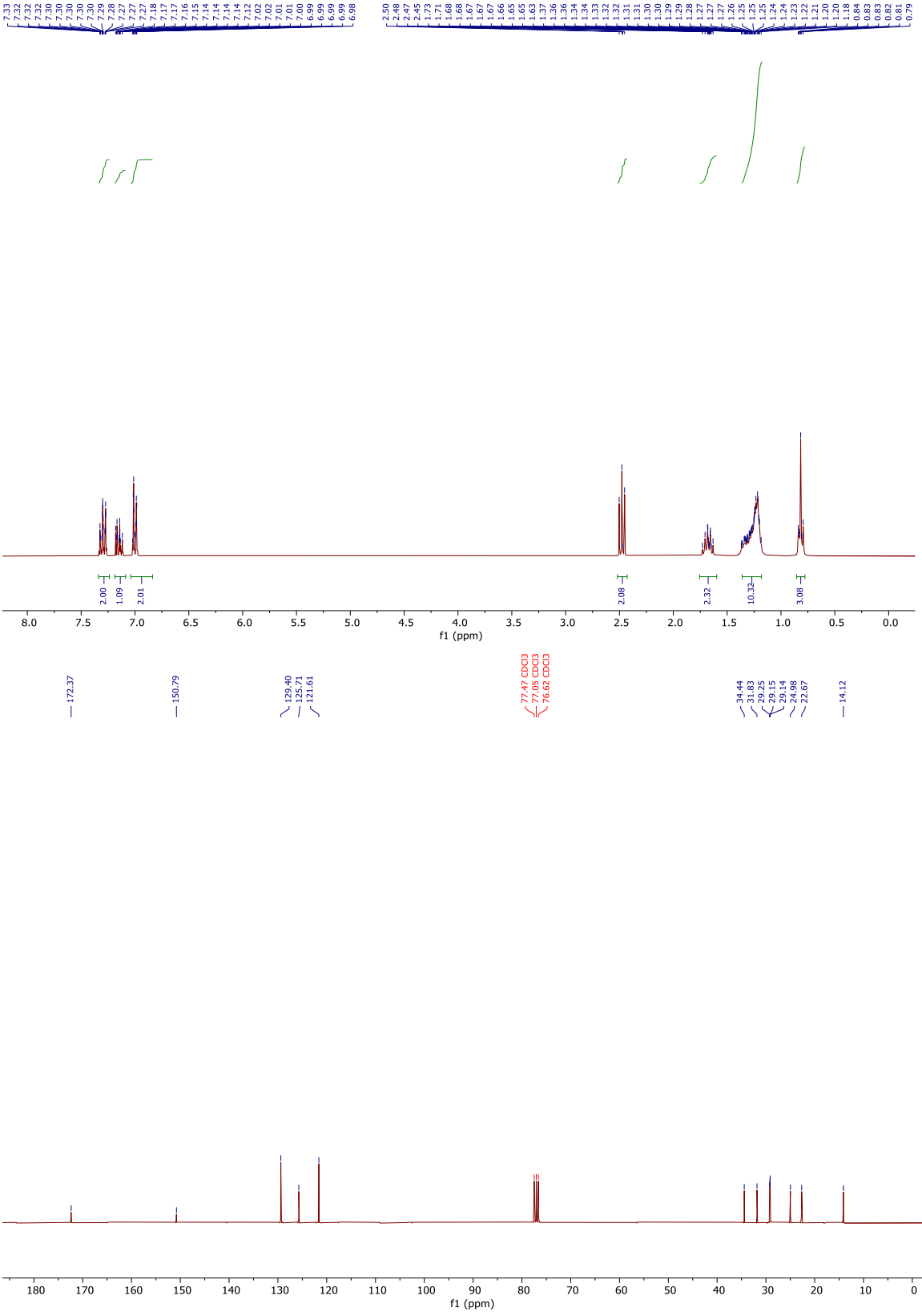
Phenyl hexanoate (**55**)



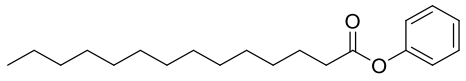


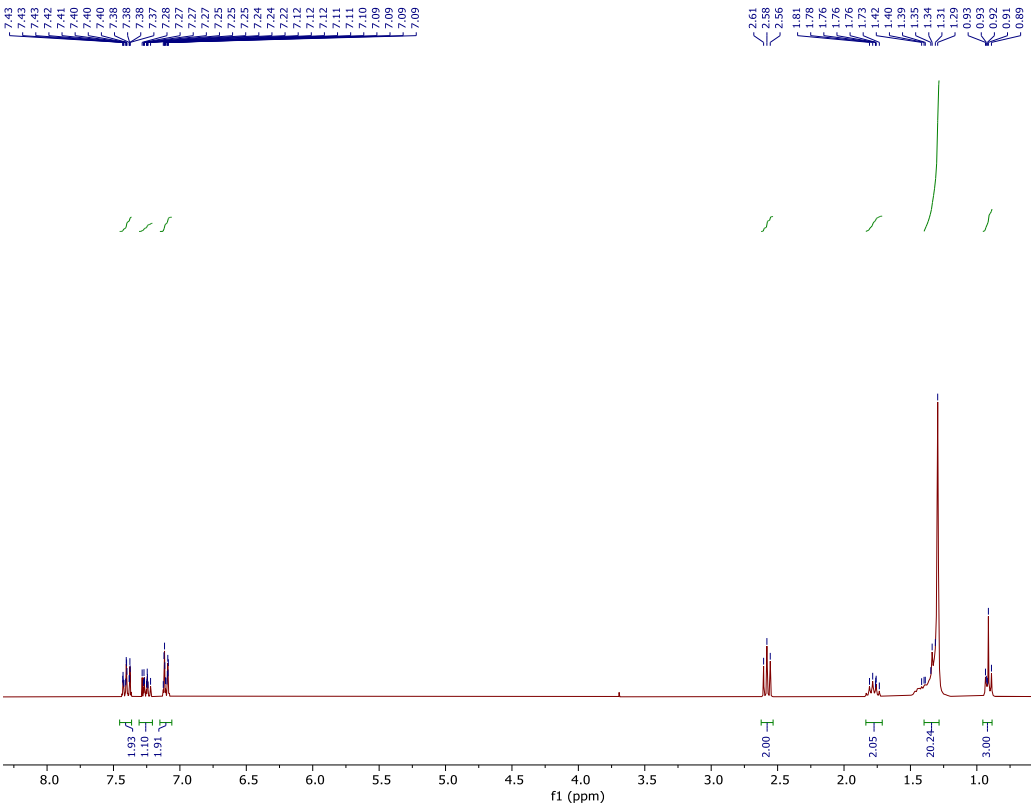
Phenyl nonanoate (**56**)

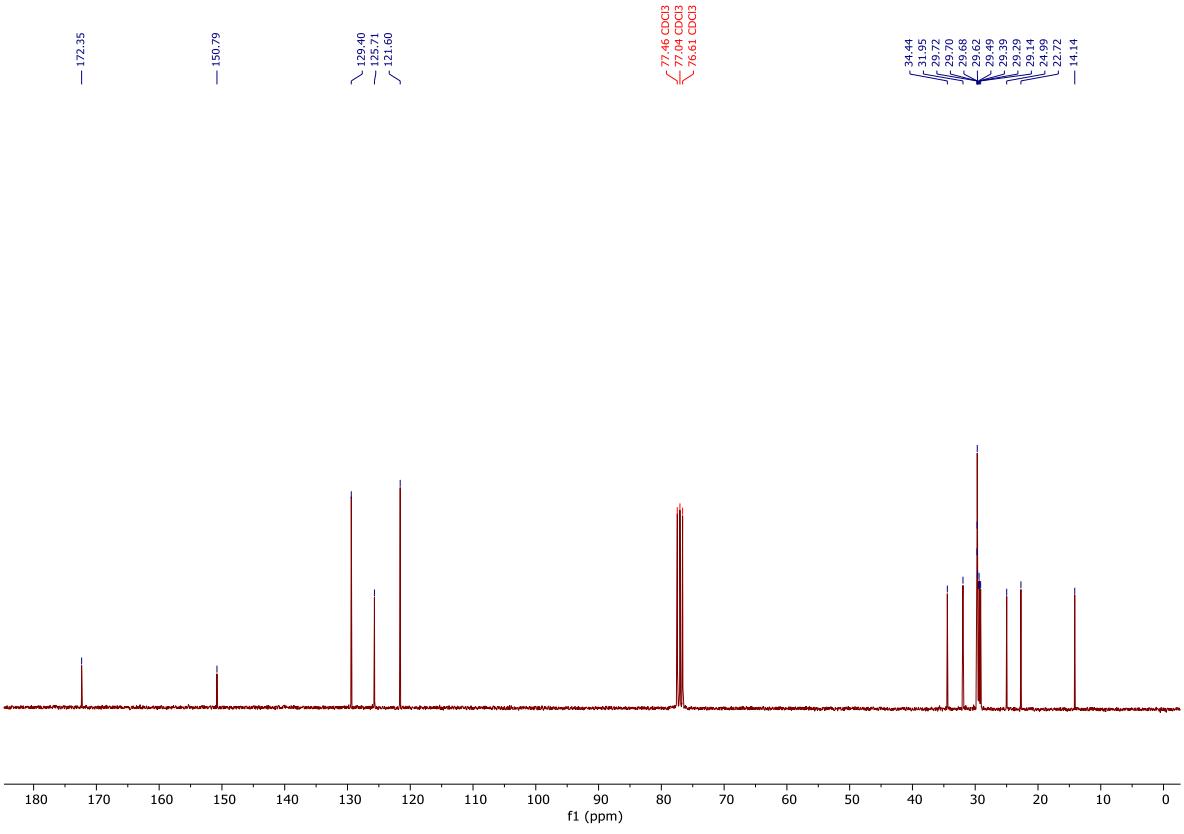




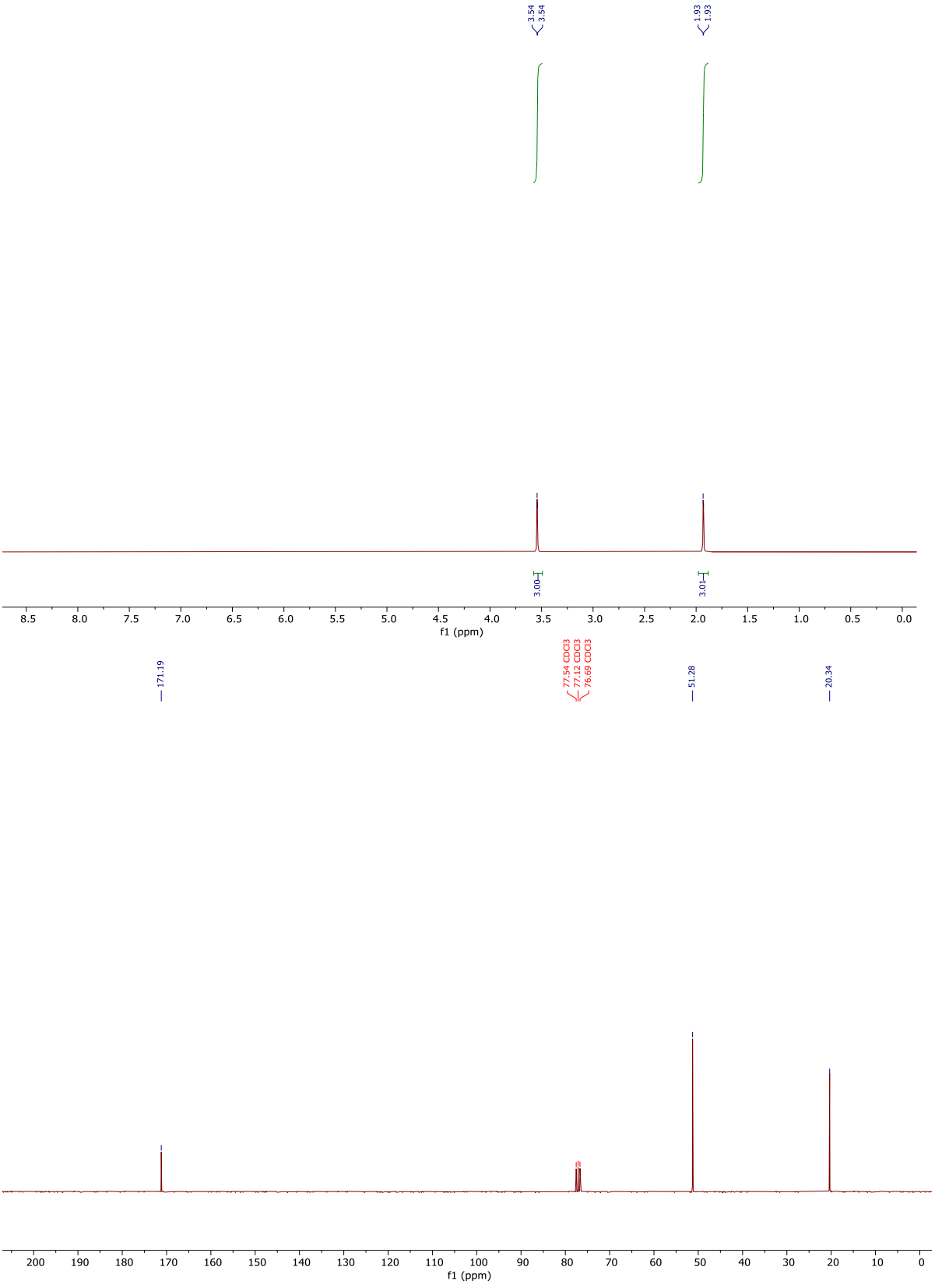
Phenyl tetradecanoate (**57**)



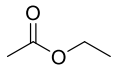


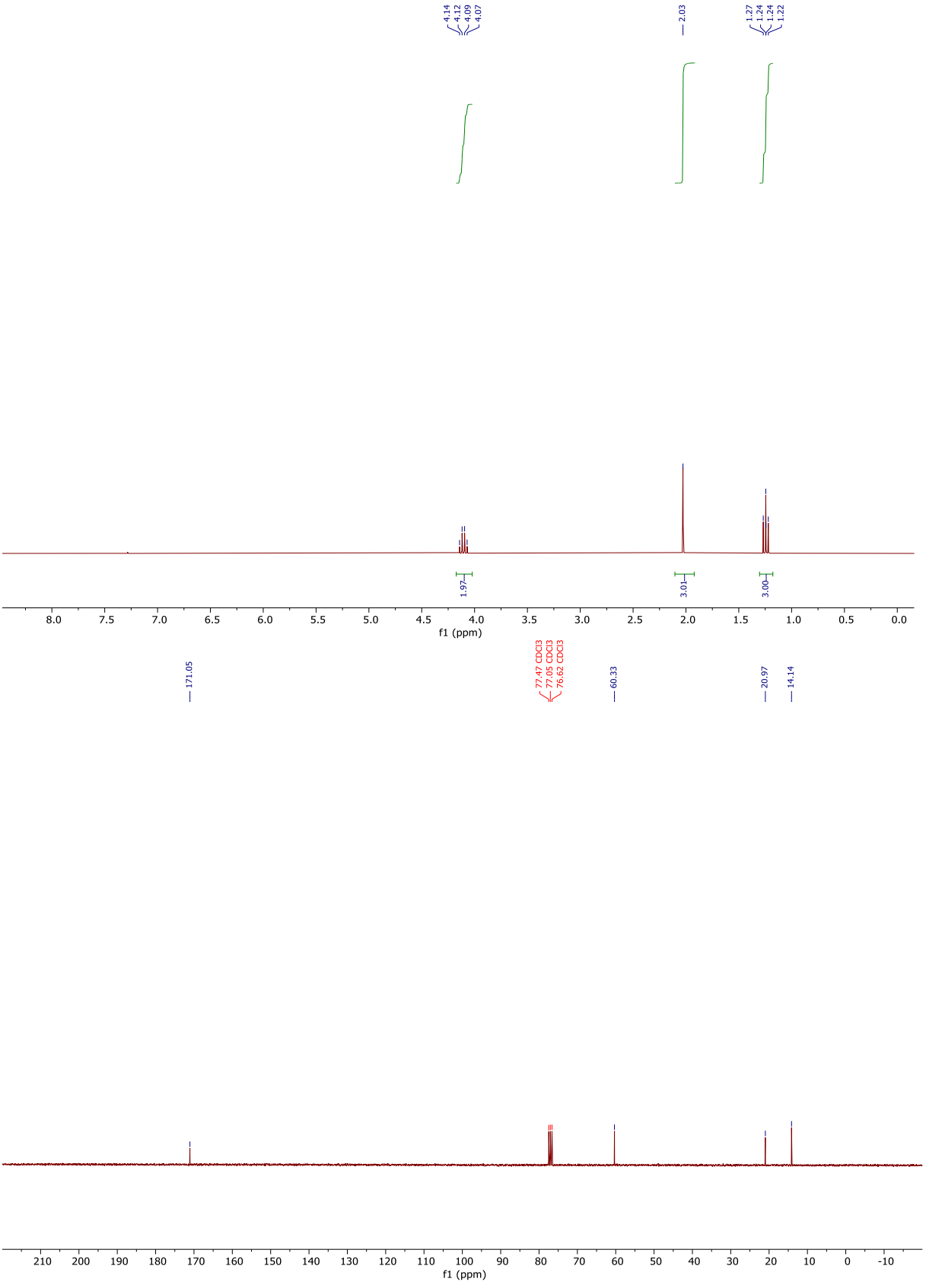


Methyl acetate (**58**)

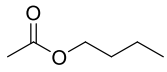


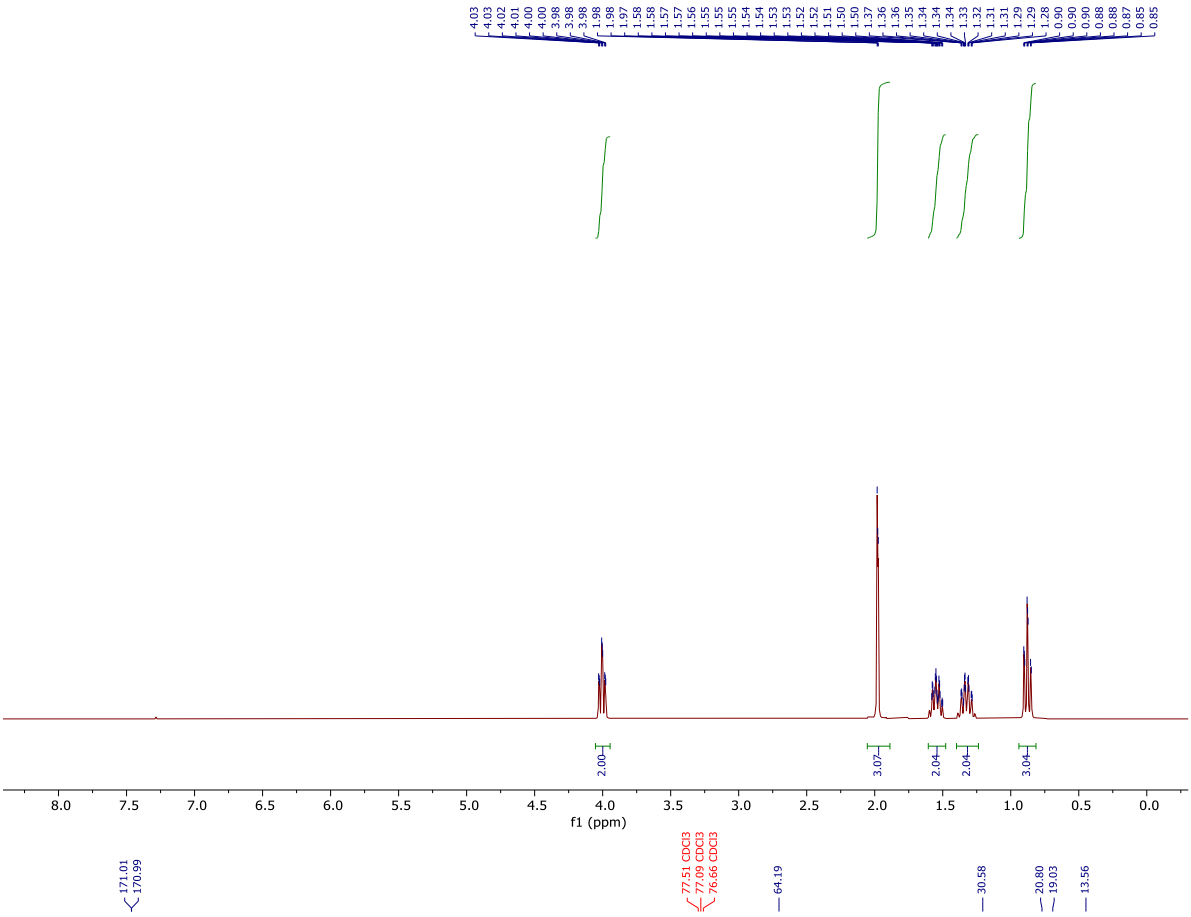
Ethyl acetate (**59**)

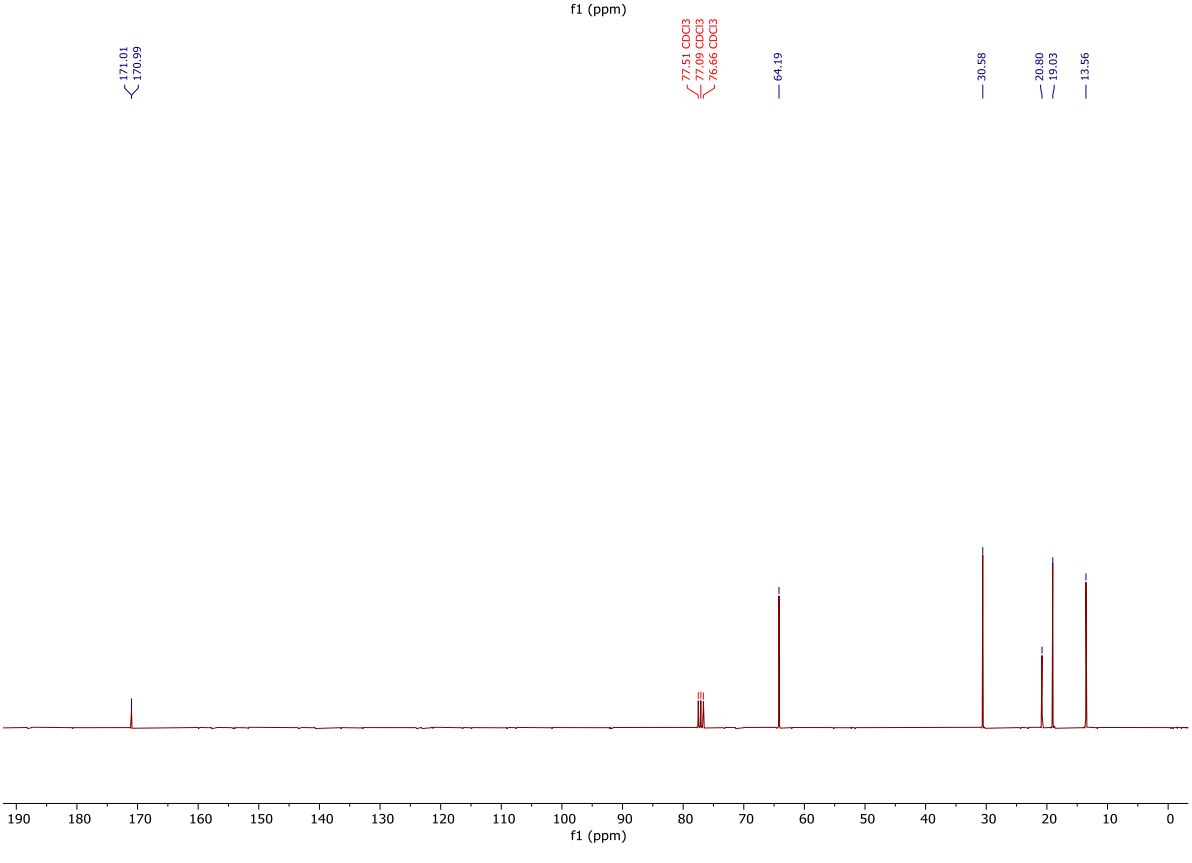




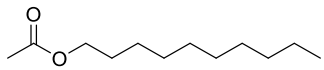
Butyl acetate (**60**)

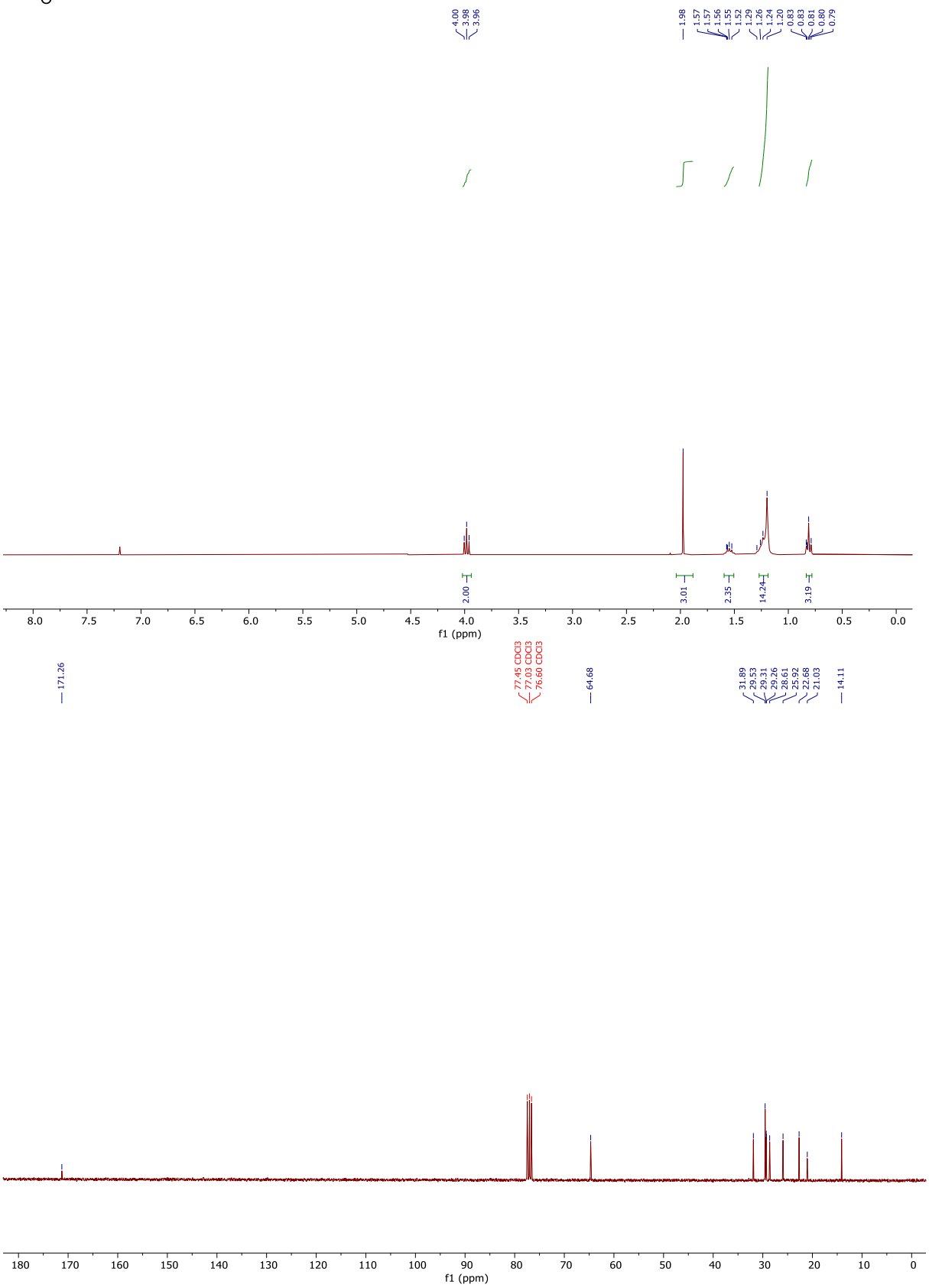




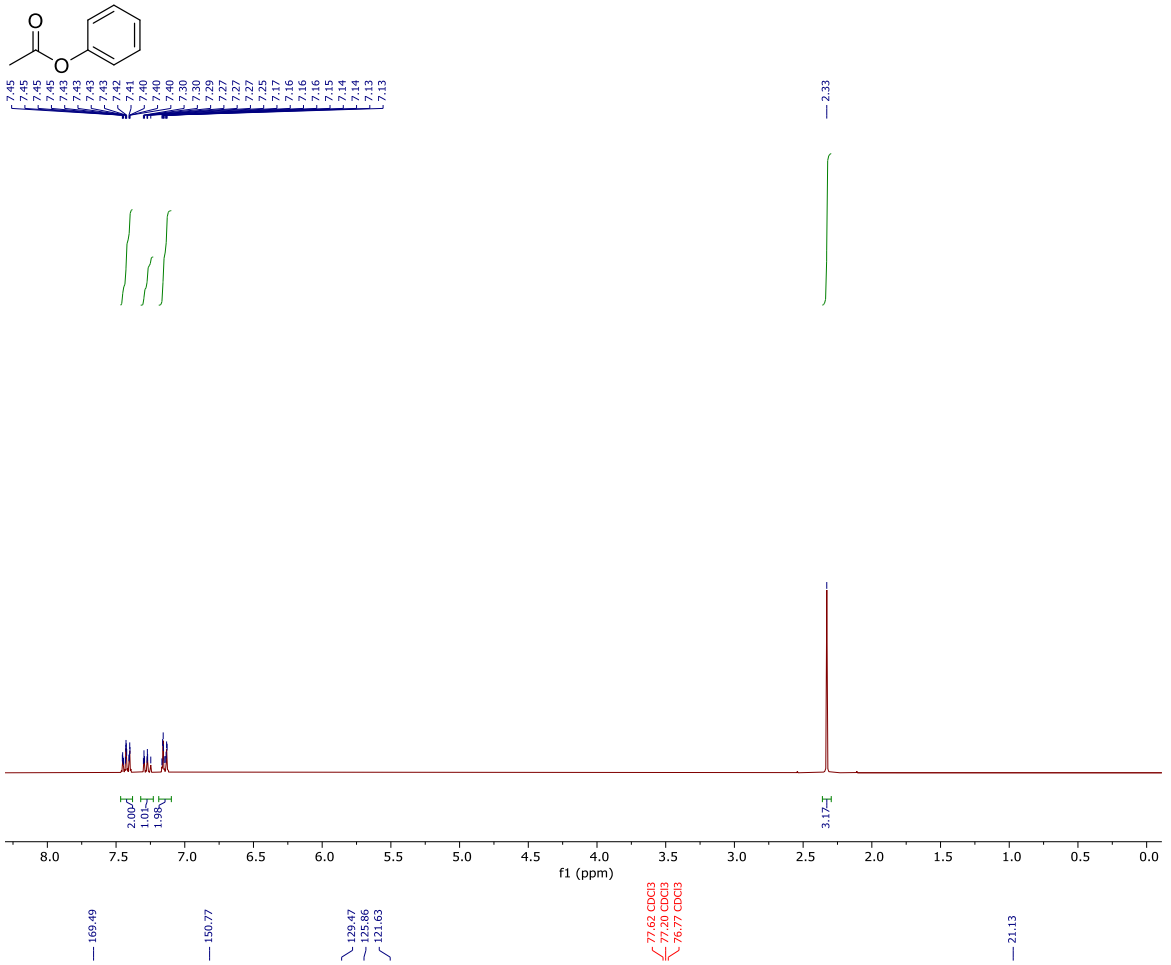


Decyl acetate (**61**)

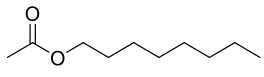


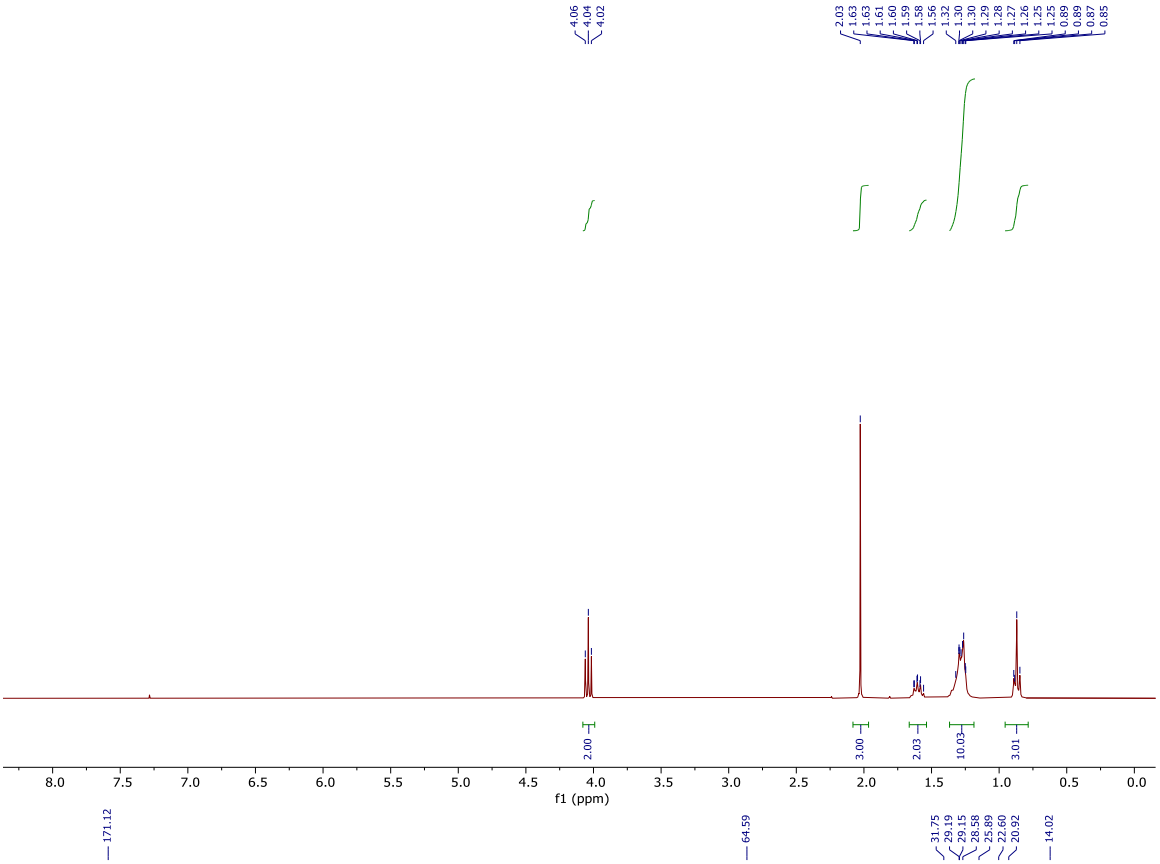


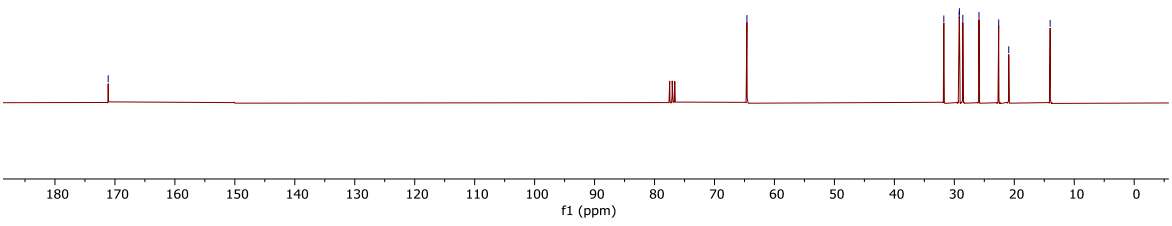
Phenyl acetate (**62**)



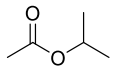
Octyl acetate (**63**)

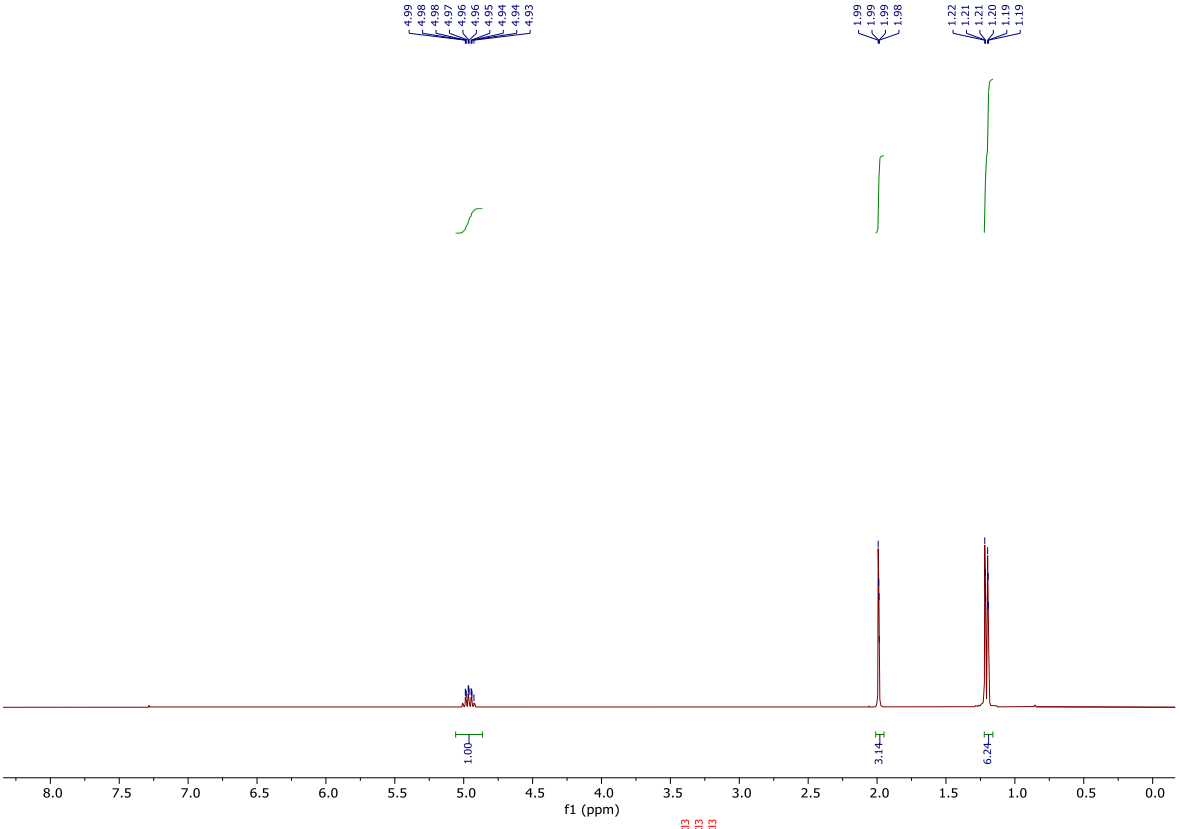


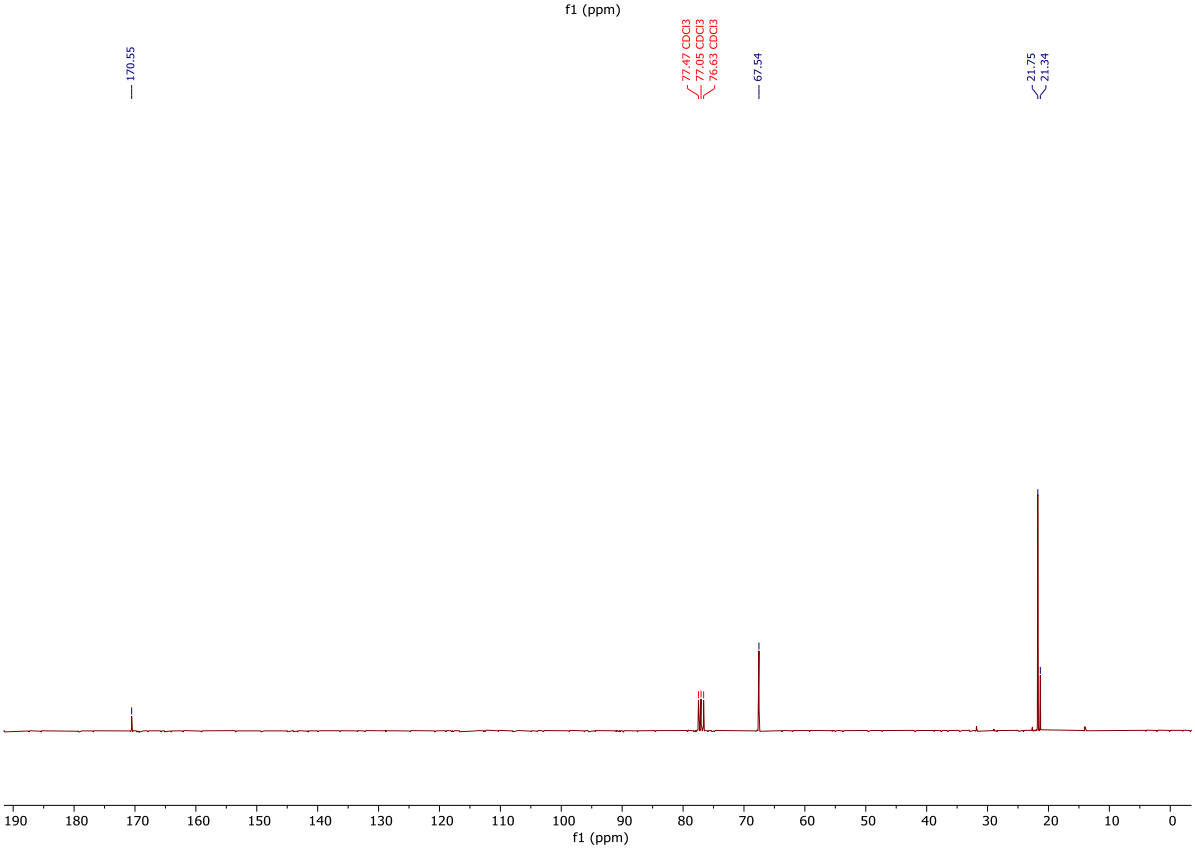




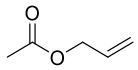
Isopropyl acetate (**64**)

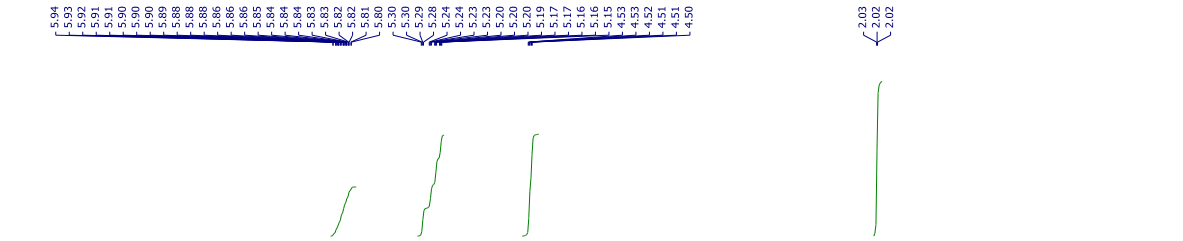


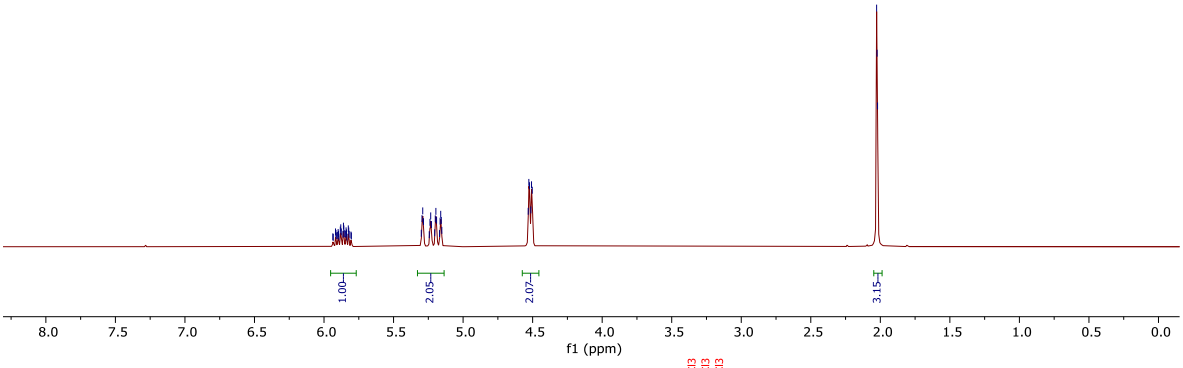


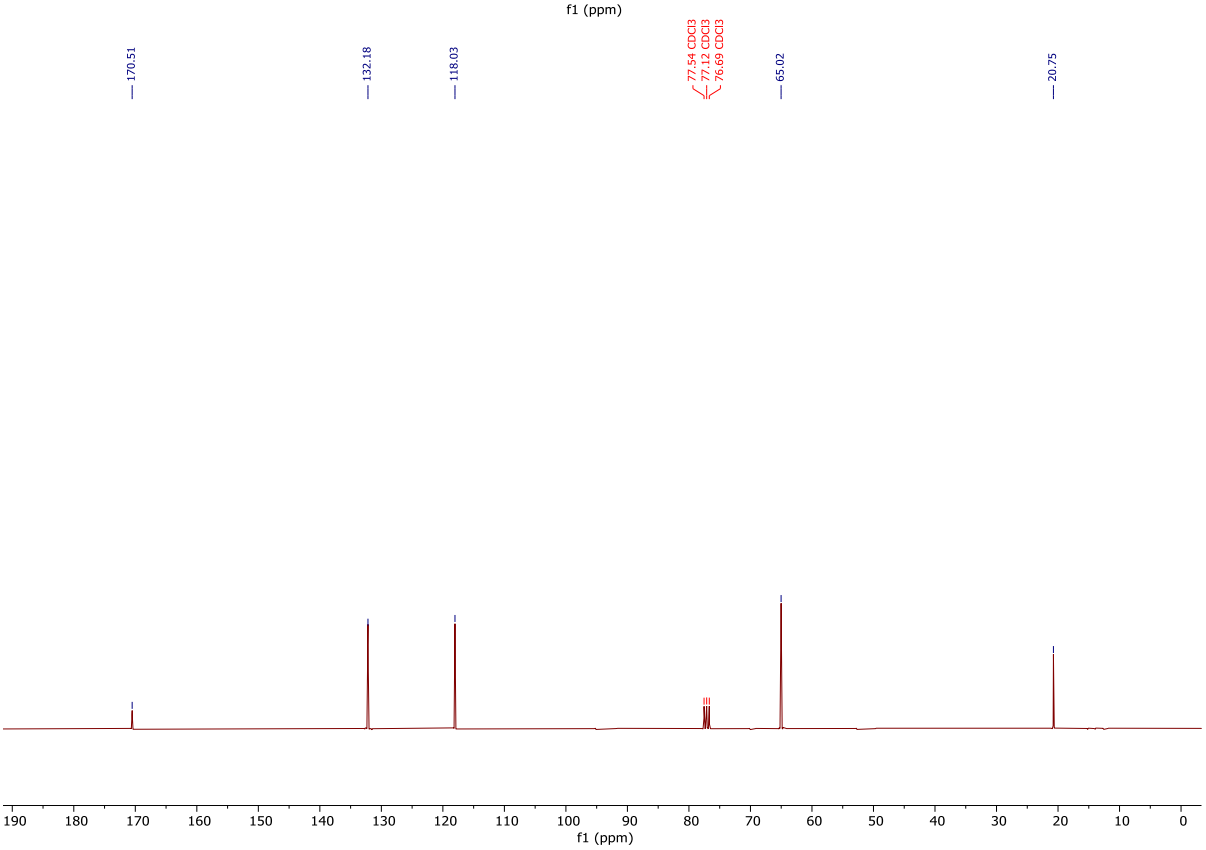


Allyl acetate (**65**)

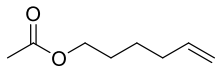


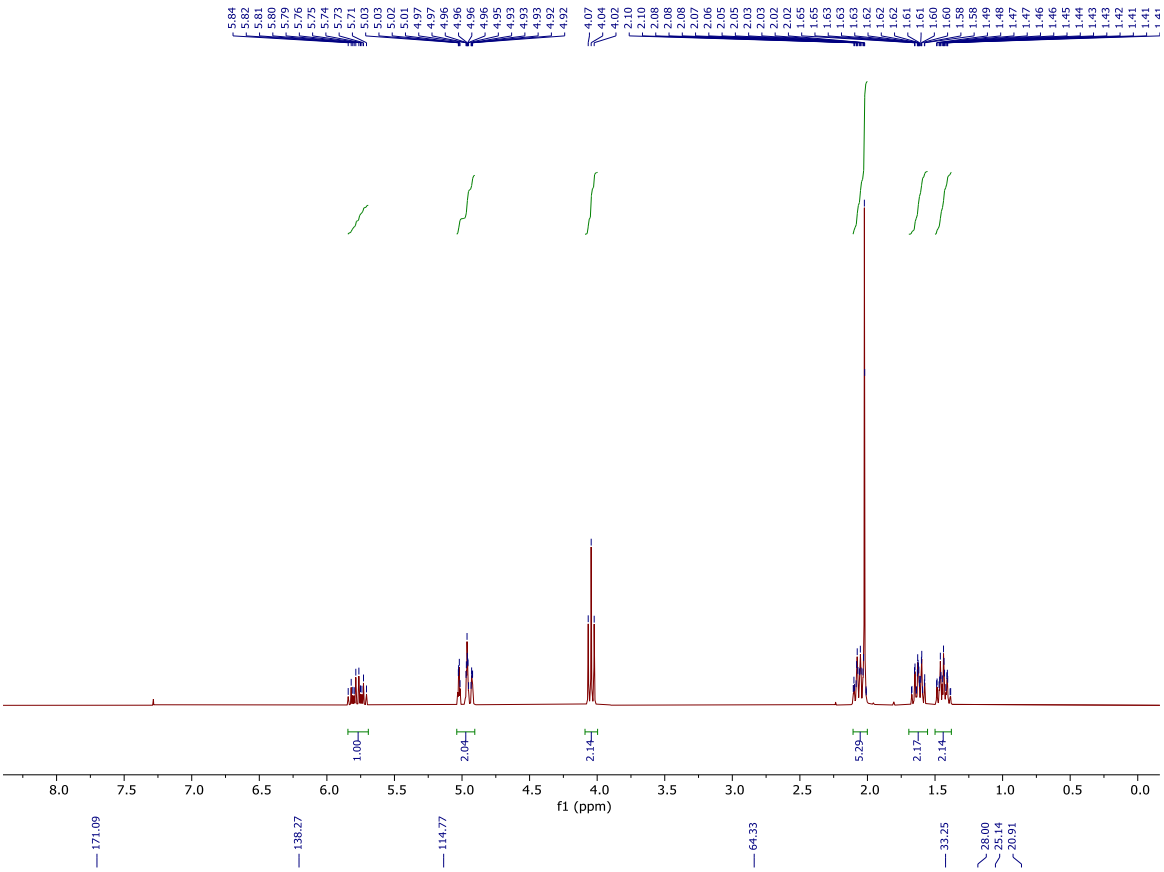


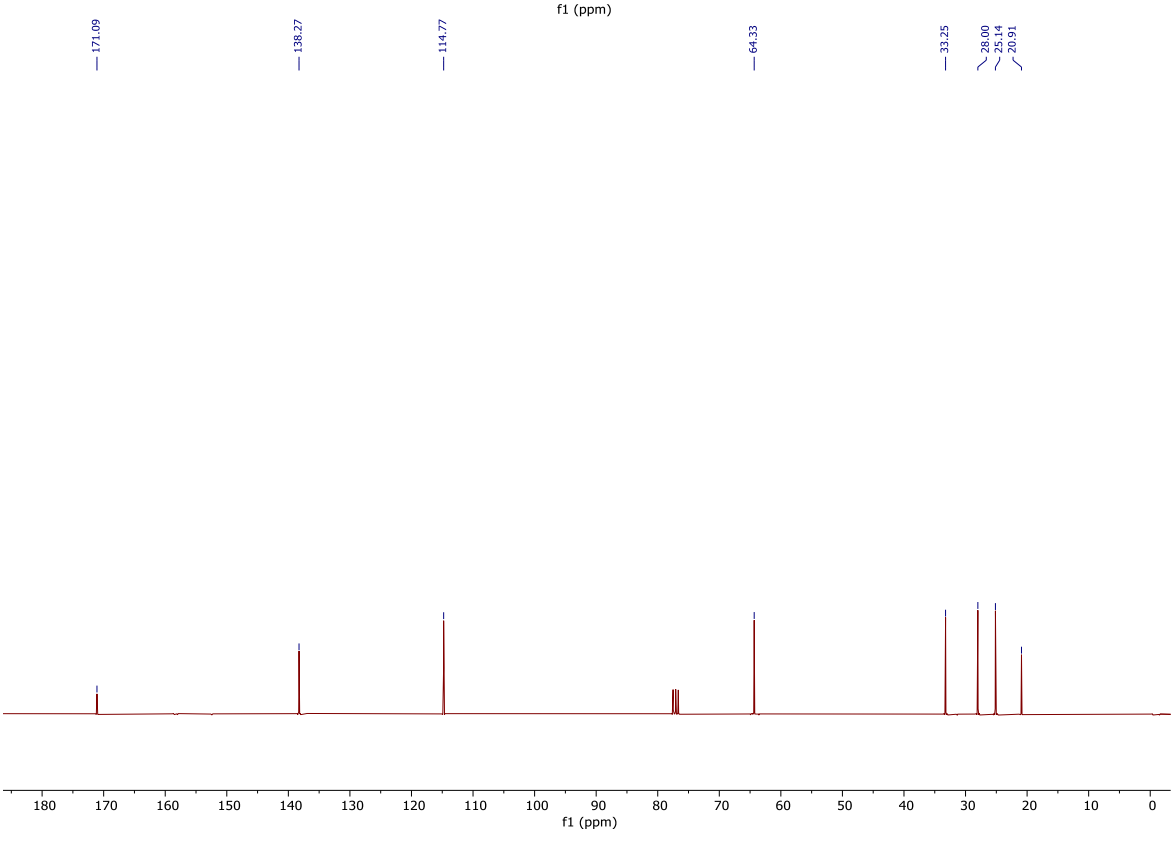




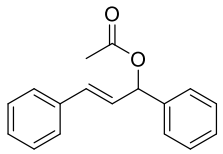
Hex-5-en-1-yl acetate (**66**)

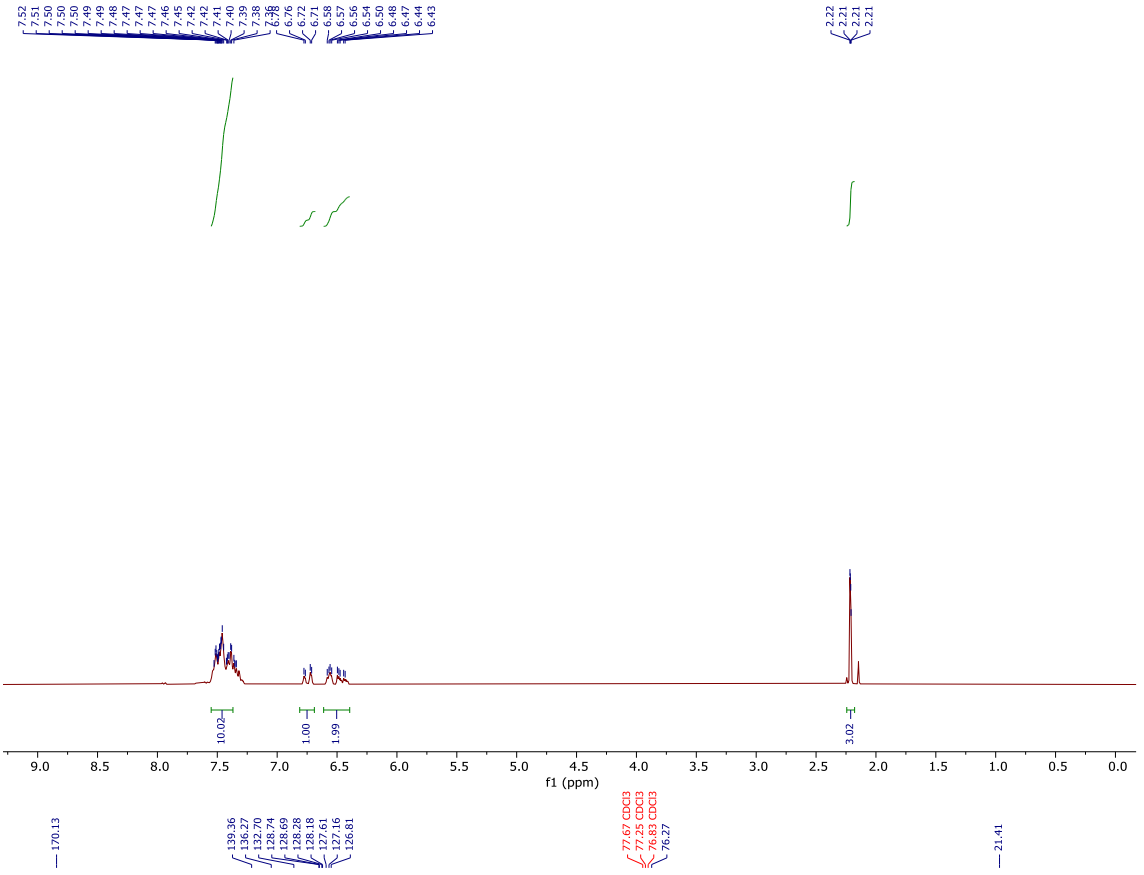


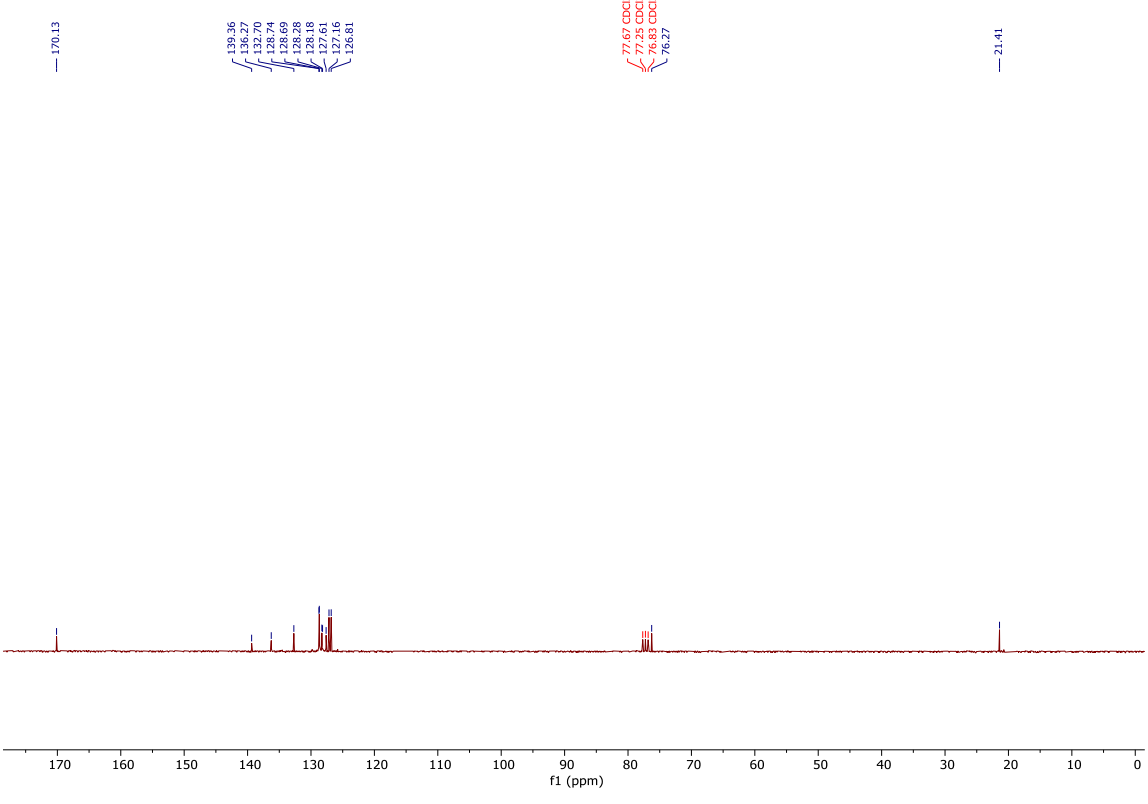




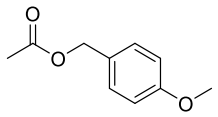
(E)-1,3-Diphenylallyl acetate (**67**)

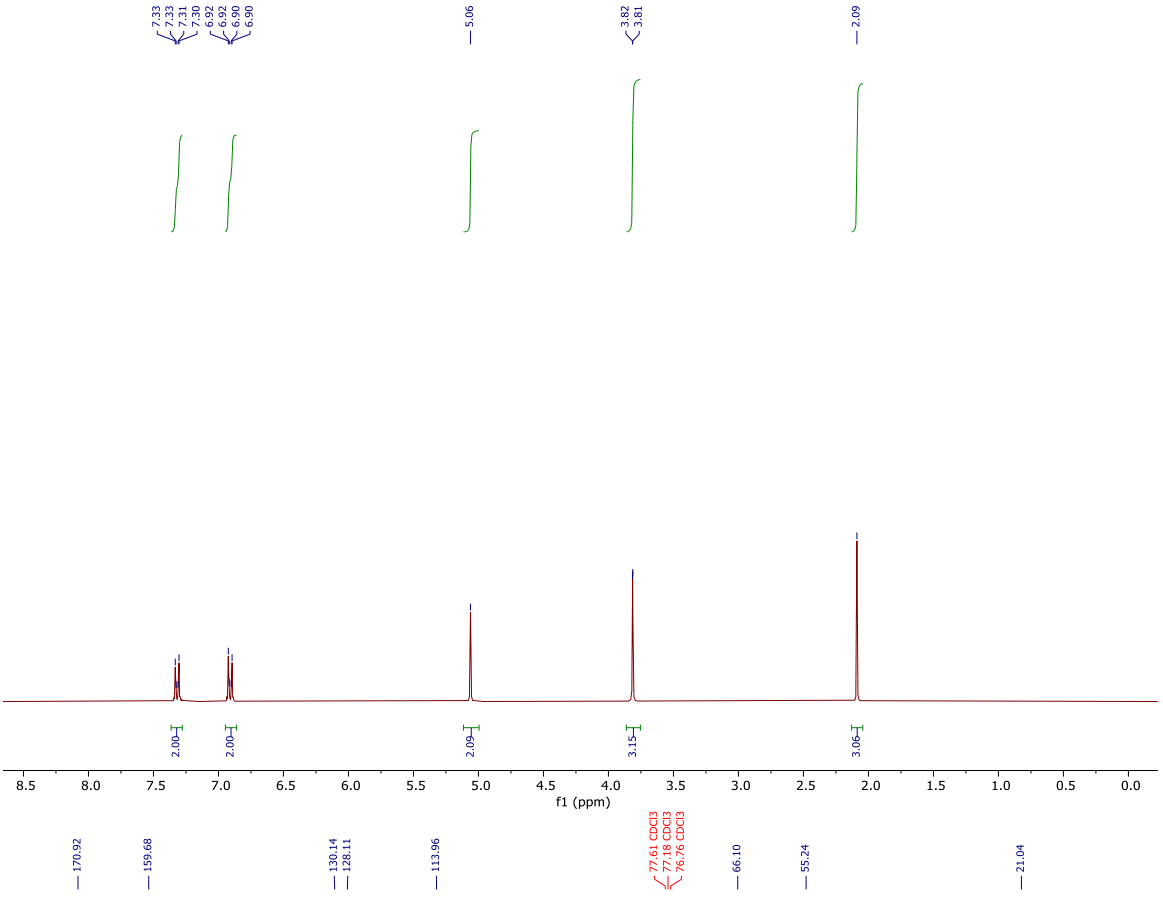


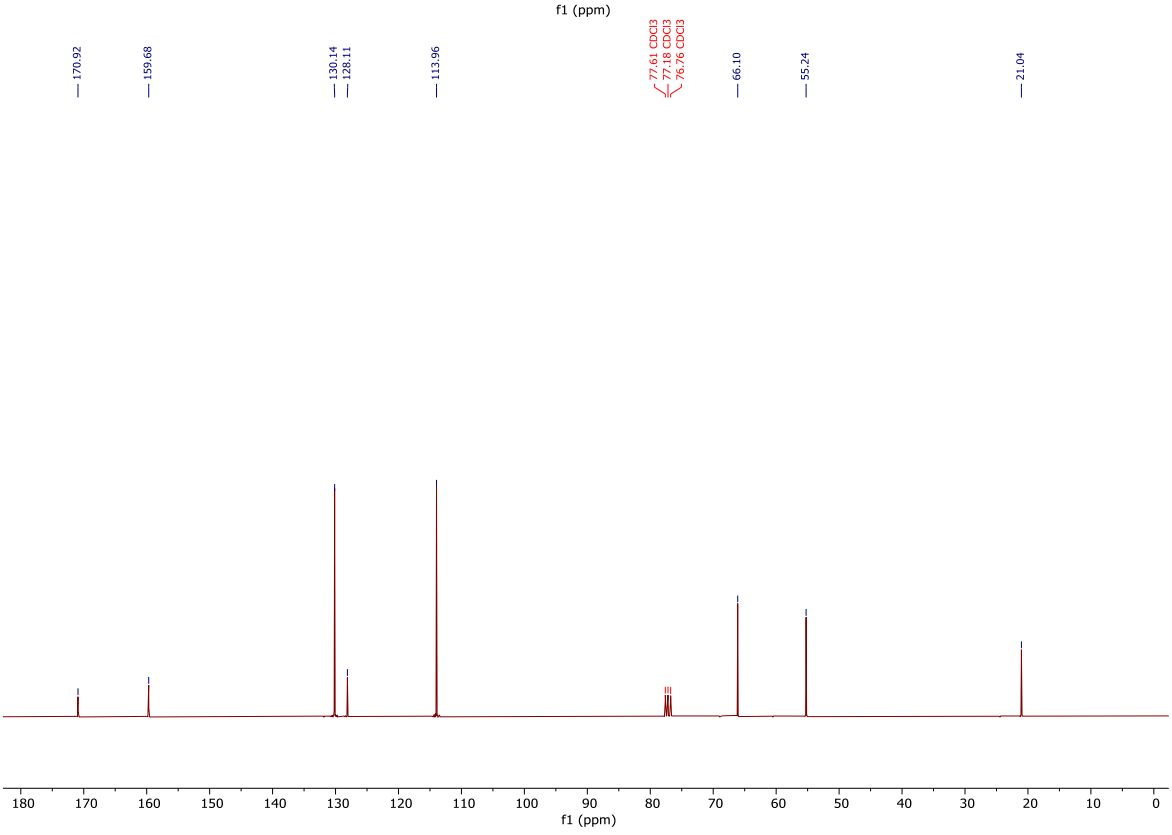




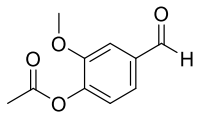
4-Methoxybenzyl acetate (**68**)

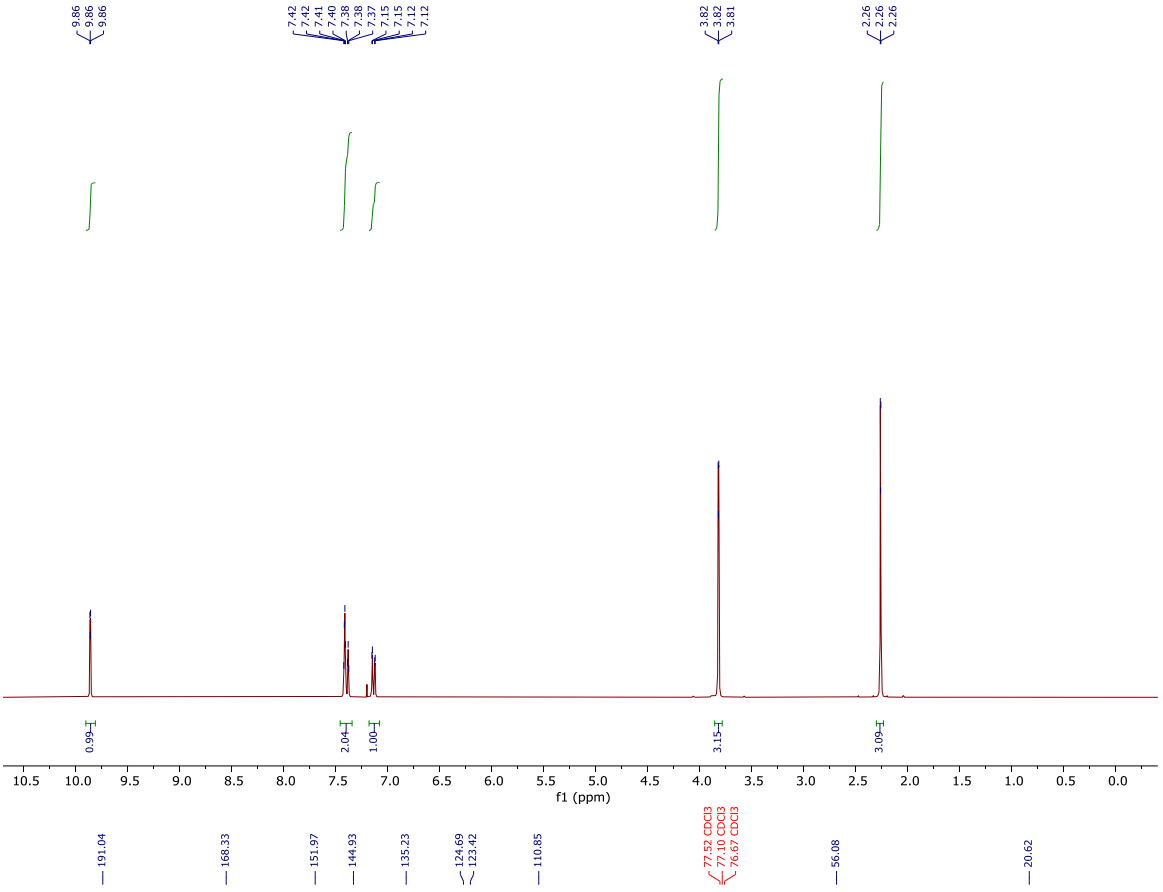


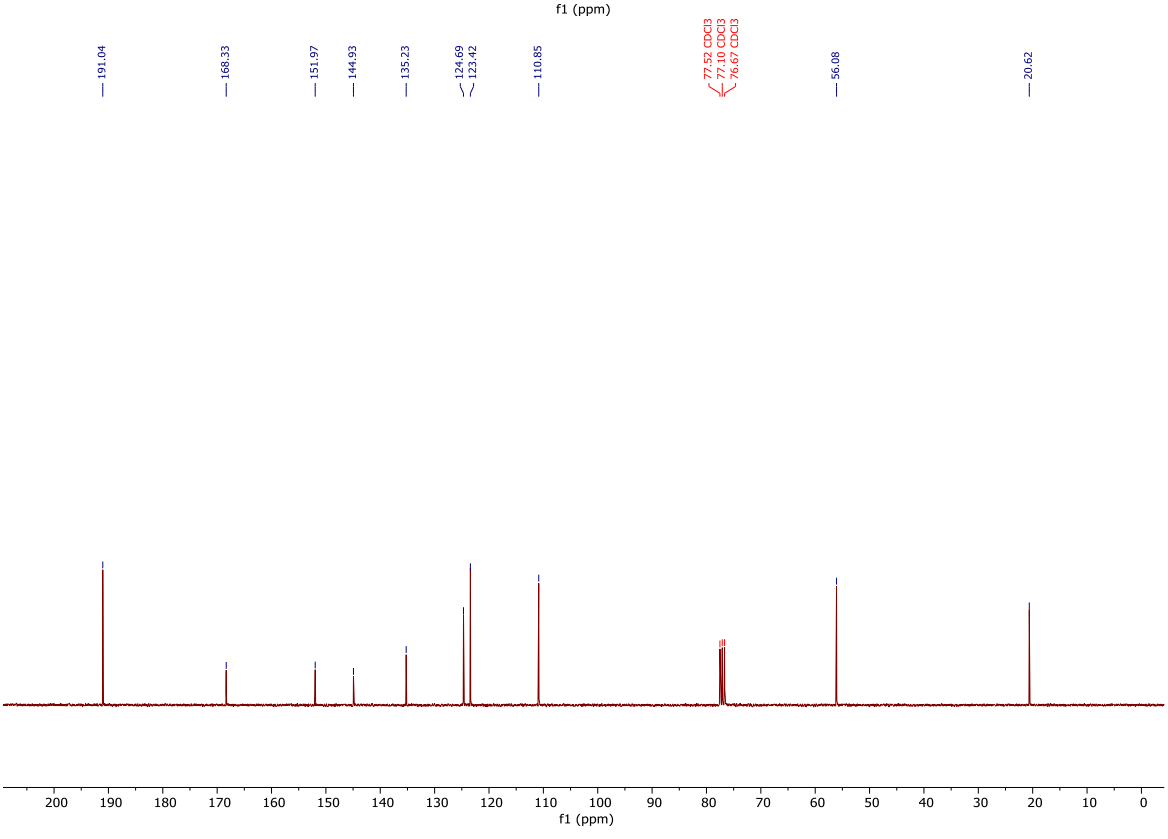




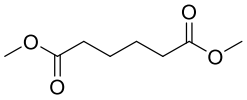
4-Formyl-2-methoxyphenyl acetate (**69**)

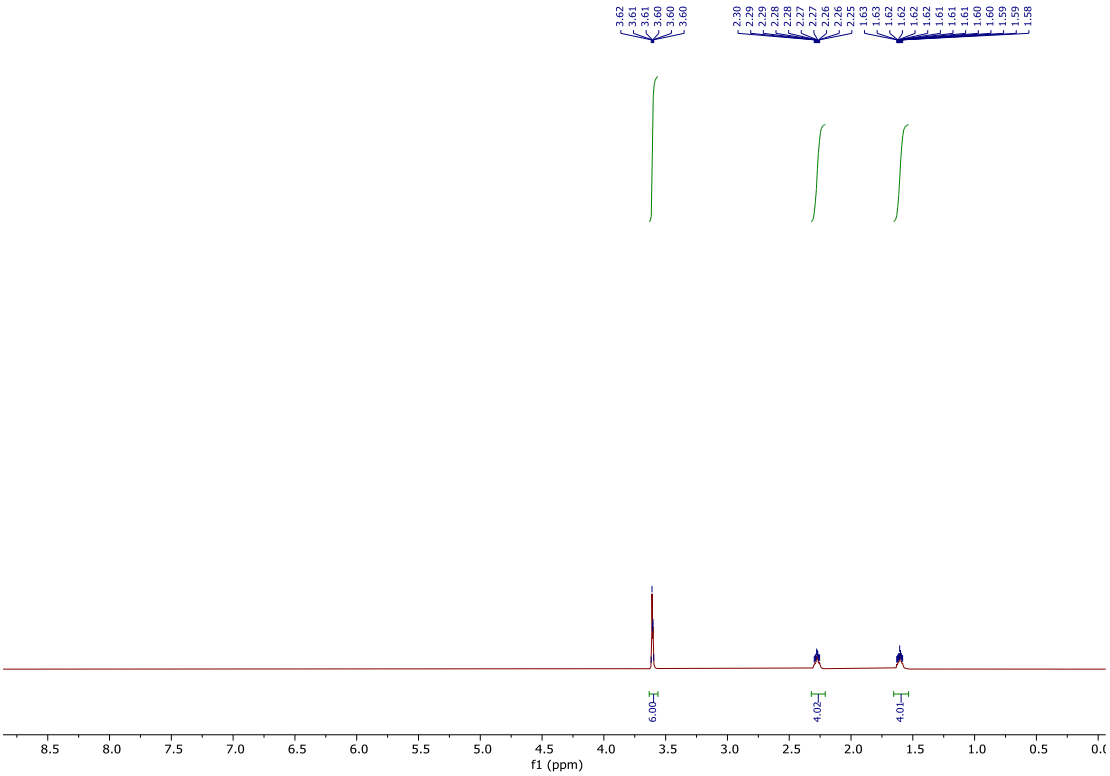


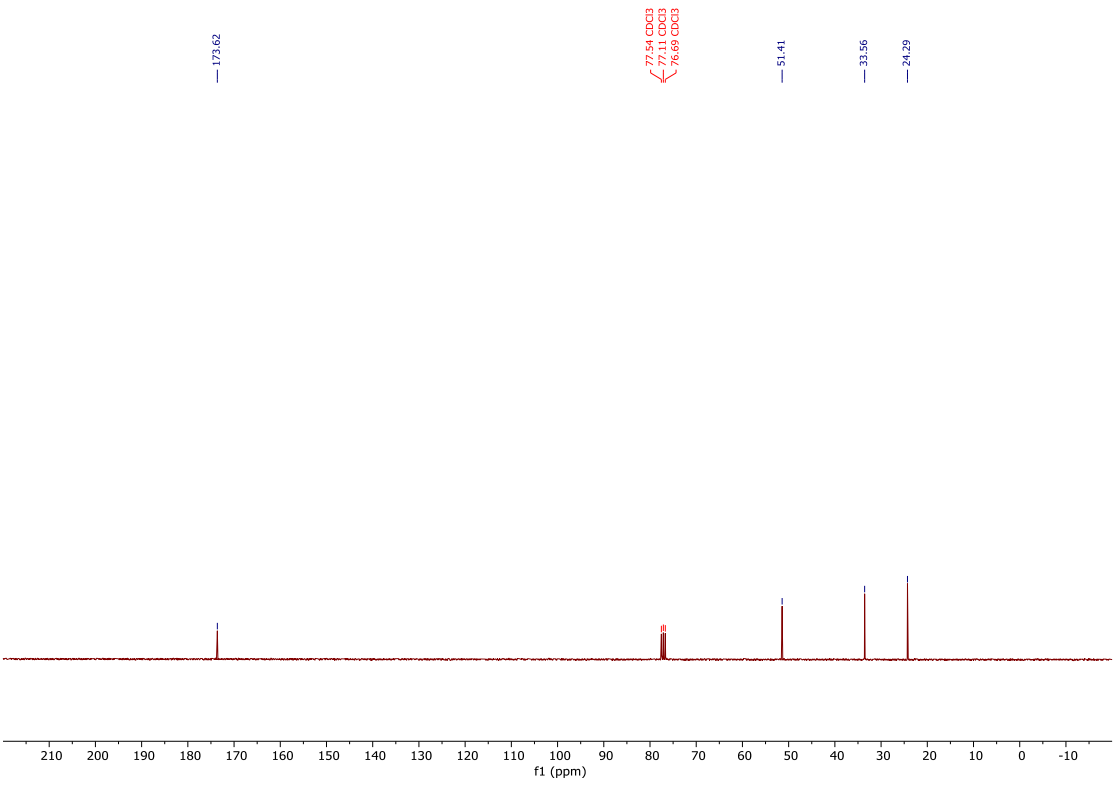




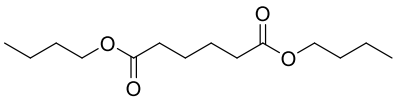
Dimethyl adipate (**70**)

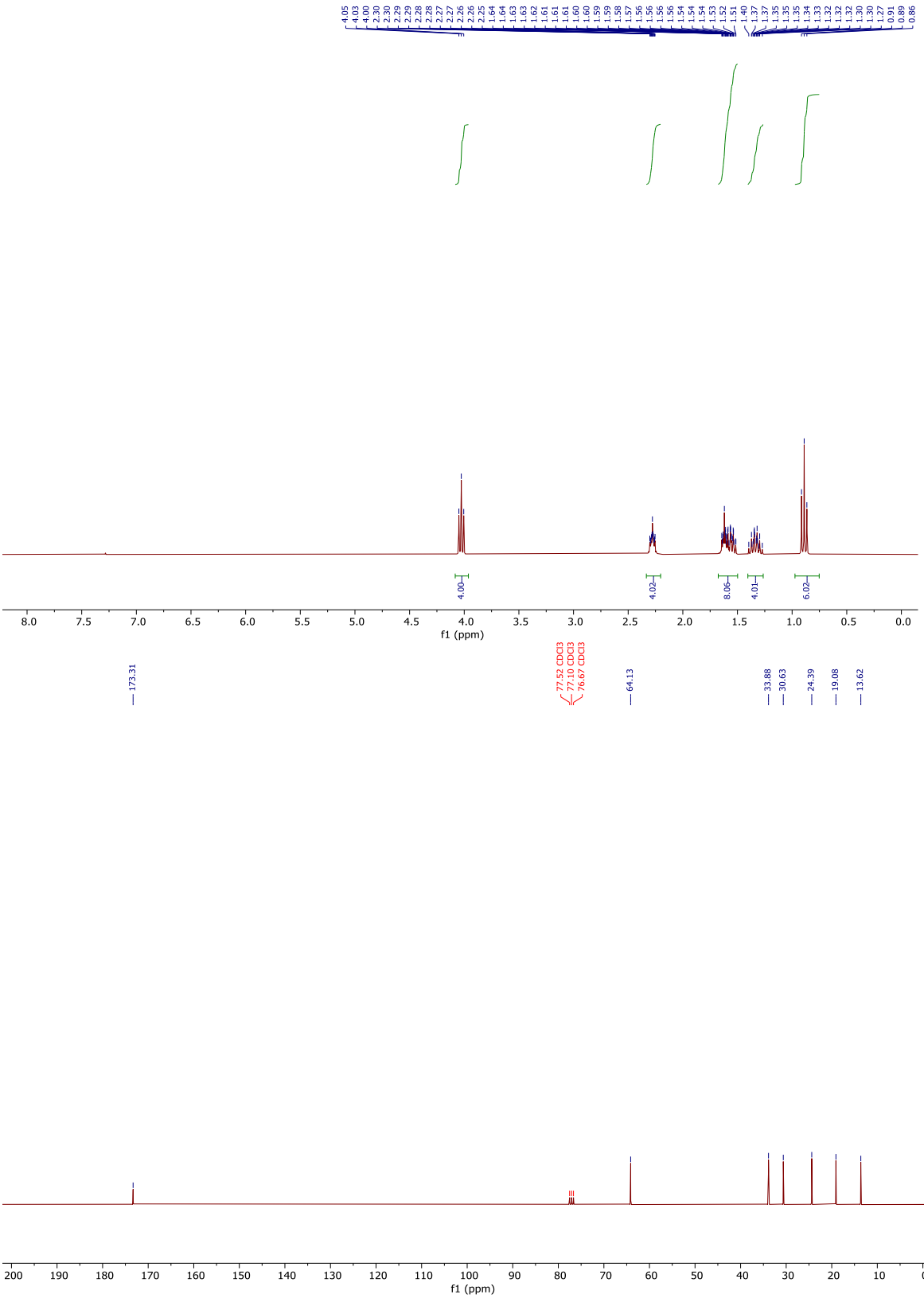




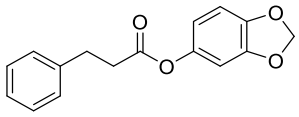


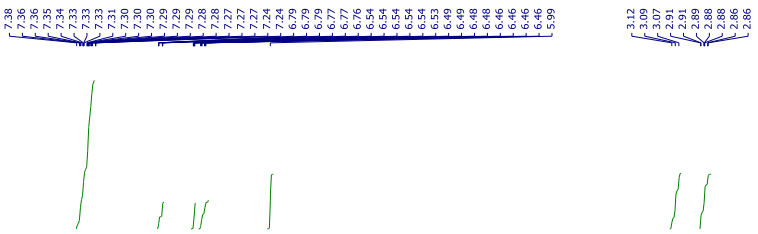
Dibutyl adipate (**71**)

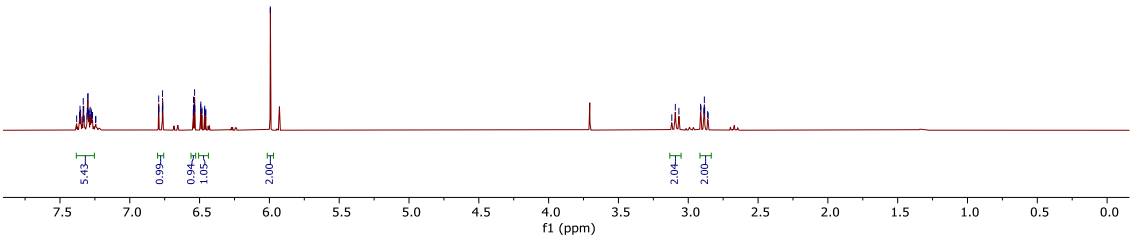


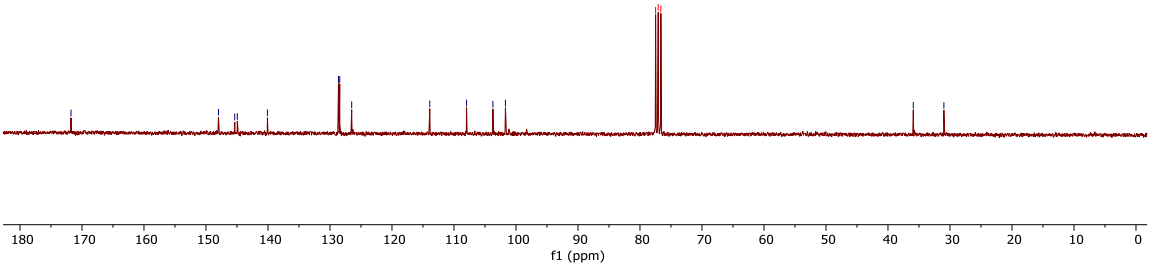


Benzo[d][1,3]dioxol-5-yl 3-phenylpropanoate (**72**)

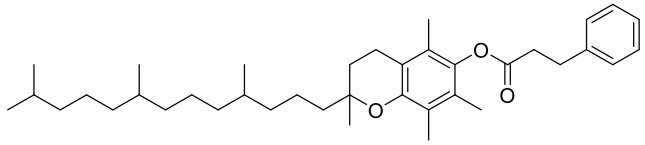


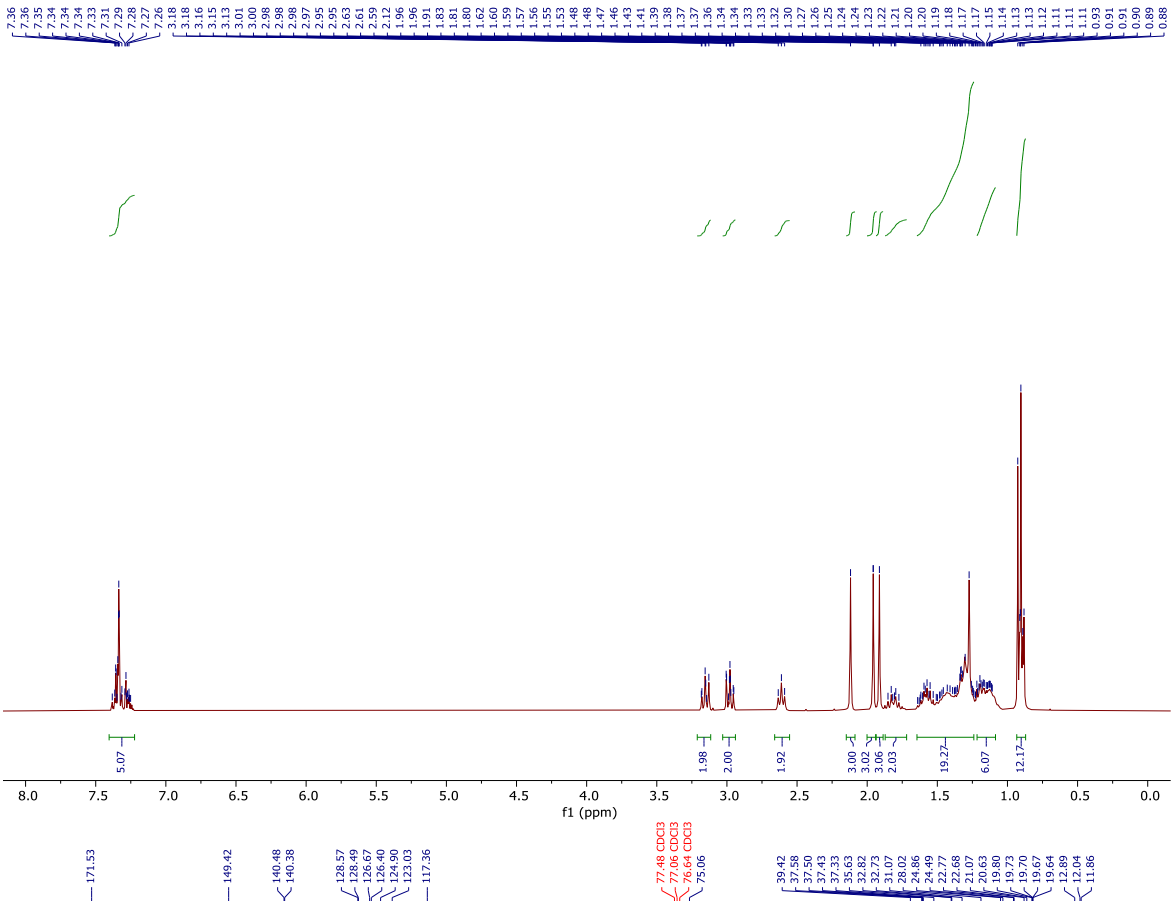


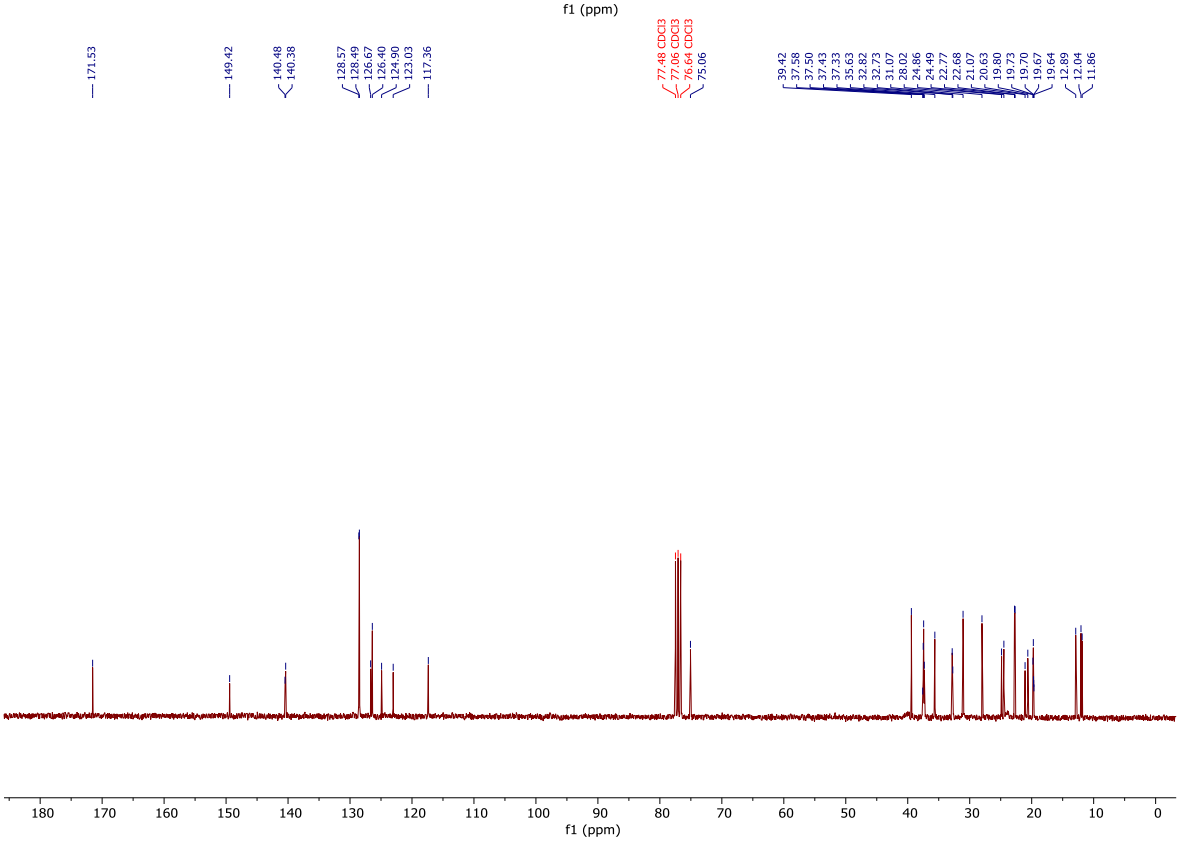




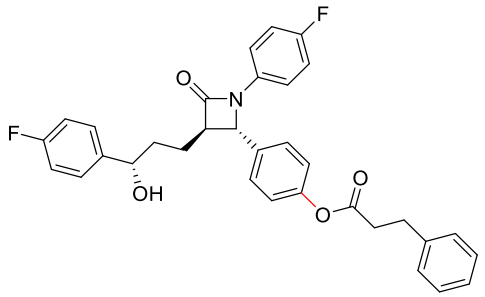
2,5,7,8-Tetramethyl-2-(4,8,12-trimethyltridecyl)chroman-6-yl 3-phenylpropanoate (**73**)

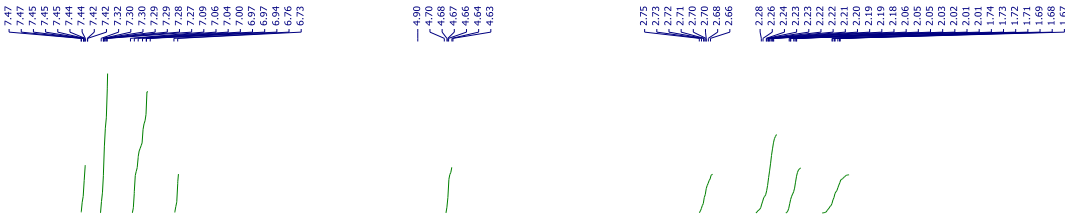


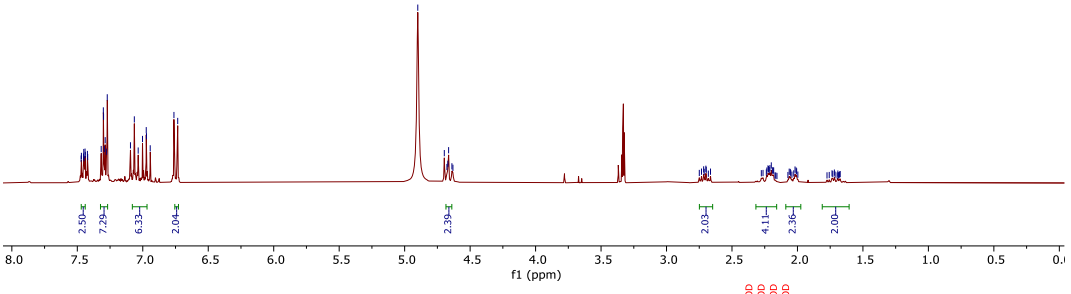


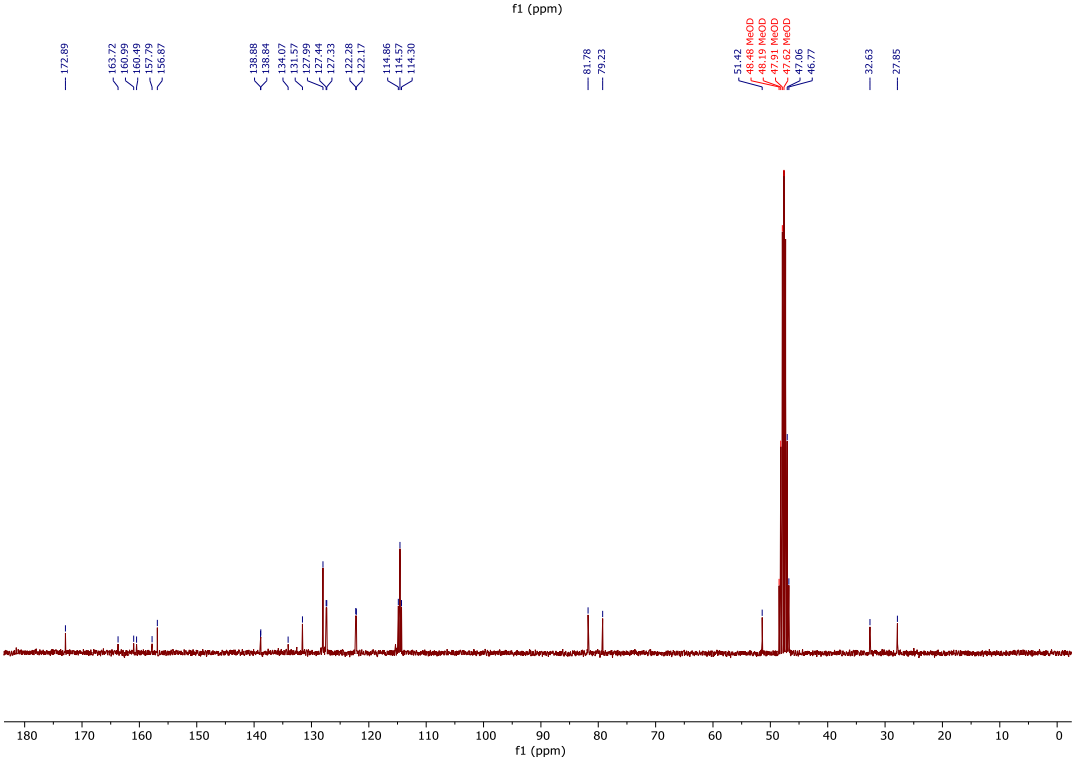


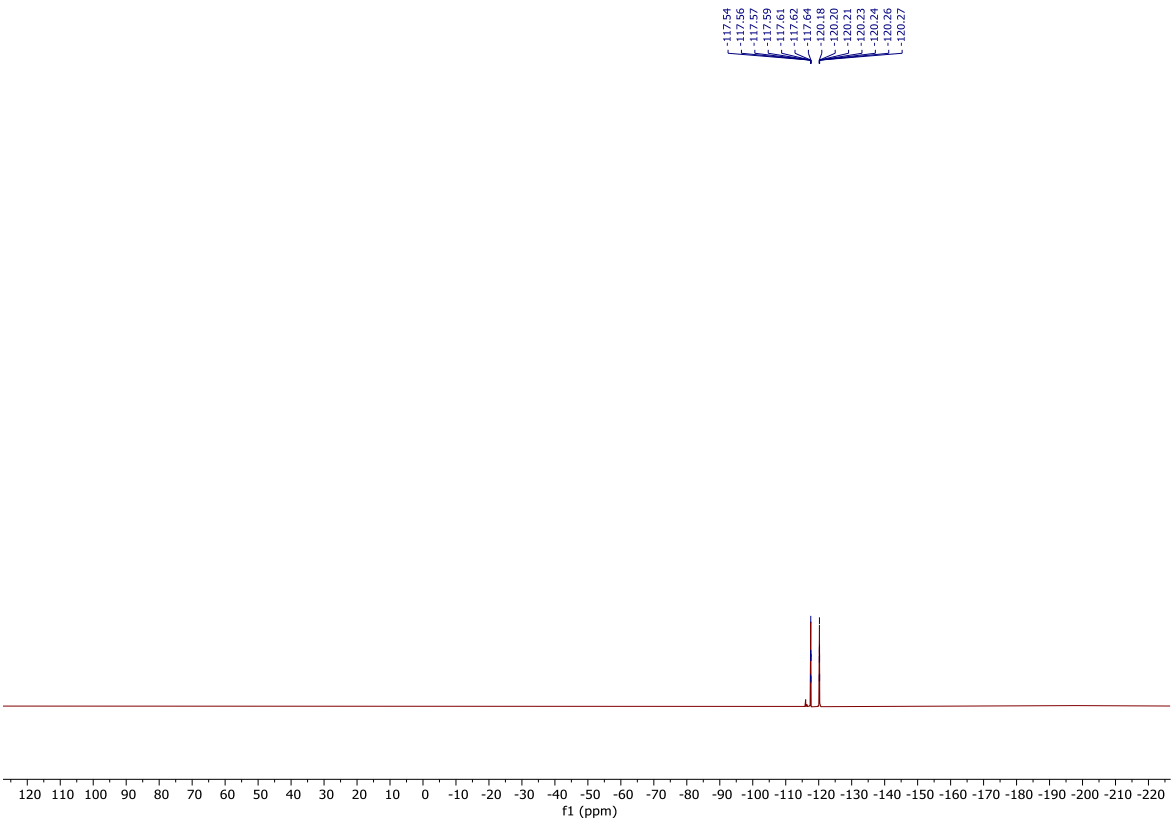
4-((2S,3R)-1-(4-Fluorophenyl)-3-((S)-3-(4-fluorophenyl)-3-hydroxypropyl)-4-oxoazetidin-2-yl)phenyl 3-phenylpropanoate (**74**)



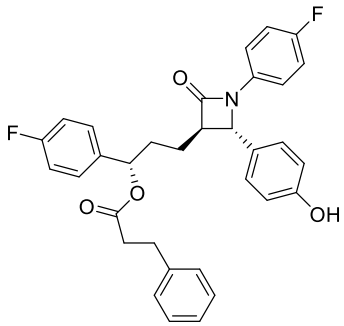


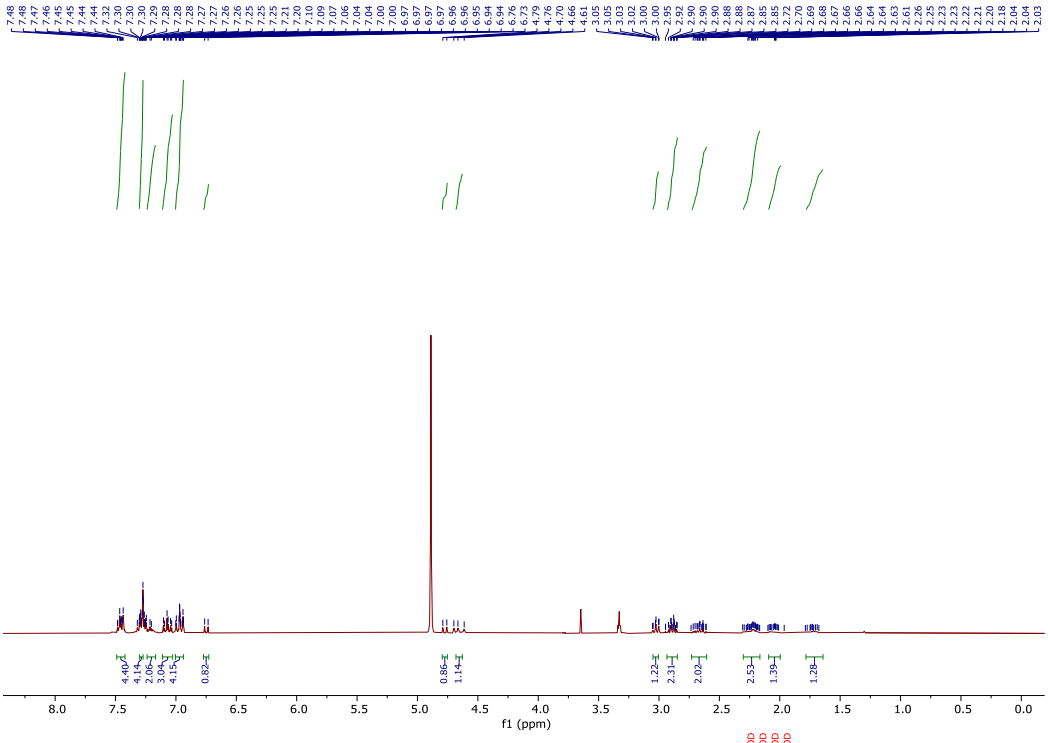


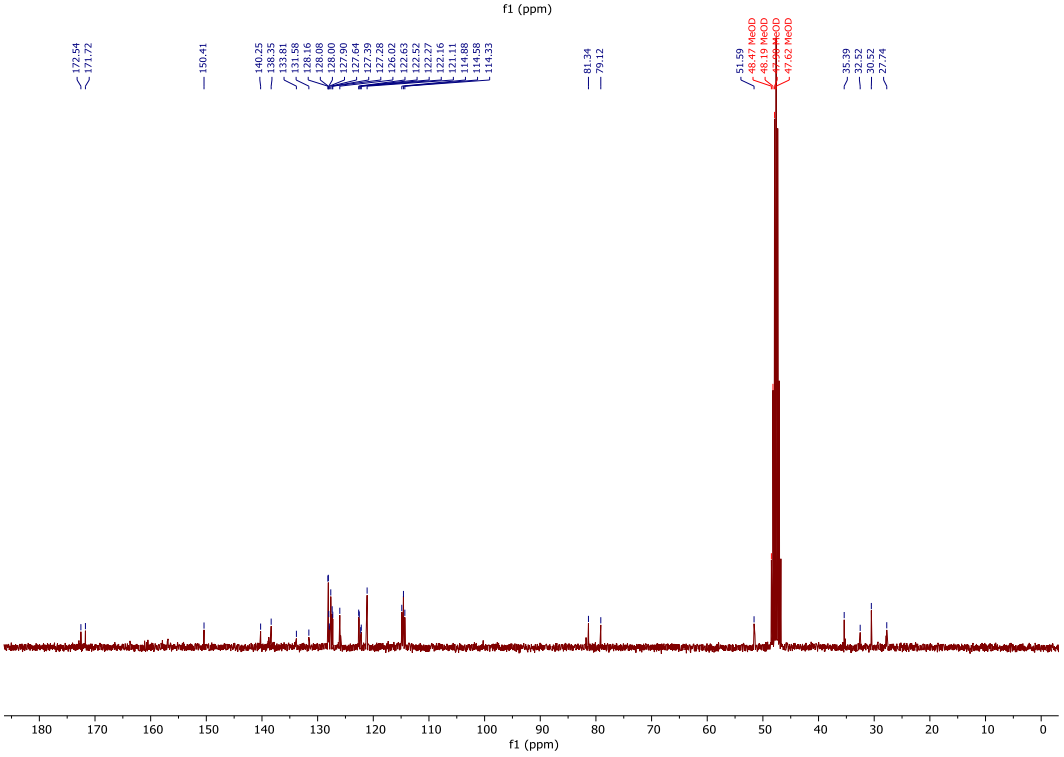


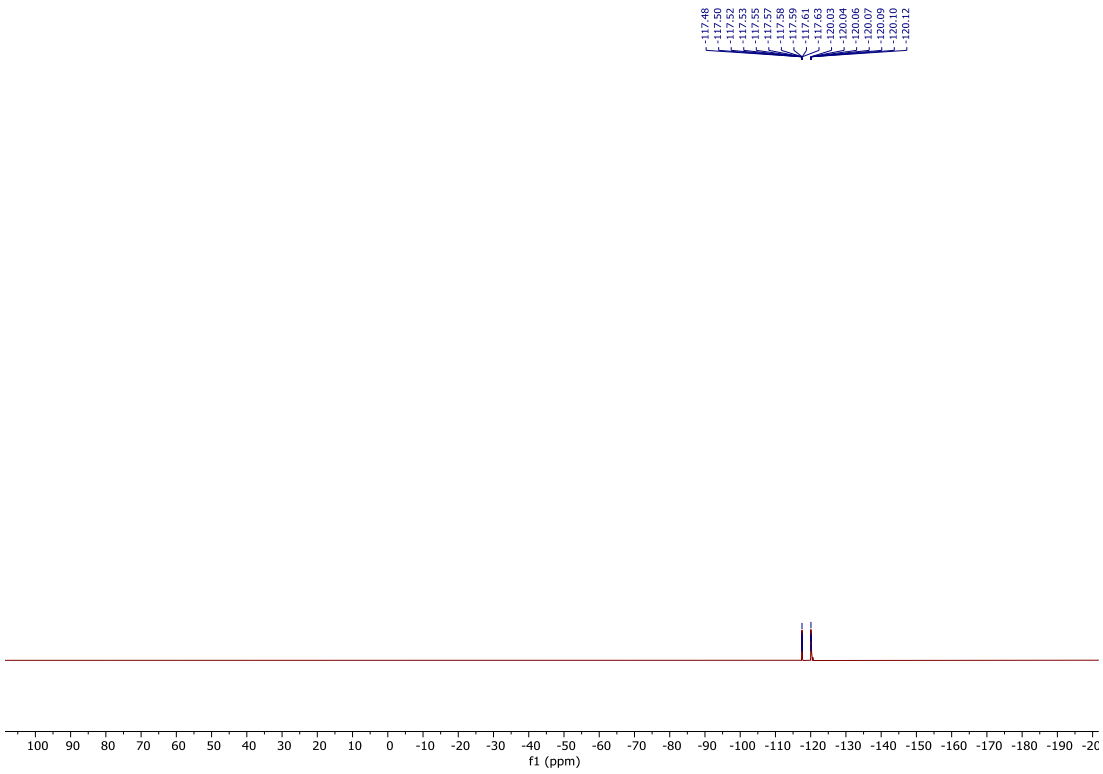

-117.54
-117.56
-117.57
-117.59
-117.61
-117.62
-117.64
-120.18
-120.20
-120.21
-120.23
-120.24
-120.26
-120.27
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

(S)-1-(4-Fluorophenyl)-3-((2S,3R)-1-(4-fluorophenyl)-2-(4-hydroxyphenyl)-4-oxoazetidin-3-yl)propyl 3-phenylpropanoate (**75**)

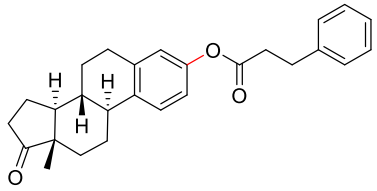


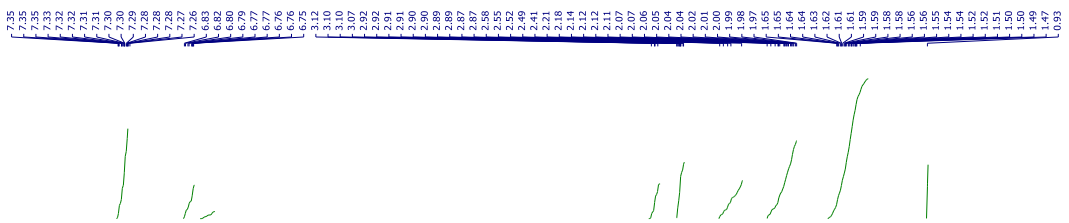


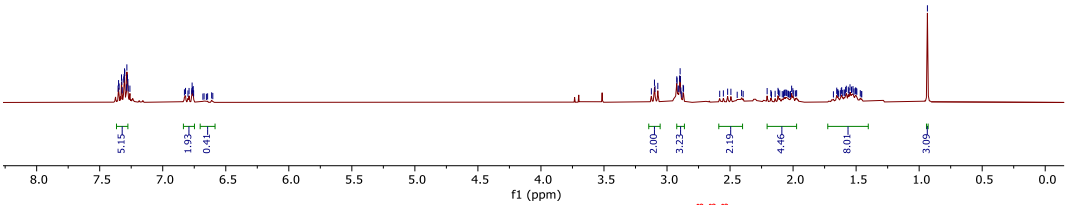


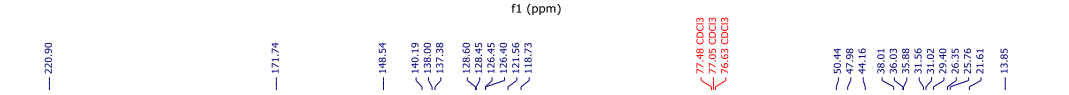

-117.48
-117.50
-117.52
-117.53
-117.55
-117.57
-117.58
-117.59
-117.61
-117.63
-120.03
-120.04
-120.06
-120.07
-120.09
-120.10
-120.12
100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -20
f1 (ppm)

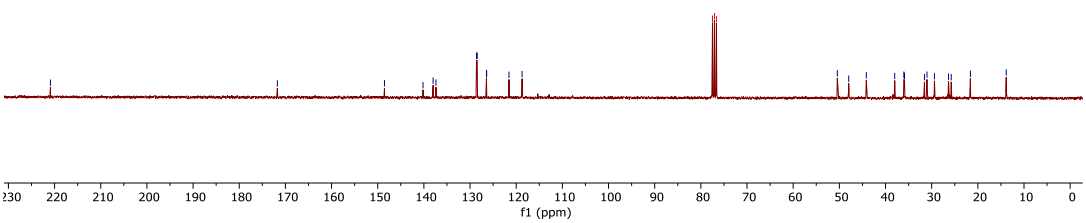
(8R,9S,13S,14S)-13-Methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl 3-phenylpropanoate (**76**)



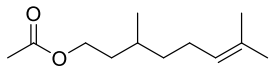


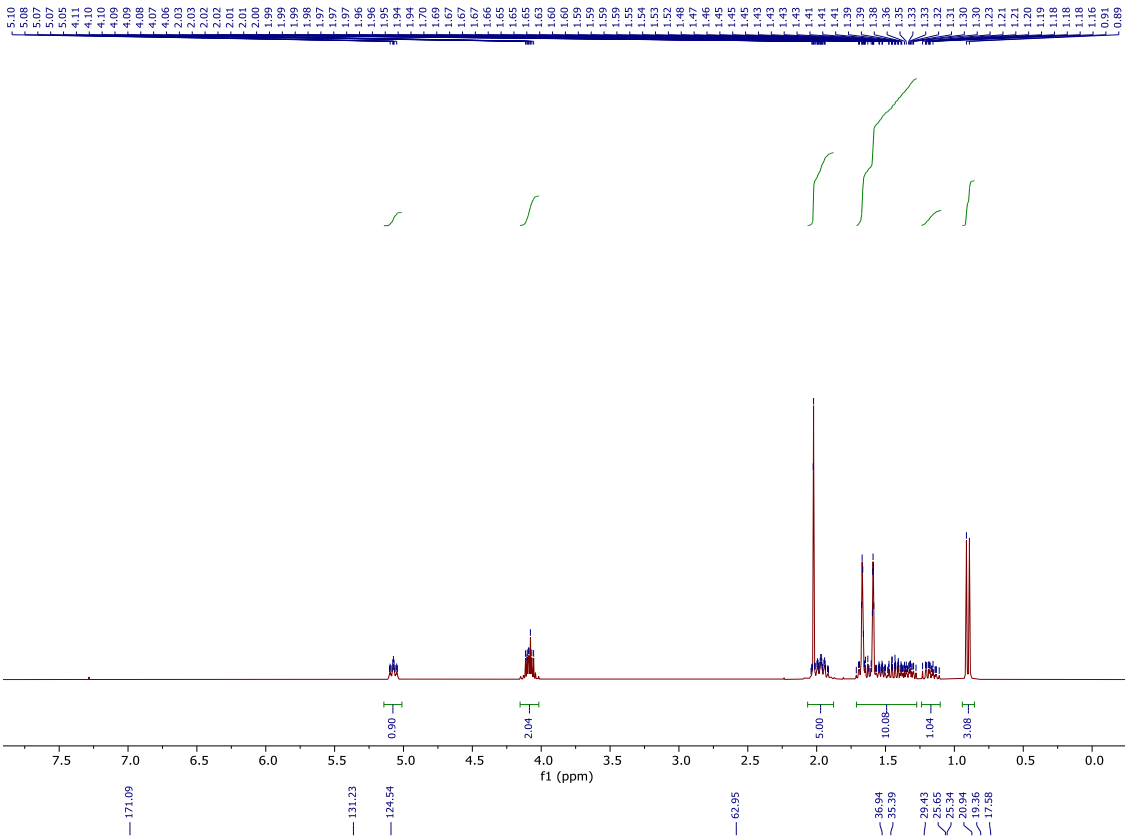


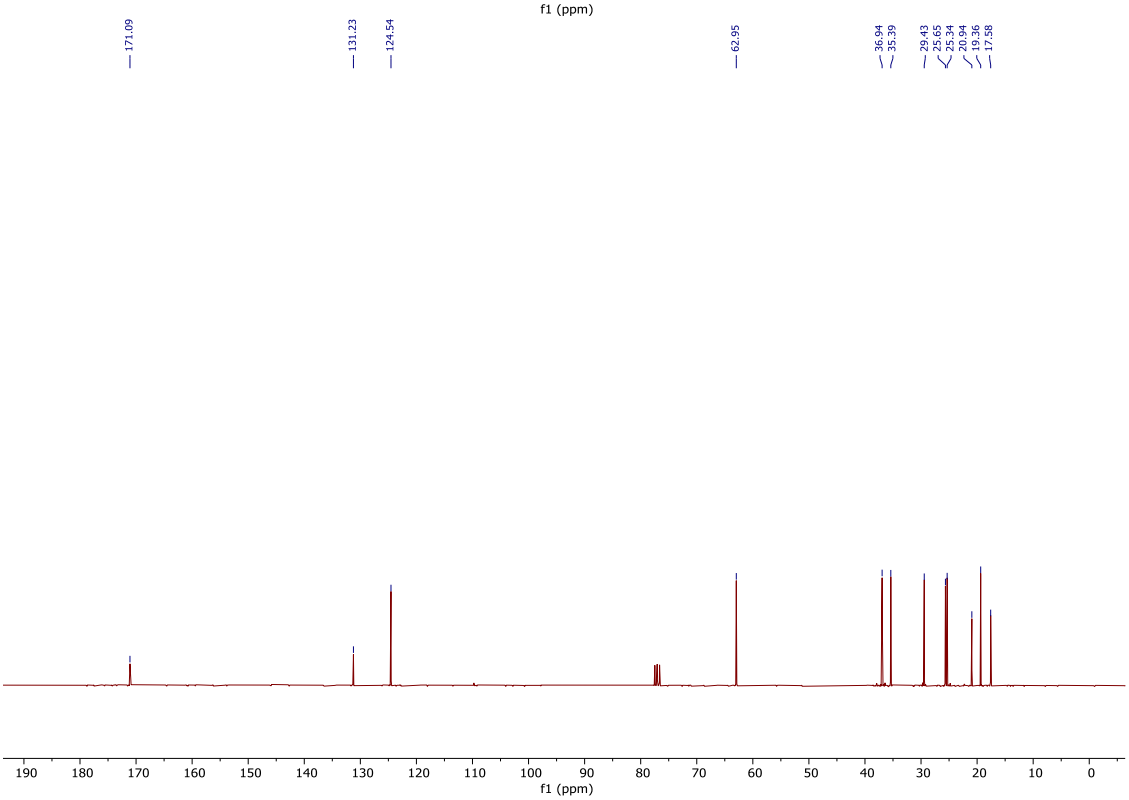




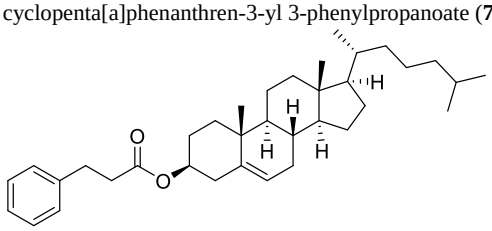
Citronellyl acetate (**77**)

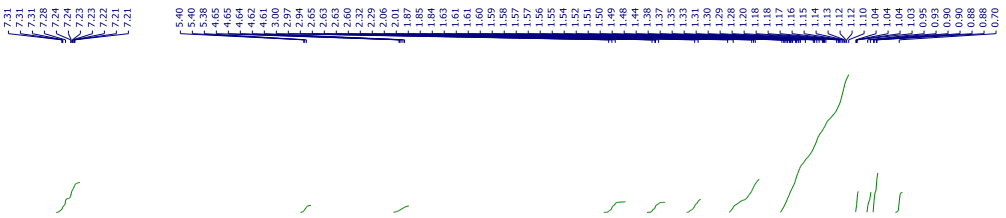


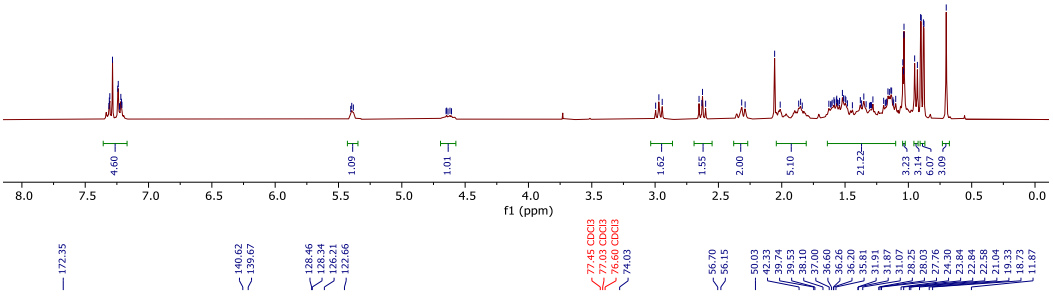


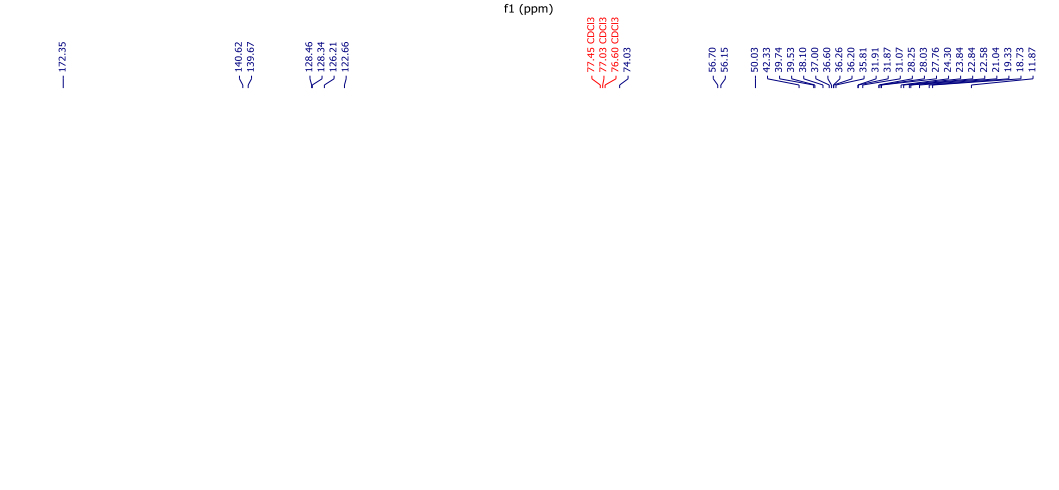


(3S,8S,9S,10R,13R,14S,17R)-10,13-Dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 3-phenylpropanoate (**78**)

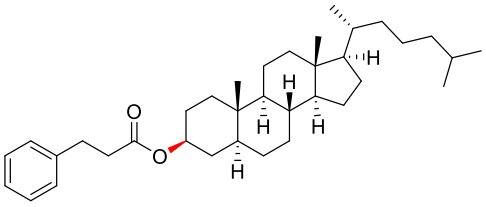


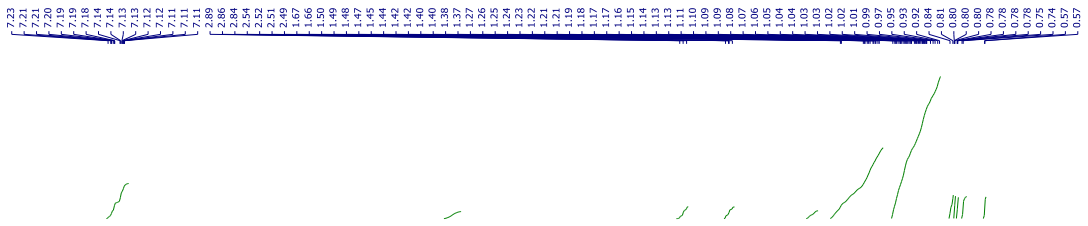


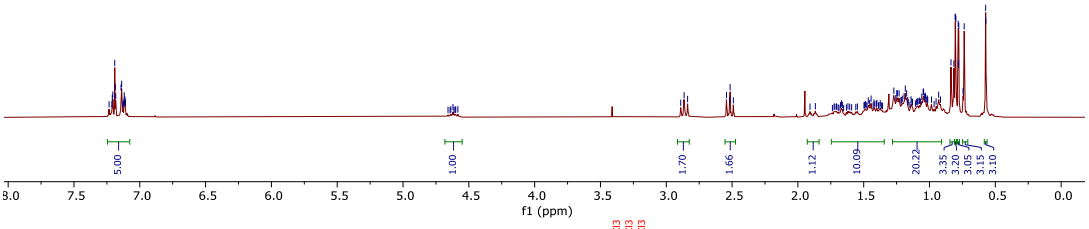


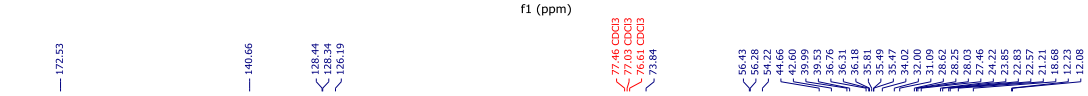


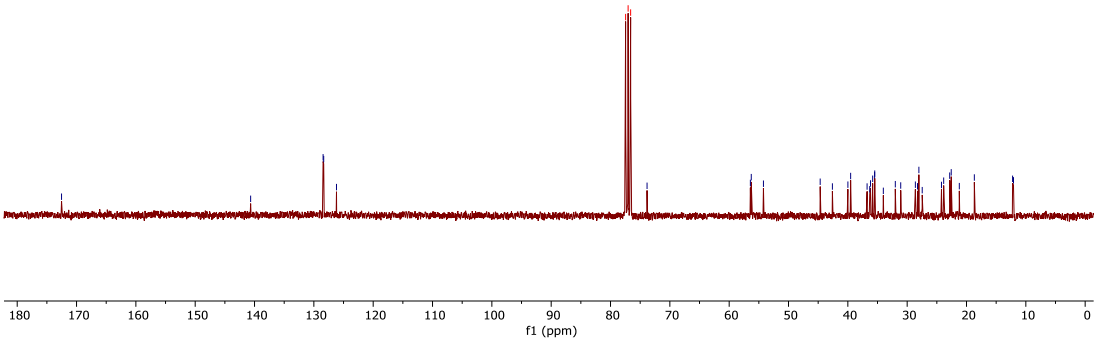
(3S,5S,8R,9S,10S,13R,14S,17R)-10,13-Dimethyl-17-((R)-6-methylheptan-2-yl)hexadecahydro-1H-cyclopenta[a]phenanthren-3-yl 3-phenylpropanoate (**79**)



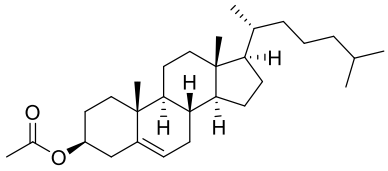


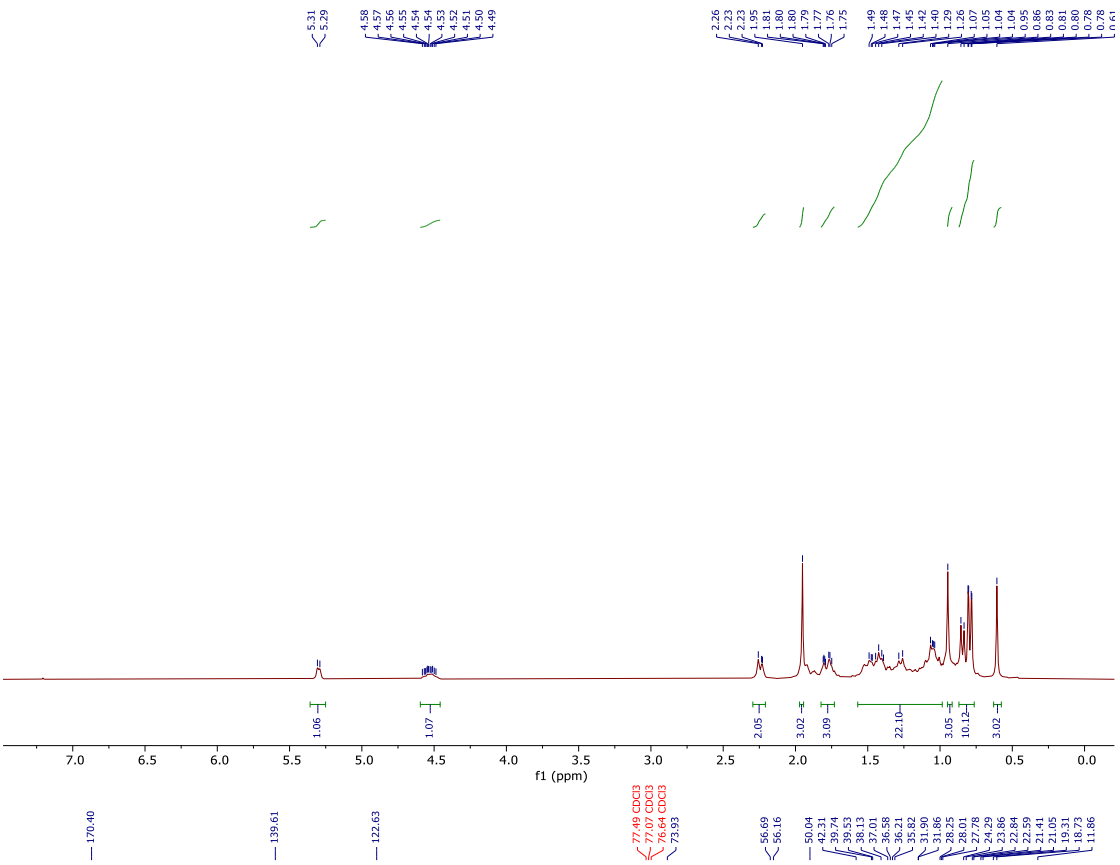


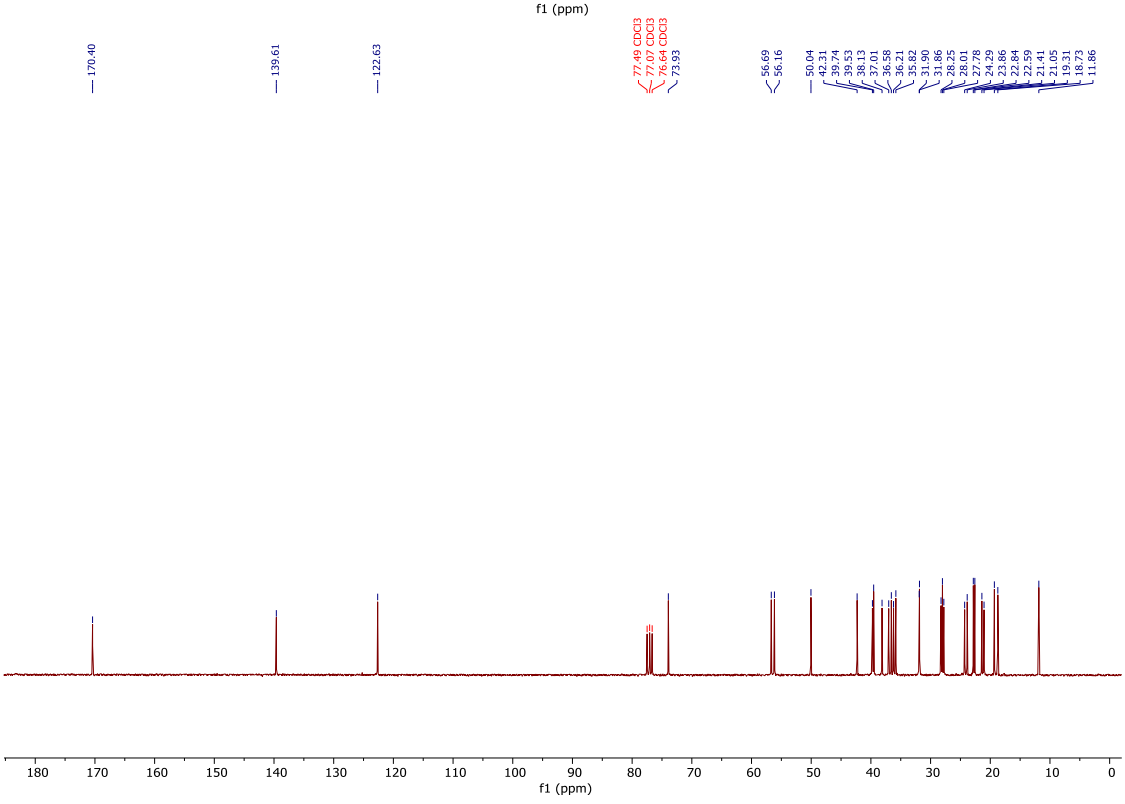




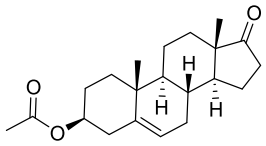
(3S,8S,9S,10R,13R,14S,17R)-10,13-Dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl acetate (**80**)

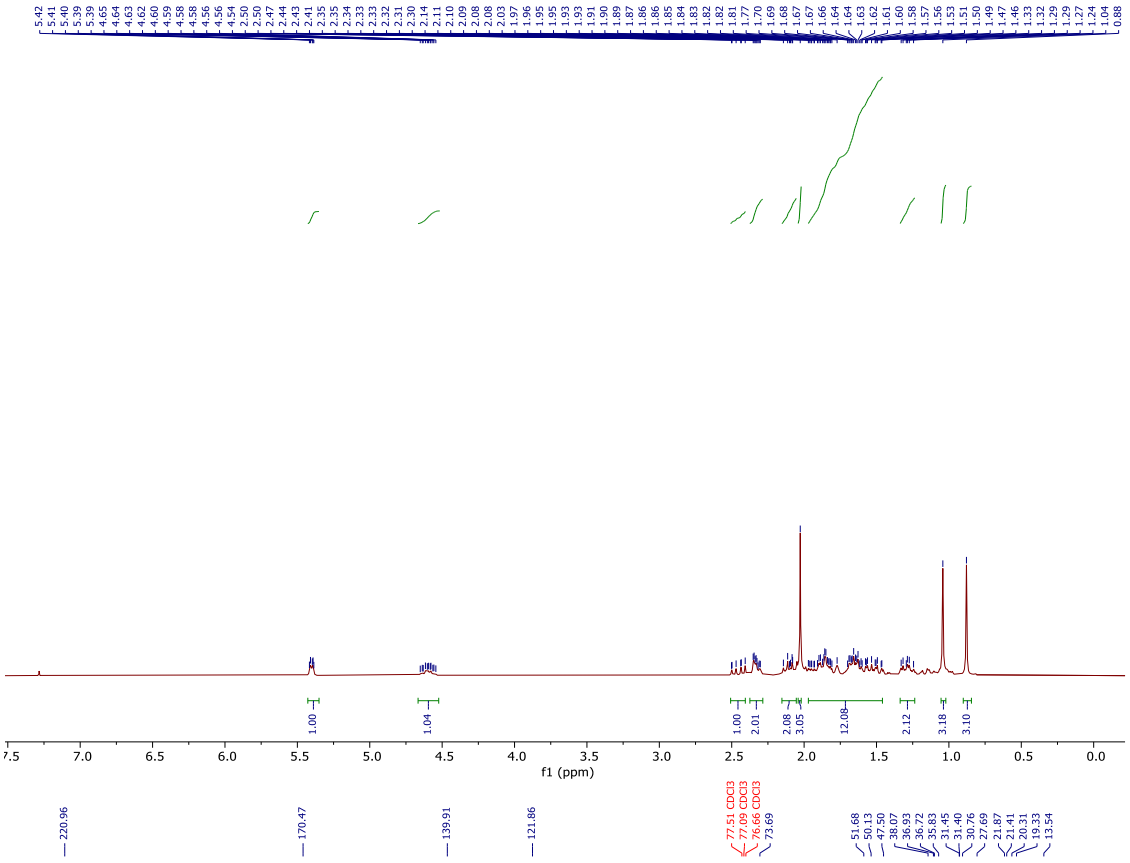


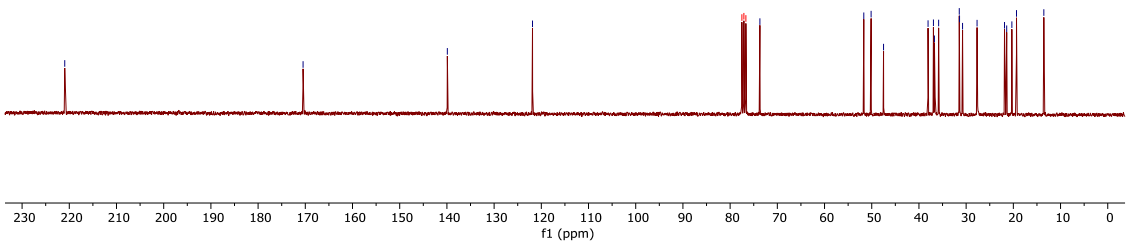




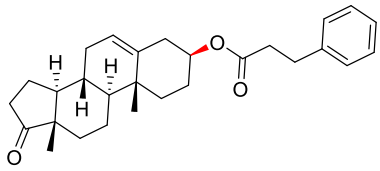
(3S,8R,9S,10R,13S,14S)-10,13-Dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl acetate (**81**)

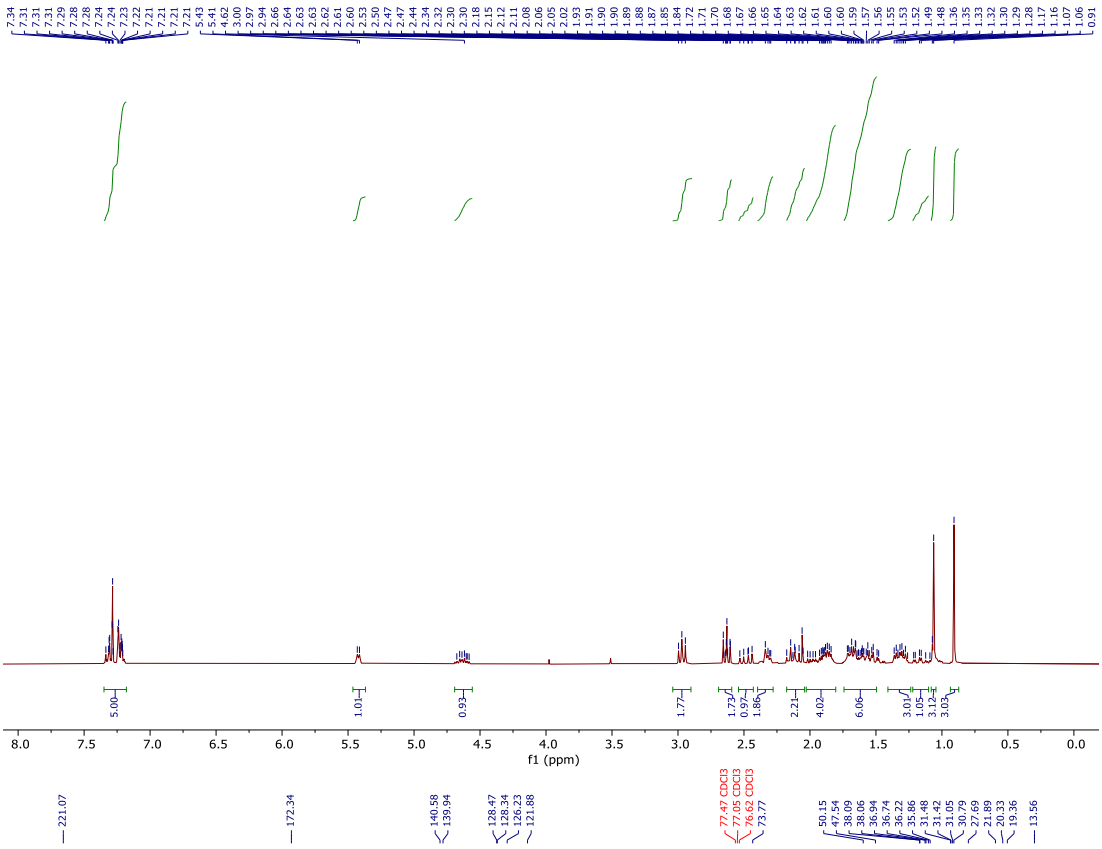


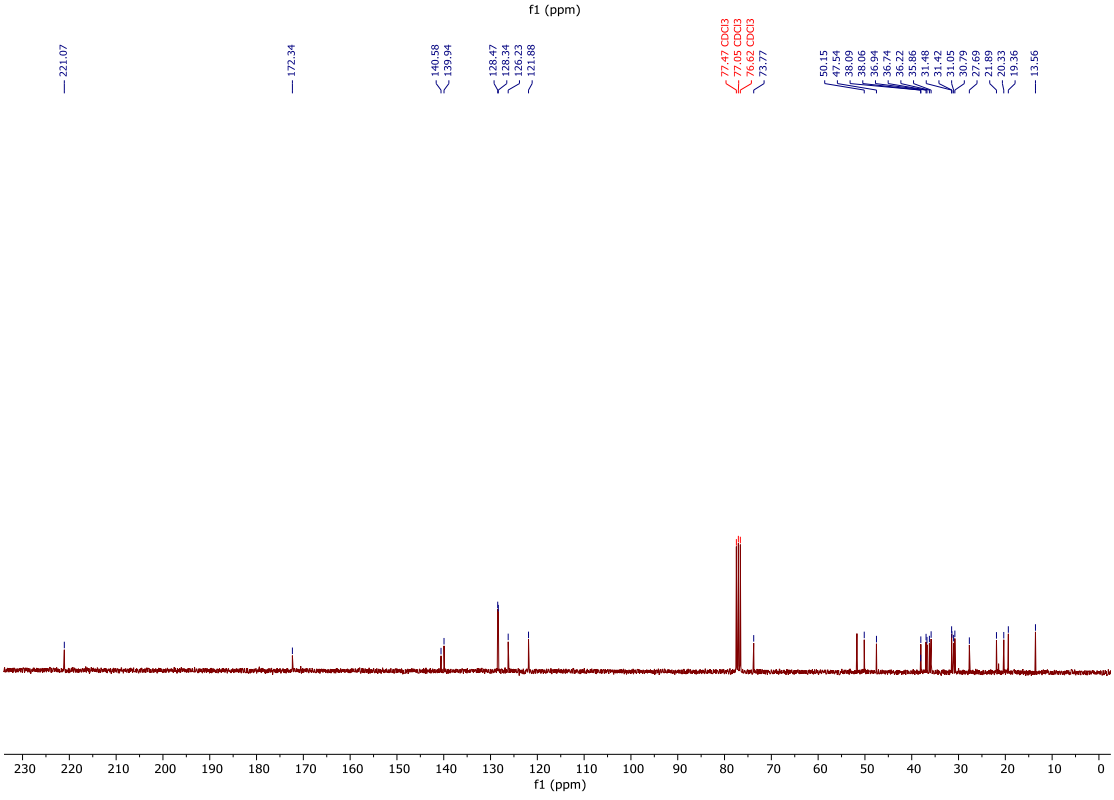




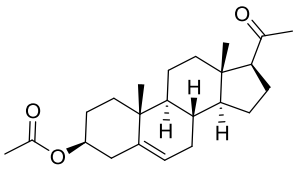
(3S,8R,9S,10R,13S,14S)-10,13-Dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 3-phenylpropanoate (**82**)

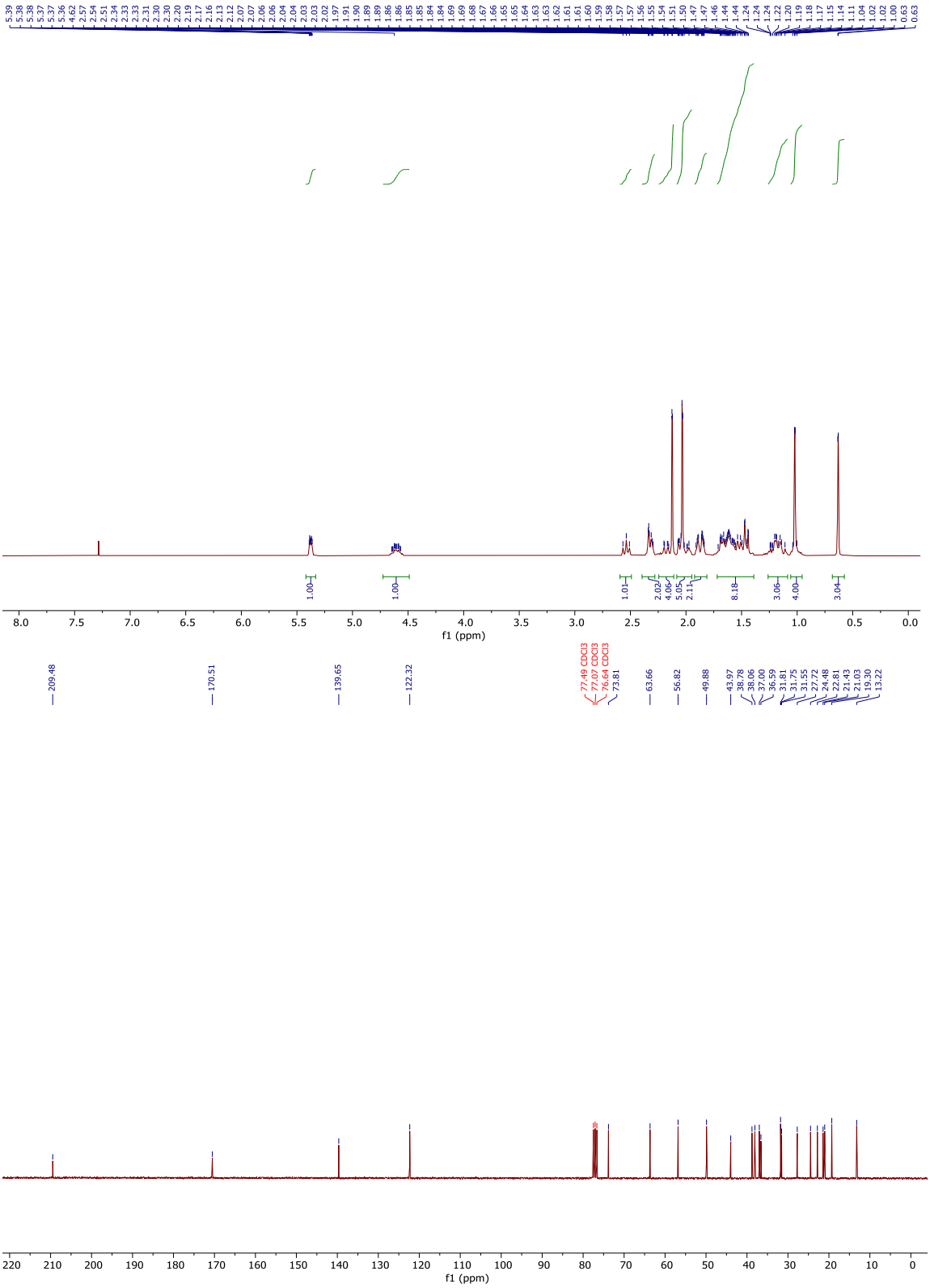




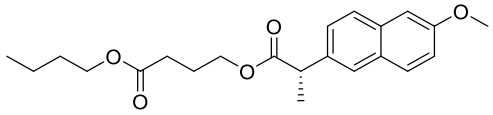


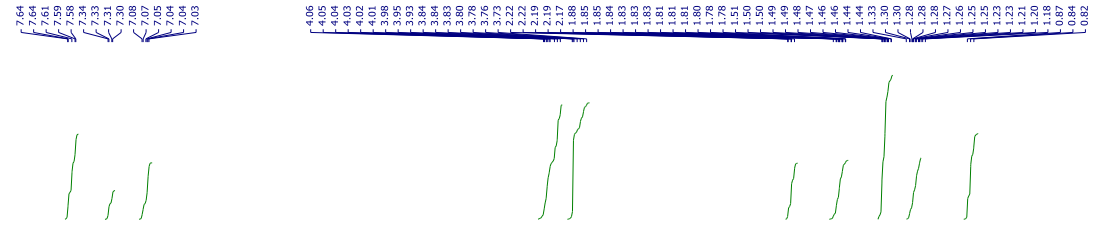
Pregnanolone acetate (**83**)

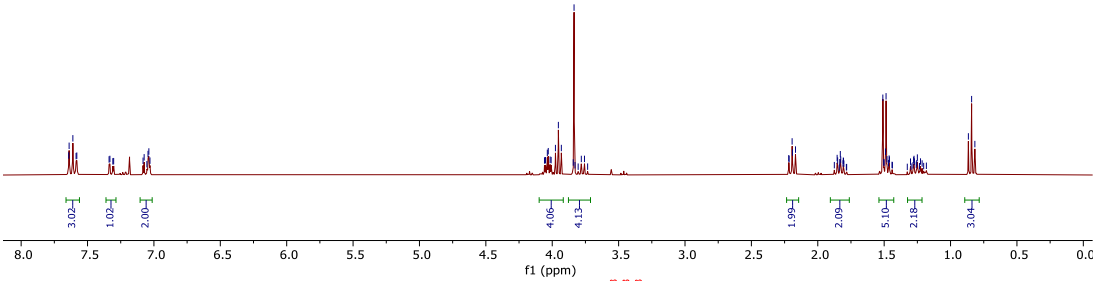


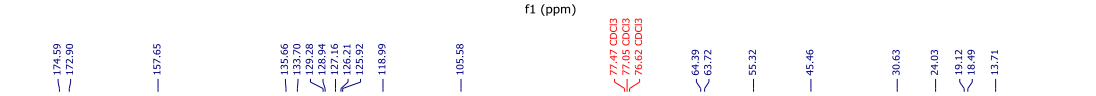


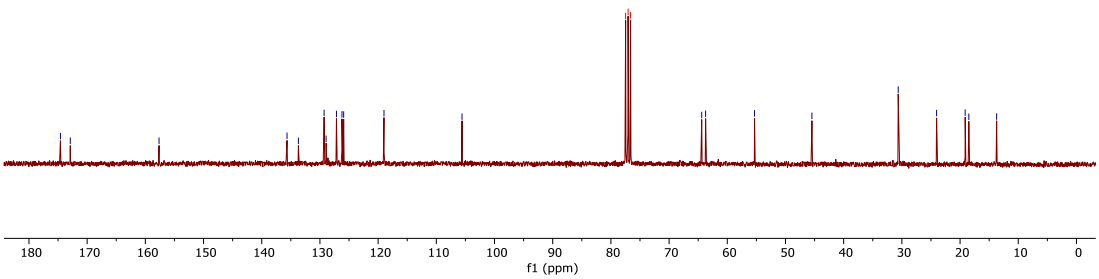
Butyl (S)-4-((2-(6-methoxynaphthalen-2-yl)propanoyl)oxy)butanoate (**84**)











Phenyl 4-(3,7-dimethyl-2,6-dioxo-2,3,6,7-tetrahydro-1H-purin-1-yl)butanoate (**85**)