Supporting Information

Rhodium-Catalyzed Synthesis of Esters from Aryl Iodides and Alcohols: Use of Alcohols with/without the Assistance of Aldehydes as Carbon Monoxide and Nucleophile Sources

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Ⅰ. General Information

Chemicals and Reagents All solvents were dried and distilled according to standard methods before use. Solvents utilized in this work were obtained from Sigma-Aldrich and Samchun Pure Chemicals (hexanes, ethyl acetate, diethyl ether, dichloromethane, and acetone). Toluene were dried over Na and distilled under nitrogen. *n*-Hexane, diethyl ether, and ethyl acetate were used without further purification. Reagents were purchased from Sigma-Aldrich, Alfa Aesar, or TCI and were used as received. $[Rh(COD)Cl]_2$ were purchased from Pressure Chem. DPEPhos((oxybis(2,1-phenylene))bis(diphenylphosphane)) were purchased from Alfa Aesar. Reactions were monitored by thin-layer chromatography on 0.25 mm E. Merck silica gel plates (60F-254). The TLC plates were visualized by UV-light (254 nm) and treatment with acidic *p*-anisaldehyde and $KMnO_4$ stain followed by gentle heating. Workup procedures were done in air. Flash column chromatography was carried out on Merck 60 silica gel (230 – 400 mesh).

Physical Methods ^1H and ^{13}C NMR spectra were recorded with Agilent 400-MR DD2 (400 MHz and 100 MHz, respectively) spectrometer. ^1H NMR spectra were taken in $CDCl_3$ and were referenced to residual TMS (7.26 ppm) and reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, dd = doublet of doublet, m = multiplet). Chemical shifts of the ^{13}C NMR spectra were measured relative to $CDCl_3$ (77.00 ppm). High-Resolution Mass Spectra were obtained at the Korea Basic Science Institute (Daegu, South Korea) on a Jeol JMS 700 high resolution mass spectrometer. GC-MS analyses were performed with a HP-6890 series with a HP-5 capillary column (30 m x 0.25 mm; coating thickness 0.25 μm) and Agilent 5973 Network Mass Selective detector. Analytical condition – initial temperature: 50 ^oC, raising temperature 10 ^oC / min, final temperature : 280 ^oC, He gas, Pressure : 7.56 psi, Total flow : 53.7 mL / min.

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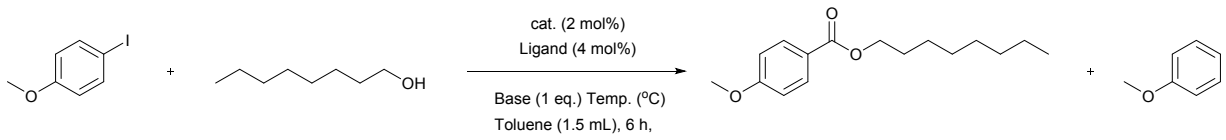
Ⅱ. General Procedure for the entries reported Table 1 from aryl iodide and alcohol

Reactions were performed in a schlenk tube equipped with a stirring bar and capped with a rubber septum. The followings were placed in the tube in order: 5 mg (c.a. 2 mol%) of catalyst, 10 mg of ligand (4 mol%) 0.5 mmol of aryl iodide, 1 equiv (86 uL) of base, 3 equiv of 1-octanol and 1.5 mL of toluene. The mixture was stirred at 120 ^oC for 18 h. The reaction mixture was extracted with aqueous NH_4Cl solution and diethyl ether and dried

over anhydrous $MgSO_4$, filtered, and finally evaporated under reduced pressure. The concentrated reaction mixture was purified by flash chromatography on silica gel (*n*-hexane/ethyl acetate) to afford the product.

Table S1. Screening reaction conditions



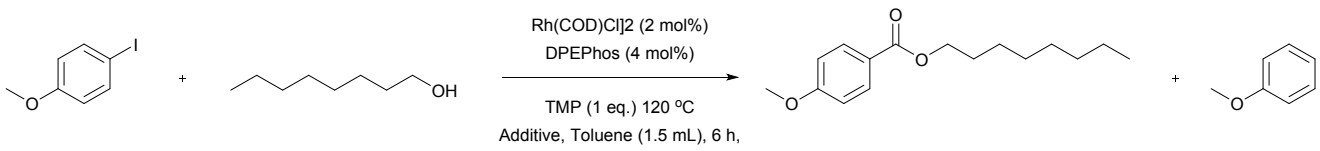
1 **2** **1a** **1b**

entry	cat (mol %)	Ligand	Base	Temperature	Yield (%)[a,b]
1	$Rh(COD)Cl]_2$	DPEPhos	TMP	120	50 (45)
2	$RhCl_3$	DPEPhos	TMP	120	40 (40)
3	$Rh(OAc)_2$	DPEPhos	TMP	120	42 (50)
4	Rh(IMes)(COD)Cl	DPEPhos	TMP	120	25 (60)
5	$Ir(COD)Cl]_2$	DPEPhos	TMP	120	N.R.
6	$Pd(OAc)_2$	DPEPhos	TMP	120	(4)[c]
7	$NiCl_2$	DPEPhos	TMP	120	N.R.
8	$PtCl_2$	DPEPhos	TMP	120	N.R.
9	$[Rh(COD)Cl]_2$	PPh_3	TMP	120	8 (75)
10	$[Rh(COD)Cl]_2$	dppm	TMP	120	trace (80)
11	$[Rh(COD)Cl]_2$	dppe	TMP	120	4 (95)
12	$[Rh(COD)Cl]_2$	dppp	TMP	120	32 (57)
13	$[Rh(COD)Cl]_2$	dppb	TMP	120	22 (60)
14	$[Rh(COD)Cl]_2$	dppf	TMP	120	29 (34)
15	$[Rh(COD)Cl]_2$	dtbpy	TMP	120	N.R.
16	$[Rh(COD)Cl]_2$	DCyOs	TMP	120	N.R.
17	$[Rh(COD)Cl]_2$	Xantphos	TMP	120	13 (51)
18	$[Rh(COD)Cl]_2$	DPEphos	DIPEA	120	3 (77)
19	$[Rh(COD)Cl]_2$	DPEPhos	Dicyclohexylamine	120	5 (82)
20	$[Rh(COD)Cl]_2$	DPEPhos	DABCO	120	18 (70)
21	$[Rh(COD)Cl]_2$	DPEPhos	PMP	120	26 (58)
22	$[Rh(COD)Cl]_2$	DPEPhos	TBD	120	(62)

23	$[Rh(COD)Cl]_2$	DPEPhos	NaOtBu	120	(99)
24	$[Rh(COD)Cl]_2$	DPEPhos	TMP	70	trace
25	$[Rh(COD)Cl]_2$	DPEPhos	TMP	100	6 (19)

[a] GC yield with 1,3,5-trimethyl as an internal standard [b] Yield of anisole are in parenthesis [c] decomposed product was obtained.

Table S2. Screening additives



1 **2** **1a** **1b**

entry	Additive	**1a**[a]	**1b**[a]	**1**[a]
1	p-Benzoquinone	trace		
2	1-dodecene	48	44	
3	nitrosobenzene			78
4	pinacolone	18	70	
5	triphenylsilane		60	
6	$Cu(OAc)_2$		99	
7	Oxone			57
8	TEMPO	trace	58	
9	BHT[b]	32	58	
10	hydroquinone	trace	61	
11	O_2 (1 atm)		80	
12	Mn(0) powder	10	90	

[a] GC yield with 1,3,5-trimethyl as an internal standard [b] 2,6-Di-*tert*-butyl-4-methylphenol

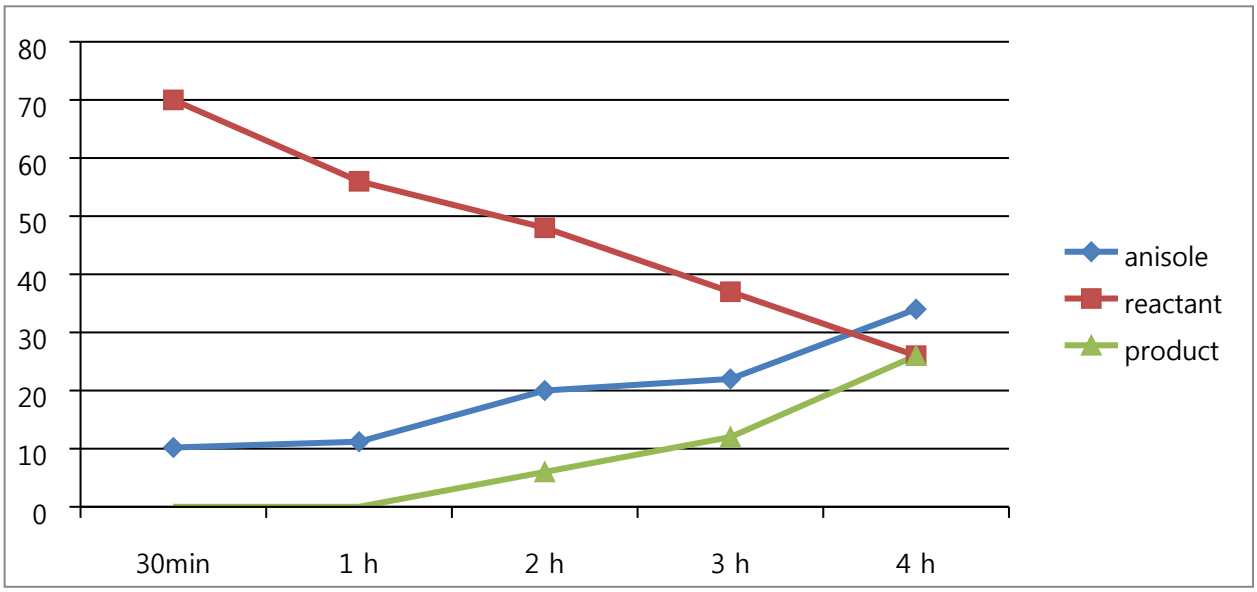
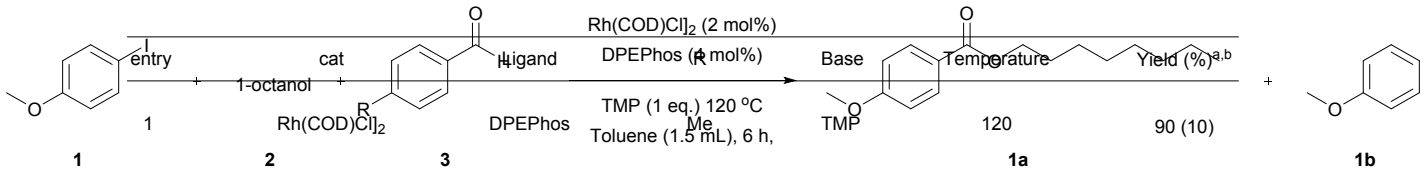


Figure S1. Time-Scale experiment

Ⅲ. General Procedure for the entries reported Table 3 from aryl iodide and alcohol with aldehyde

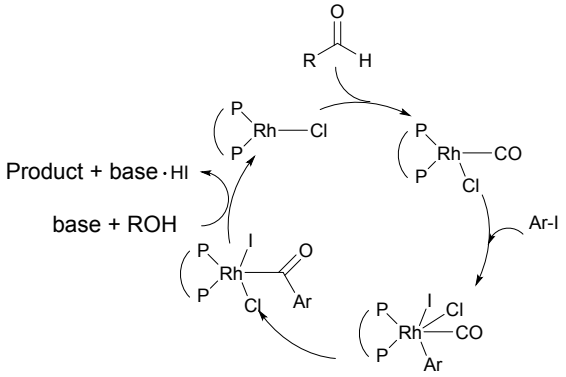
Reactions were performed in a schlenk tube equipped with a stirring bar and capped with a rubber septum. The followings were placed in the tube in order: 5 mg (c.a. 2 mol%) of catalyst, 10 mg of ligand (4 mol%) 0.5 mmol of aryl iodide, 1 equiv (86 uL) of base, 1equiv. of aldehyde, 3 equiv of 1-octanol and 1.5 mL of toluene. The mixture was stirred at 130 ^{o}C for 18 h. The reaction mixture was extracted with aqueous NH_4Cl solution and diethyl ether and dried over anhydrous $MgSO_4$, filtered, and finally evaporated under reduced pressure. The concentrated reaction mixture was purified by flash chromatography on silica gel (*n*-hexane/ethyl acetate) to afford the product.

Table S3. Screening reaction conditions with aldehyde



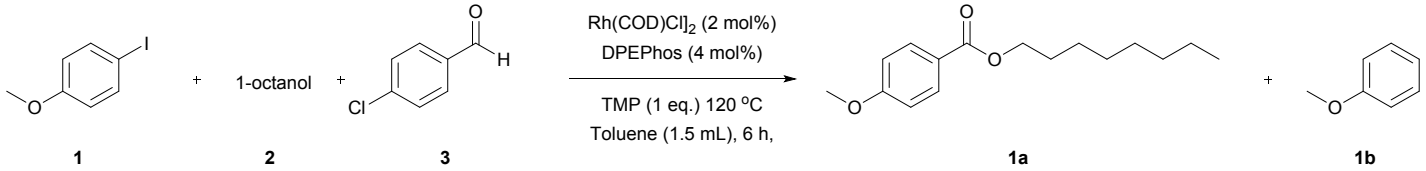
entry	cat	ligand	R	Base	Temperature	Yield (%)[a,b]
1	$Rh(COD)Cl]_2$	DPEPhos	Me	TMP	120	90 (10)
2	$RhCl_3$	DPEPhos	Me	TMP	120	7 (2)
3	$Rh(OAc)_2$	DPEPhos	Me	TMP	120	75 (17)
4	$Rh(COD)Cl]_2$ (4 mol%)	DPEPhos	Me	TMP	120	51 (18)
5	$Ir(COD)Cl]_2$	DPEPhos	TMP	TMP	120	N.R.
6	$Pd(OAc)_2$	DPEPhos	TMP	TMP	120	(4)[c]
7	$NiCl_2$	DPEPhos	TMP	TMP	120	N.R.
8	$Rh(COD)Cl]_2$	PPh_3	Me	TMP	120	7 (46)
9	$[Rh(COD)Cl]_2$	dppm	Me	TMP	120	trace (67)
10	$[Rh(COD)Cl]_2$	dppe	Me	TMP	120	3 (54)
11	$[Rh(COD)Cl]_2$	dppp	Me	TMP	120	52 (43)
12	$[Rh(COD)Cl]_2$	dppb	Me	TMP	120	58 (39)
13	$[Rh(COD)Cl]_2$	dpppent	Me	TMP	120	49 (31)
14	$Rh(COD)Cl]_2$	dppbenz	Me	TMP	120	trace (48)
15	$Rh(COD)Cl]_2$	BINAP	Me	TMP	120	52 (13)
16	$Rh(COD)Cl]_2$	DPEPhos	Cl	TMP	120	75 (5)
17	$Rh(COD)Cl]_2$	DPEPhos	Br	TMP	120	45 (12)
18	$Rh(COD)Cl]_2$	DPEPhos	NO_2	TMP	120	70 (4)
19	$Rh(COD)Cl]_2$	DPEPhos	dodecyl aldehyde	TMP	120	73 (19)
20	$Rh(COD)Cl]_2$	DPEPhos	propionaldehyde	TMP	120	2 (24)
21	$Rh(COD)Cl]_2$	DPEPhos	Me	DIPEA	120	27 (56)
22	$Rh(COD)Cl]_2$	DPEPhos	Me	DABCO	120	10 (32)
23	$Rh(COD)Cl]_2$	DPEPhos	Me	K_2CO_3	120	37 (2)
24	$Rh(COD)Cl]_2$	DPEPhos	Me	DIPEA	110	52 (9)

[a] GC yield using 1,3,5-trimethylbenzene as an internal standard. [b] Reduction product yield are in parenthesis. [c] Decomposed product were observed



Scheme S1. Proposed mechanism with aldehyde.

Table S4. Control Experiment for proposed mechanism



1 **2** **3** **1a** **1b**

entry	Variation from initial conditions	Yield[b]
1	Without $[Rh(COD)Cl]_2$	trace
2	Without alcohol	No Reaction
3	Without Ligand	No Reaction
4	Without Aldehyde	44
5	Without Base	No Reaction

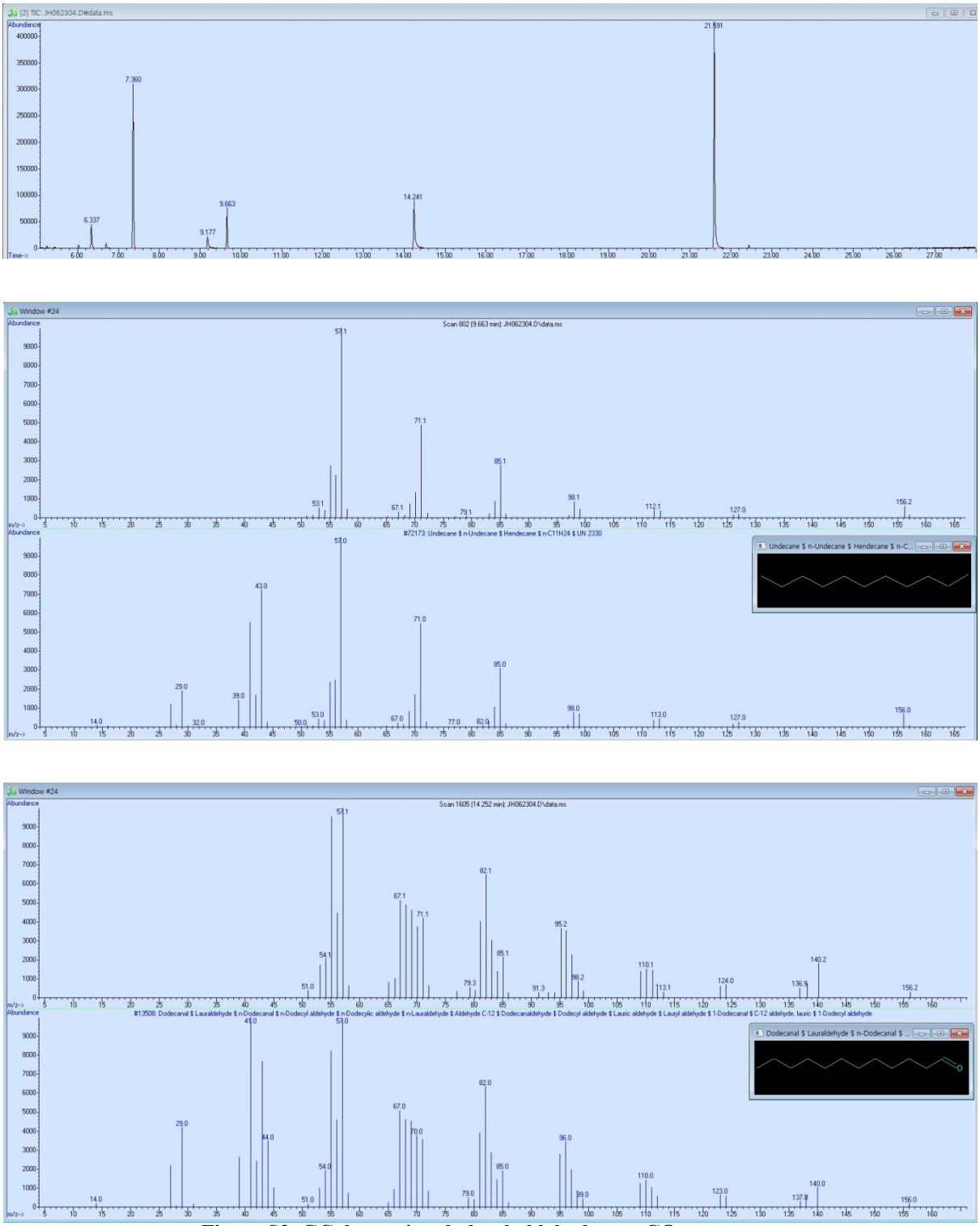


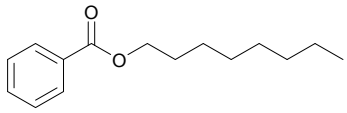
Figure S2. GC data using dodecyl aldehyde as a CO source

Retention time – 9.663 min : undecane (R-H moiety)

14.241 min : dodecyl aldehyde (CO surrogate)

21.591 min : product

Characterization Data for the Isolated Products

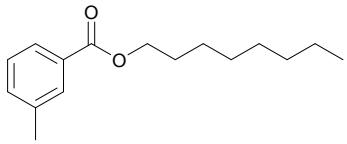


Octyl benzoate: colorless liquid (Table 3, **4ba**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.3 Hz, 2 H), 7.47 (t, *J* = 7.4 Hz, 1 H), 7.36 (t, *J* = 7.7 Hz, 2 H), 4.24 (t, *J* = 6.7 Hz, 2 H), 1.83 – 1.59 (m, 2 H), 1.57 – 1.32 (m, 2 H), 1.24 (m, 8 H), 0.81 (t, *J* = 6.6 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 132.7, 130.5, 129.5, 128.3, 65.1, 31.7, 29.2, 29.1, 28.7, 26.0, 22.6, 14.1.

IR (ATR): 1723 cm^{-1}, HRMS (EI) calc. for $[C_{15}H_{22}O_2, M]^+$ 234.1620, found 234.1620

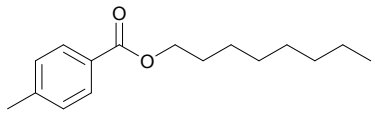


Octyl 3-methylbenzoate: colorless liquid (Table 3, **4ca**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.7 Hz, 2 H), 7.25 (m, 2 H), 4.23 (t, *J* = 6.7 Hz, 2 H), 2.32 (s, 3 H), 1.72 – 1.65 (m, 2 H), 1.40 – 1.33 (m, 2 H), 1.28 – 1.19 (m, 8 H), 0.81 (t, *J* = 6.5 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 138.0, 133.5, 130.4, 130.0, 128.2, 126.6, 65.1, 31.8, 29.22, 29.16, 28.7, 26.0, 22.6, 21.2, 14.1.

IR (ATR): 1721 cm^{-1}, HRMS (EI) calc. for $[C_{16}H_{24}O_2, M]^+$ 248.1776, found 248.1777

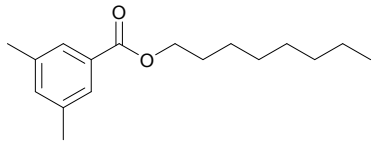


Octyl 4-methylbenzoate: colorless liquid (Table 3, **4da**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.1 Hz, 2 H), 7.15 (d, *J* = 8.0 Hz, 2 H), 4.22 (t, *J* = 6.7 Hz, 2 H), 2.33 (s, 3 H), 1.72 – 1.63 (m, 2 H), 1.41 – 1.32 (m, 2 H), 1.24 (m, 8 H), 0.81 (t, *J* = 6.7 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 143.4, 129.5, 129.0, 127.8, 64.9, 31.8, 29.23, 29.17, 28.7, 26.0, 22.6, 21.6, 14.1.

IR (ATR): 1721 cm^{-1}, HRMS (EI) calc. for $[C_{16}H_{24}O_2, M]^+$ 248.1776, found 248.1777

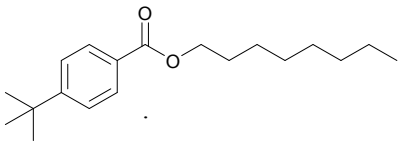


Octyl 3,5-dimethylbenzoate: colorless liquid. (Table3, **4ea**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (s, 2 H), 7.09 (s, 1 H), 4.21 (t, *J* = 6.7 Hz, 2 H), 2.27 (s, 6 H), 1.71 – 1.65 (m, 2 H), 1.39 – 1.32 (m, 2H), 1.27 – 1.16 (m, 8 H), 0.80 (t, *J* = 6.4 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 137.9, 134.4, 130.4, 127.2, 65.0, 31.8, 29.23, 29.16, 28.7, 26.0, 22.6, 21.1, 14.1.

IR (ATR): 1719 cm^{-1}, HRMS (EI) calc. for $[C_{17}H_{26}O_2, M]^+$ 262.1933, found 262.1933

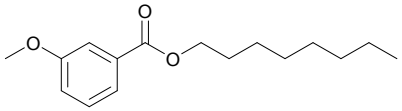


Octyl 4-(tert-butyl)benzoate: colorless liquid. (Table3, **4fa**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.4 Hz, 2 H), 7.37 (d, *J* = 8.4 Hz, 2 H), 4.22 (t, *J* = 6.6 Hz, 2 H), 1.68 (dd, *J* = 14.2, 7.1 Hz, 2 H), 1.39 – 1.32 (m, 2 H), 1.26 (s, 9 H), 1.29 – 1.22 (m, 8 H), 0.81 (t, *J* = 6.6 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 156.4, 129.4, 127.7, 125.2, 64.9, 35.0, 31.8, 31.1, 29.23, 29.18, 28.7, 26.0, 22.6, 14.1.

IR (ATR): 1721 cm^{-1}, HRMS (EI) calc. for $[C_{19}H_{30}O_2, M]^+$ 290.2246, found 290.2246

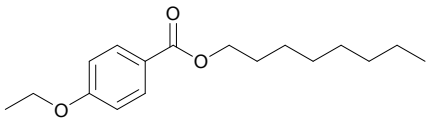


Octyl 3-methoxybenzoate: colorless liquid. (Table3, **4ga**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.3 Hz, 1 H), 7.49 (s, 1 H), 7.26 (t, *J* = 8.4 Hz, 1 H), 7.01 (d, *J* = 8.2 Hz, 1 H), 4.23 (t, *J* = 7.3 Hz, 2 H), 3.77 (s, 3 H), 1.72 – 1.65 (m, 2 H), 1.35 (m, 2 H), 1.22 (m, 8 H), 0.80 (t, *J* = 5.0 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 159.5, 131.8, 129.4, 121.9, 119.2, 114.0, 65.2, 55.4, 31.8, 29.21, 29.16, 28.7, 26.0, 22.6, 14.1.

IR (ATR): 1700 cm^{-1}, HRMS (EI) calc. for $[C_{16}H_{24}O_2, M]^+$ 264.1725, found 264.1727

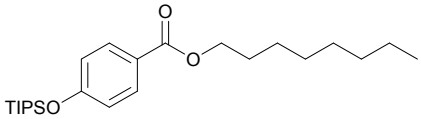


Octyl 4-ethoxybenzoate: colorless liquid. (Table3, **4ha**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.7 Hz, 2 H), 6.79 (d, *J* = 8.7 Hz, 2 H), 4.18 (t, *J* = 6.6 Hz, 2 H), 3.96 (q, *J* = 6.9 Hz, 2 H), 1.68 – 1.61 (m, 2 H), 1.34 – 1.30(m, 5 H), 1.28 – 1.12 (m, 8 H), 0.79 (t, *J* = 6.4 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 162.5, 131.4, 122.6, 113.8, 64.7, 63.5, 31.7, 29.17, 29.11, 28.7, 26.0, 22.5, 14.5, 14.0.

IR (ATR): 1717 cm^{-1}, HRMS (EI) calc. for $[C_{17}H_{26}O_3, M]^+$ 278.1882, found 278.1884



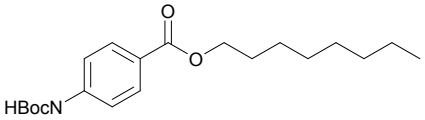
Octyl 4-((triisopropylsilyl)oxy)benzoate: colorless liquid. (Table3, **4ia**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.9 Hz, 2 H), 6.82 (d, *J* = 8.8 Hz, 2 H), 4.20 (t, *J* = 6.7 Hz, 2 H), 1.71 – 1.63 (m, 2H), 1.40 – 1.32 (m, 2H), 1.23 (m, 10 H), 1.04 (s, 9 H), 1.02 (s, 7 H), 0.81 (t, *J* = 6.7 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 160.3, 131.5, 123.3, 119.6, 64.8, 31.8, 29.26, 29.20, 28.8, 26.1, 22.6, 17.9,

14.1, 12.7.

IR (ATR): 1705 cm^{-1}, HRMS (EI) calc. for $[C_{24}H_{42}O_3Si, M]^+$ 406.2903, found 406.2906

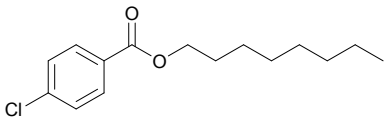


Octyl 4-((tert-butoxycarbonyl)amino)benzoate: colorless liquid. (Table3, **4ja**)

^1H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.4 Hz, 2 H), 7.37 (d, *J* = 8.4 Hz, 2 H), 6.86 (s, 1 H), 4.21 (t, *J* = 6.6 Hz, 2 H), 1.70 – 1.63 (m, 2 H), 1.43 (s, 9 H), 1.37 – 1.33 (m, 2 H), 1.23 – 1.20 (m, 8 H), 0.79 (t, *J* = 6.8 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 152.2, 142.7, 130.8, 124.6, 117.3, 81.0, 64.9, 31.7, 29.19, 29.13, 28.7, 28.2, 26.0, 22.6, 14.0.

IR (ATR): 1704 cm^{-1}, HRMS (EI) calc. for $[C_{20}H_{31}O_4N, M]^+$ 349.2253, found 349.2255

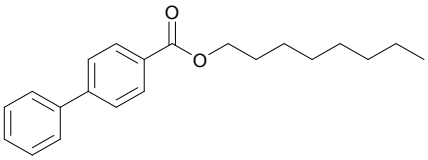


Octyl 4-chlorobenzoate: colorless liquid. (Table3, **4ka**) with octyl ester impurities

^1H NMR (400 MHz, $cdcl_3$) δ 7.90 (d, *J* = 8.2 Hz, 2 H), 7.33 (d, *J* = 8.5 Hz, 2 H), 4.23 (t, *J* = 6.7 Hz, 2 H), 1.72 – 1.64 (m, 2 H), 1.38 – 1.32 (m, 2 H), 1.23 – 1.20 (m, 8 H), 0.81 (t, *J* = 4.5 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 139.2, 130.9, 128.9, 128.6, 65.4, 31.8, 29.20, 29.15, 28.6, 26.0, 22.6, 14.1.

IR (ATR): 1700 cm^{-1}, HRMS (EI) calc. for $[C_{15}H_{21}O_2Cl, M]^+$ 268.1230, found 268.1233

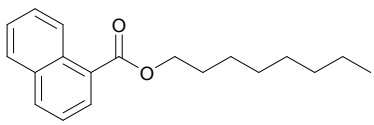


Octyl [1,1'-biphenyl]-4-carboxylate: colorless liquid. (Table3, **4la**)

^1H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.0 Hz, 2 H), 7.57 (dd, *J* = 13.8, 7.8 Hz, 4 H), 7.40 (t, *J* = 7.4 Hz, 2 H), 7.32 (t, *J* = 7.2 Hz, 1 H), 4.27 (t, *J* = 6.6 Hz, 2 H), 1.76 – 1.67 (m, 2 H), 1.42 – 1.35 (m, 2 H), 1.31 – 1.18 (m, 8 H), 0.82 (t, *J* = 6.3 Hz, 3 H).

^{13}C NMR (100 MHz, $cdcl_3$) δ 166.6, 145.5, 140.1, 130.0, 129.3, 128.9, 128.1, 127.3, 127.0, 65.2, 31.8, 29.26, 29.20, 28.8, 26.1, 22.6, 14.1.

IR (ATR): 1720 cm^{-1}, HRMS (EI) calc. for $[C_{21}H_{26}O_2, M]^+$ 310.1933, found 310.1934

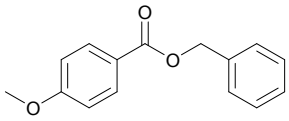


Octyl 1-naphthoate: colorless liquid. (Table3, **4ma**)

^1H NMR (400 MHz, $CDCl_3$) δ 8.83 (d, *J* = 8.6 Hz, 1 H), 8.08 (d, *J* = 6.9 Hz, 1 H), 7.90 (d, *J* = 8.2 Hz, 1 H), 7.77 (d, *J* = 8.1 Hz, 1), 7.51 (t, *J* = 7.6 Hz, 1 H), 7.41 (dt, *J* = 14.1, 7.6 Hz, 2 H), 4.32 (t, *J* = 6.6 Hz, 2 H), 1.78 – 1.68 (m, 2 H), 1.42 – 1.35 (m, 2 H), 1.31 – 1.15 (m, 8 H), 0.80 (t, *J* = 5.8 Hz, 3 H).

^{13}C NMR (100 MHz, cdcl$_3$) δ 167.6, 133.8, 133.1, 131.3, 130.0, 128.4, 127.6, 127.4, 126.1, 125.8, 124.4, 65.2, 31.7, 29.20, 29.15, 28.7, 26.1, 22.6, 14.0.

IR (ATR): 1716 cm^{-1}, HRMS (EI) calc. for [$C_{19}H_{24}O_2$, M]$^+$ 284.1776, found 284.1779

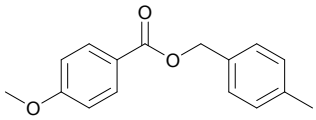


Benzyl 4-methoxybenzoate: colorless liquid. (Table 4, **4ab**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.8 Hz, 2 H), 7.36 (d, *J* = 7.2 Hz, 2 H), 7.33 – 7.22 (m, 3 H), 6.83 (d, *J* = 8.8 Hz, 2 H), 5.26 (s, 2 H), 3.77 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 163.4, 136.3, 131.7, 128.5, 128.10, 128.06, 122.5, 113.6, 66.4, 55.4.

IR (ATR): 1715 cm^{-1}, HRMS (EI) calc. for [$C_{15}H_{14}O_3$, M]$^+$ 242.0943, found 242.0941

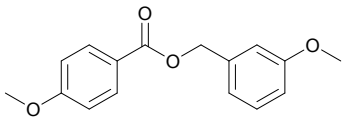


4-Methylbenzyl 4-methoxybenzoate: white crystal. (Table 4, **4ac**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.5 Hz, 2 H), 7.23 (d, *J* = 7.7 Hz, 2 H), 7.08 (d, *J* = 7.6 Hz, 2 H), 6.79 (d, *J* = 8.3 Hz, 2 H), 5.19 (s, 2 H), 3.72 (s, 3 H), 2.25 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 163.3, 137.9, 133.2, 131.6, 129.1, 128.2, 122.6, 113.5, 66.3, 55.4, 21.1.

IR (ATR): 1708 cm^{-1}, HRMS (EI) calc. for [$C_{16}H_{16}O_3$, M]$^+$ 256.1099, found 256.1102, m.p. 38.4 ^{o}C

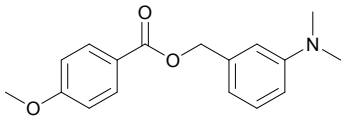


3-Methoxybenzyl 4-methoxybenzoate: colorless liquid. (Table 4, **4ad**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.7 Hz, 2 H), 7.20 (t, *J* = 7.9 Hz, 1 H), 6.98 – 6.85 (m, 2 H), 6.85 – 6.71 (m, 3 H), 5.21 (s, 2 H), 3.74 (s, 3 H), 3.71 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 163.4, 159.7, 137.8, 131.7, 129.5, 122.4, 120.2, 113.6, 113.5, 113.6, 66.2, 55.3, 55.2.

IR (ATR): 1712 cm^{-1}, HRMS (EI) calc. for [$C_{16}H_{16}O_4$, M]$^+$ 272.1049, found 272.1051



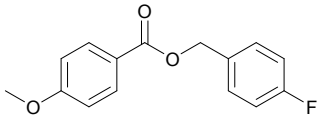
3-(Dimethylamino)benzyl 4-methoxybenzoate: dark green liquid. (Table 4, **4ae**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.8 Hz, 2 H), 7.15 (t, *J* = 7.8 Hz, 1 H), 6.80 (d, *J* = 8.8 Hz, 2 H), 6.70 (d, *J* = 7.8 Hz, 2 H), 6.60 (d, *J* = 8.5 Hz, 1 H), 5.19 (s, 2 H), 3.73 (s, 3 H), 2.85 (s, 6 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 163.3, 150.7, 137.0, 131.7, 129.2, 122.6, 116.2, 113.5, 112.2, 112.1, 67.0,

55.3, 40.5.

IR (ATR): 1709 cm^{-1}, HRMS (EI) calc. for $[C_{17}H_{19}O_3N, M]^+$ 285.1365, found 285.1366

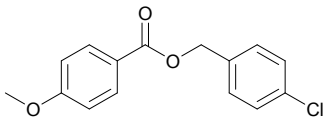


4-Fluorobenzyl 4-methoxybenzoate: white solid. (Table 4, **4af**)

^1H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.9 Hz, 2 H), 7.31 (dd, *J* = 8.5, 5.5 Hz, 2 H), 6.96 (t, *J* = 8.7 Hz, 2 H), 6.81 (d, *J* = 8.9 Hz, 2 H), 5.19 (s, 2 H), 3.74 (s, 3 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.1, 163.8, 163.4, 161.3, 132.11, 132.08, 131.7, 130.9, 130.02, 122.4, 115.5, 115.3, 113.6, 65.6, 55.4.

IR (ATR): 1711 cm^{-1}, HRMS (EI) calc. for $[C_{15}H_{13}O_3F, M]^+$ 260.0849, found 260.0850, m.p.: 54 °C

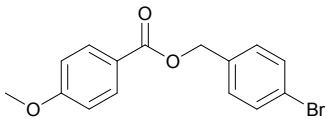


4-Chlorobenzyl 4-methoxybenzoate: white solid. (Table 4, **4ag**)

^1H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.8 Hz, 2 H), 7.24 (q, *J* = 8.6 Hz, 4 H), 6.80 (d, *J* = 8.8 Hz, 2 H), 5.18 (s, 2 H), 3.73 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9, 163.4, 134.7, 133.9, 131.6, 129.4, 128.6, 122.2, 113.6, 65.4, 55.3.

IR (ATR): 1712 cm^{-1}, HRMS (EI) calc. for $[C_{15}H_{13}O_3Cl, M]^+$ 276.0553, found 276.0552, m.p. : 86 °C

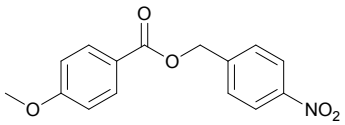


4-Bromobenzyl 4-methoxybenzoate: white solid. (Table 4, **4ah**)

^1H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.9 Hz, 2 H), 7.39 (d, *J* = 8.3 Hz, 2 H), 7.20 (d, *J* = 8.3 Hz, 2 H), 6.81 (d, *J* = 8.9 Hz, 2 H), 5.17 (s, 2 H), 3.74 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9, 163.4, 135.3, 131.64, 131.61, 129.7, 122.2, 122.1, 113.6, 65.5, 55.3.

IR (ATR): 1713 cm^{-1}, HRMS (EI) calc. for $[C_{15}H_{13}O_3Br, M]^+$ 320.0048, found 320.0049, m.p. : 94 °C

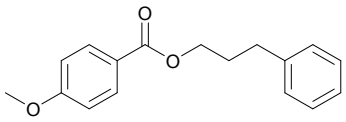


4-Nitrobenzyl 4-methoxybenzoate: yellow crystal. (Table 4, **4ai**)

^1H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.4 Hz, 2 H), 7.94 (d, *J* = 8.6 Hz, 2 H), 7.49 (d, *J* = 8.3 Hz, 2 H), 6.84 (d, *J* = 8.6 Hz, 2 H), 5.33 (s, 2 H), 3.76 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 163.6, 147.5, 143.6, 131.7, 128.1, 123.7, 121.7, 113.7, 64.8, 55.4.

IR (ATR): 1714 cm^{-1}, HRMS (EI) calc. for $[C_{15}H_{13}O_5N, M]^+$ 287.0794, found 287.0795, m.p. : 132 °C

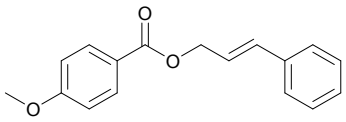


3-Phenylpropyl 4-methoxybenzoate: colorless liquid. (Table 4, **4aj**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.5 Hz, 2 H), 7.17 (d, *J* = 7.0 Hz, 2 H), 7.10 (d, *J* = 6.5 Hz, 3 H), 6.80 (d, *J* = 8.2 Hz, 2 H), 4.20 (t, *J* = 6.1 Hz, 2 H), 3.72 (s, 3 H), 2.67 (t, *J* = 7.4 Hz, 2 H), 1.98 (t, *J* = 5.2 Hz 2 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 163.2, 141.2, 131.6, 131.5, 128.3, 125.9, 122.7, 113.5, 63.9, 55.3, 32.2, 30.3.

IR (ATR): 1716 cm^{-1}, HRMS (EI) calc. for $[C_{17}H_{18}O_3, M]^+$ 270.1256, found 270.1253,

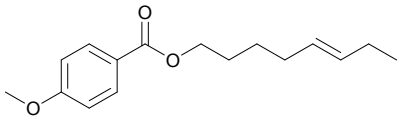


Cinnamyl 4-methoxybenzoate: colorless liquid. (Table 4, **4ak**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.6 Hz, 2 H), 7.30 (d, *J* = 7.5 Hz, 2 H), 7.21 (t, *J* = 7.4 Hz, 2 H), 7.15 (d, *J* = 7.0 Hz, 1 H), 6.81 (d, *J* = 8.5 Hz, 2 H), 6.62 (d, *J* = 15.9 Hz, 1 H), 6.29 (dt, *J* = 13.1, 6.3 Hz, 1 H), 4.84 (d, *J* = 6.2 Hz, 2 H), 3.72 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 163.3, 136.2, 133.9, 131.6, 128.5, 127.9, 126.5, 123.5, 122.5, 113.5, 65.1, 55.3.

IR (ATR): 1709 cm^{-1}, HRMS (EI) calc. for $[C_{17}H_{16}O_3, M]^+$ 268.1099 found 268.1097

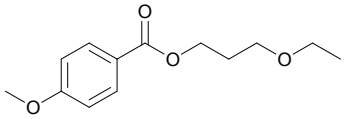


(E)-Oct-5-en-1-yl 4-methoxybenzoate: colorless liquid. (Table 4, **4al**) with regioisomer

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.4 Hz, 2 H), 6.82 (d, *J* = 8.3 Hz, 2 H), 5.42 – 5.20 (m, 2 H), 4.20 (t, *J* = 6.5 Hz, 2 H), 3.75 (s, 6 H), 2.04 – 1.92 (m, 4 H), 1.73 – 1.63 (m, 2 H), 1.45 – 1.37 (m, 2 H), 0.87 (t, *J* = 7.5 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 163.2, 132.1, 131.4, 128.4, 122.8, 113.4, 64.5, 55.3, 28.2, 26.6, 26.1, 20.5, 14.3.

IR (ATR): 1702 cm^{-1}, HRMS (EI) calc. for $[C_{16}H_{22}O_3, M]^+$ 262.1569 found 262.1568

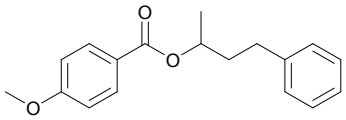


3-Ethoxypropyl 4-methoxybenzoate: colorless liquid. (Table 4, **4am**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.1 Hz, 2 H), 6.81 (d, *J* = 8.1 Hz, 2 H), 4.29 (t, *J* = 6.0 Hz, 2 H), 3.75 (s, 3 H), 3.47 (t, *J* = 5.9 Hz, 2 H), 3.40 (d, *J* = 6.8 Hz, 2 H), 1.98 – 1.90 (m, 2 H), 1.10 (t, *J* = 6.7 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 163.2, 131.4, 122.7, 113.4, 67.0, 66.1, 61.8, 55.3, 29.1, 15.0.

IR (ATR): 1713 cm^{-1}, HRMS (EI) calc. for $[C_{13}H_{18}O_4, M]^+$ 238.1205 found 238.1206

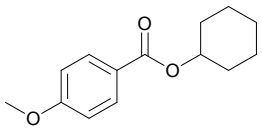


4-Phenylbutan-2-yl 4-methoxybenzoate: colorless liquid. (Table 4, **4an**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.7 Hz, 2 H), 7.16 (t, *J* = 7.4 Hz, 2 H), 7.08 (d, *J* = 7.5 Hz, 3 H), 6.81 (d, *J* = 8.7 Hz, 2 H), 5.06 (dd, *J* = 12.4, 6.2 Hz, 1 H), 3.73 (s, 3 H), 2.68 – 2.56 (m, 2 H), 2.02 – 1.94 (m, 1 H), 1.86 – 1.79 (m, 1 H), 1.26 (d, *J* = 6.2 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 163.2, 141.5, 131.4, 128.3, 128.2, 125.8, 123.1, 113.5, 70.7, 55.3, 37.7, 31.8, 20.1.

IR (ATR): 1700 cm^{-1}, HRMS (EI) calc. for $[C_{18}H_{20}O_3, M]^+$ 284.1412 found 284.1414

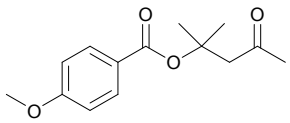


Cyclohexyl 4-methoxybenzoate: colorless liquid. (Table 4, **4ao**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.7 Hz, 2 H), 6.81 (d, *J* = 8.7 Hz, 2 H), 4.94 – 4.85 (m, 1 H), 3.74 (s, 3 H), 1.87 – 1.83 (m, 2 H), 1.73 – 1.65 (m, 2 H), 1.53 – 1.44 (m, 3 H), 1.38 – 1.22 (m, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 163.1, 131.4, 123.3, 113.4, 72.5, 55.3, 31.6, 25.4, 23.6.

IR (ATR): 1704 cm^{-1}, HRMS (EI) calc. for $[C_{14}H_{18}O_3, M]^+$ 234.1256 found 234.1258

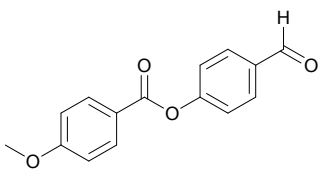


2-Methyl-4-oxopentan-2-yl 4-methoxybenzoate: colorless liquid. (Table 4, **4ap**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 5.3 Hz, 2 H), 6.82 (d, *J* = 5.3 Hz, 2 H), 3.77 (s, 3 H), 3.09 (s, 2 H), 2.08 (s, 3 H), 1.57 (s, 6 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 206.0, 165.6, 163.2, 131.4, 123.8, 113.5, 80.4, 55.4, 52.4, 31.7, 26.6.

IR (ATR): 1703 cm^{-1}, HRMS (EI) calc. for $[C_{14}H_{18}O_4, M]^+$ 250.1205 found 250.1205



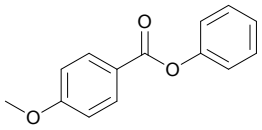
4-Formylphenyl 4-methoxybenzoate: colorless liquid. (Table 4, **4aq**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.94 (s, 1 H), 8.08 (d, *J* = 8.7 Hz, 2 H), 7.88 (d, *J* = 8.3 Hz, 2 H), 7.32 (d, *J* = 8.3

Hz, 2 H), 6.92 (d, *J* = 8.7 Hz, 2 H), 3.83 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 191.0, 164.2, 164.1, 155.8, 133.9, 132.4, 131.2, 122.6, 121.1, 114.0, 55.5.

IR (ATR): 1724, 1695 cm^{-1}, HRMS (EI) calc. for $[C_{15}H_{12}O_4, M]^+$ 256.0736 found 256.0733

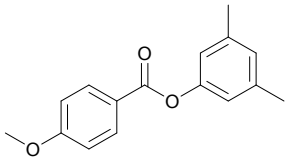


Phenyl 4-methoxybenzoate: pale brown crystal. (Table 4, **4ar**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.7 Hz, 2 H), 7.32 (t, *J* = 6.7 Hz, 2 H), 7.18 – 7.09 (m, 3 H), 6.89 (d, *J* = 7.7 Hz, 2 H), 3.78 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 163.8, 151.0, 132.2, 129.4, 125.6, 121.8, 121.7, 113.8, 55.4.

IR (ATR): 1732 cm^{-1}, HRMS (EI) calc. for $[C_{14}H_{12}O_3, M]^+$ 228.0786 found 228.0782, m.p.: 74 °C

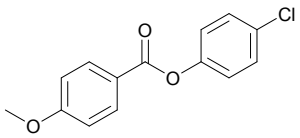


3,5-Dimethylphenyl 4-methoxybenzoate: pale brown solid. (Table 4, **4as**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.4 Hz, 2 H), 6.86 (d, *J* = 8.5 Hz, 2 H), 6.78 (s, 1 H), 6.72 (s, 2 H), 3.76 (s, 3 H), 2.23 (s, 6 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 163.7, 150.9, 139.1, 132.1, 127.4, 121.9, 119.3, 113.7, 55.4, 21.2.

IR (ATR): 1725 cm^{-1}, HRMS (EI) calc. for $[C_{16}H_{16}O_3, M]^+$ 256.1099 found 256.1103, m.p.: 62 °C

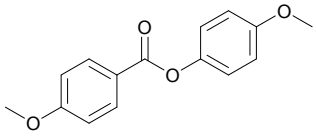


4-Chlorophenyl 4-methoxybenzoate: pale brown crystal. (Table 4, **4at**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 5.7 Hz, 2 H), 7.23 (d, *J* = 5.6 Hz, 2 H), 7.02 (d, *J* = 5.6 Hz, 2 H), 6.84 (d, *J* = 5.8 Hz, 2 H), 3.74 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 163.9, 149.4, 132.2, 130.9, 129.3, 123.1, 121.3, 113.8, 55.4.

IR (ATR): 1728 cm^{-1}, HRMS (EI) calc. for $[C_{14}H_{11}O_3Cl, M]^+$ 262.0397 found 262.0400, m.p.: 96 °C

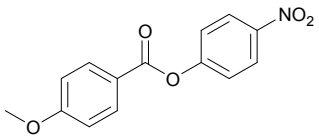


4-Methoxyphenyl 4-methoxybenzoate: pale brown crystal. (Table 4, **4au**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.6 Hz, 2 H), 7.02 (d, *J* = 8.7 Hz, 2 H), 6.85 (dd, *J* = 16.4, 8.7 Hz, 4 H), 3.77 (s, 3 H), 3.70 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 163.7, 157.1, 144.4, 132.1, 122.4, 121.8, 114.4, 113.7, 55.46, 55.40.

IR (ATR): 1728 cm^{-1}, HRMS (EI) calc. for $[C_{15}H_{14}O_4, M]^+$ 258.0892 found 258.0890, m.p.: 124 °C

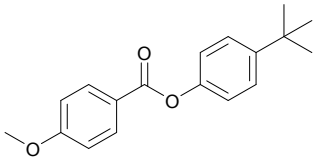


4-Nitrophenyl 4-methoxybenzoate: pale brown crystal. (Table 4, **4av**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 9.0 Hz, 2 H), 8.07 (d, *J* = 8.8 Hz, 2 H), 7.33 (d, *J* = 9.0 Hz, 2 H), 6.93 (d, *J* = 8.8 Hz, 2 H), 3.83 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 163.9, 155.9, 145.2, 132.5, 125.2, 122.6, 120.7, 114.0, 55.6.

IR (ATR): 1735 cm^{-1}, HRMS (EI) calc. for $[C_{14}H_{11}O_5N, M]^+$ 273.0637 found 273.0639, m.p.: 167 °C

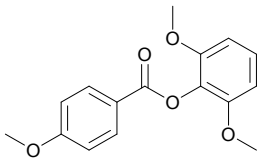


4-(tert-Butyl)phenyl 4-methoxybenzoate: pale brown crystal. (Table 4, **4aw**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.9 Hz, 2 H), 7.34 (d, *J* = 7.6 Hz, 2 H), 7.04 (d, *J* = 7.4 Hz, 2 H), 6.89 (d, *J* = 7.9 Hz, 2 H), 3.79 (s, 3 H), 1.25 (s, 9 H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 163.8, 148.6, 148.4, 132.2, 126.3, 122.0, 121.0, 113.7, 55.4, 34.4, 31.4.

IR (ATR): 1729 cm^{-1}, HRMS (EI) calc. for $[C_{18}H_{20}O_3, M]^+$ 284.1412 found 284.1411, m.p.: 103 °C



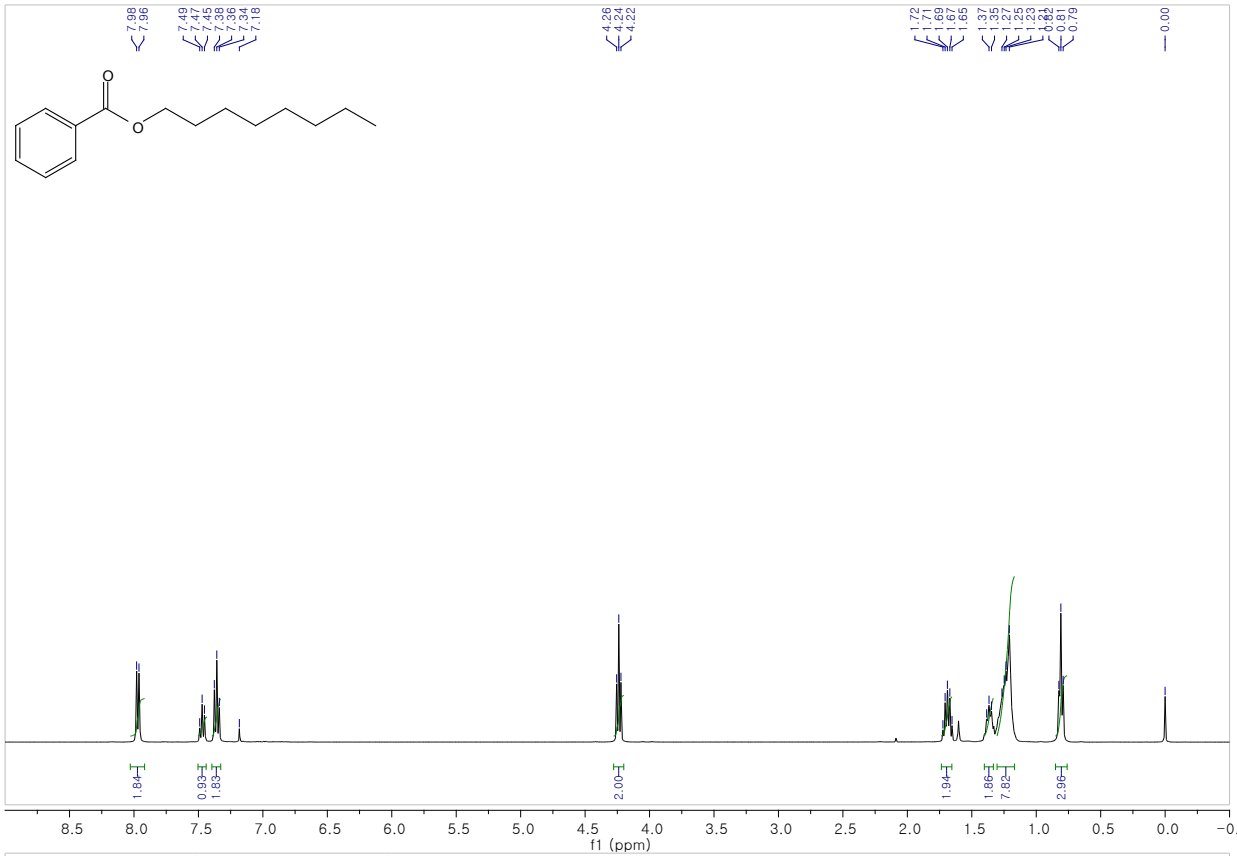
2,6-Dimethoxyphenyl 4-methoxybenzoate: pale brown crystal. (Table 4, **4ax**)

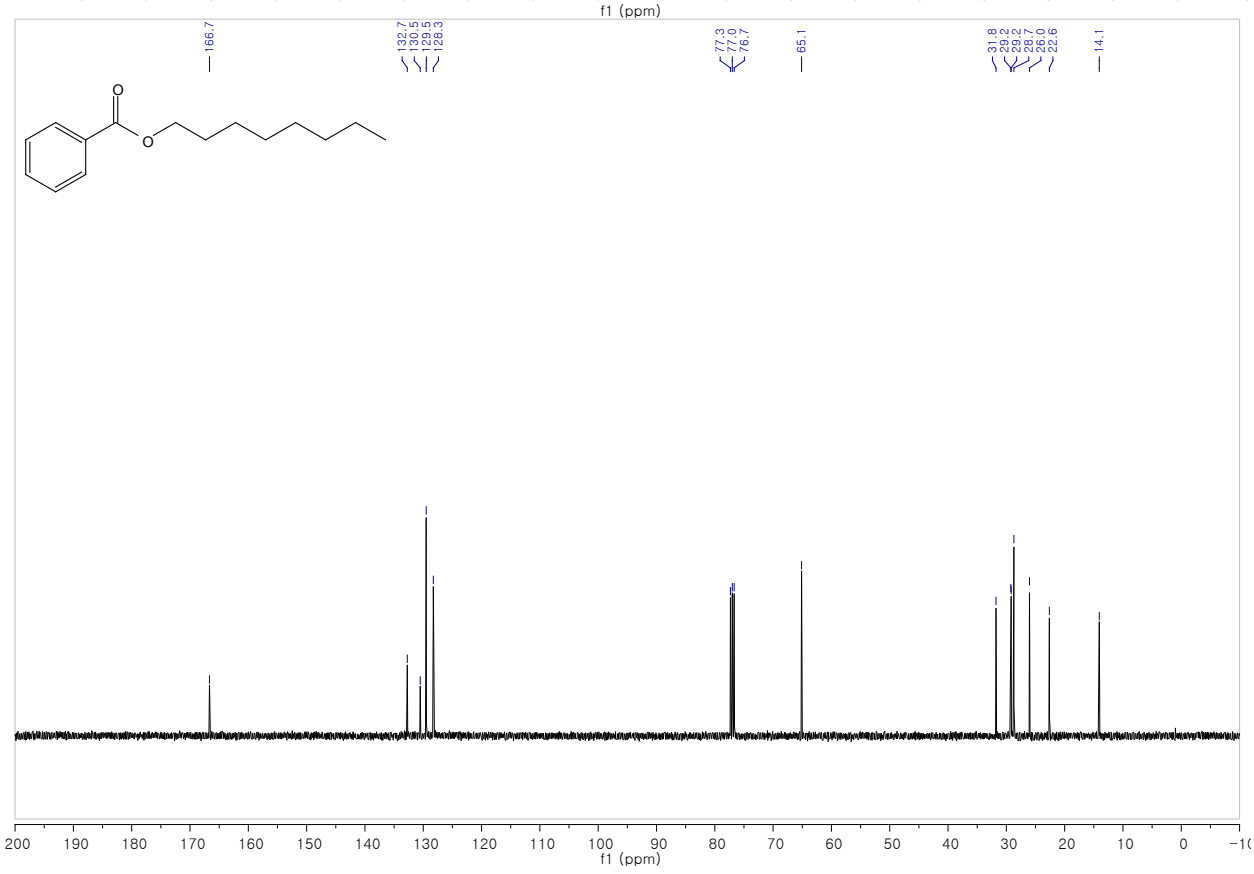
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.7 Hz, 2H), 7.07 (d, *J* = 8.4 Hz, 1H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.55 (d, *J* = 8.4 Hz, 2H), 3.77 (s, 3H), 3.70 (s, 6H).

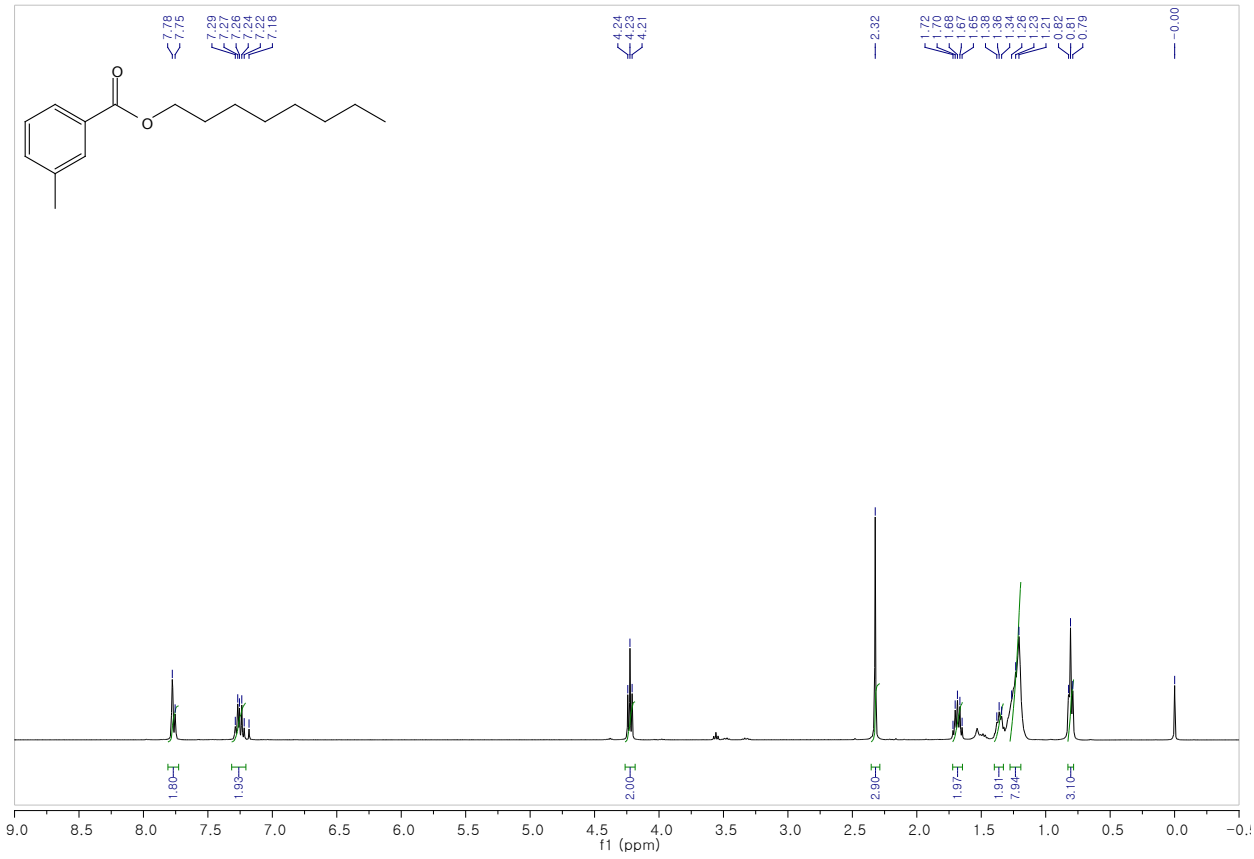
^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2, 163.6, 152.5, 132.4, 128.9, 126.1, 121.7, 113.6, 104.9, 56.1, 55.4.

IR (ATR): 1734 cm^{-1}, HRMS (EI) calc. for $[C_{16}H_{16}O_5, M]^+$ 288.0998 found 288.0999, m.p.: 119 °C

VI. NMR Spectra of Isolated Products



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7.24
7.22
7.18
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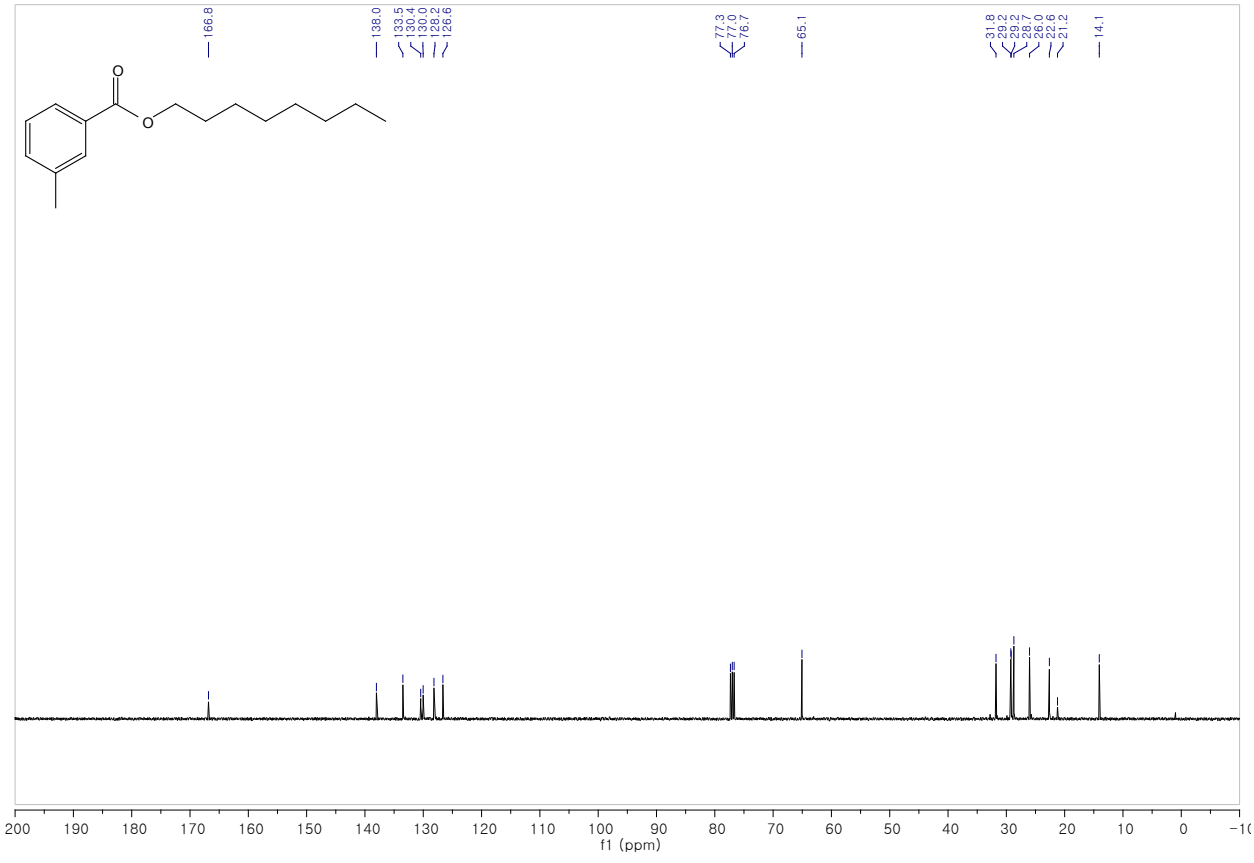
4.23
4.21
2.32
1.72
1.70
1.69
1.67
1.65
1.38
1.36
1.34
1.26
1.23
1.21
0.82
0.81
0.79
0.00
1.80
1.93
2.00
2.90
1.97
1.91
7.94
3.10
f1 (ppm)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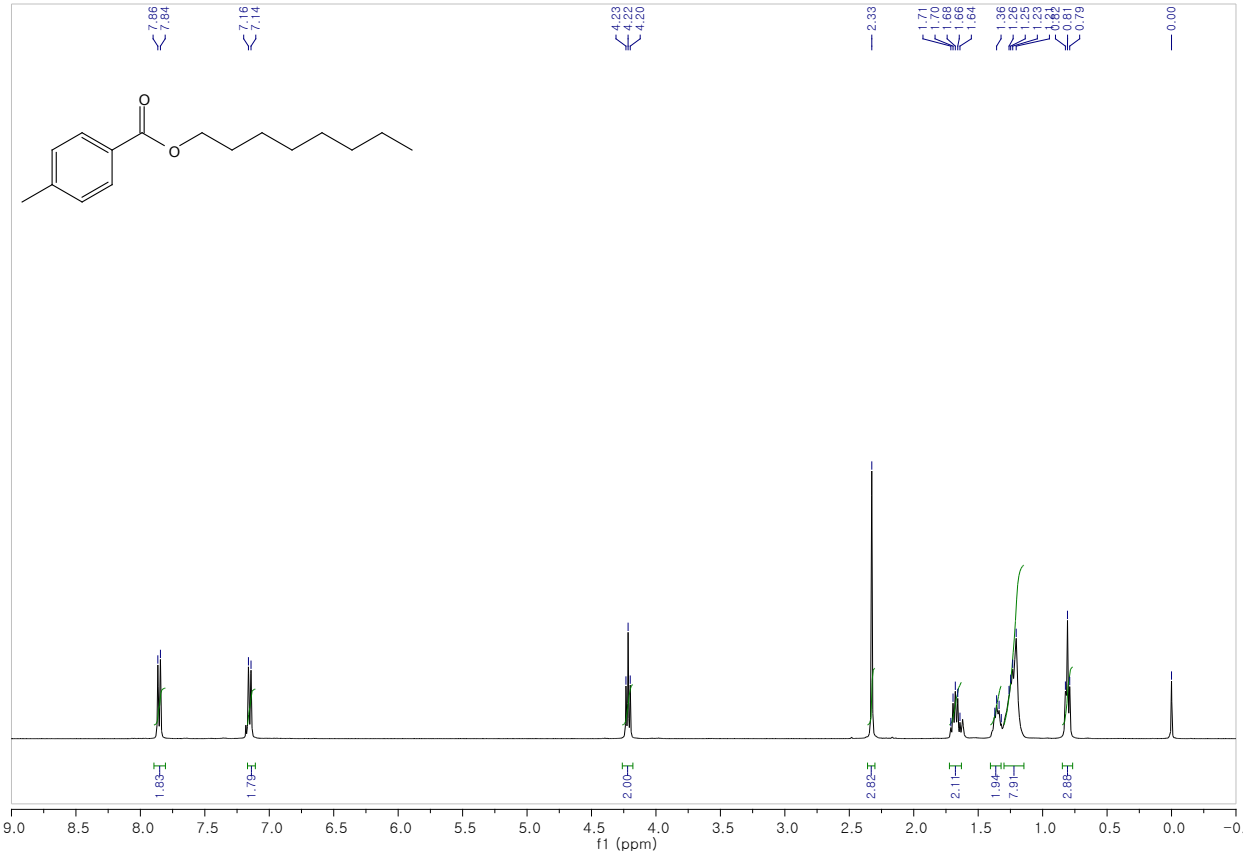
138.0
133.5
130.4
130.0
128.2
126.6
77.3
77.0
76.7
65.1
31.8
29.2
29.2
28.7
25.6
22.6
21.2
14.1
f1 (ppm)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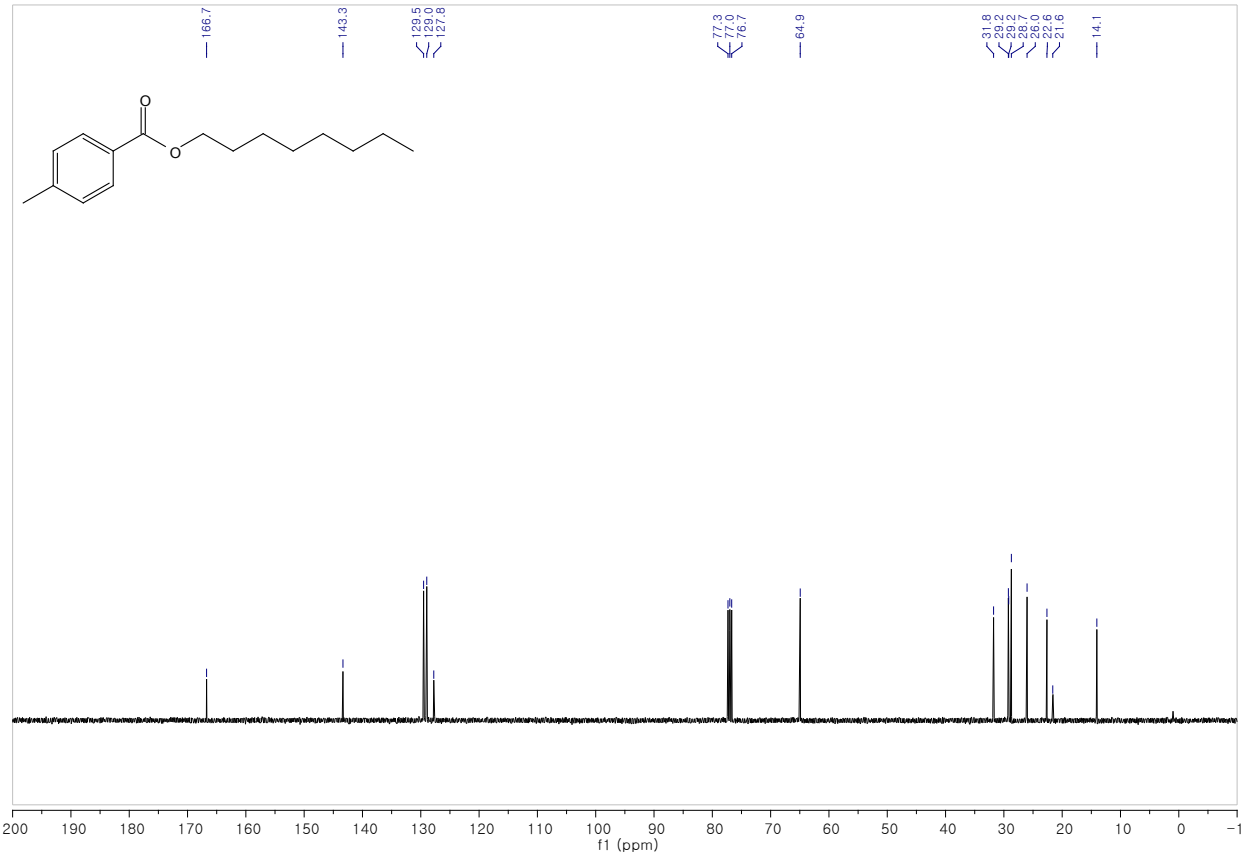
7.84
7.16
7.14
4.23
4.22
4.20
2.33
1.71
1.70
1.68
1.66
1.64
1.36
1.26
1.25
1.23
0.82
0.81
0.79
0.00
1.83
1.79
2.00
2.82
2.11
1.94
7.91
2.88
f1 (ppm)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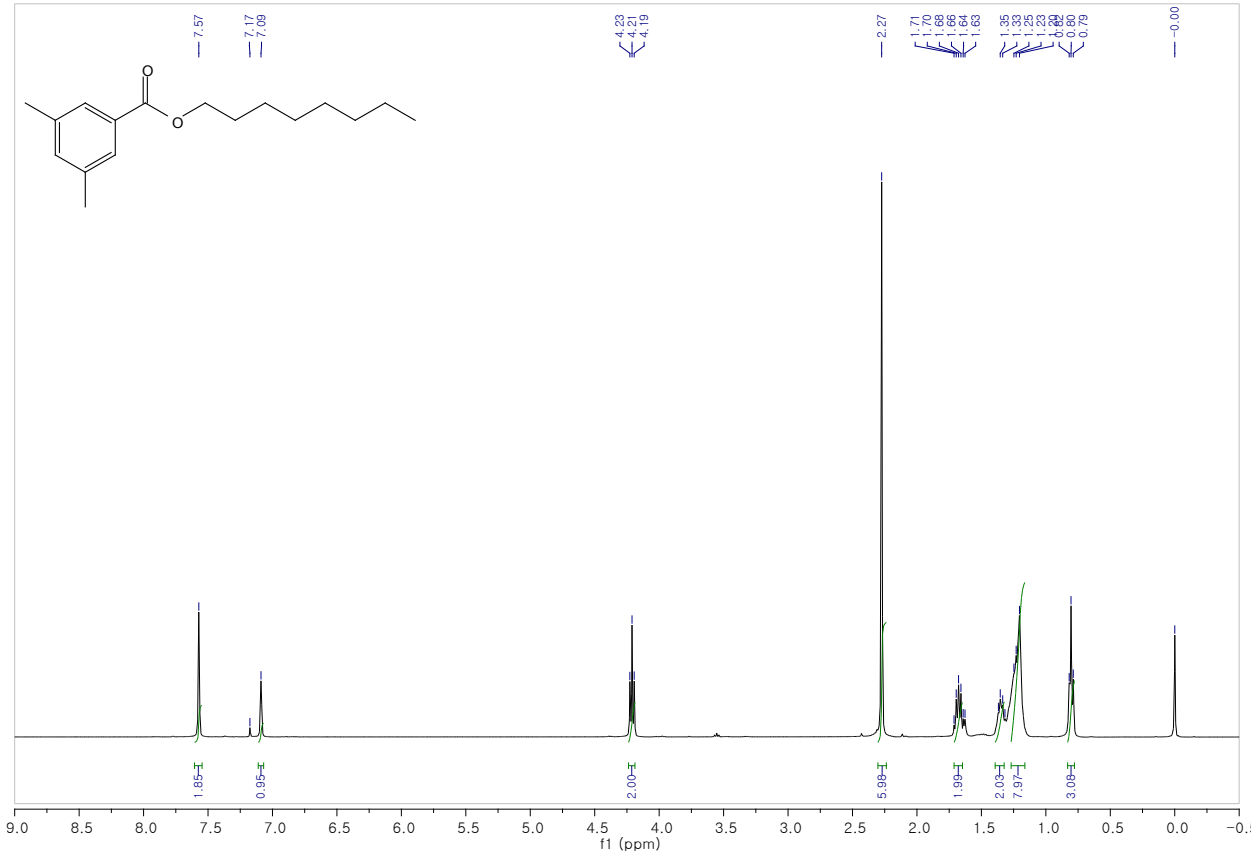
143.3
129.5
129.0
127.8
77.3
77.0
76.7
64.9
31.8
29.2
28.7
26.0
22.6
21.6
14.1
f1 (ppm)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4.19
2.27
1.71
1.70
1.68
1.66
1.64
1.63
1.35
1.33
1.25
1.23
0.82
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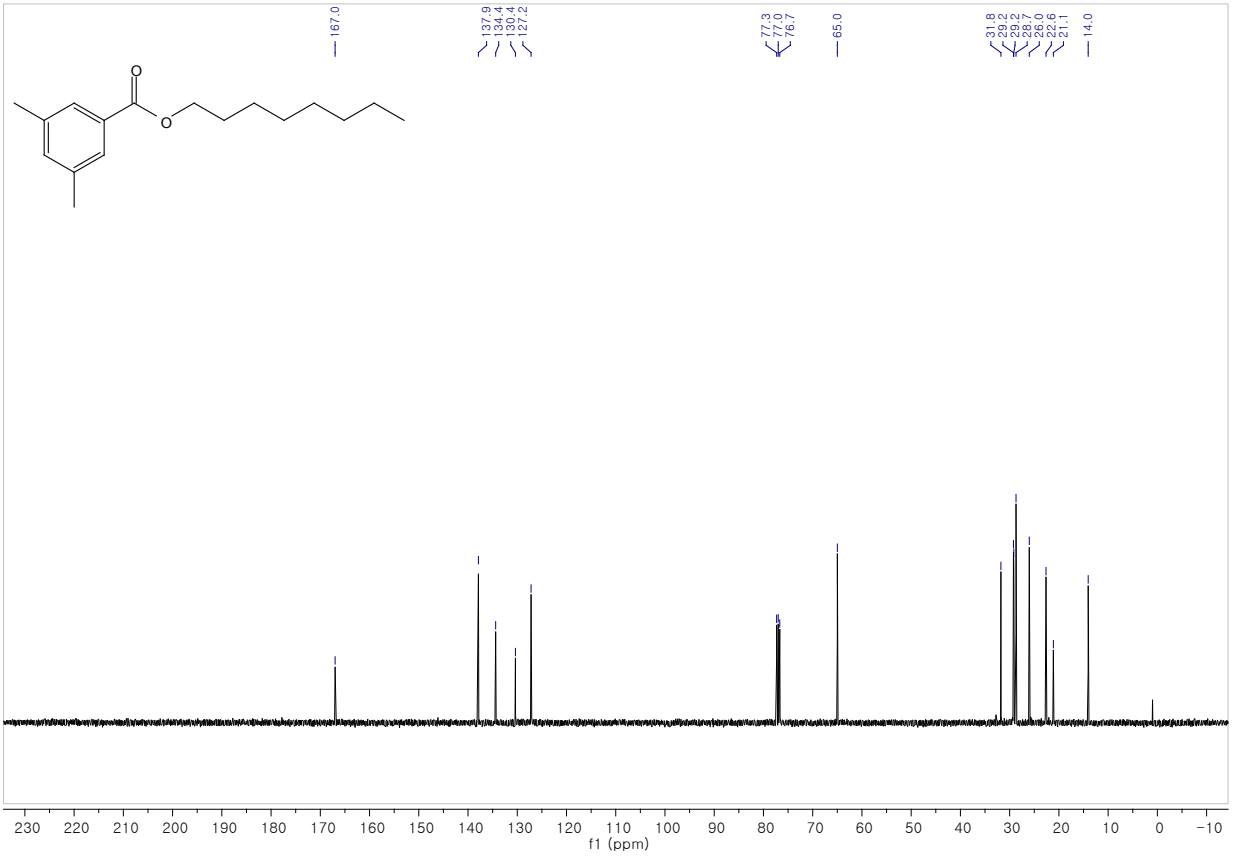
0.95
2.00
5.98
1.99
2.03
7.97
3.08
f1 (ppm)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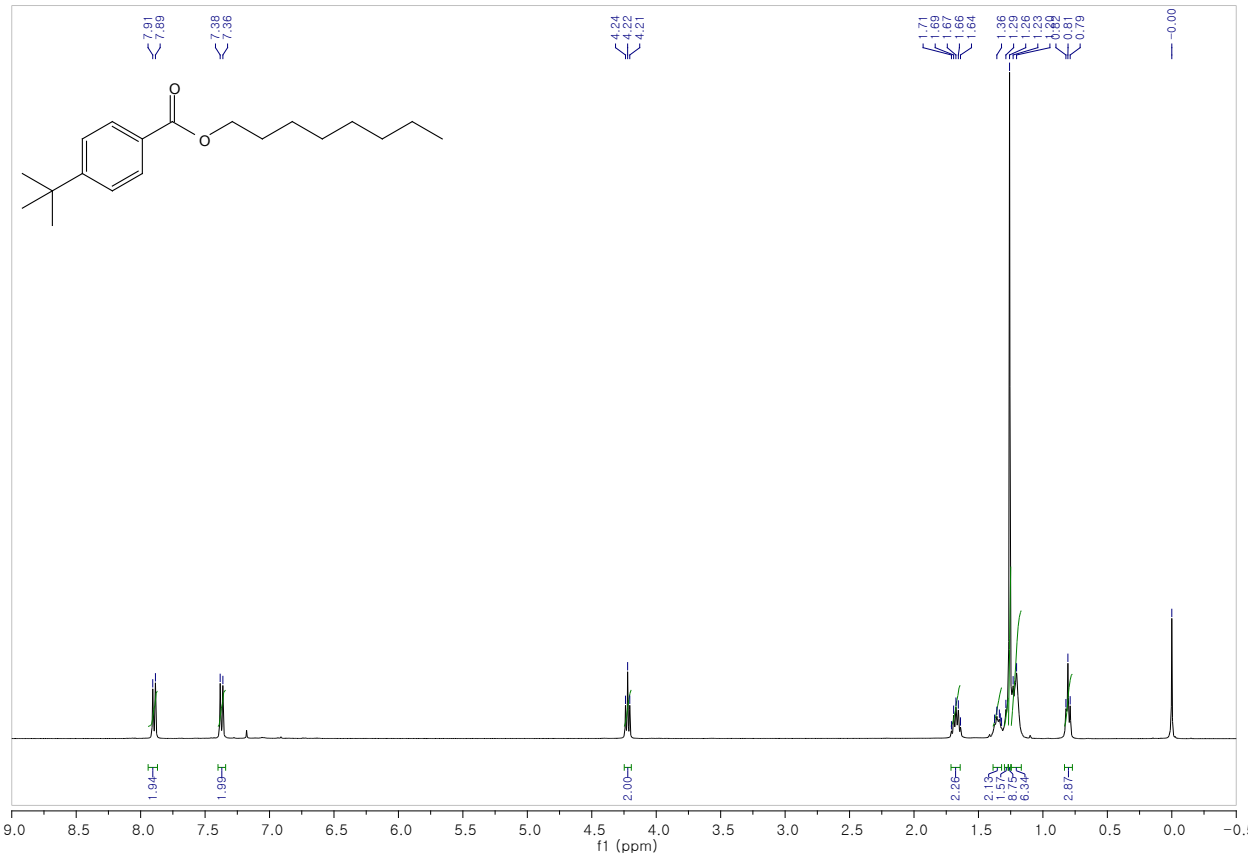
137.9
134.4
130.4
127.2
77.3
77.0
76.7
65.0
31.8
29.2
29.2
28.7
26.0
22.6
21.1
14.0
f1 (ppm)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4.24
4.22
4.21
1.71
1.69
1.67
1.66
1.64
1.36
1.29
1.26
1.23
0.81
0.79
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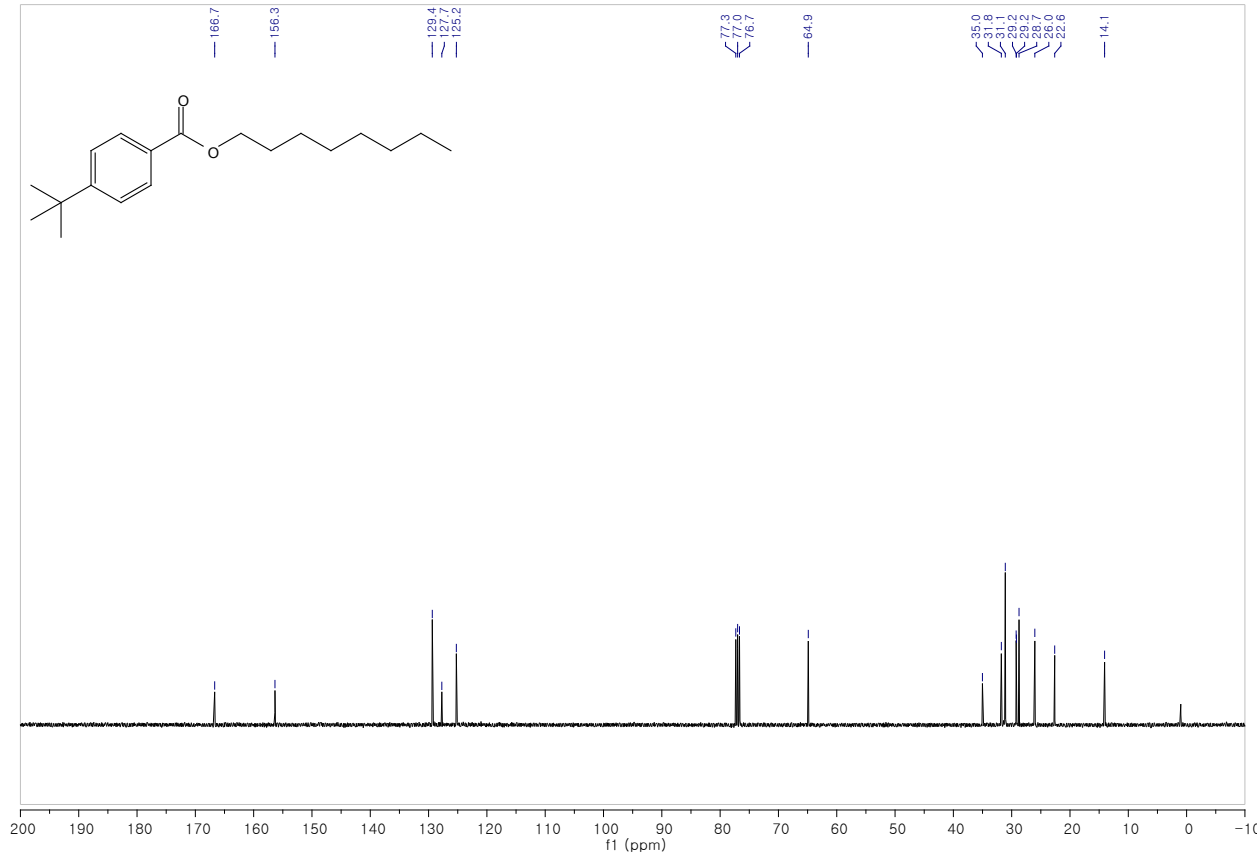
1.99
2.00
2.26
2.13
1.57
8.75
6.34
2.87
f1 (ppm)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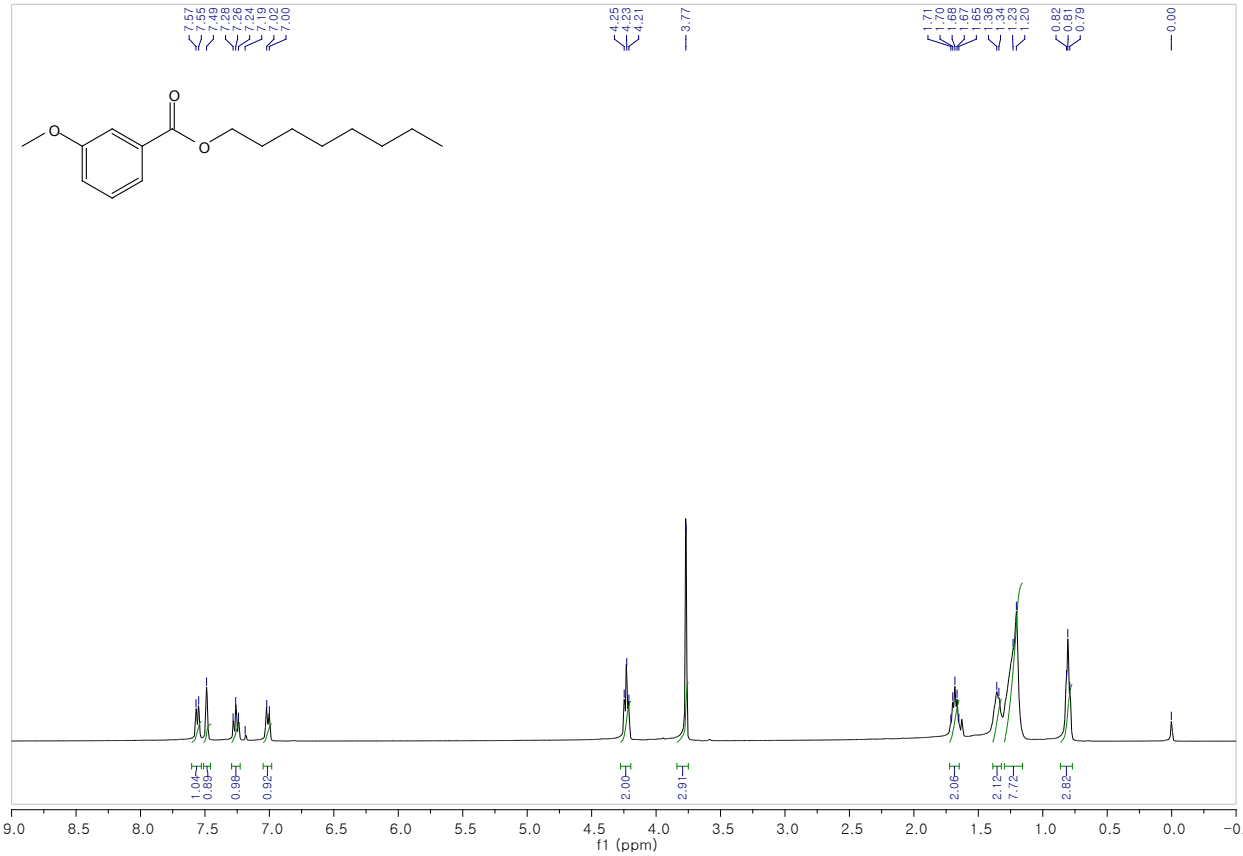
156.3
129.4
127.7
125.2
77.3
77.0
76.7
64.9
35.0
31.8
31.1
29.2
29.2
28.7
28.0
22.6
14.1
f1 (ppm)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4.21
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1.70
1.68
1.67
1.65
1.36
1.34
1.23
1.20
0.82
0.81
0.79
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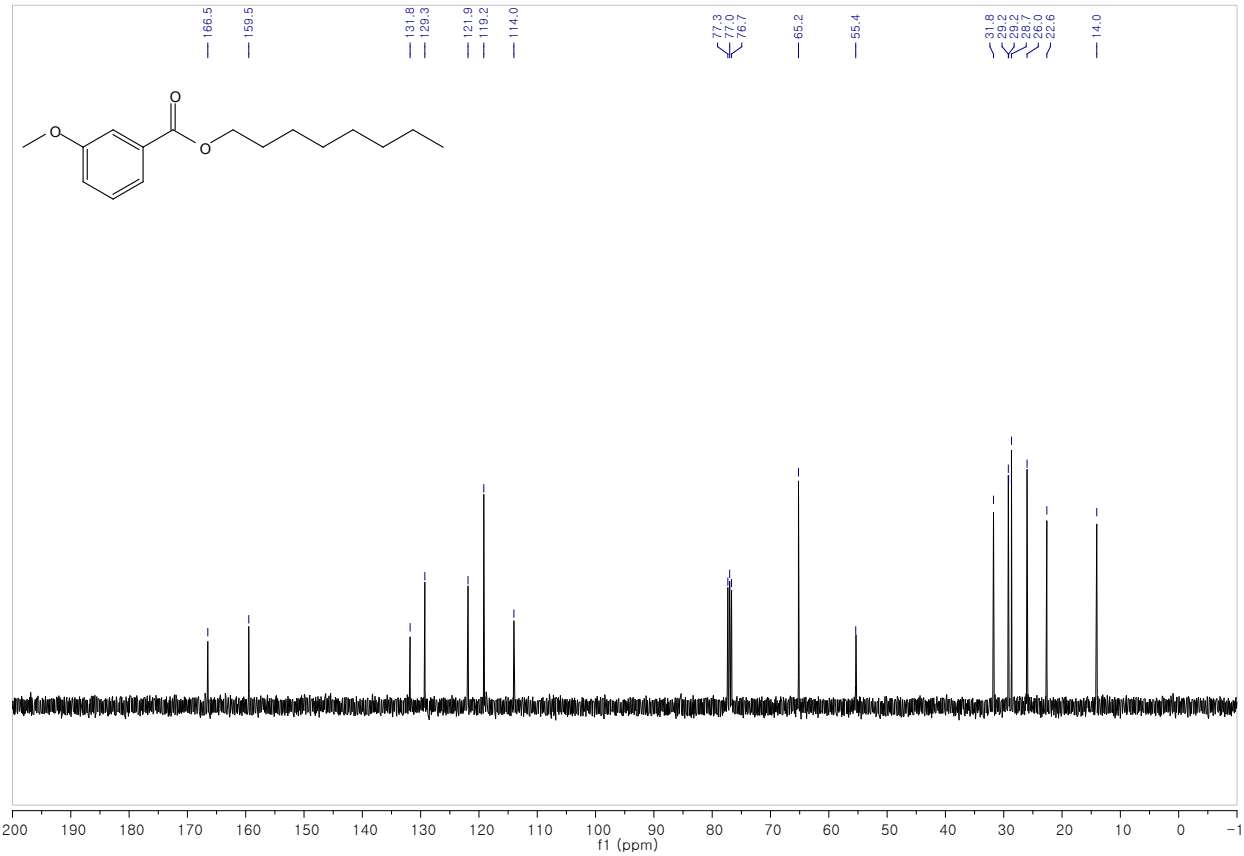
0.98
0.92
2.00
2.91
2.06
2.12
7.72
2.82
f1 (ppm)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129.3
121.9
119.2
114.0
77.3
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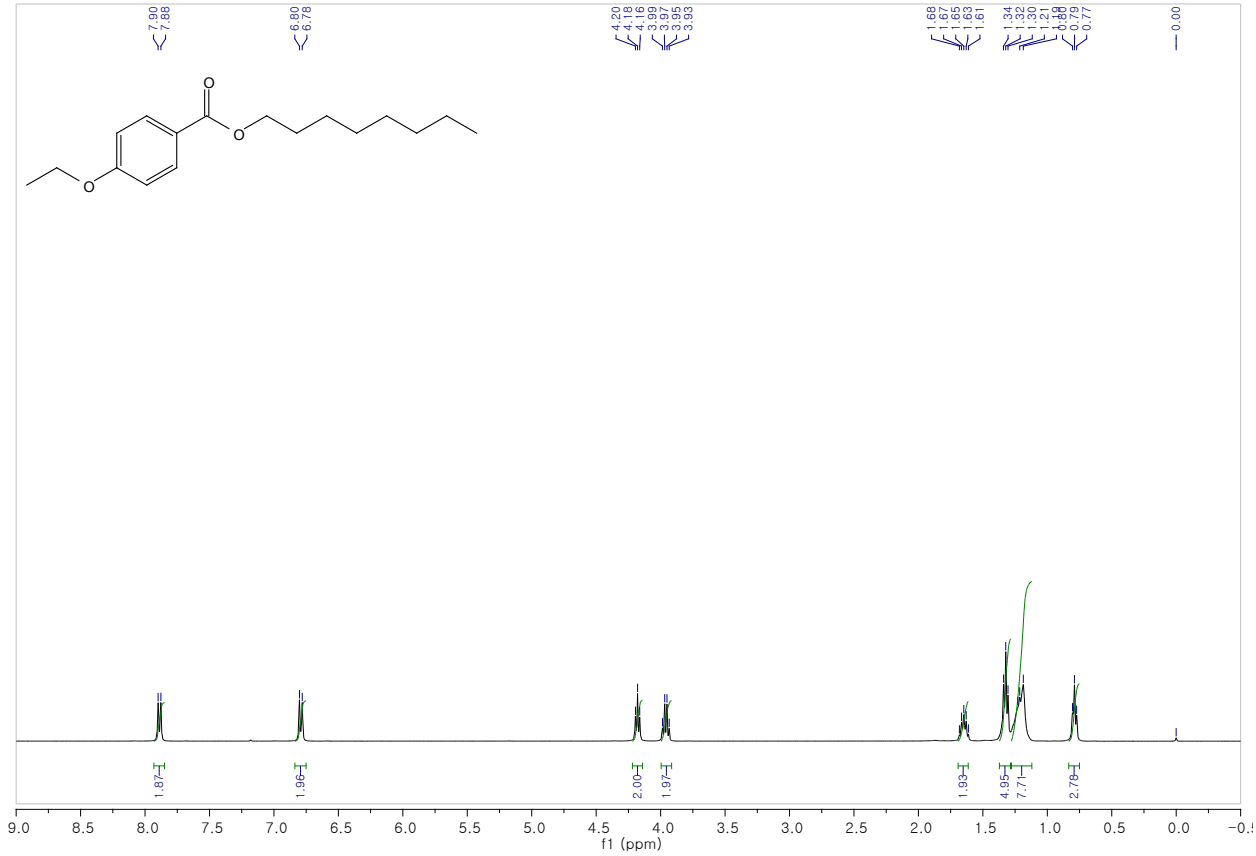
31.8
29.2
29.2
28.7
28.0
22.6
14.0
f1 (ppm)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3.95
3.93
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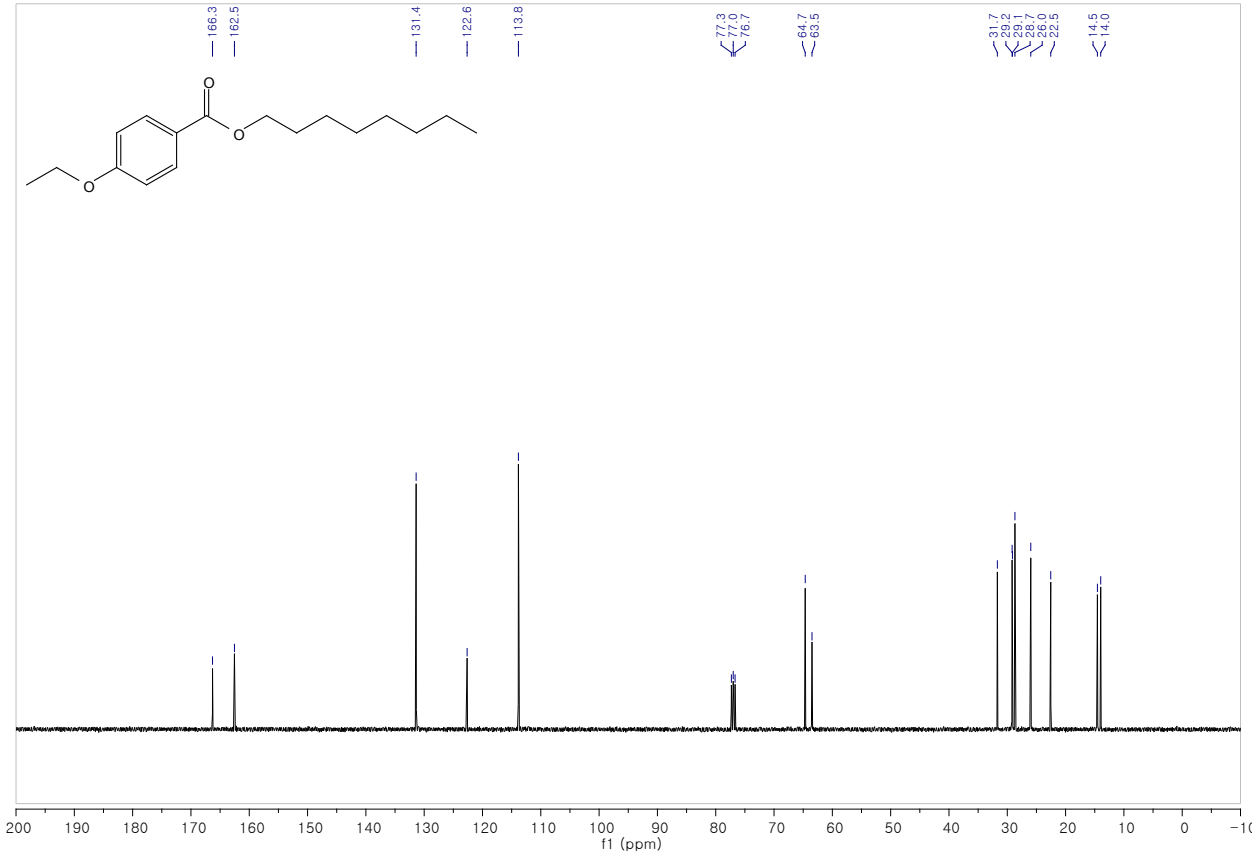
1.67
1.65
1.63
1.61
1.34
1.32
1.30
1.21
0.79
0.77
0.00
O
O
O
1.87
1.96
2.00
1.97
1.93
4.95
7.71
2.78
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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122.6
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77.3
77.0
76.7
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63.5
31.7
29.2
29.1
28.7
26.0
22.5
14.5
14.0
O
O
O
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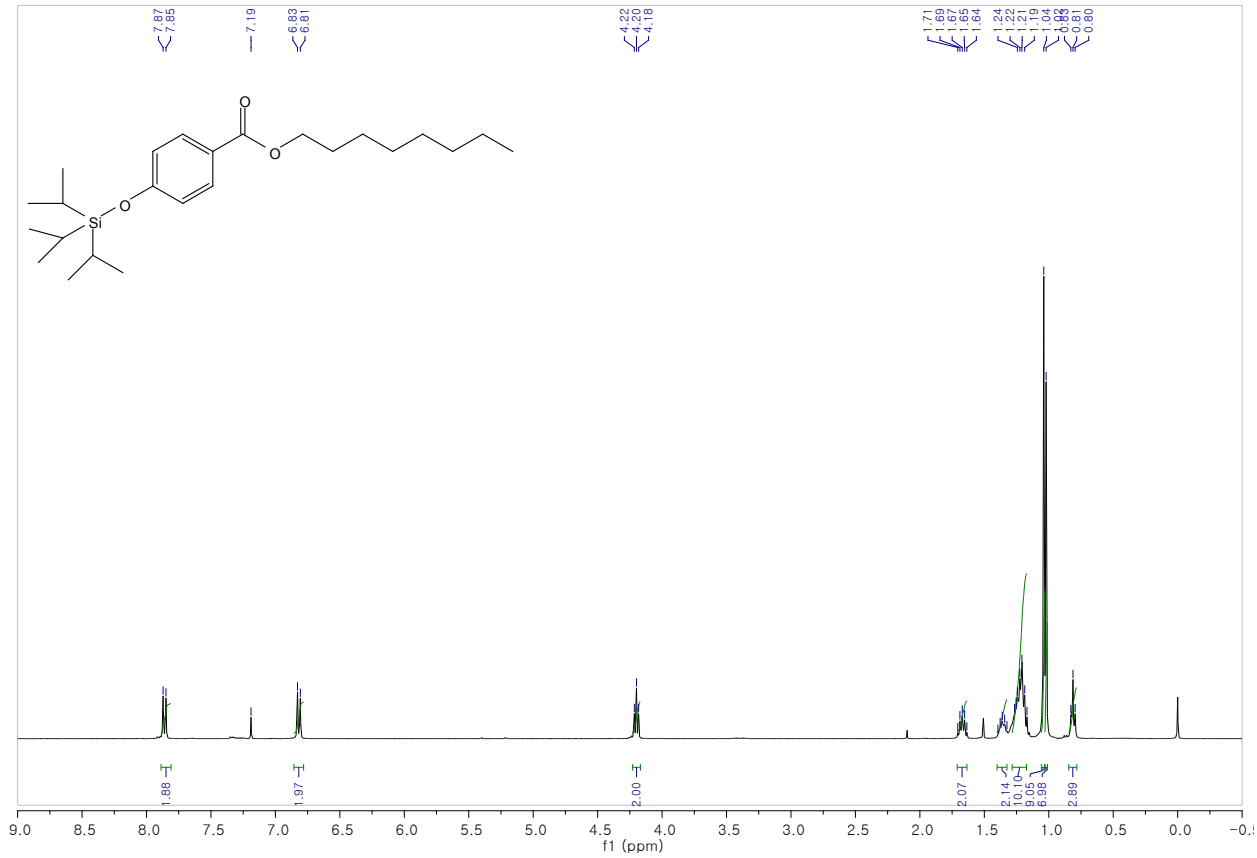
f1 (ppm)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1.24
1.22
1.21
1.19
1.04
0.83
0.81
0.80
O
O
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9.05
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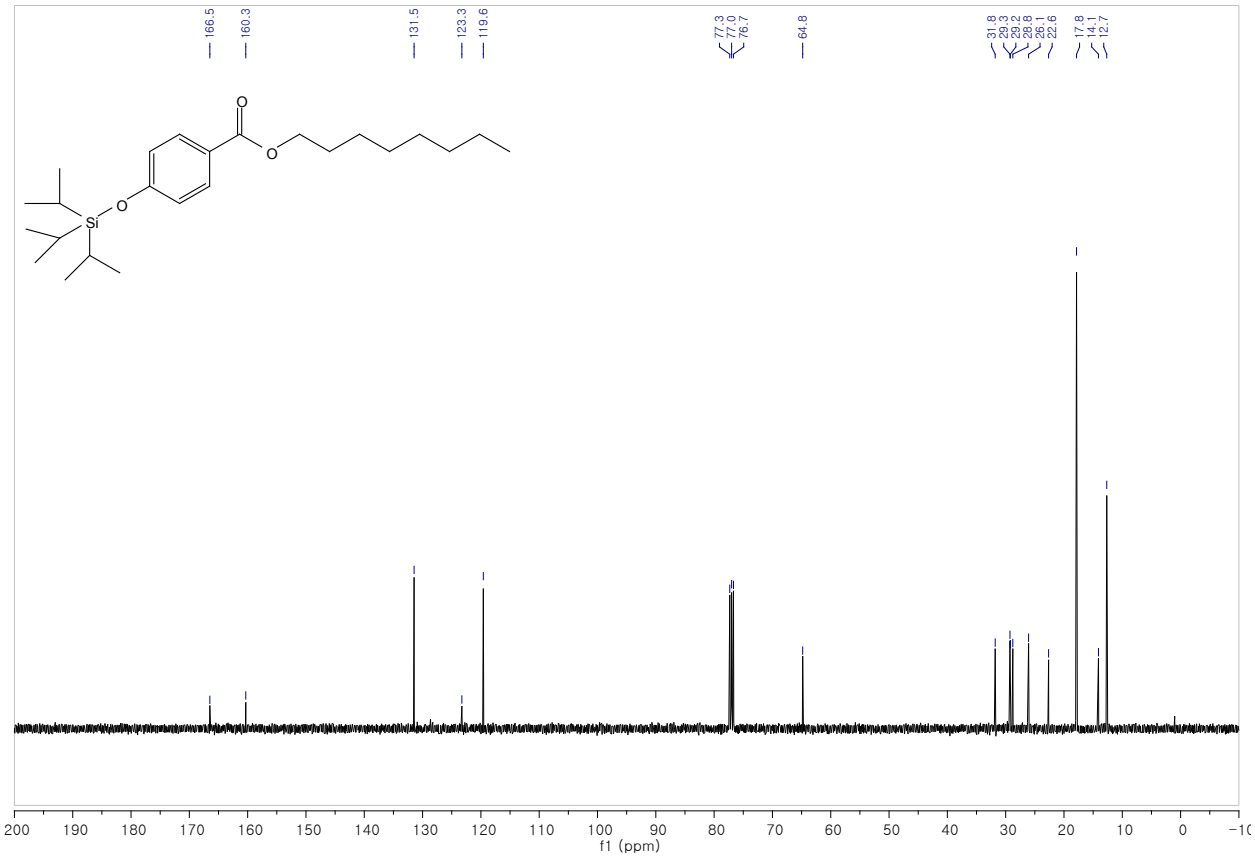
2.89
f1 (ppm)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26.1
22.6
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14.1
12.7
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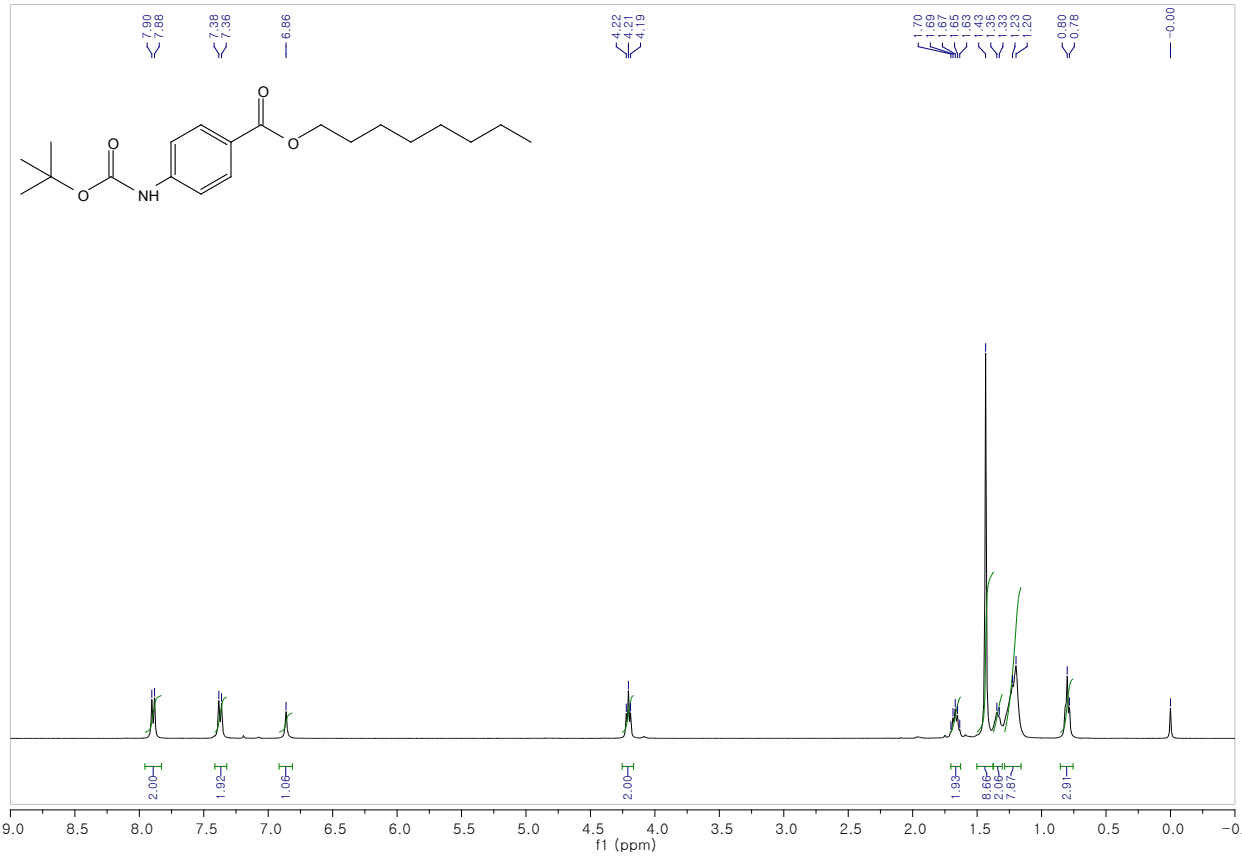
O
O
Si
f1 (ppm)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1.43
1.35
1.33
1.23
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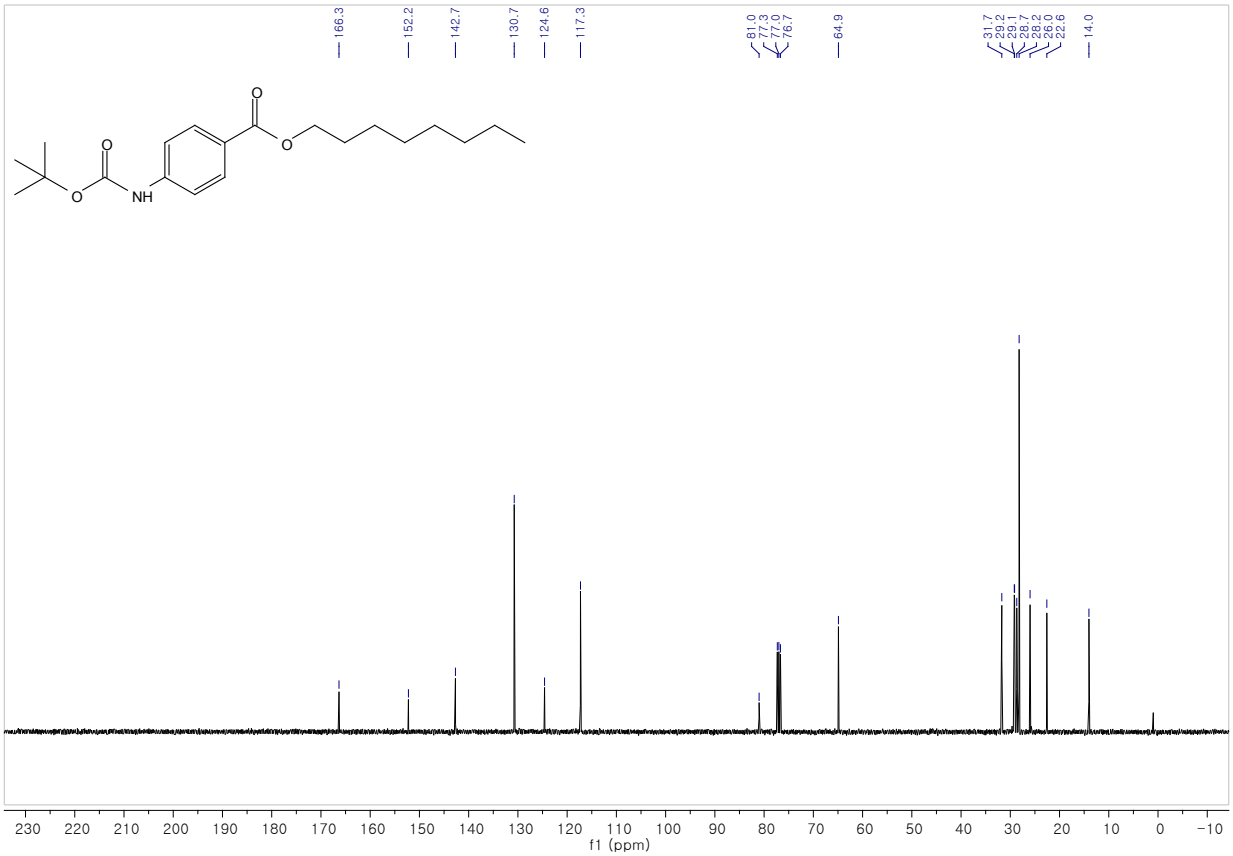
0.80
0.78
-0.00
O
O
O
NH
O
2.00
1.92
1.06
2.00
1.93
8.66
2.06
7.87
2.91
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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76.7
64.9
31.7
29.2
29.1
28.7
28.2
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22.6
14.0
O
O
O
NH
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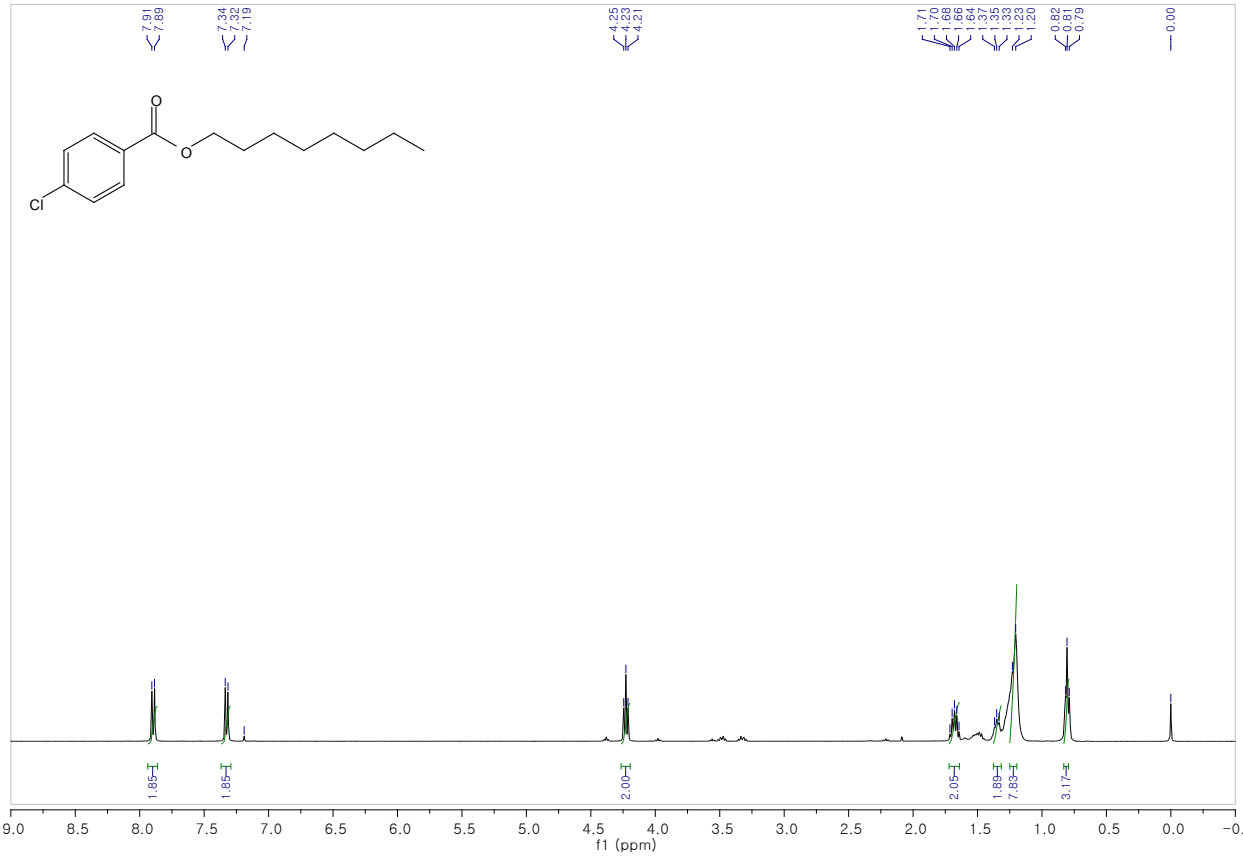
f1 (ppm)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1.68
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1.37
1.35
1.33
1.23
1.20
0.82
0.81
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O
Cl
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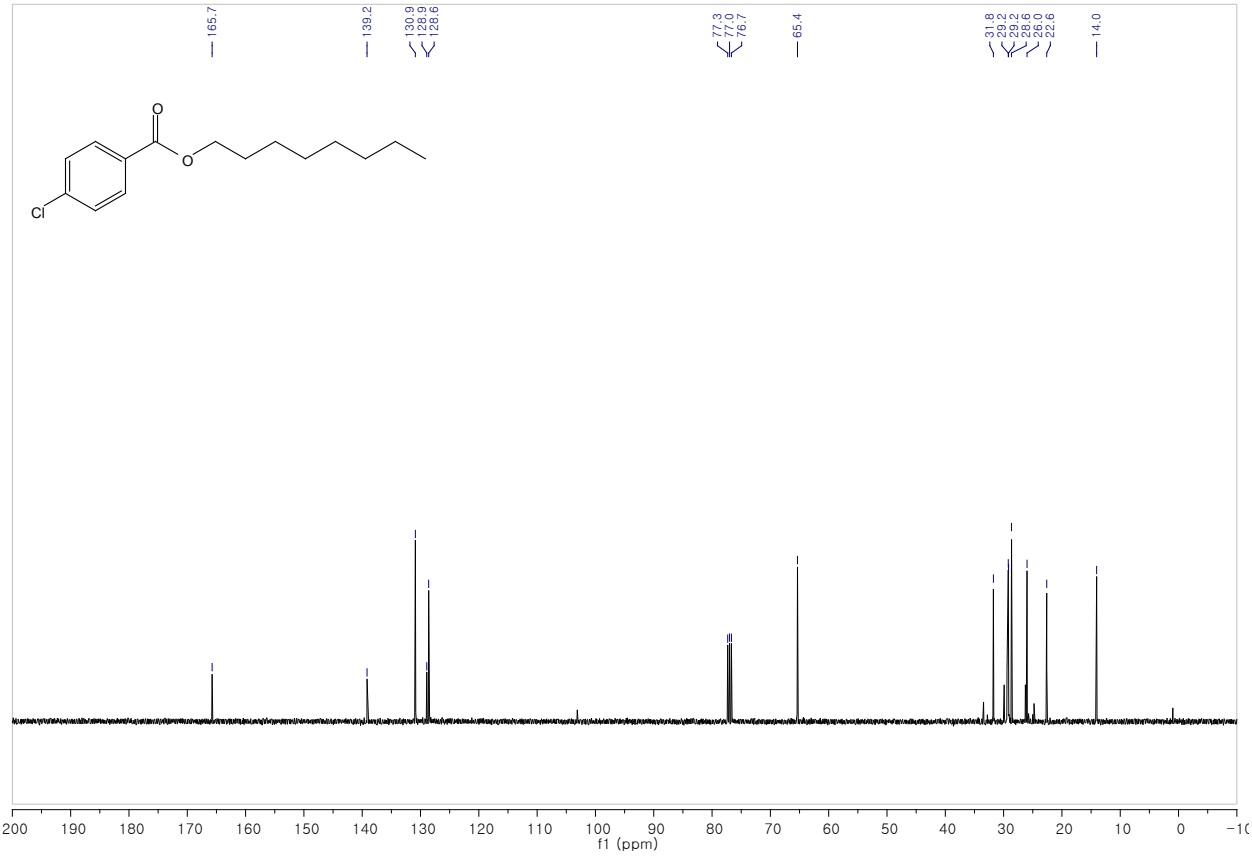
3.17
f1 (ppm)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28.6
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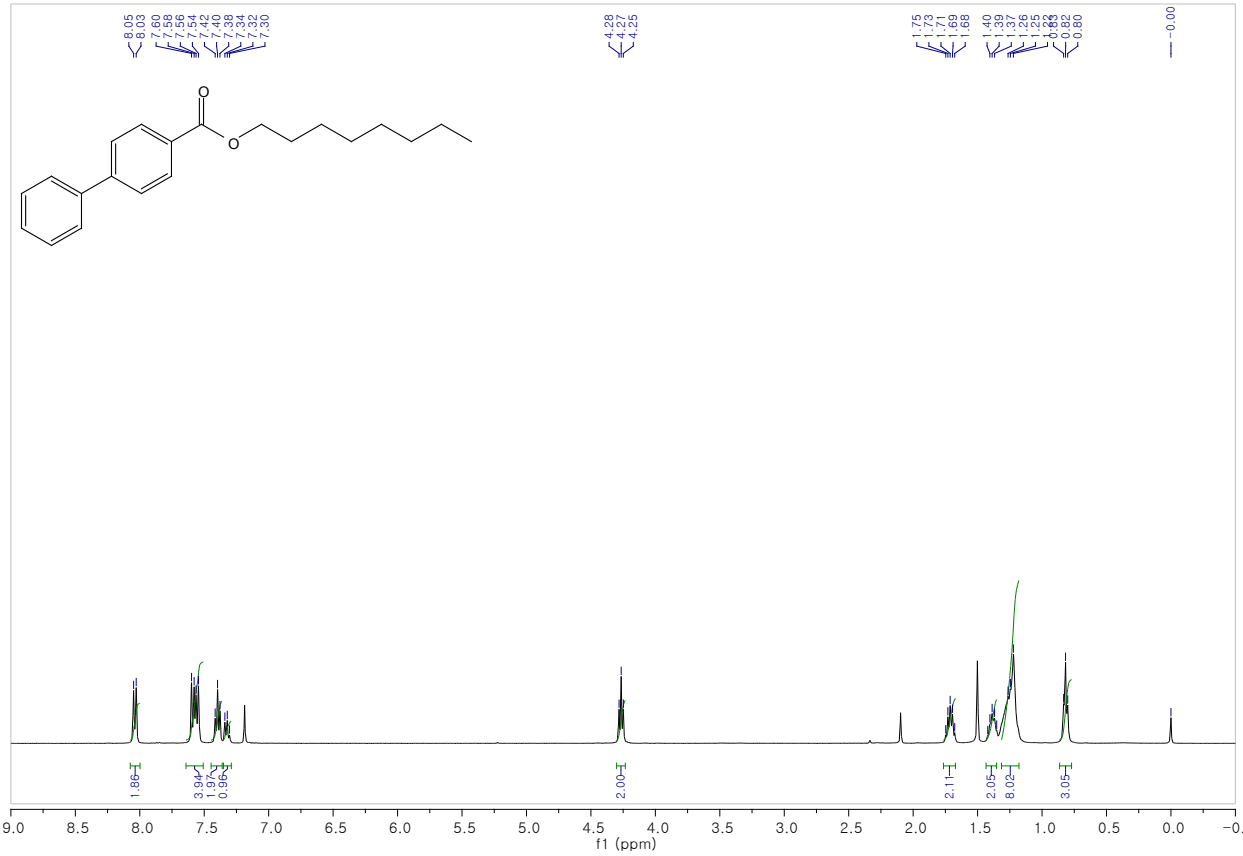
22.6
14.0
O
O
Cl
f1 (ppm)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1.73
1.71
1.69
1.68
1.40
1.39
1.37
1.36
1.25
1.22
0.88
0.82
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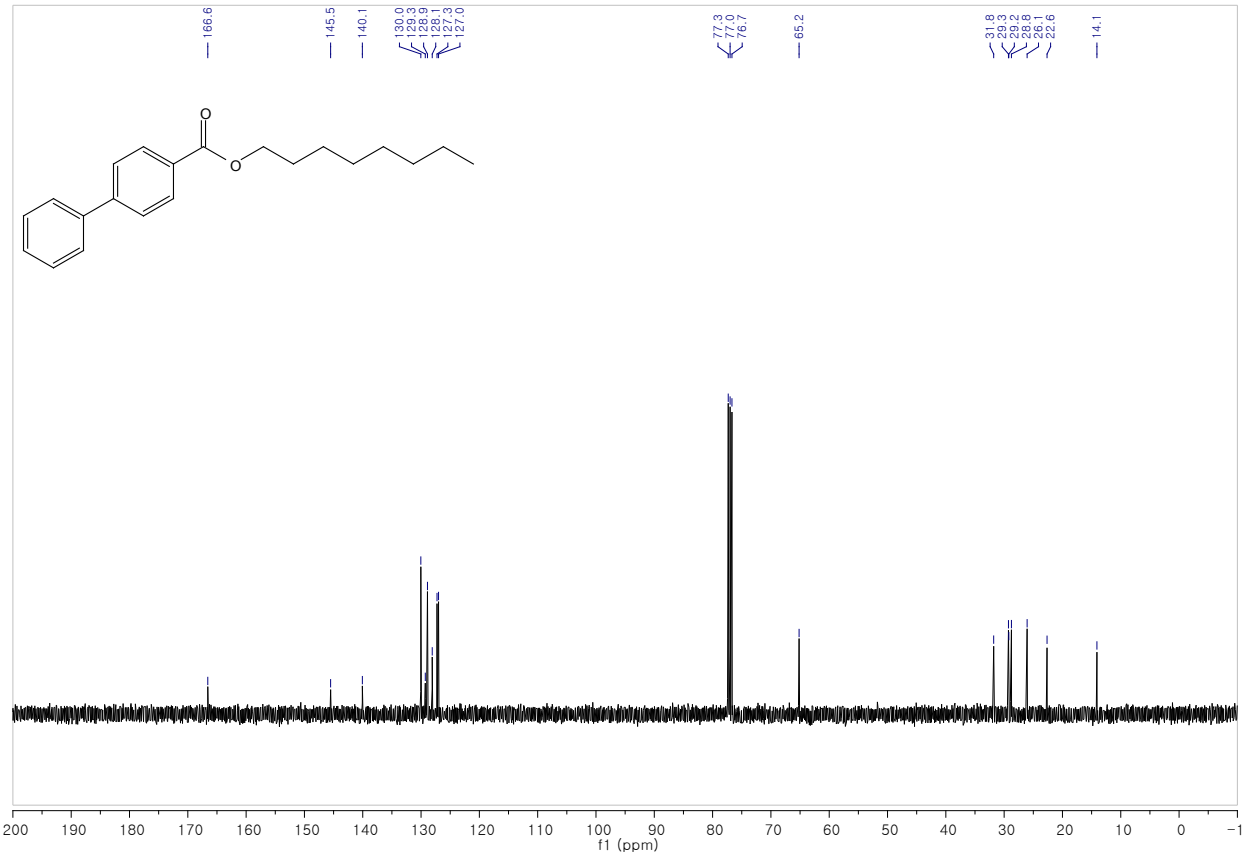
f1 (ppm)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127.3
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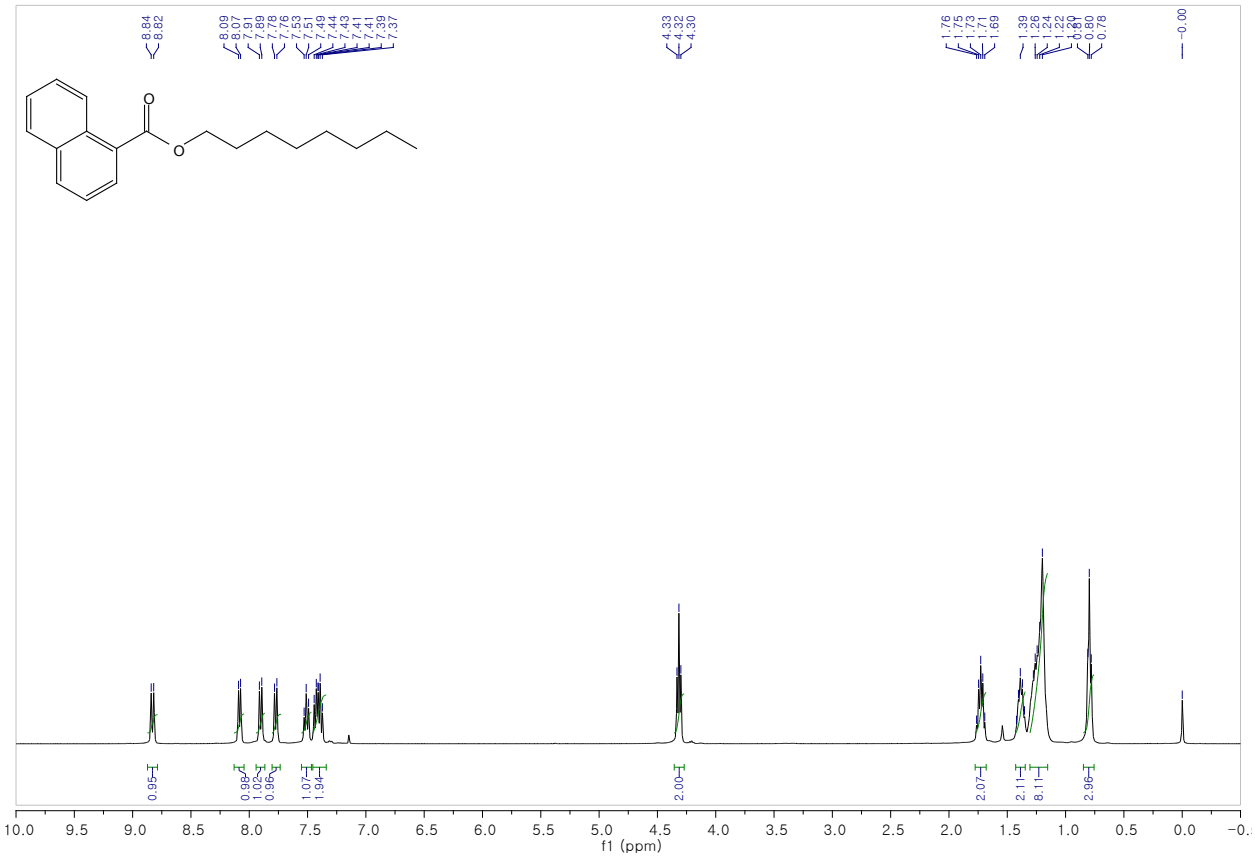
77.3
77.0
76.7
65.2
31.8
29.3
29.2
28.8
28.1
22.6
14.1
f1 (ppm)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8.82
8.09
8.07
7.91
7.89
7.78
7.76
7.53
7.51
7.49
7.44
7.43
7.41
7.41
7.39
7.37
4.33
4.32
4.30
1.76
1.75
1.73
1.71
1.69
1.39
1.26
1.24
1.22
1.20
0.81
0.80
0.78
-0.00
0.95
0.98
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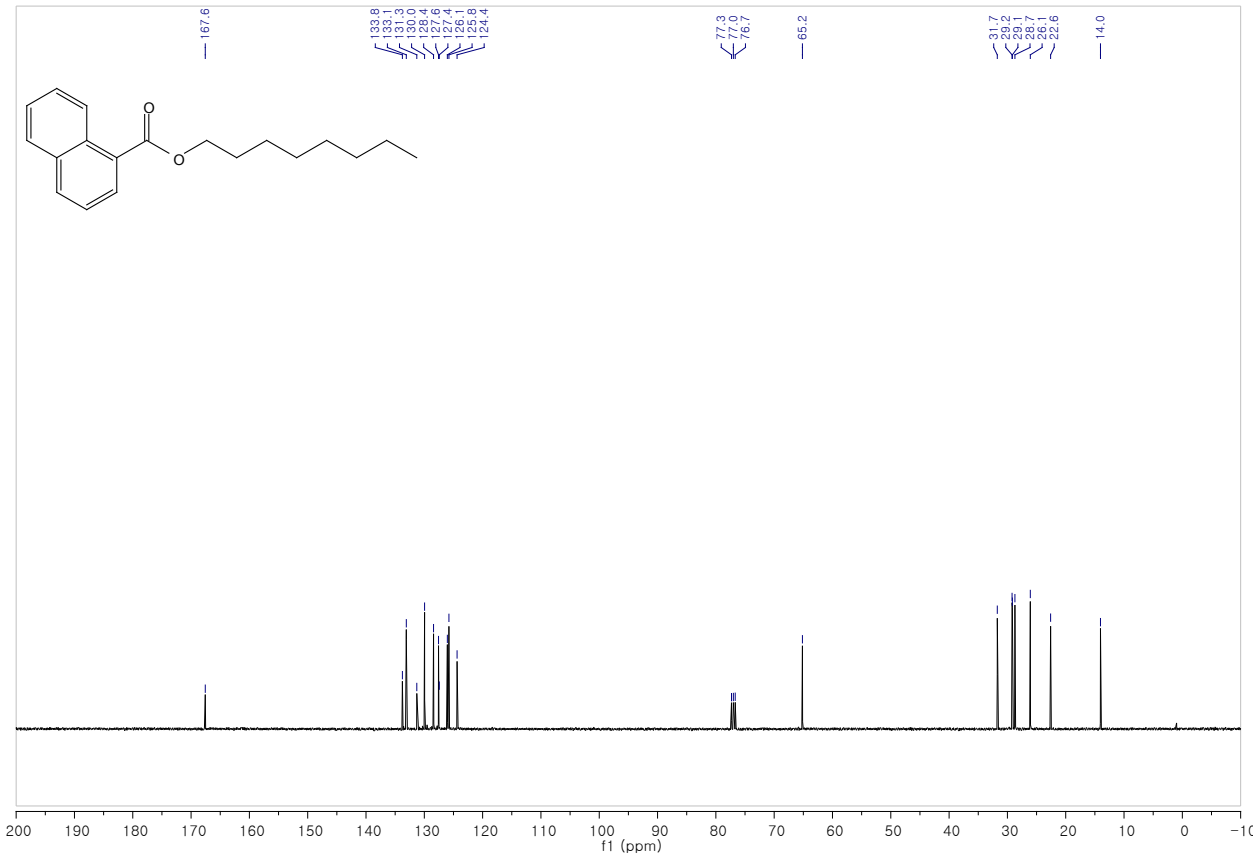
0.96
1.07
1.94
2.00
2.07
2.11
8.11
2.96
f1 (ppm)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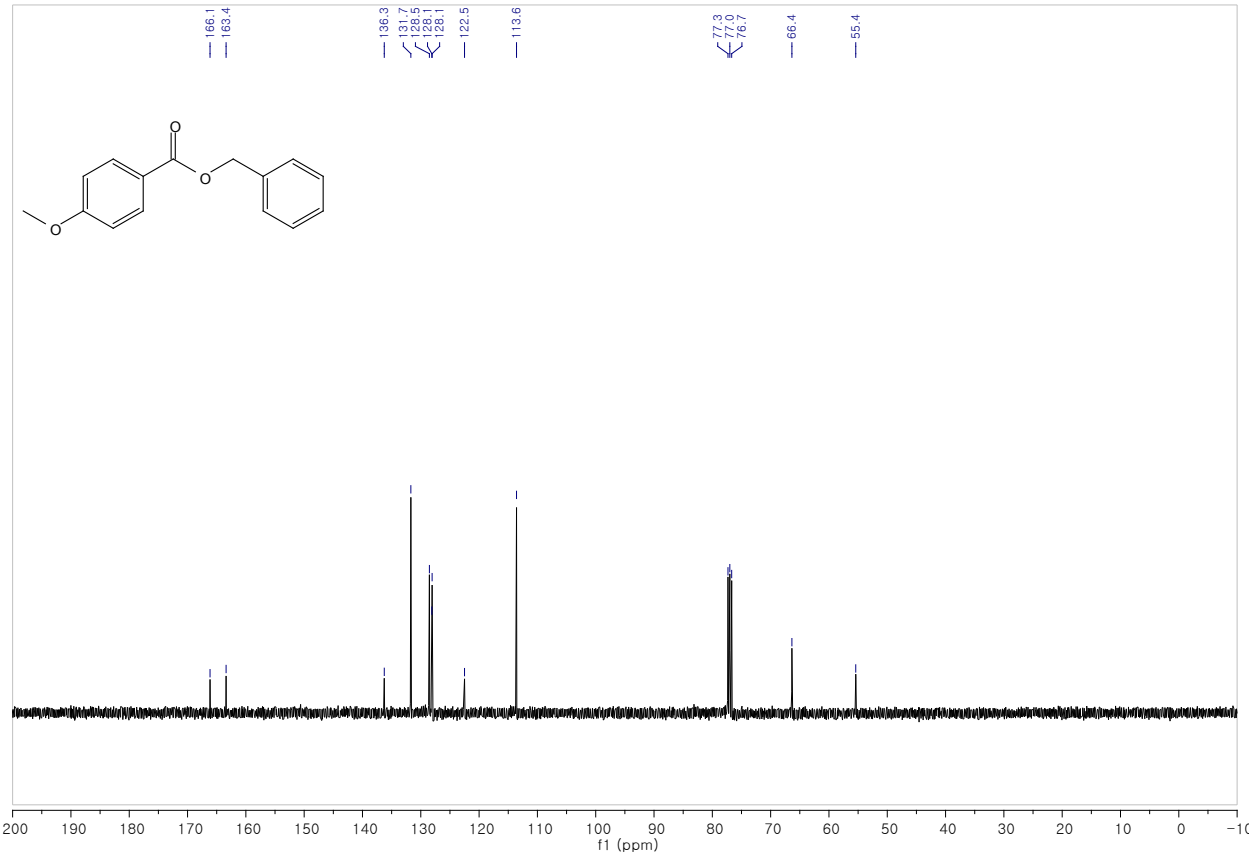
133.8
133.1
131.3
130.0
128.4
127.6
127.4
126.1
125.8
124.4
77.3
77.0
76.7
65.2
31.7
29.2
29.1
28.7
26.1
22.6
14.0
f1 (ppm)


7.97
7.95
7.37
7.35
7.32
7.30
7.29
7.27
7.25
6.84
6.82
5.26
3.77
0.00
O
O
O
1.92
1.94
2.82
1.96
1.99
3.00
f1 (ppm)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136.3
131.7
128.5
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128.1
122.5
113.6
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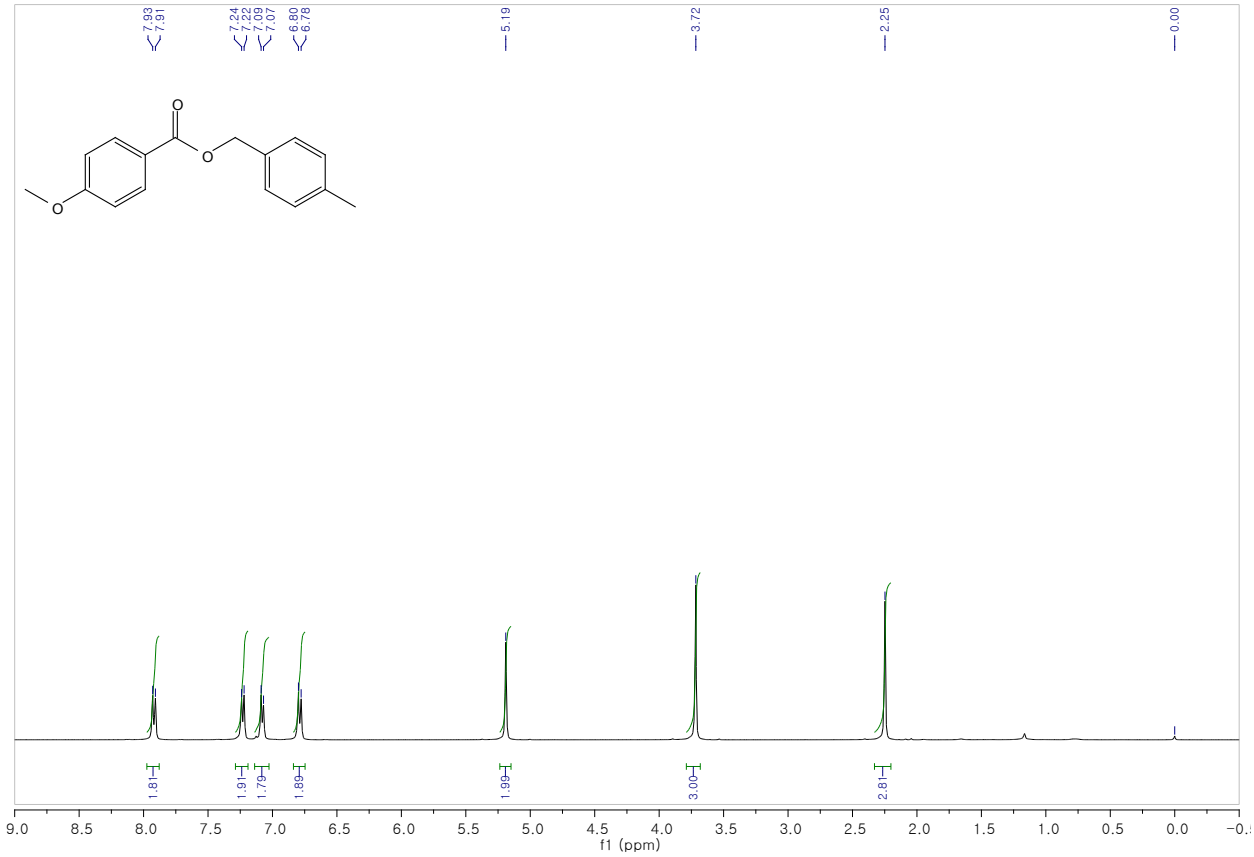
77.0
76.7
66.4
55.4
O
O
O
f1 (ppm)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7.91
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7.22
7.09
7.07
6.80
6.78
5.19
3.72
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O
O
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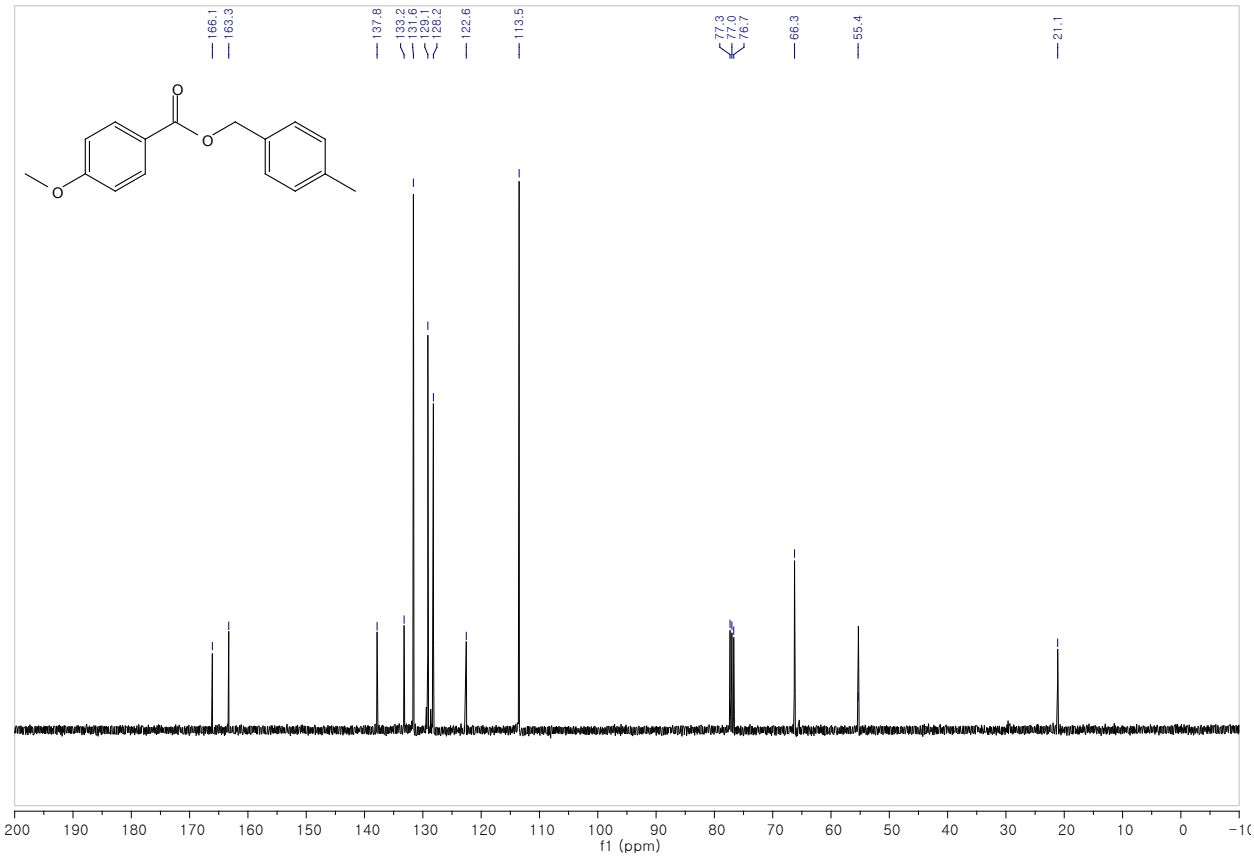
1.91
1.79
1.89
1.99
3.00
2.81
f1 (ppm)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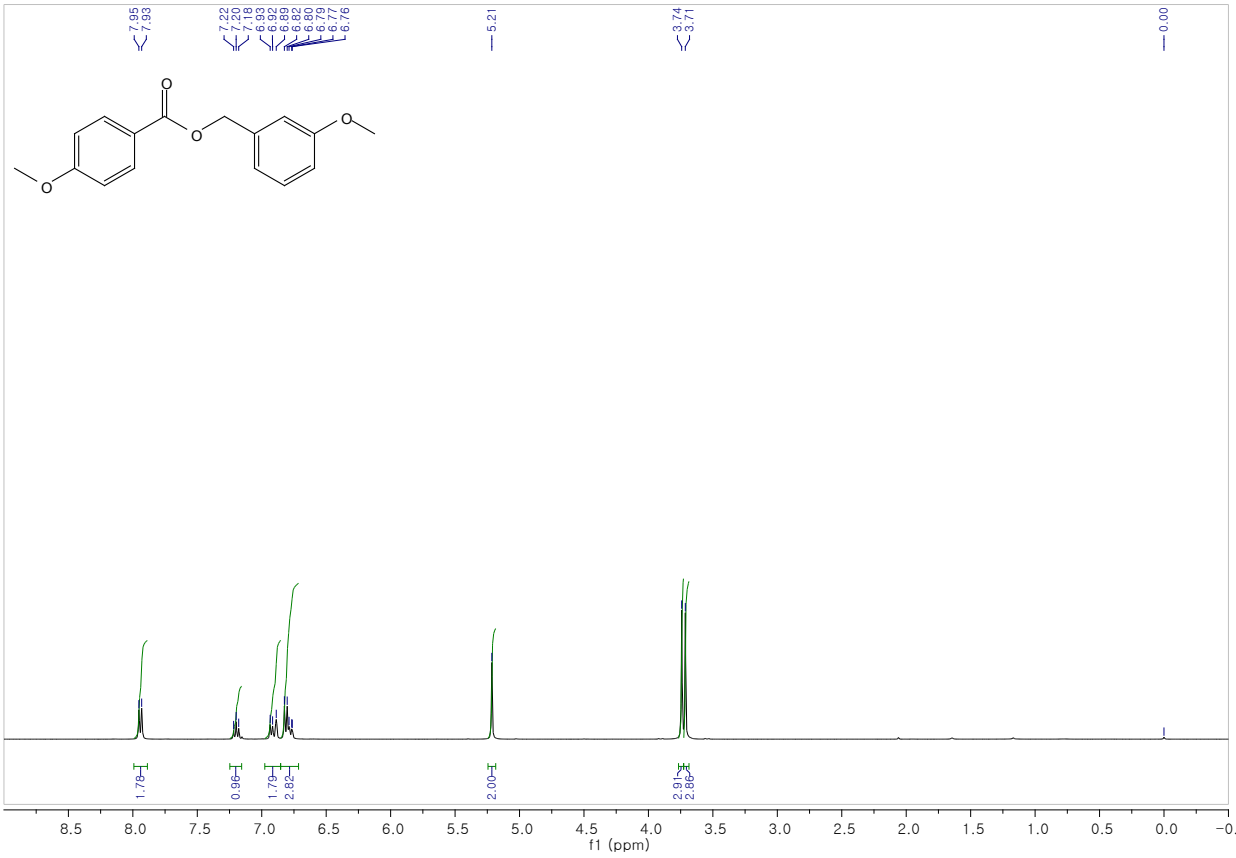
163.3
137.8
133.2
131.6
129.1
128.2
122.6
113.5
77.3
77.0
76.7
66.3
55.4
21.1
O
O
O
f1 (ppm)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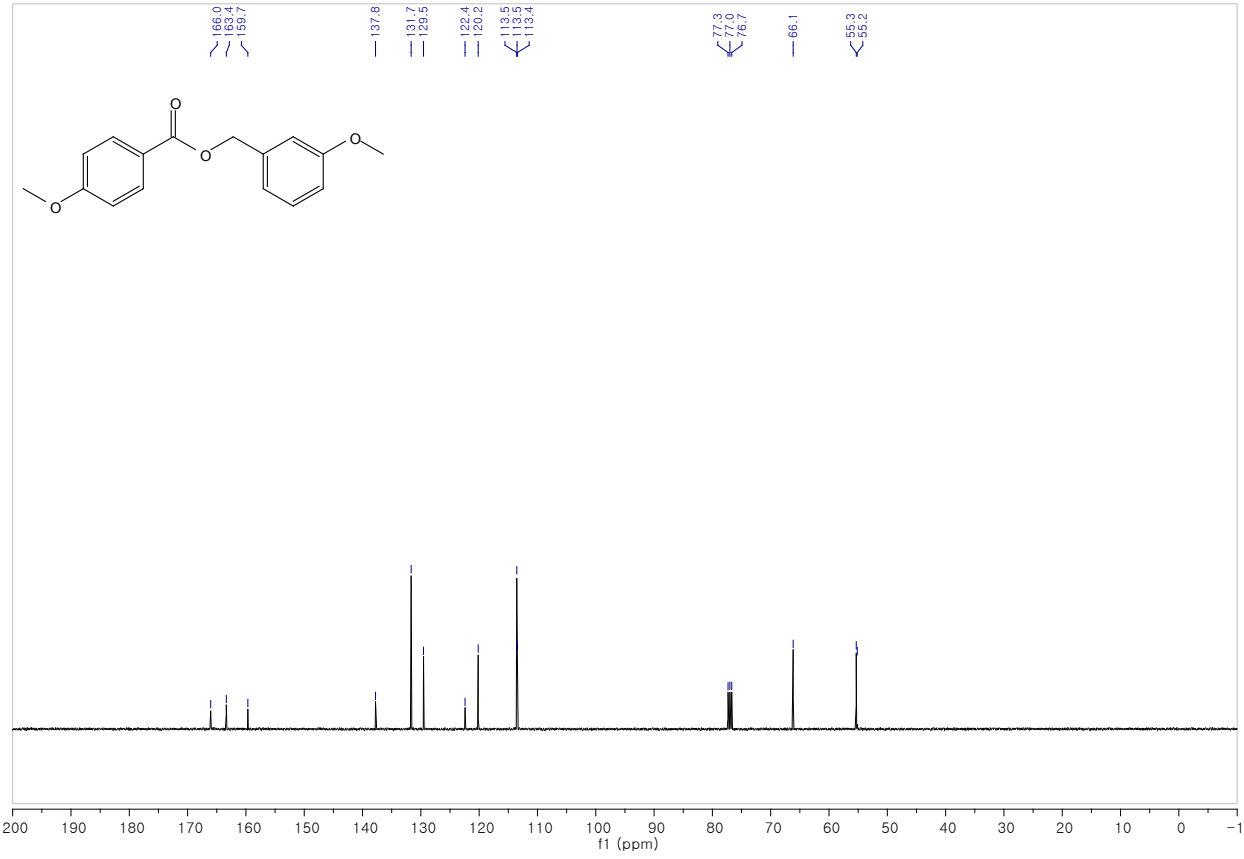
7.93
7.22
7.20
7.18
6.93
6.92
6.89
6.82
6.80
6.79
6.77
6.76
5.21
3.74
3.71
0.00
1.78
0.96
1.79
2.82
2.00
2.91
2.86
f1 (ppm)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159.7
137.8
131.7
129.5
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120.2
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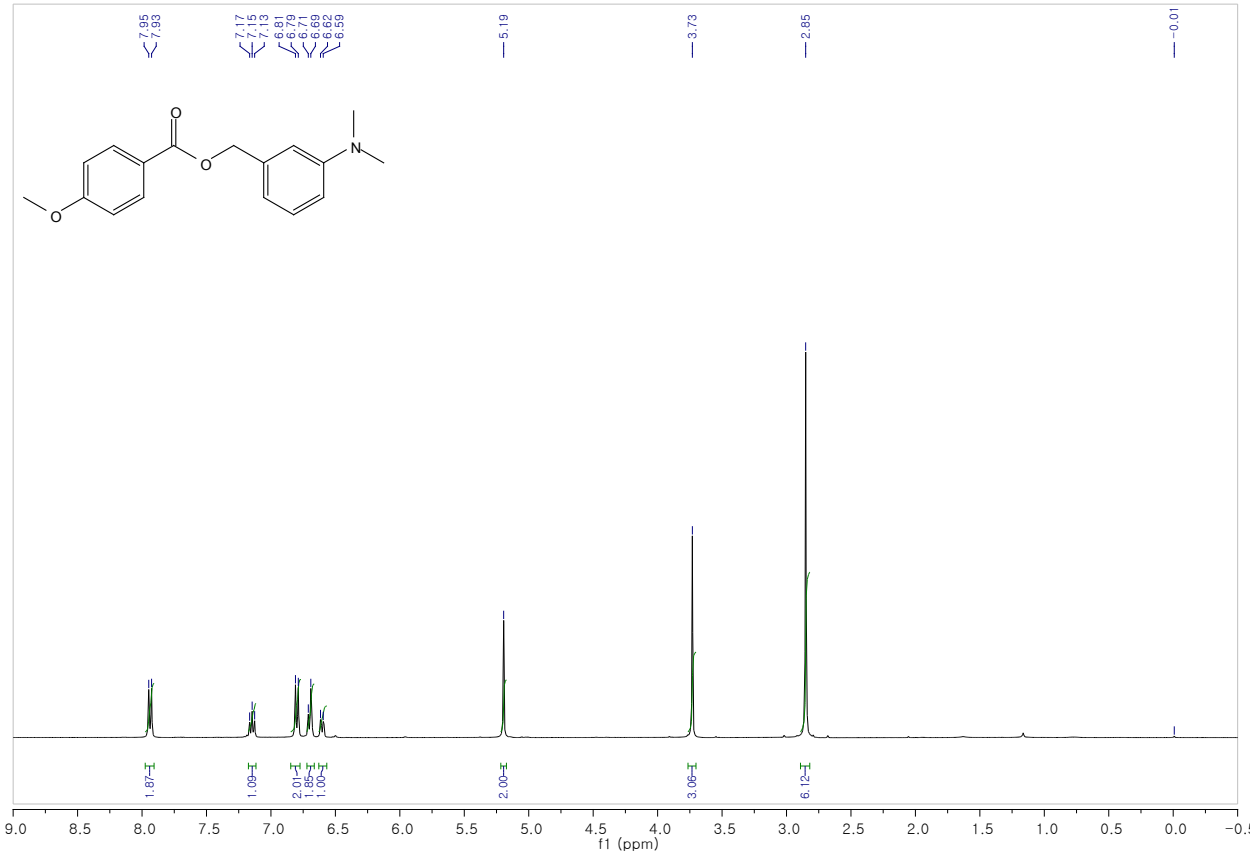
113.5
113.4
77.3
77.0
76.7
66.1
55.3
55.2
f1 (ppm)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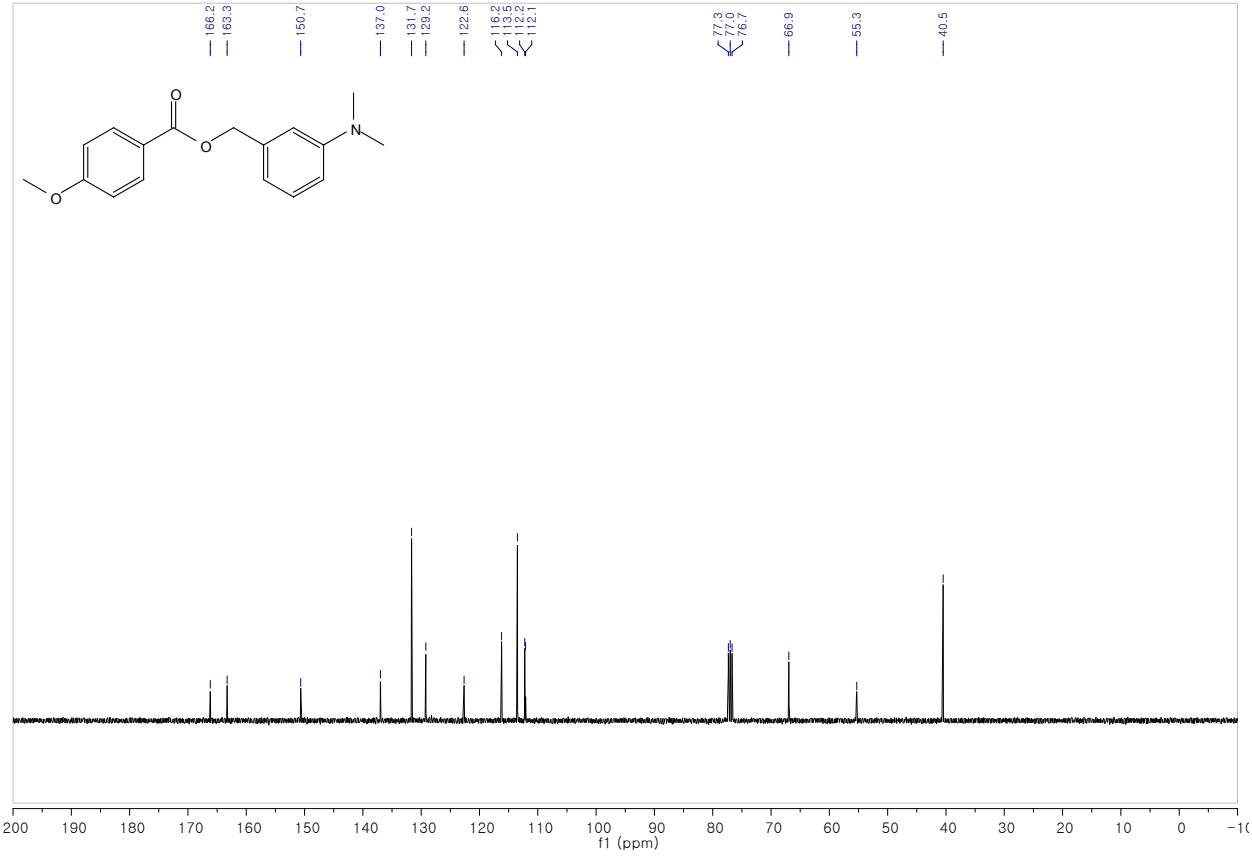
7.15
7.13
6.81
6.79
6.71
6.69
6.62
6.59
5.19
3.73
2.85
-0.01
1.87
1.09
2.01
1.85
1.00
2.00
3.06
6.12
O
O
O
N
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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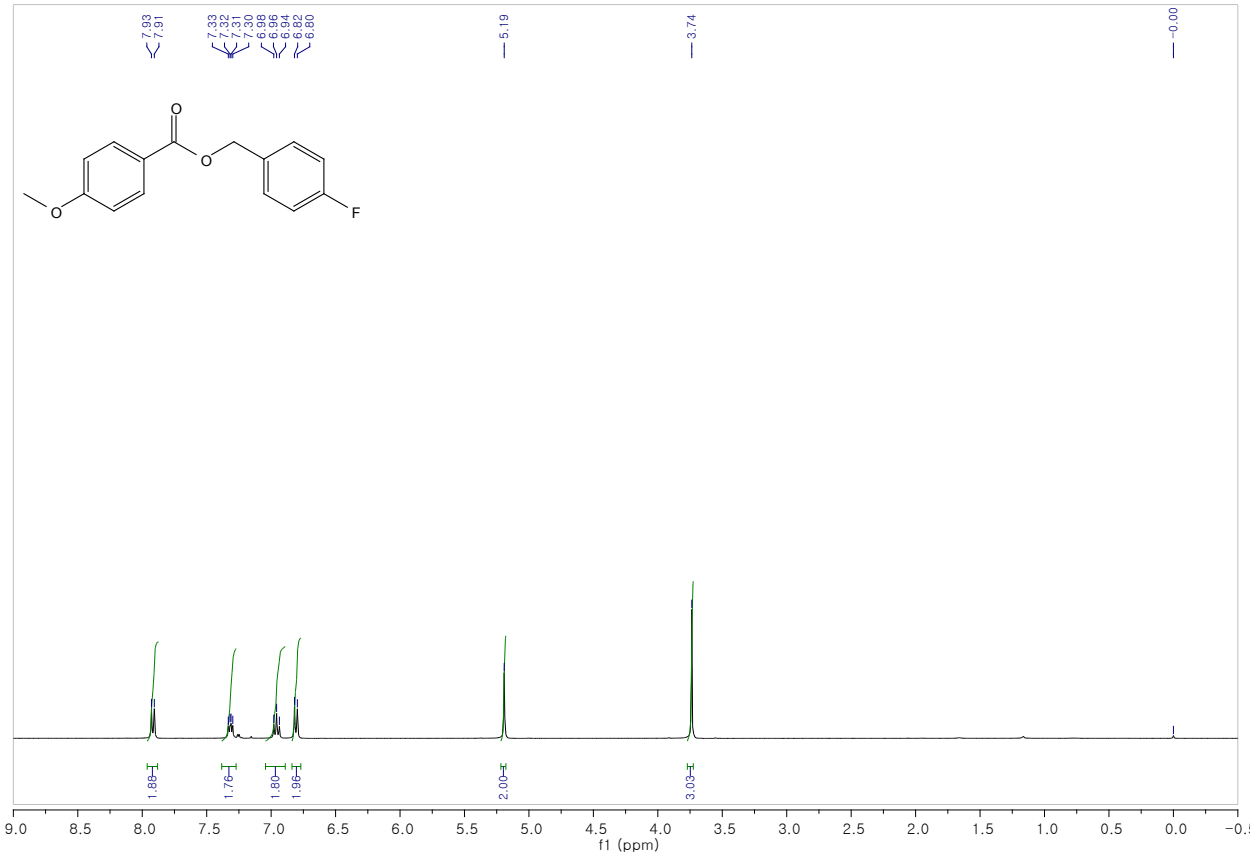
163.3
150.7
137.0
131.7
129.2
122.6
116.2
113.5
112.2
112.1
77.3
77.0
76.7
66.9
55.3
40.5
O
O
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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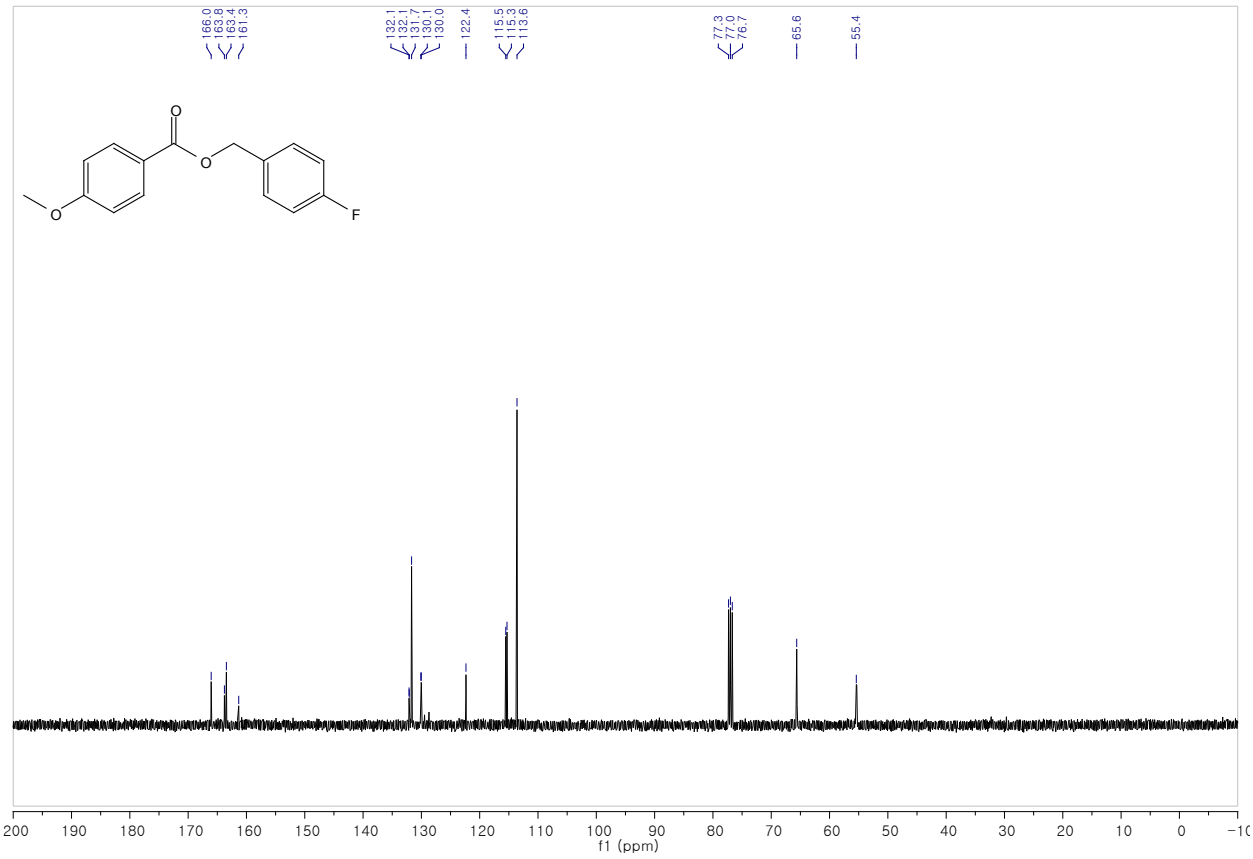
7.91
7.33
7.32
7.31
7.30
6.98
6.96
6.94
6.82
6.80
5.19
3.74
0.00
O
O
O
F
1.86
1.76
1.80
1.96
2.00
3.03
f1 (ppm)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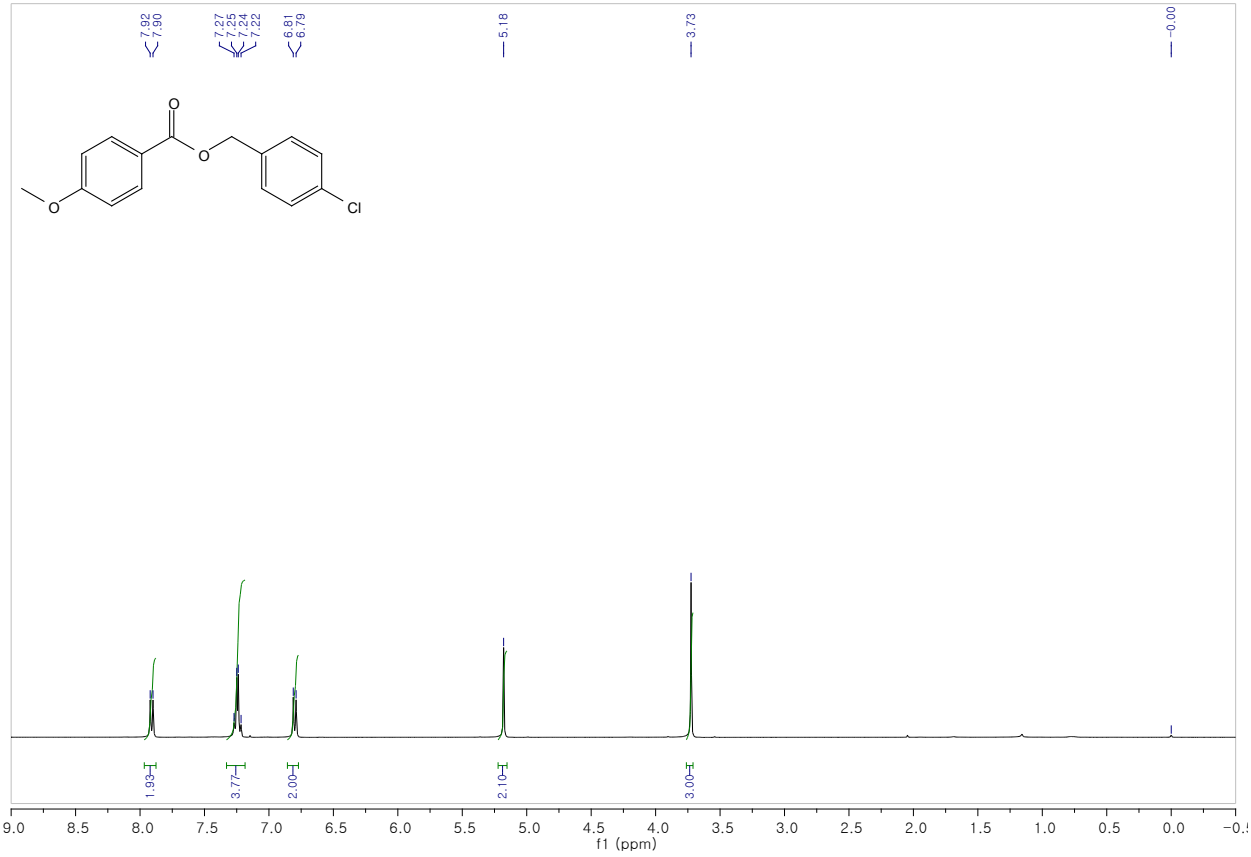
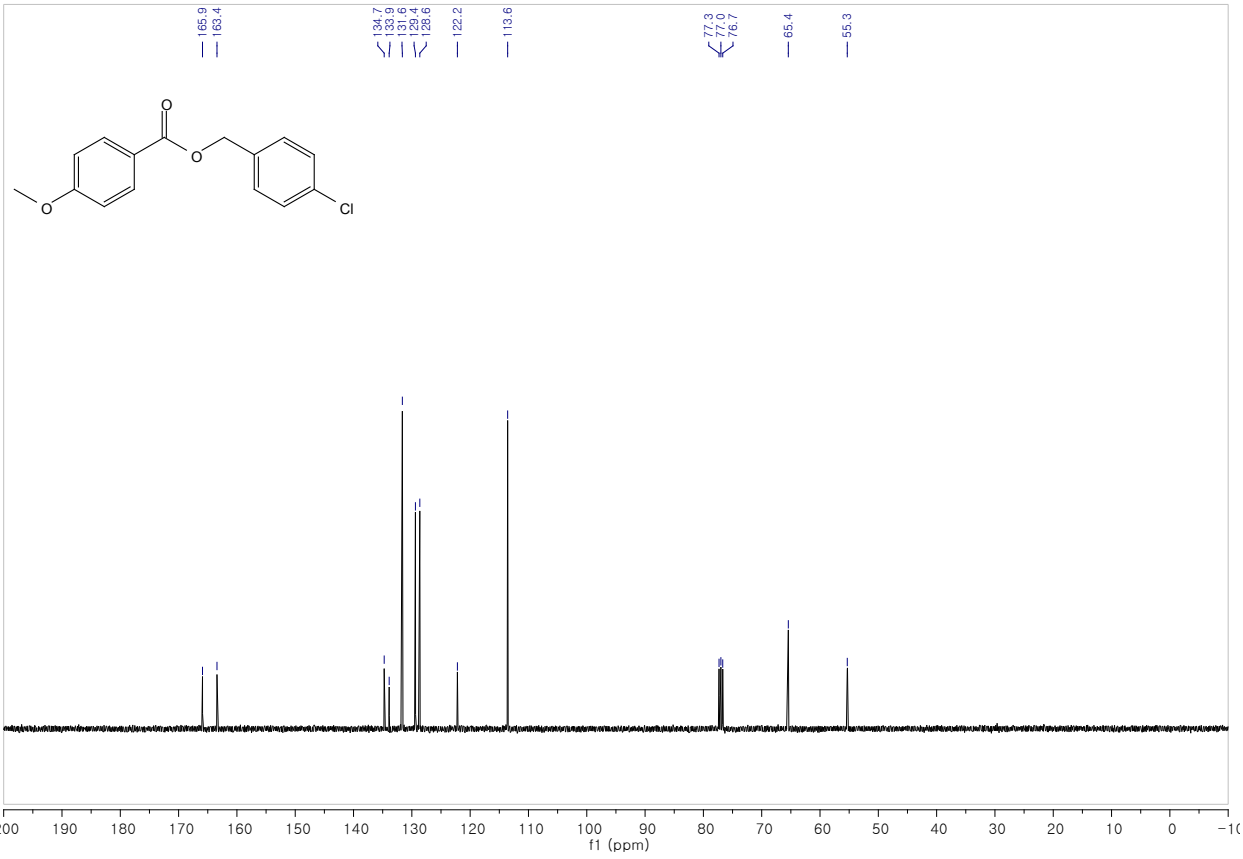
163.8
163.4
161.3
132.1
132.1
131.7
130.1
130.0
122.4
115.5
115.3
113.6
77.3
77.0
76.7
65.6
55.4
O
O
O
F
f1 (ppm)


7.92
7.90
7.27
7.25
7.24
7.22
6.81
6.79
5.18
3.73
0.00
O
O
O
Cl
1.93
3.77
2.00
2.10
3.00
f1 (ppm)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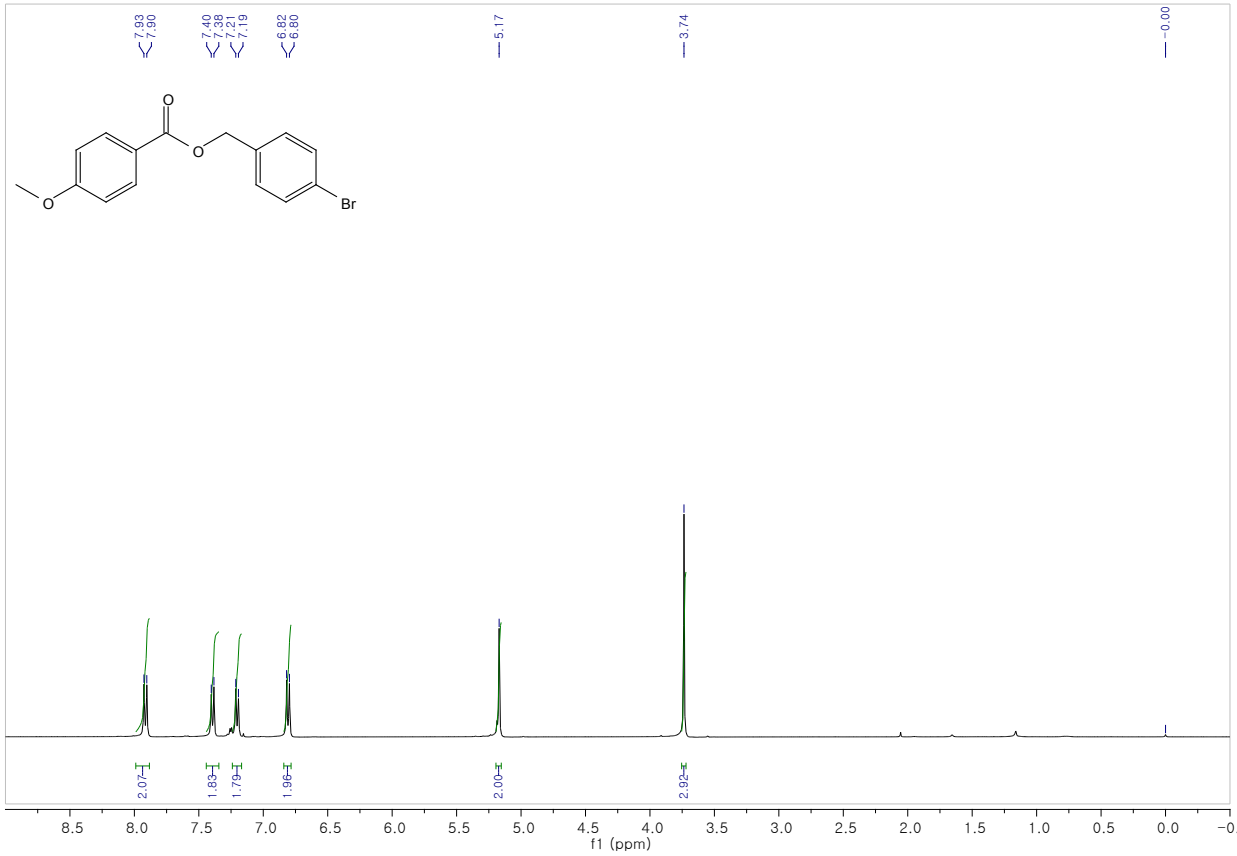
163.4
134.7
133.9
131.6
129.4
128.6
122.2
113.6
77.3
77.0
76.7
65.4
55.3
O
O
O
Cl
f1 (ppm)


7.93
7.90
7.40
7.38
7.21
7.19
6.82
6.80
5.17
3.74
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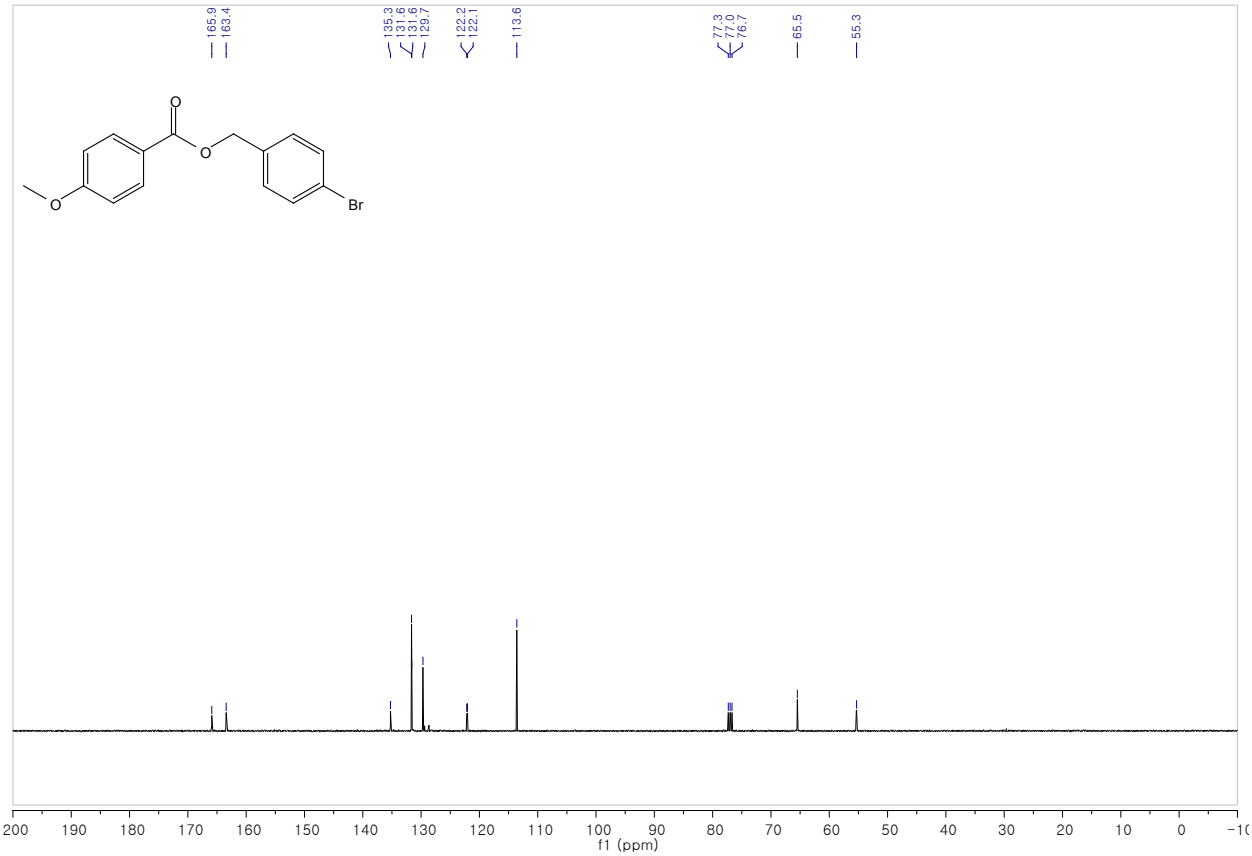
O
O
O
Br
2.07
1.83
1.79
1.96
2.00
2.92
f1 (ppm)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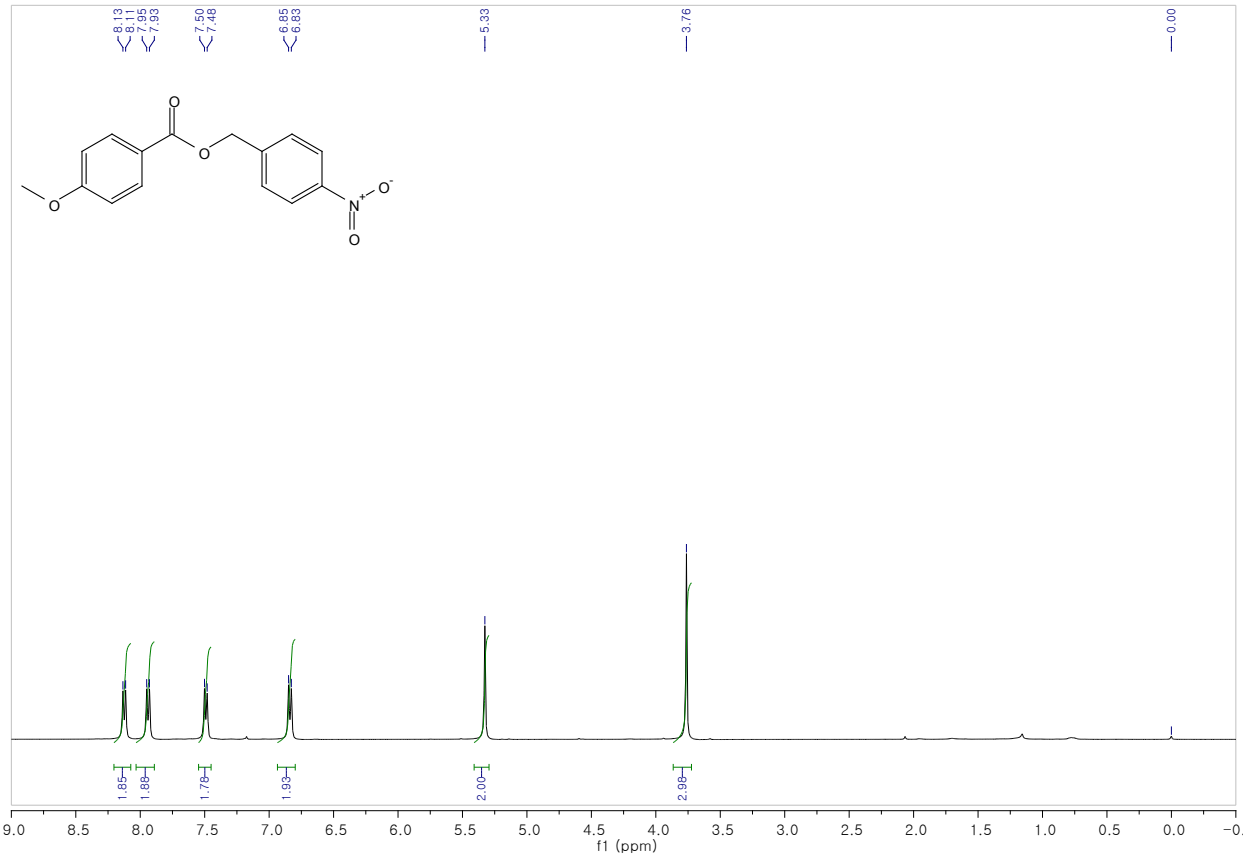
163.4
135.3
131.6
129.7
122.2
122.1
113.6
77.3
77.0
76.7
65.5
55.3
O
O
O
Br
f1 (ppm)


8.13
8.11
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7.50
7.48
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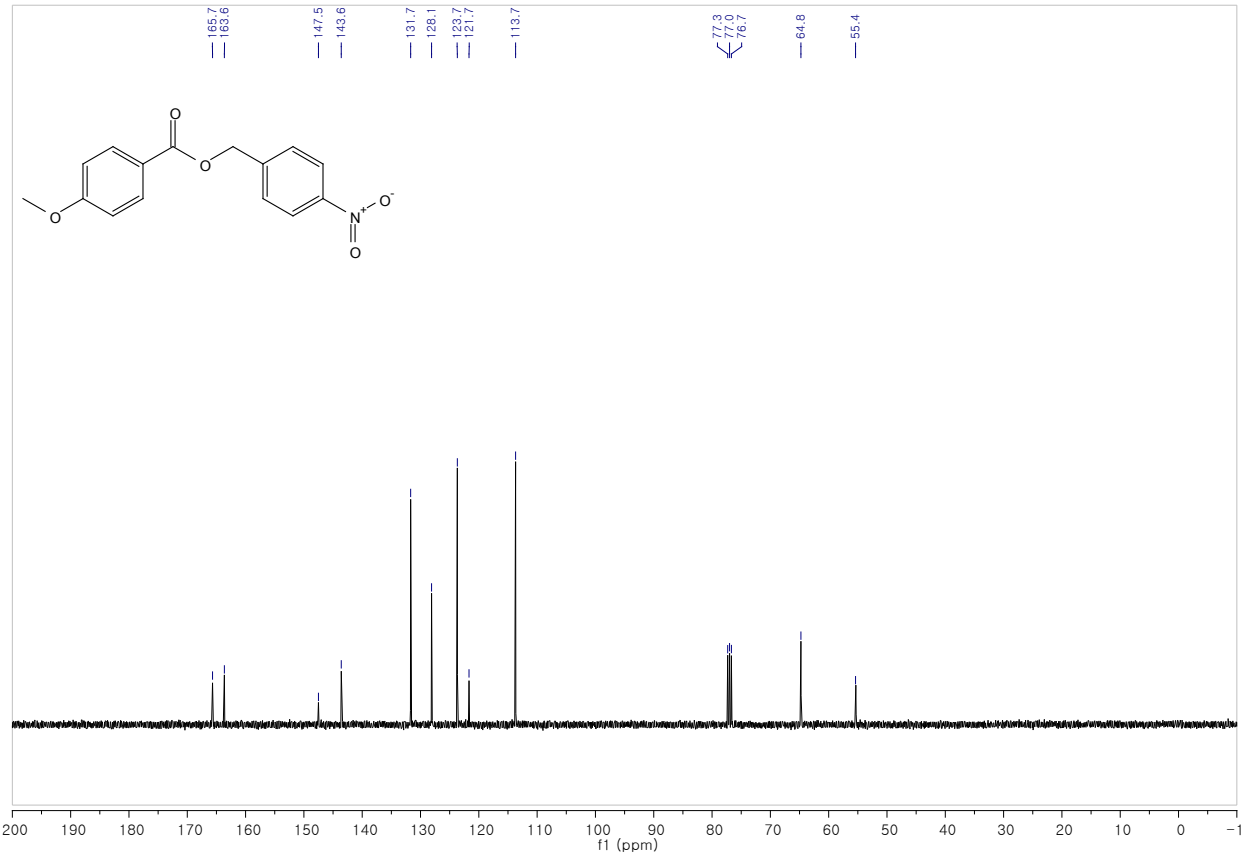
6.83
5.33
3.76
0.00
1.85
1.88
1.78
1.93
2.00
2.98
f1 (ppm)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163.6
147.5
143.6
131.7
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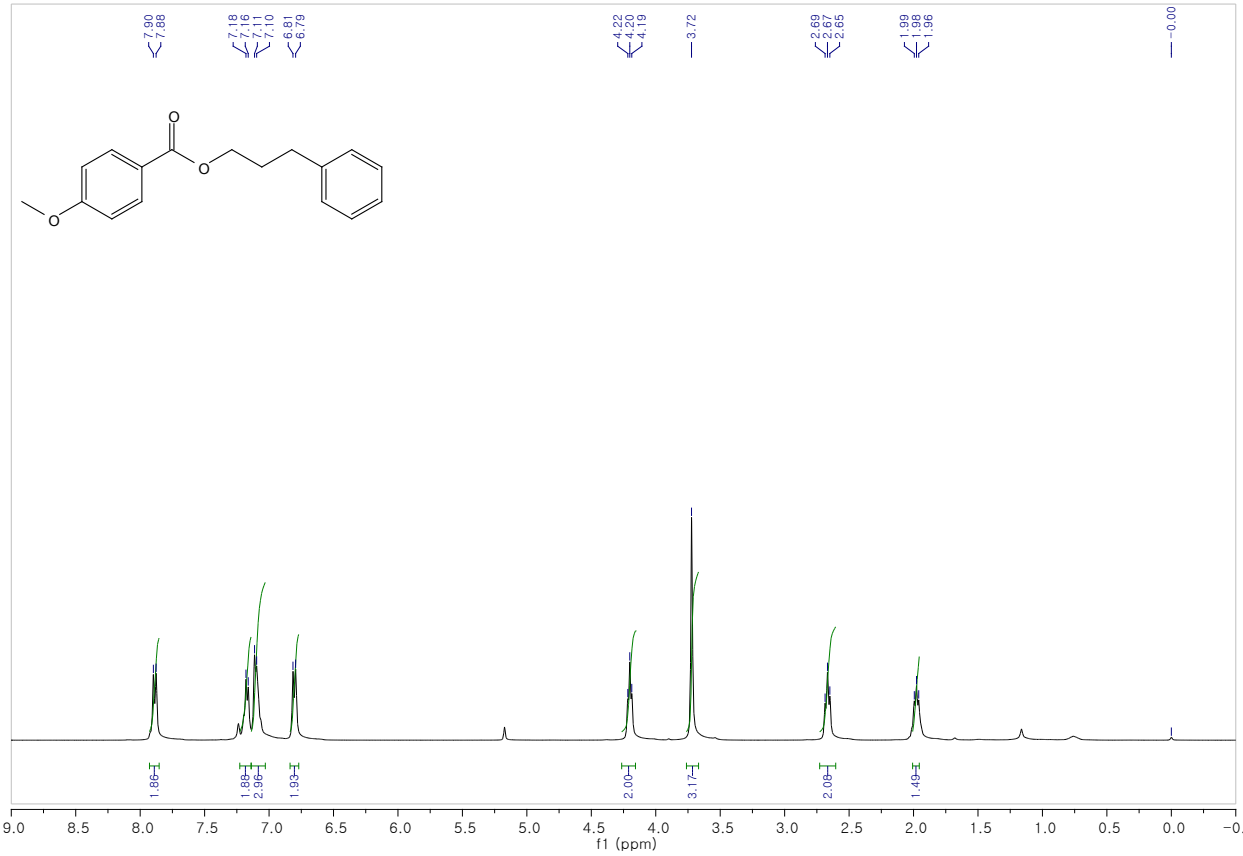
123.7
121.7
113.7
77.3
77.0
76.7
64.8
55.4
f1 (ppm)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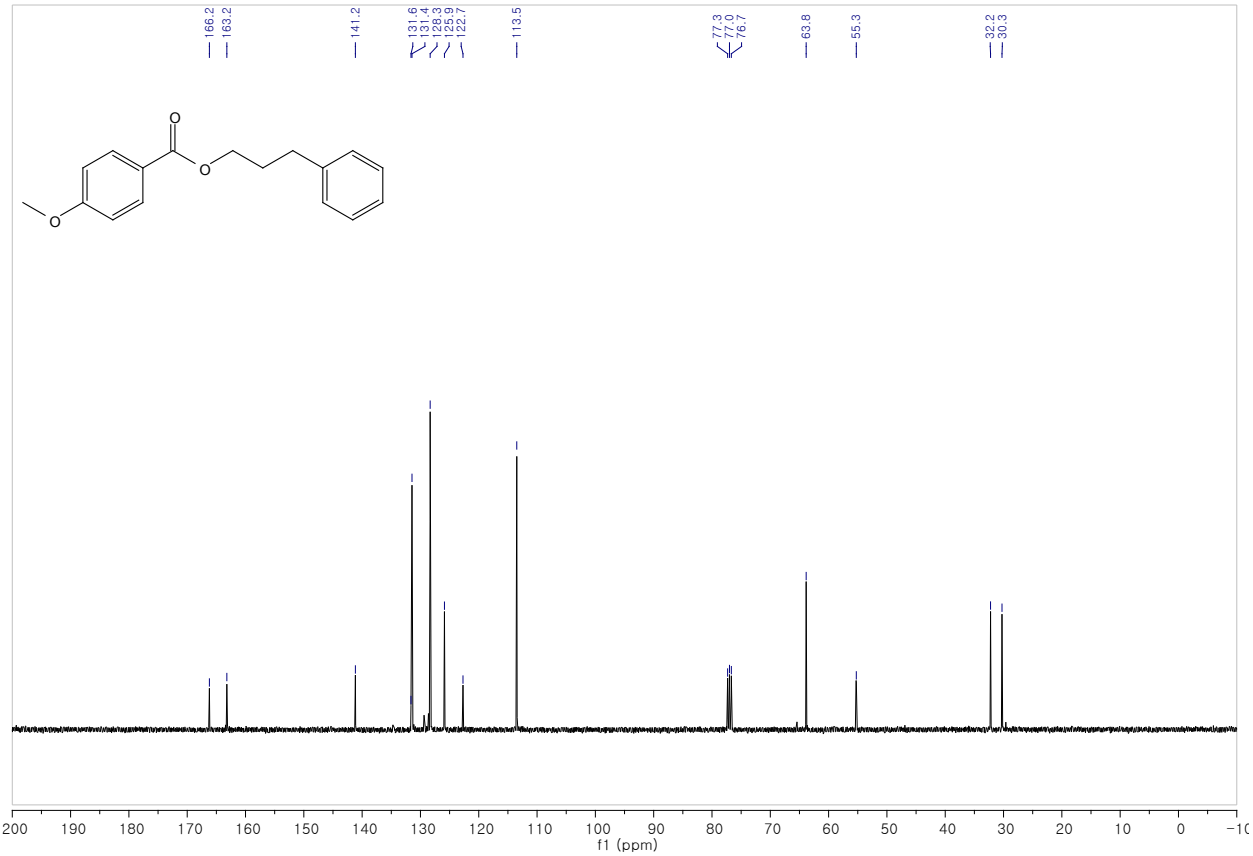
7.88
7.18
7.16
7.11
7.10
6.81
6.79
4.22
4.20
4.19
3.72
2.69
2.67
2.65
1.99
1.98
1.96
0.00
O
O
O
1.86
1.88
2.96
1.93
2.00
3.17
2.08
1.49
f1 (ppm)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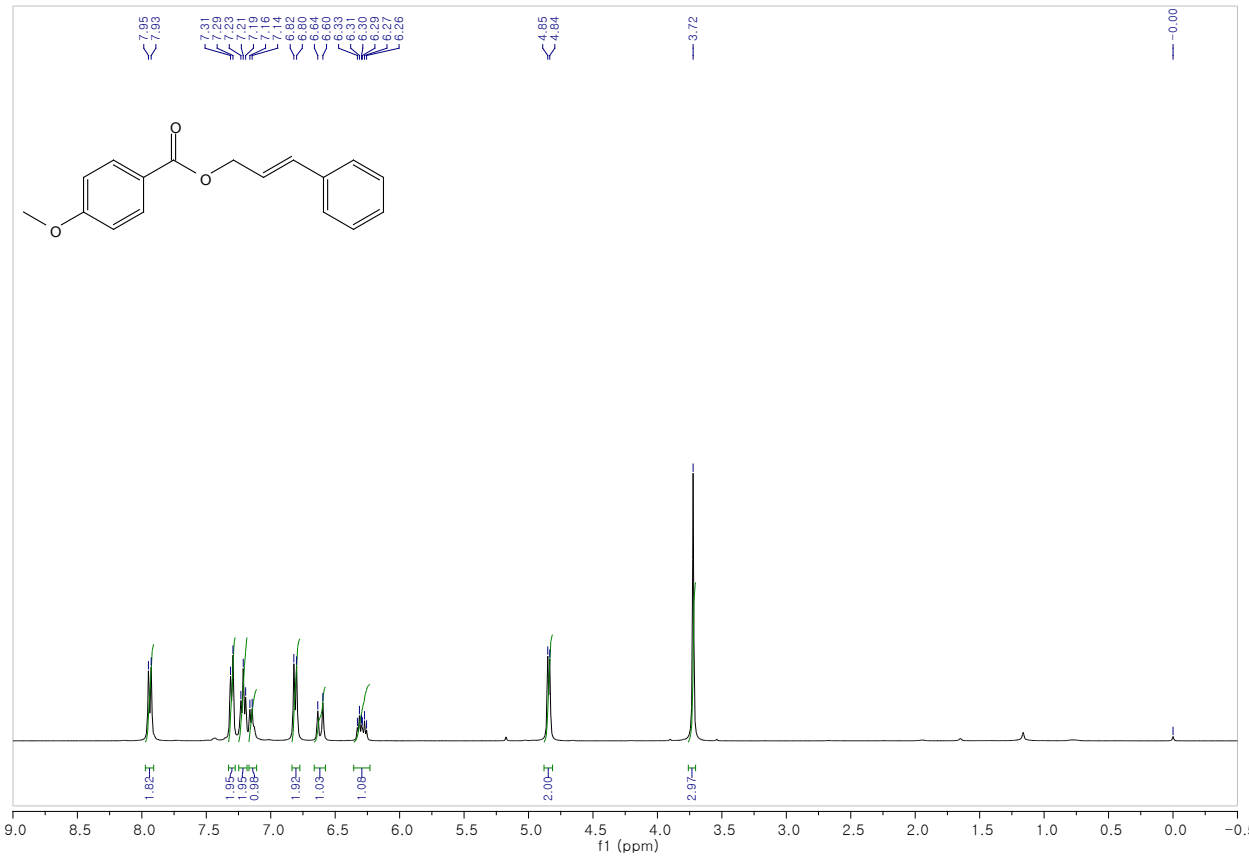
163.2
141.2
131.6
131.4
128.3
125.9
122.7
113.5
77.3
77.0
76.7
63.8
55.3
32.2
30.3
O
O
O
f1 (ppm)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7.31
7.29
7.23
7.21
7.19
7.16
7.14
6.82
6.80
6.64
6.60
6.33
6.31
6.30
6.29
6.27
6.26
4.85
4.84
3.72
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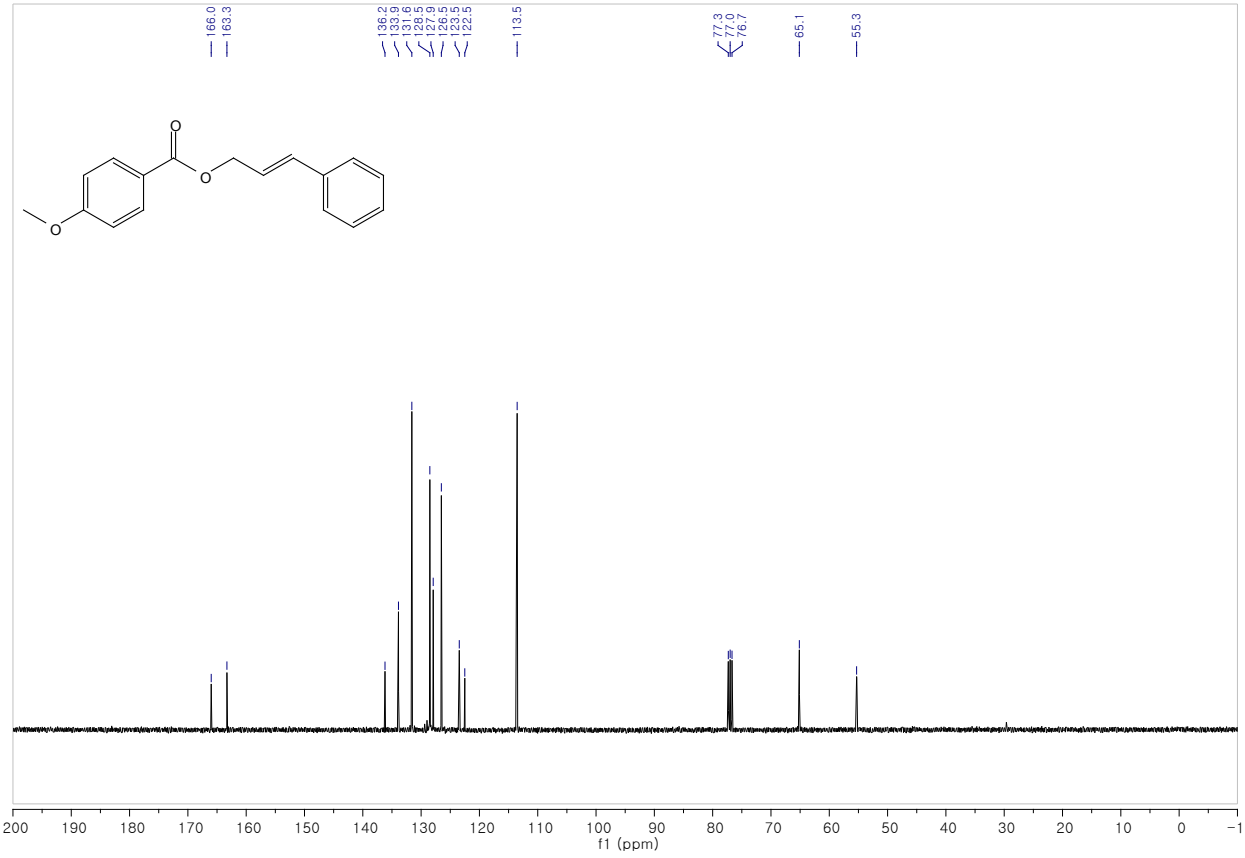
1.95
1.95
0.98
1.92
1.03
1.08
2.00
2.97
f1 (ppm)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163.3
136.2
133.9
131.6
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127.9
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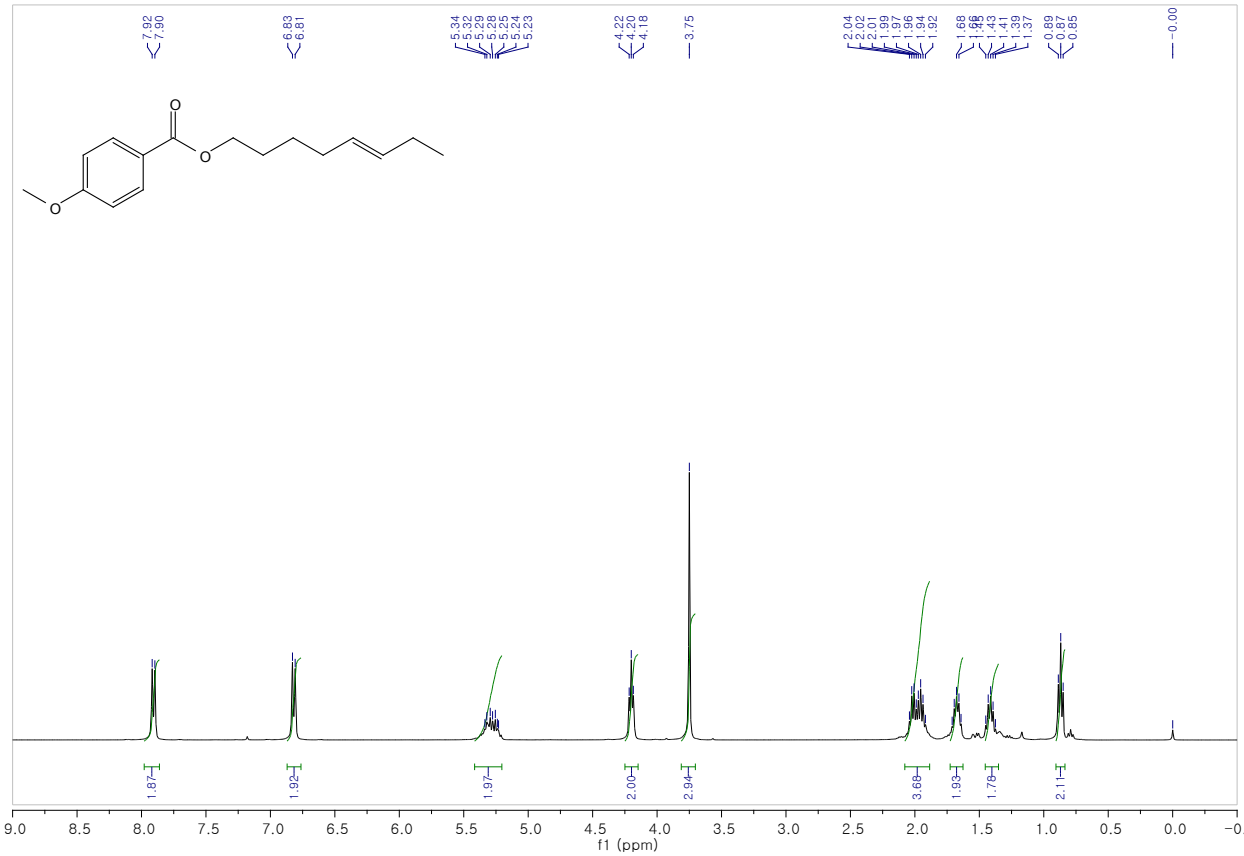
123.5
122.5
113.5
77.3
77.0
76.7
65.1
55.3
f1 (ppm)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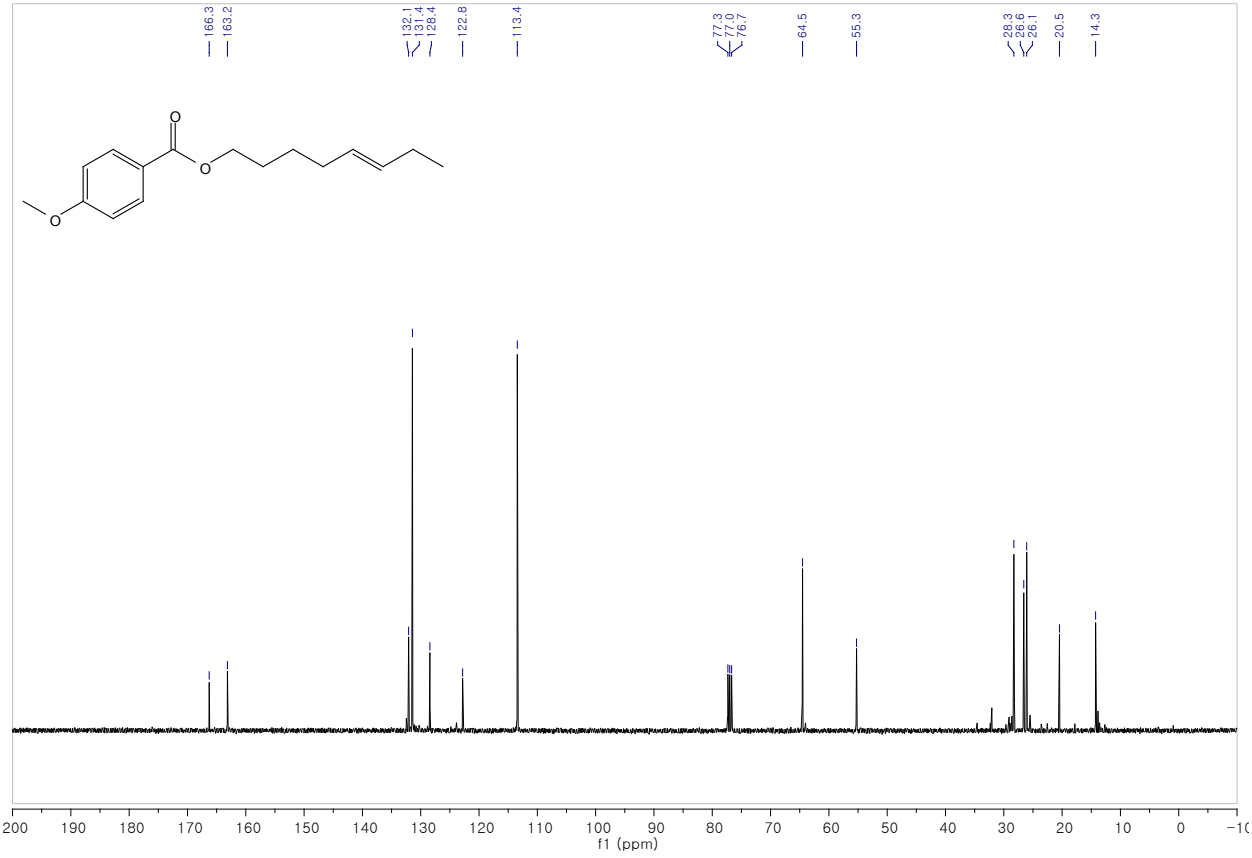
7.90
6.83
6.81
5.34
5.32
5.29
5.28
5.25
5.24
5.23
4.22
4.20
4.18
3.75
2.04
2.02
2.01
1.99
1.97
1.96
1.94
1.92
1.68
1.66
1.43
1.41
1.39
1.37
0.89
0.87
0.85
0.00
1.87
1.92
1.97
2.00
2.94
3.68
1.93
1.78
2.11
f1 (ppm)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131.4
128.4
122.8
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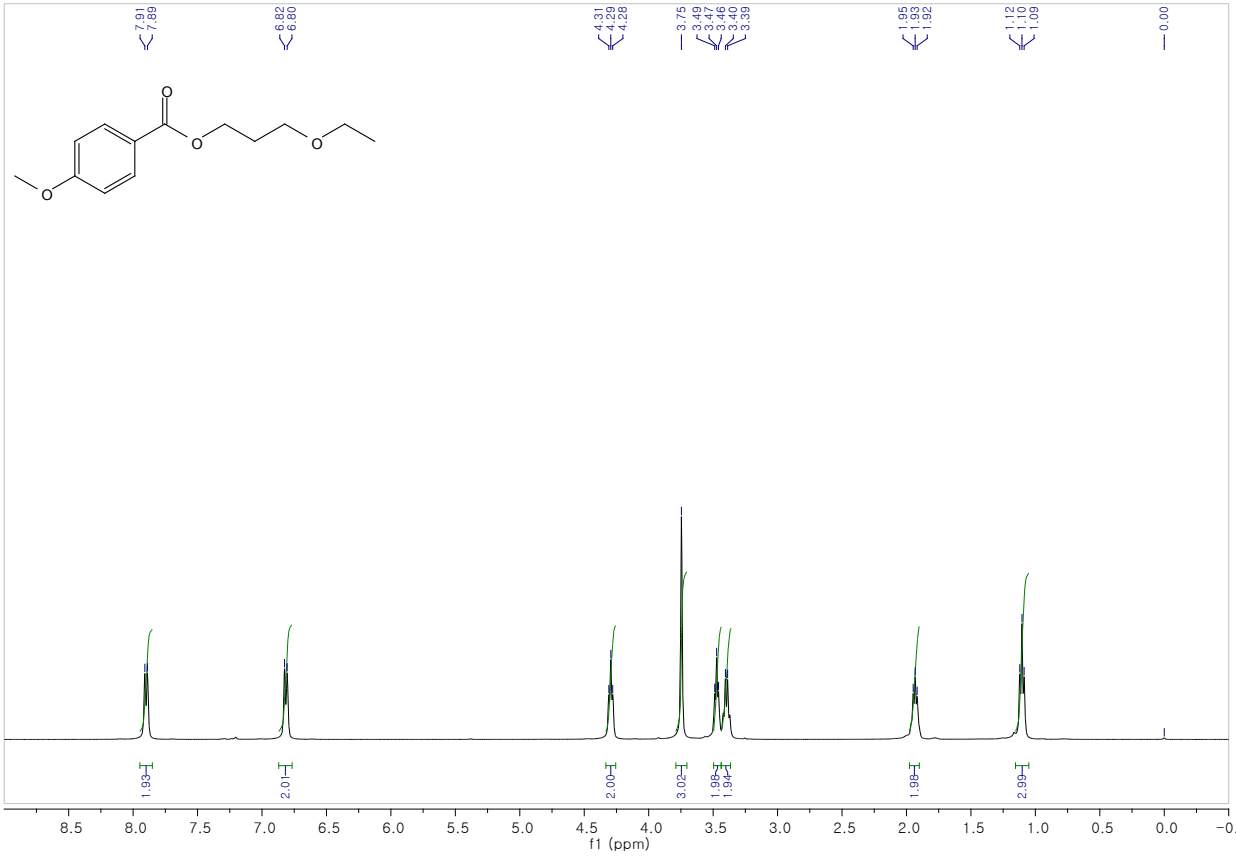
64.5
55.3
28.3
26.6
26.1
20.5
14.3
f1 (ppm)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6.80
4.31
4.29
4.28
3.75
3.49
3.47
3.46
3.40
3.39
1.95
1.93
1.92
1.12
1.10
1.09
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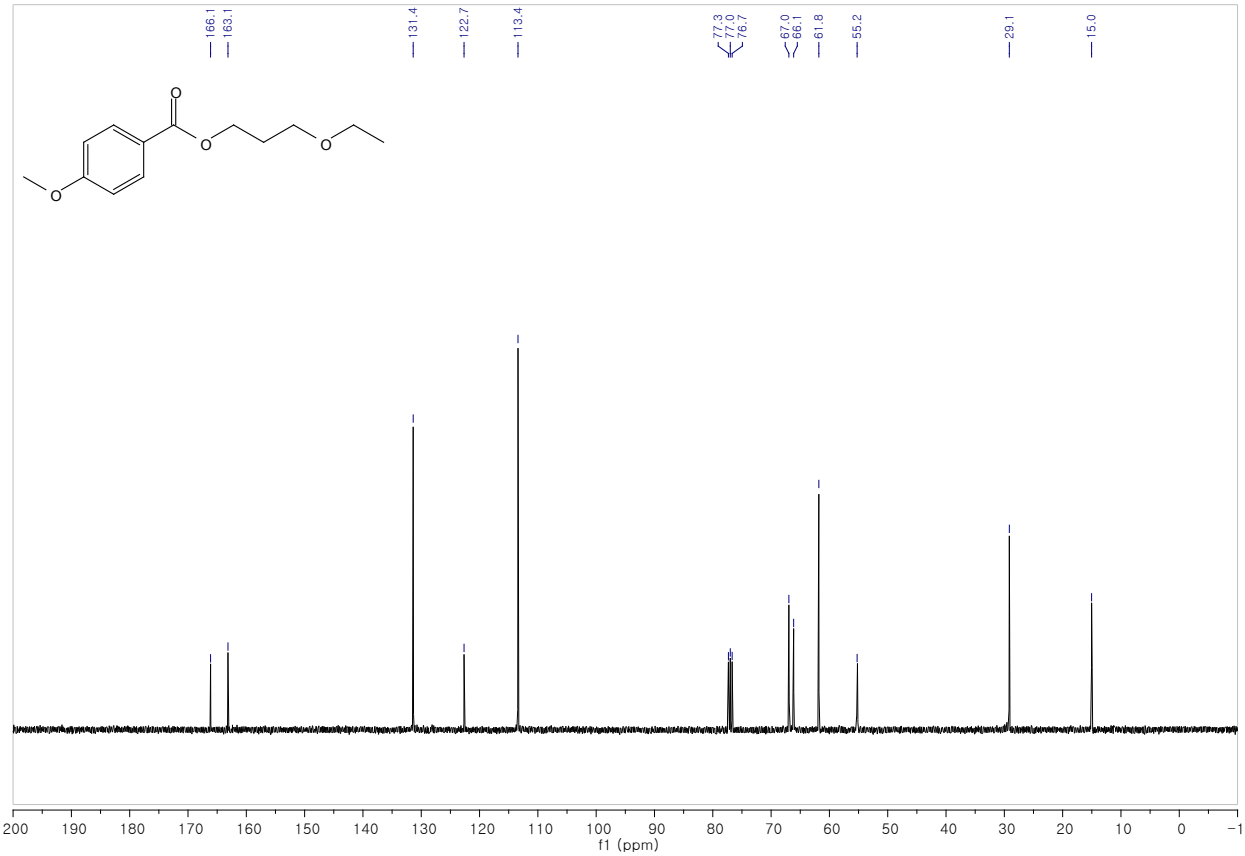
1.93
2.01
2.00
3.02
1.98
1.94
1.98
2.99
f1 (ppm)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131.4
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113.4
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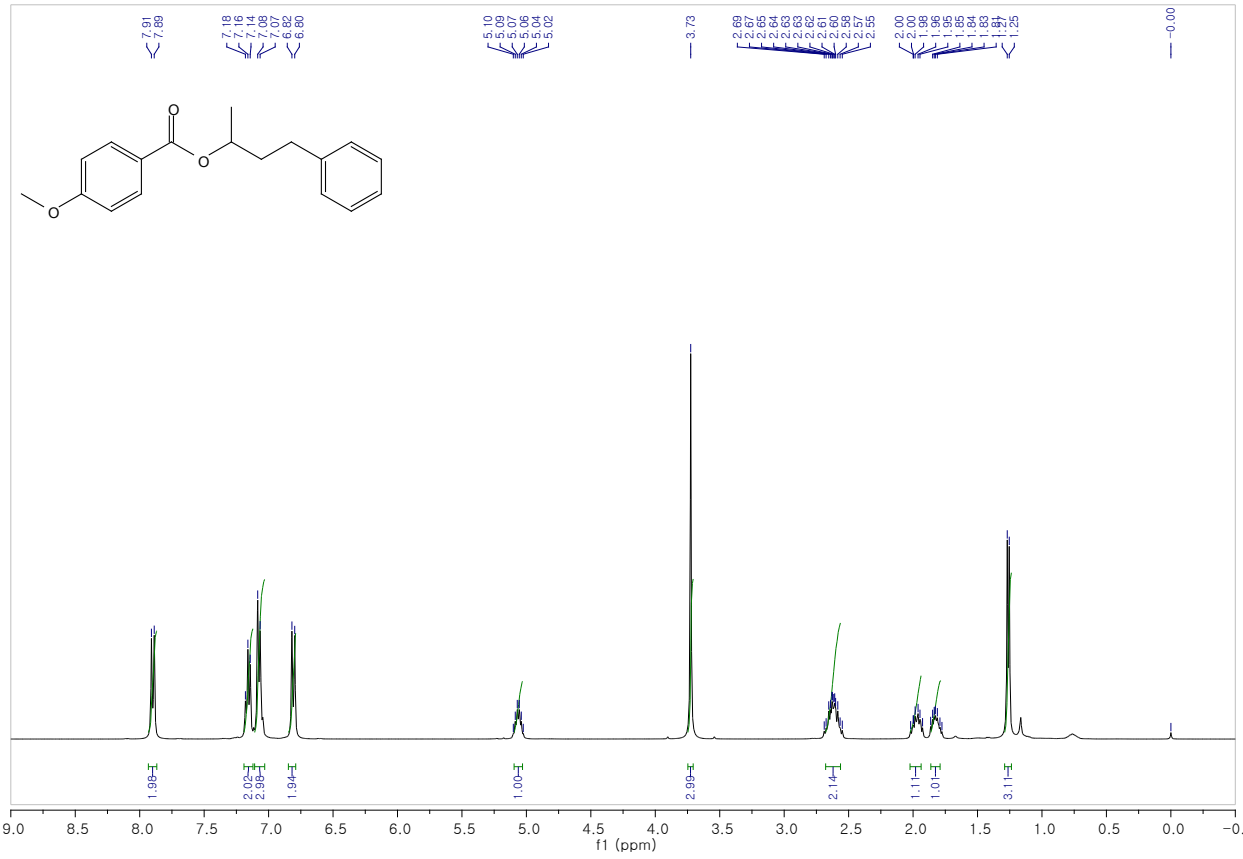
76.7
67.0
66.1
61.8
55.2
29.1
15.0
f1 (ppm)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7.89
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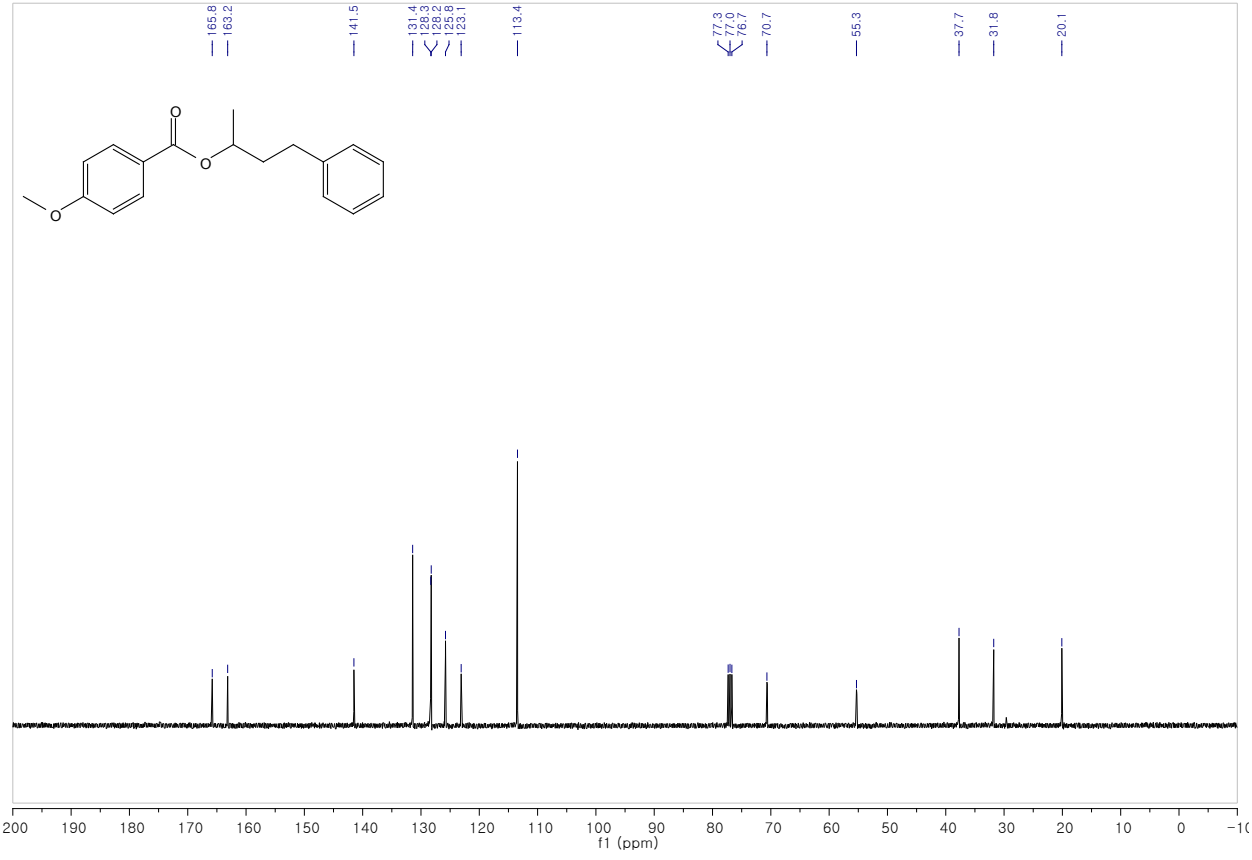
7.16
7.14
7.09
7.07
6.82
6.80
5.10
5.09
5.07
5.06
5.04
5.02
3.73
2.69
2.67
2.65
2.64
2.63
2.62
2.61
2.60
2.58
2.57
2.55
2.00
2.00
1.98
1.96
1.95
1.85
1.84
1.83
1.41
1.27
1.25
0.00
1.98
2.02
2.98
1.94
1.00
2.90
2.14
1.11
1.01
3.11
f1 (ppm)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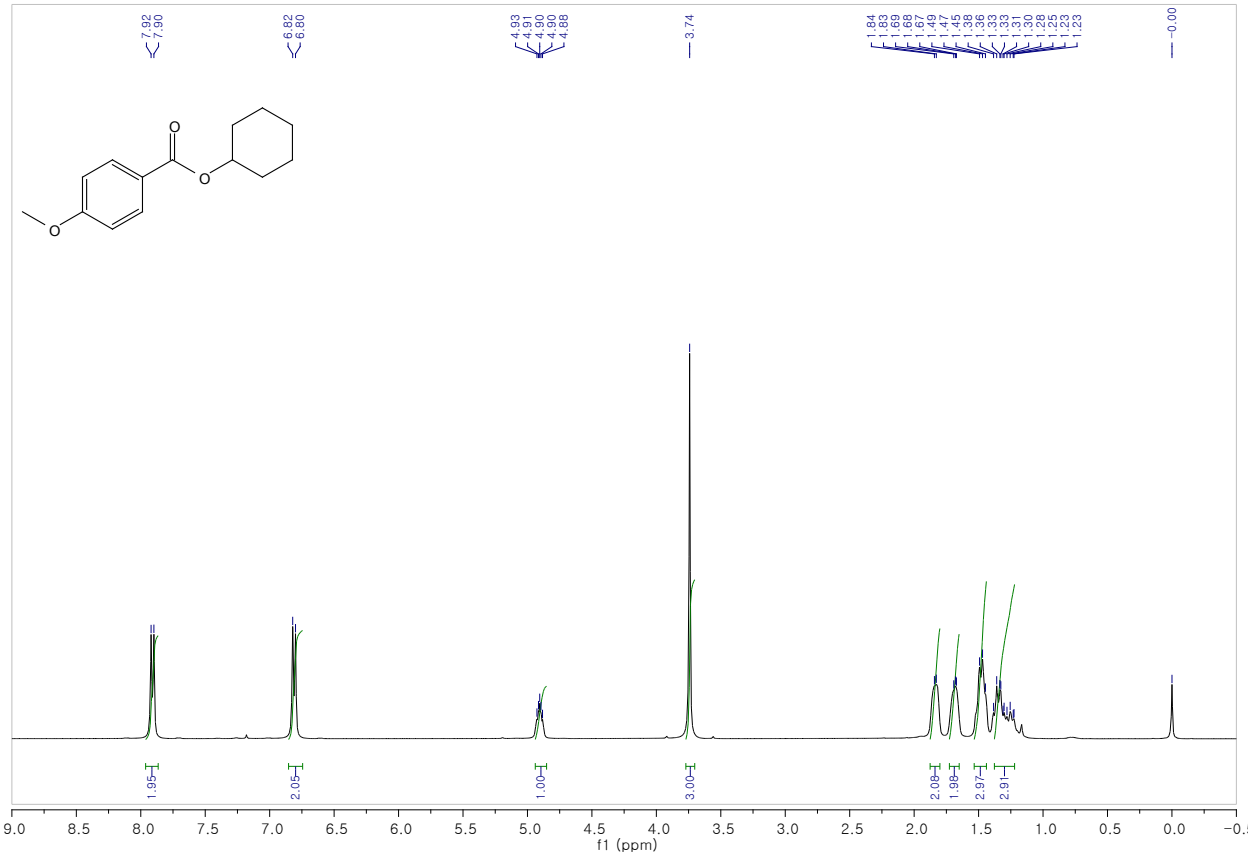
163.2
141.5
131.4
128.3
128.2
125.8
123.1
113.4
77.3
77.0
76.7
70.7
55.3
37.7
31.8
20.1
f1 (ppm)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7.90
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6.80
4.93
4.91
4.90
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4.88
3.74
1.84
1.83
1.68
1.68
1.67
1.49
1.47
1.45
1.38
1.36
1.33
1.33
1.31
1.30
1.28
1.25
1.23
1.23
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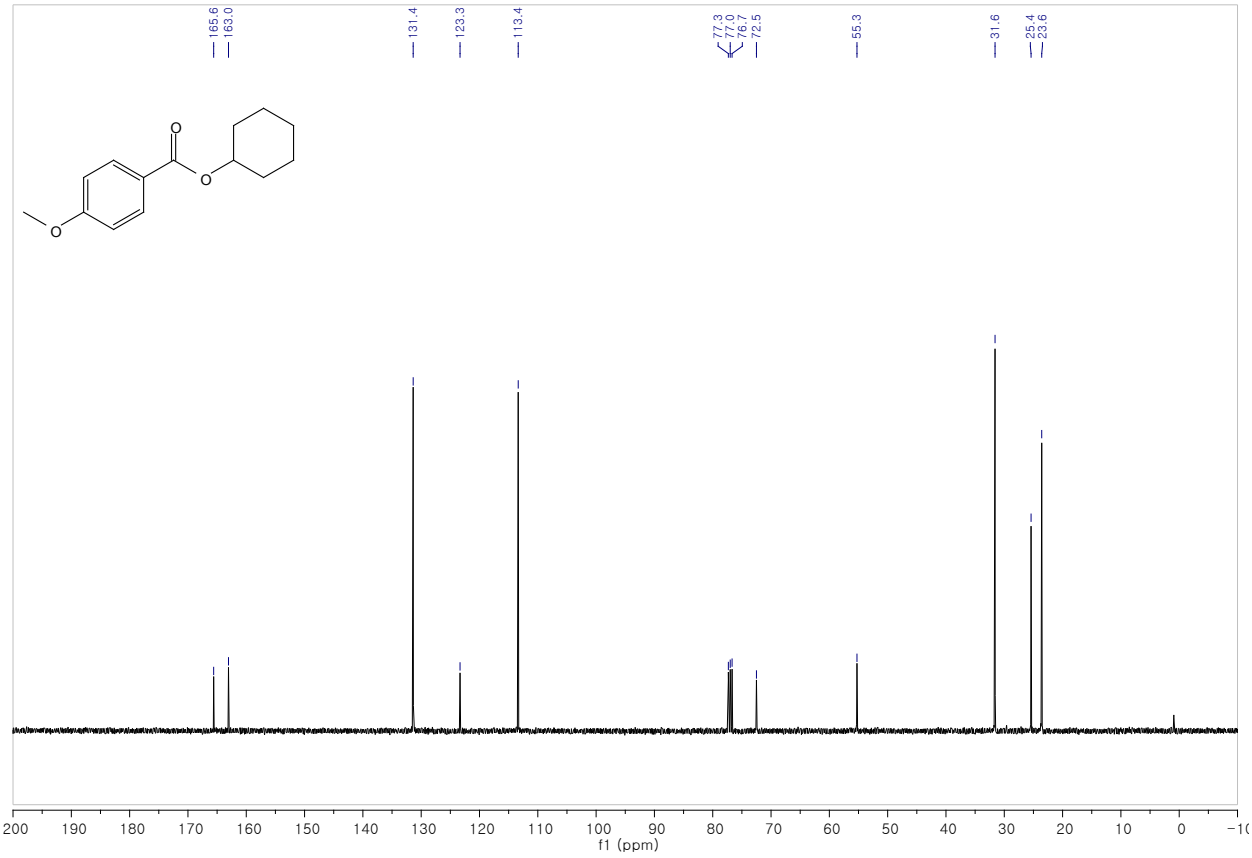
1.95
2.05
1.00
3.00
2.08
1.98
2.97
2.91
f1 (ppm)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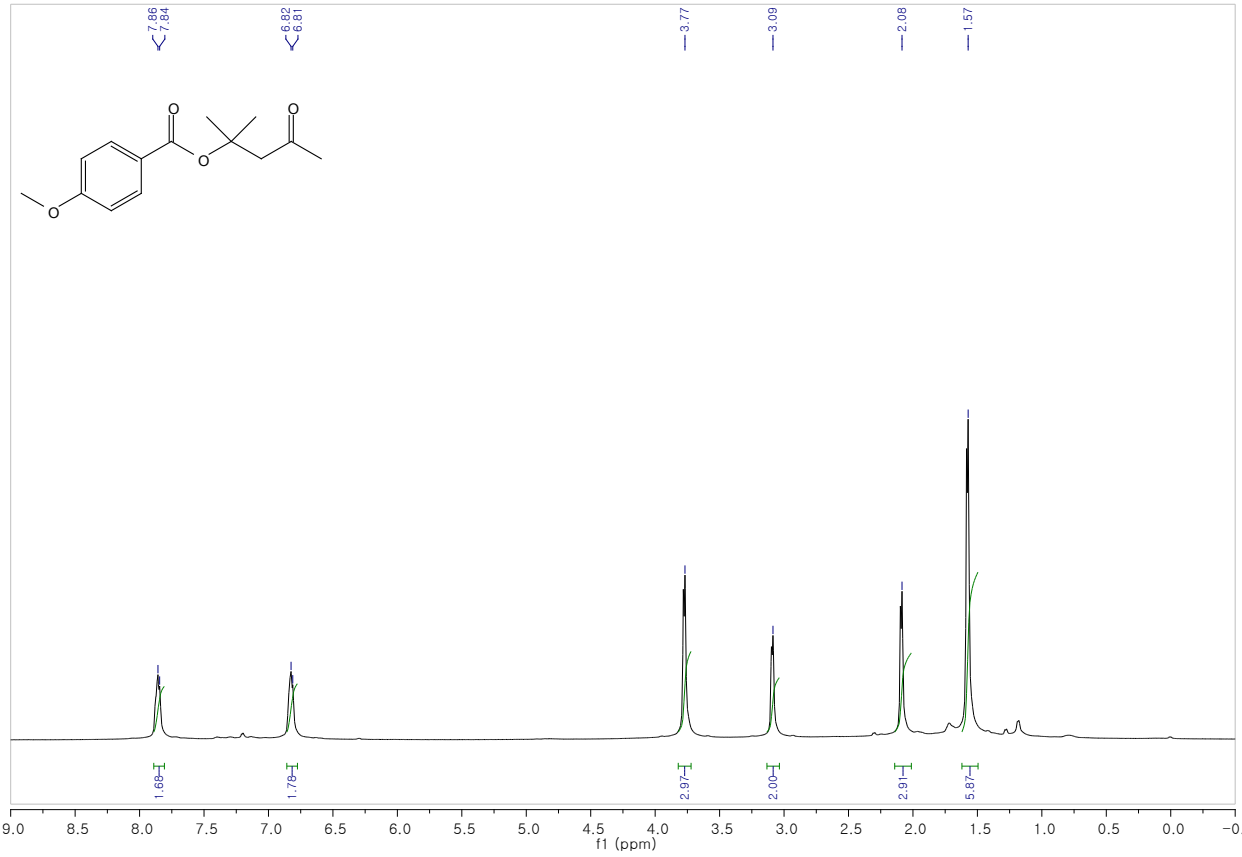
123.3
113.4
77.3
77.0
76.7
72.5
55.3
31.6
25.4
23.6
f1 (ppm)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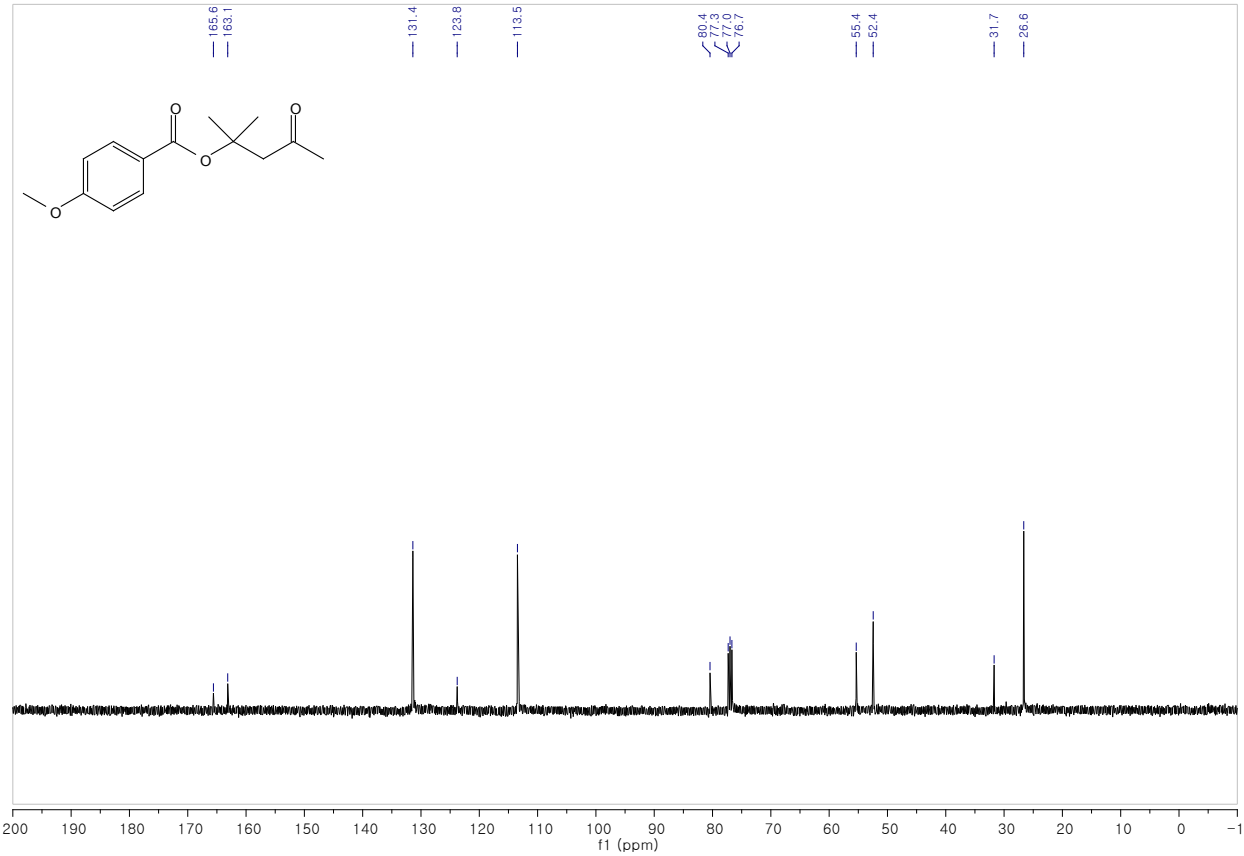
3.77
3.09
2.08
1.57
O
O
O
O
1.68
1.78
2.97
2.00
2.91
5.87
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


165.6
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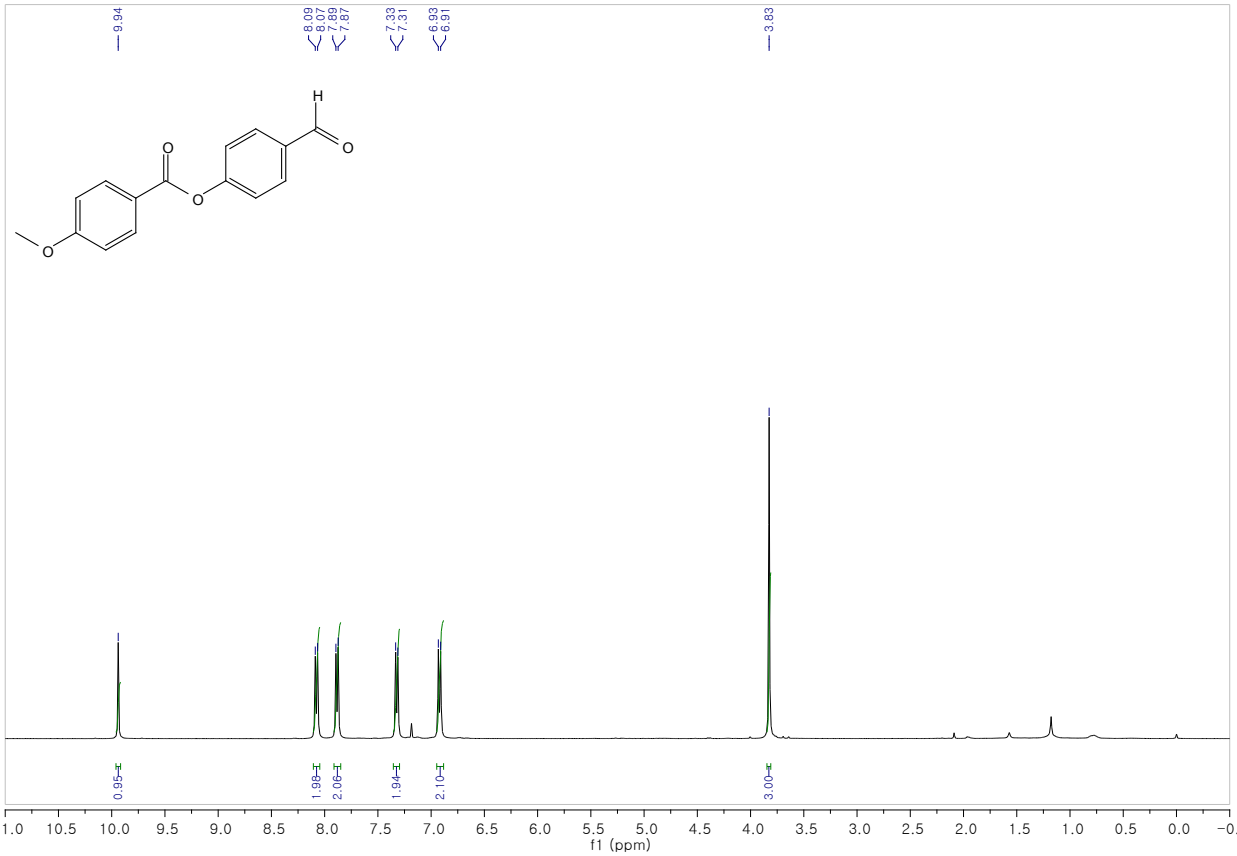
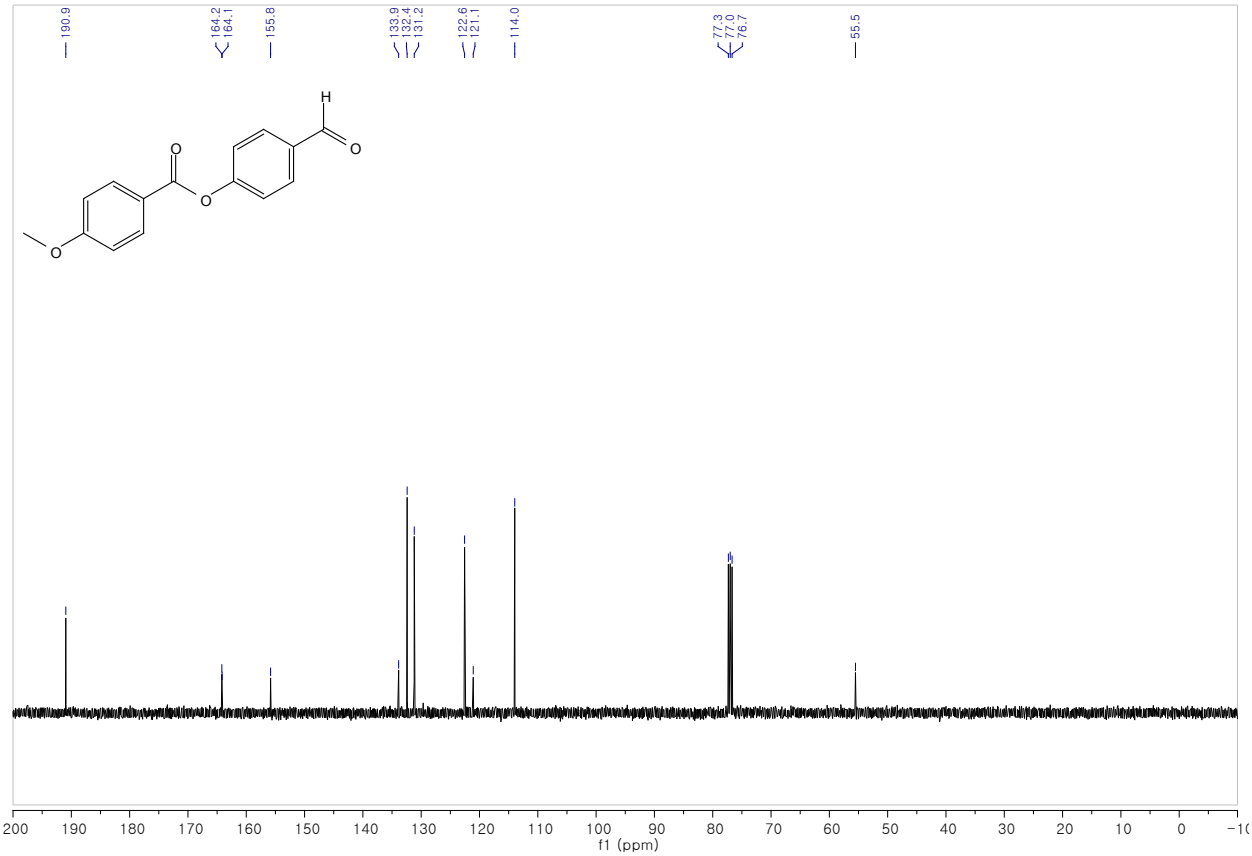
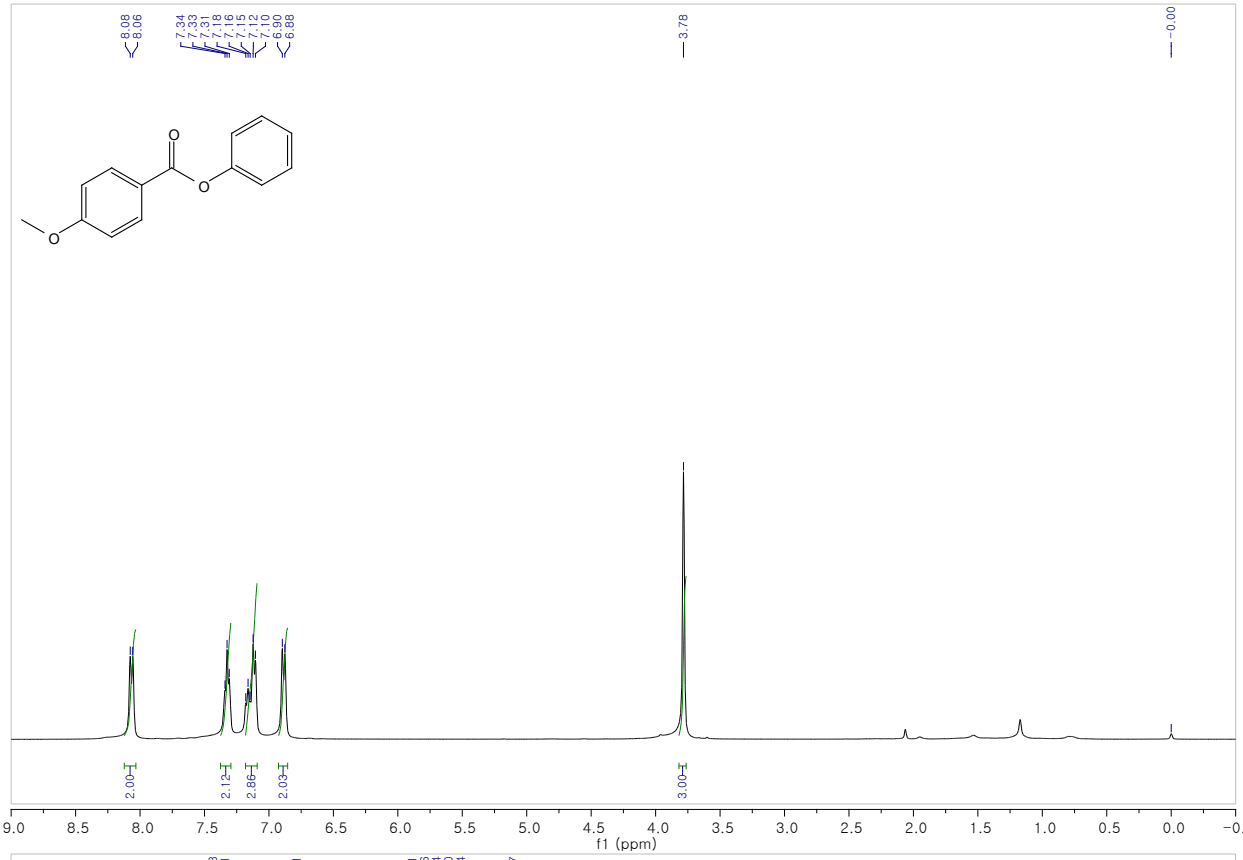
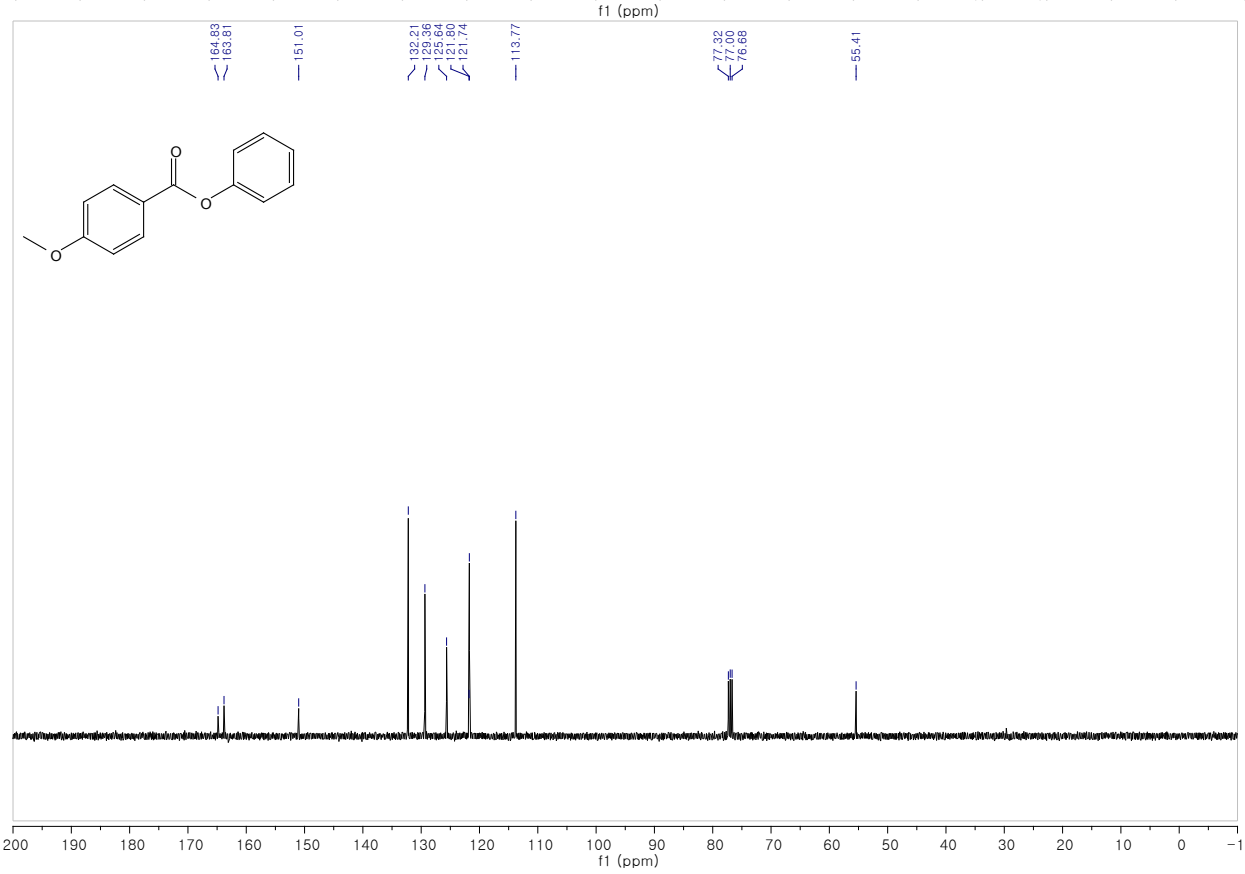
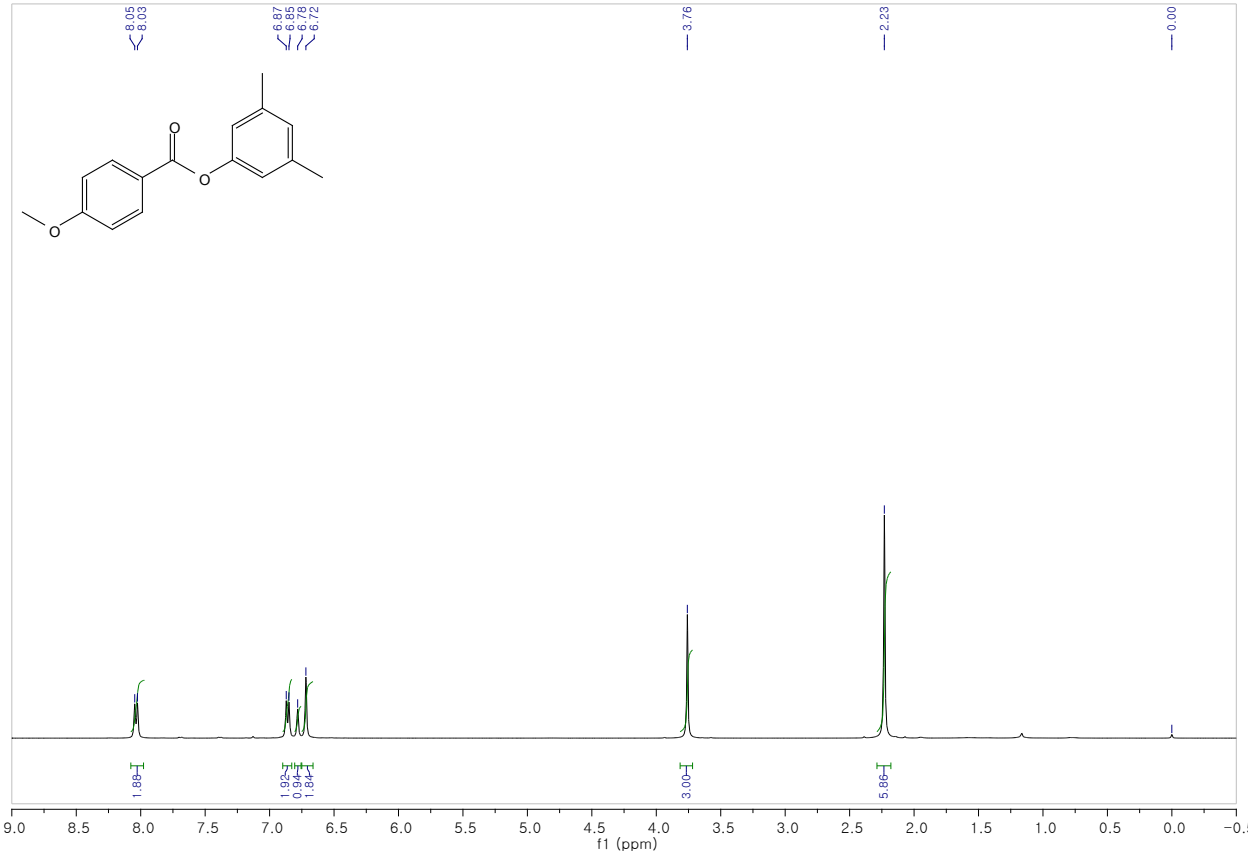
131.4
123.8
113.5
80.4
77.3
77.0
76.7
55.4
52.4
31.7
26.6
O
O
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

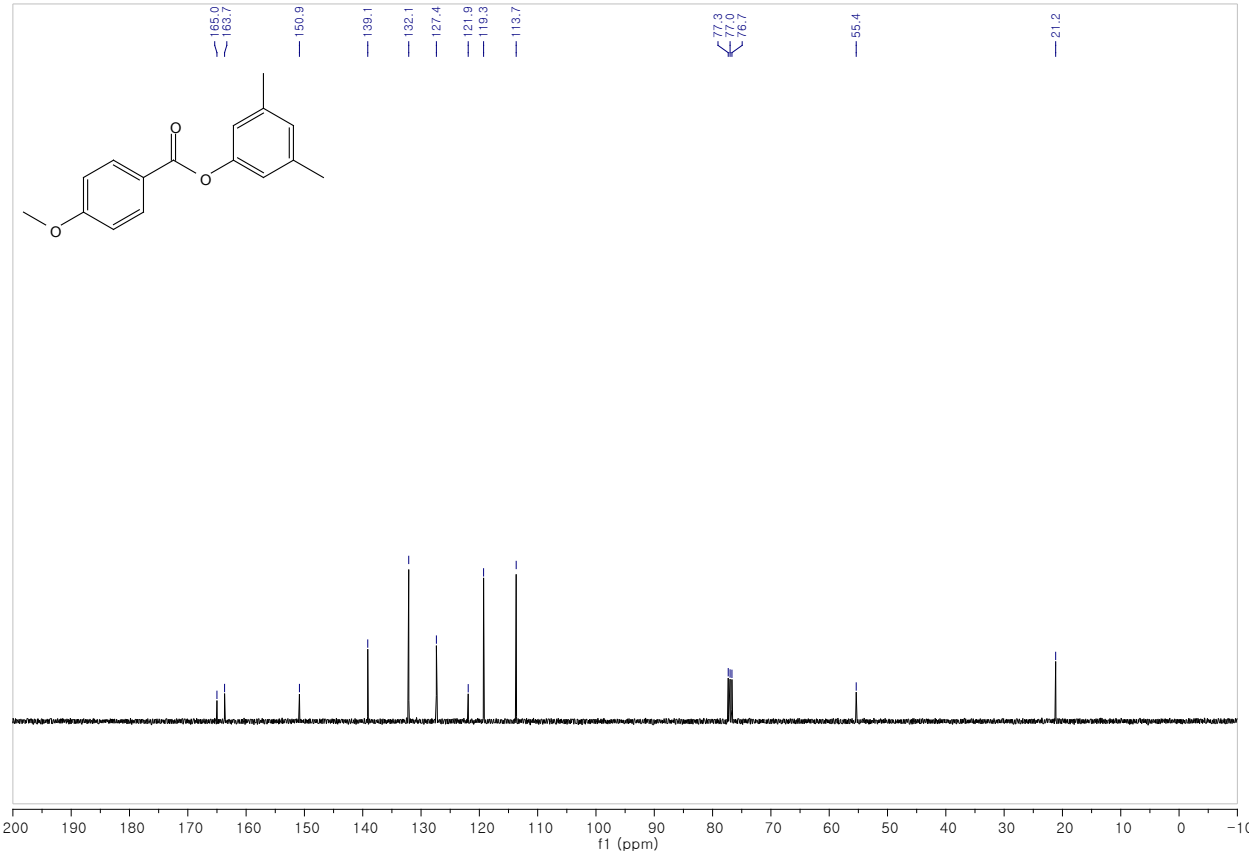

9.94
8.09
8.07
7.89
7.87
7.33
7.31
6.93
6.91
3.83
H
O
O
O
O
0.95
1.98
2.06
1.94
2.10
3.00
f1 (ppm)

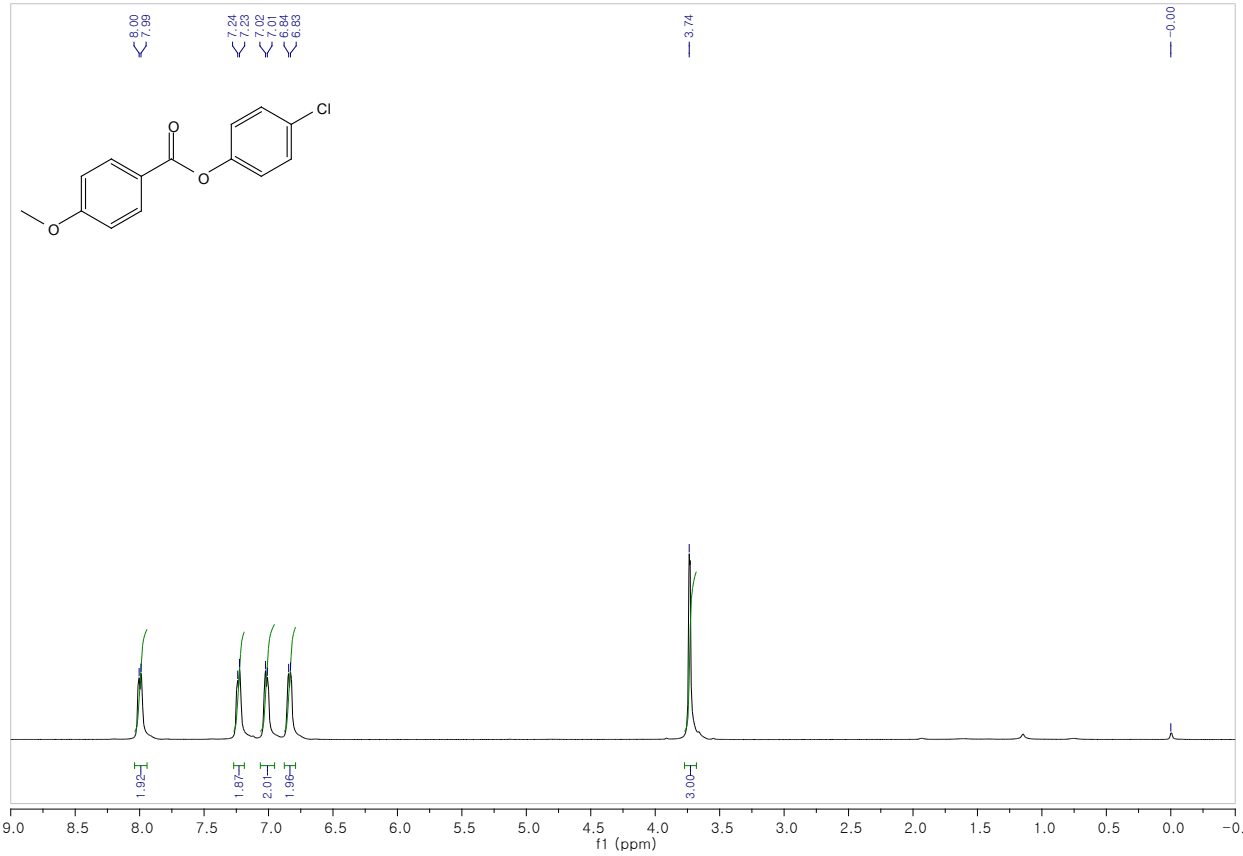

190.9
164.2
164.1
155.8
133.9
132.4
131.2
122.6
121.1
114.0
77.3
77.0
76.7
55.5
H
O
O
O
O
f1 (ppm)

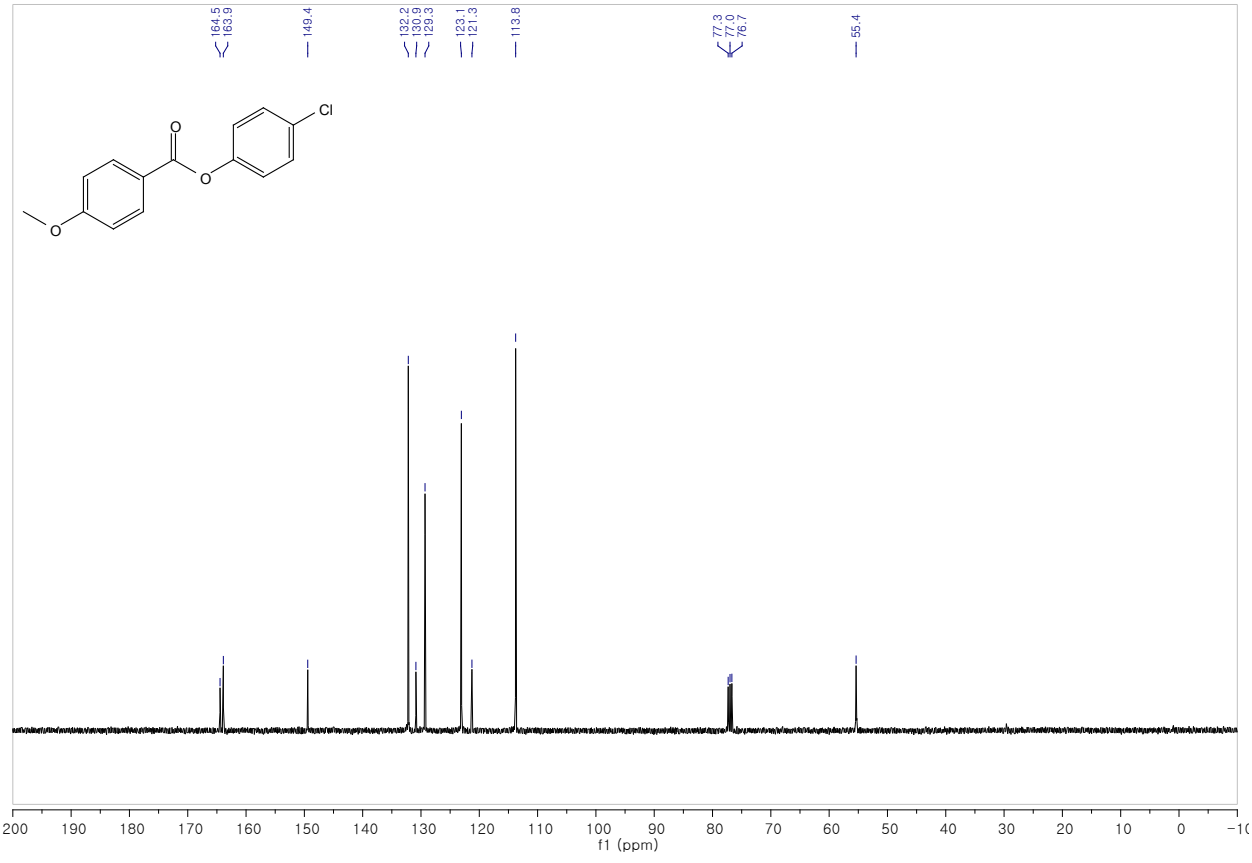

8.08
8.06
7.34
7.33
7.31
7.18
7.16
7.15
7.12
7.10
6.90
6.88
3.78
0.00
O
O
O
2.00
2.12
2.86
2.03
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

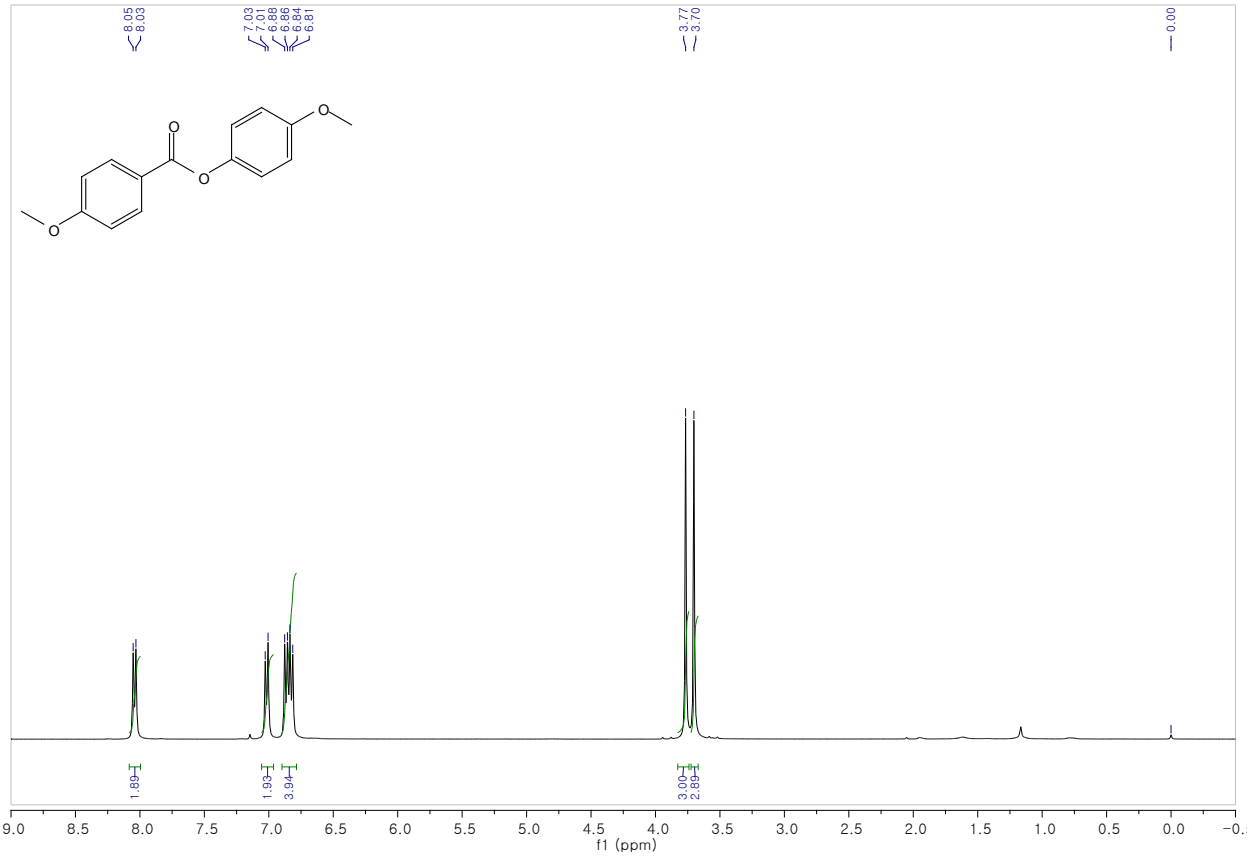

164.83
163.81
151.01
132.21
129.36
125.64
121.80
121.74
113.77
77.32
77.00
76.68
55.41
O
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

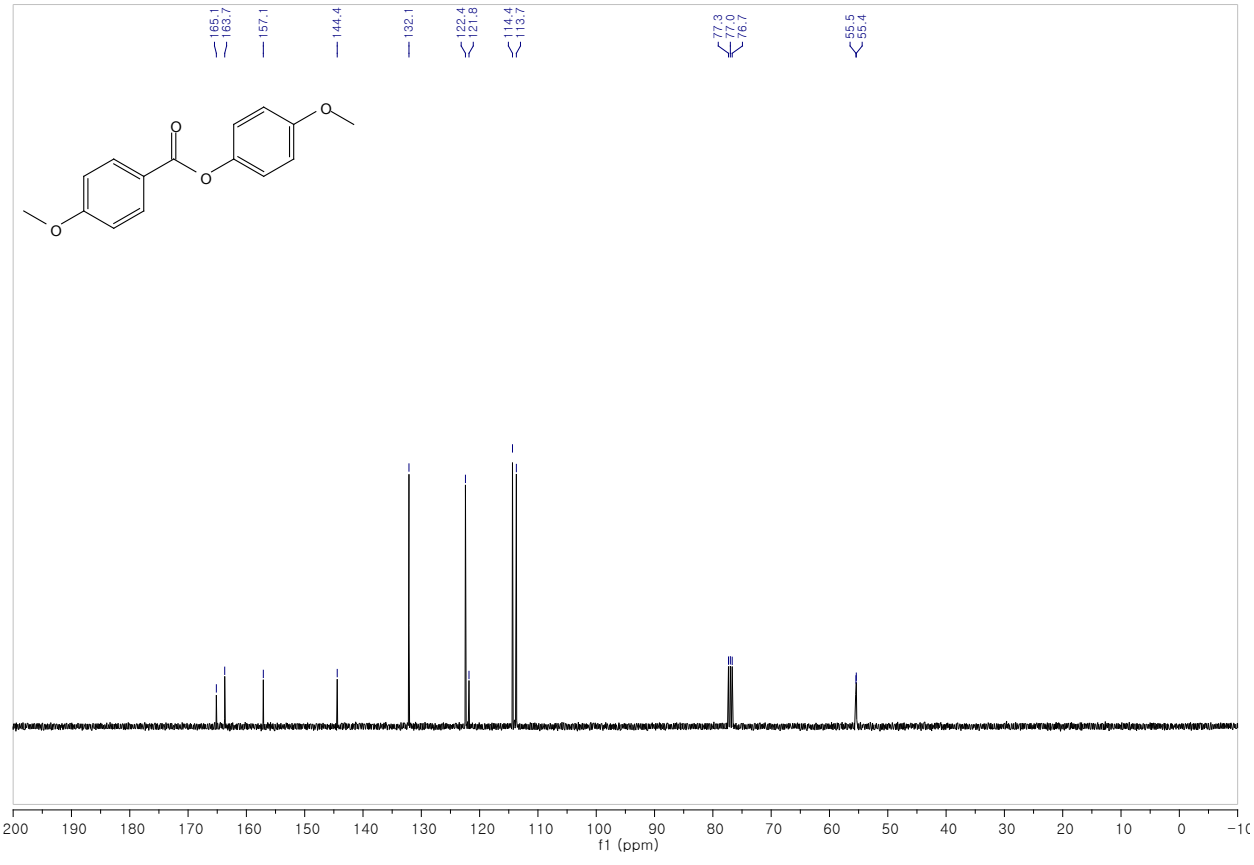

8.05
8.03
6.87
6.85
6.75
6.72
3.76
2.23
0.00
O
O
O
1.88
1.92
0.94
1.84
3.00
5.86
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

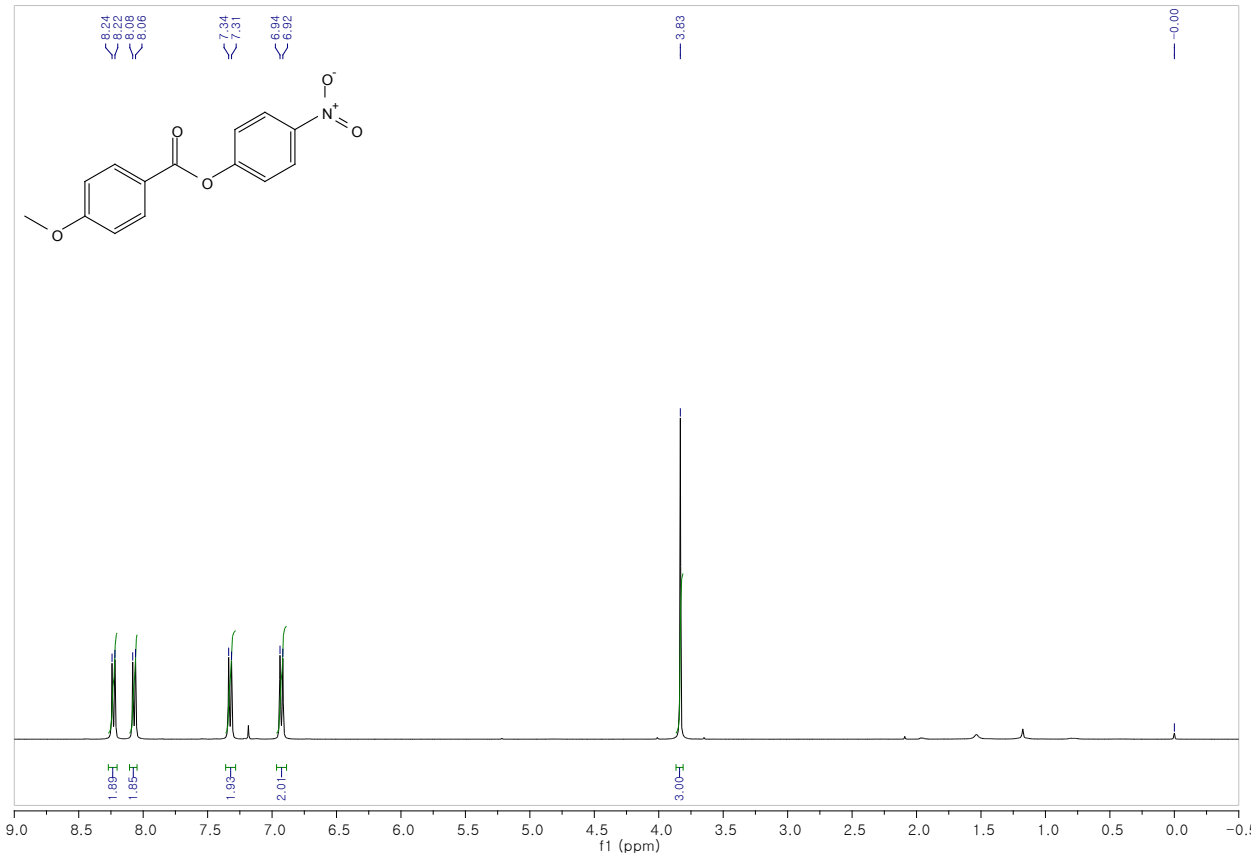

165.0
163.7
150.9
139.1
132.1
127.4
121.9
119.3
113.7
77.3
77.0
76.7
55.4
21.2
O
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

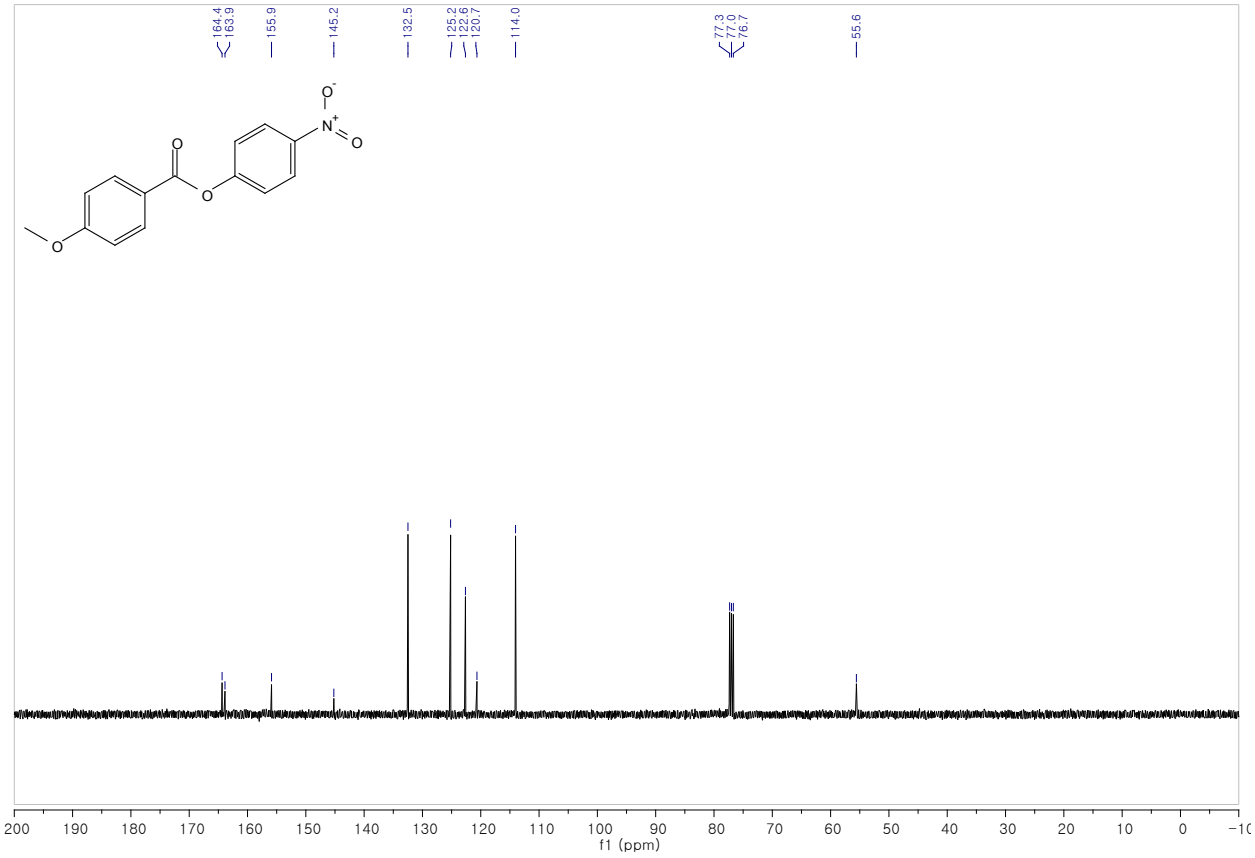

8.00
7.99
7.24
7.23
7.02
7.01
6.84
6.83
3.74
0.00
Cl
O
O
O
1.92
1.87
2.01
1.96
3.00
f1 (ppm)

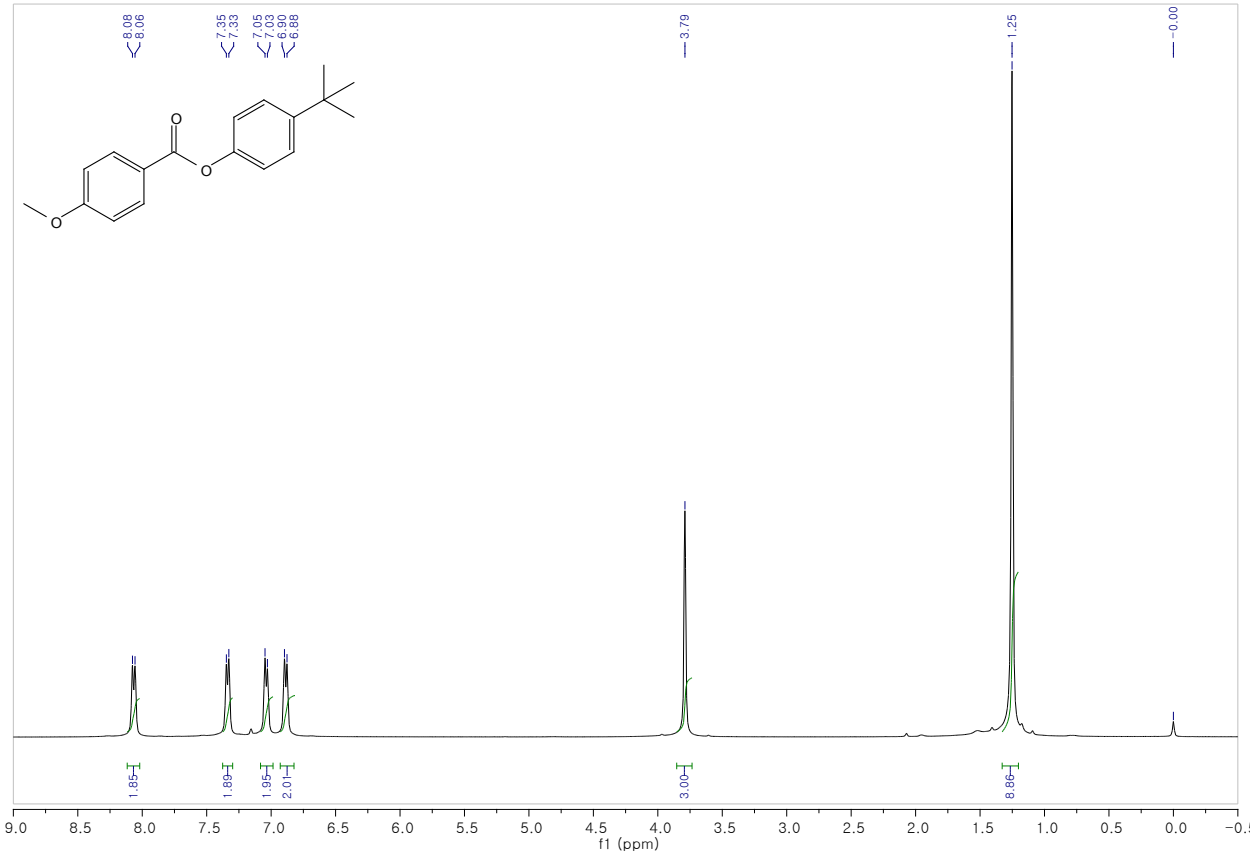

164.5
163.9
149.4
132.2
130.9
129.3
123.1
121.3
113.8
77.3
77.0
76.7
55.4
Cl
O
O
O
f1 (ppm)

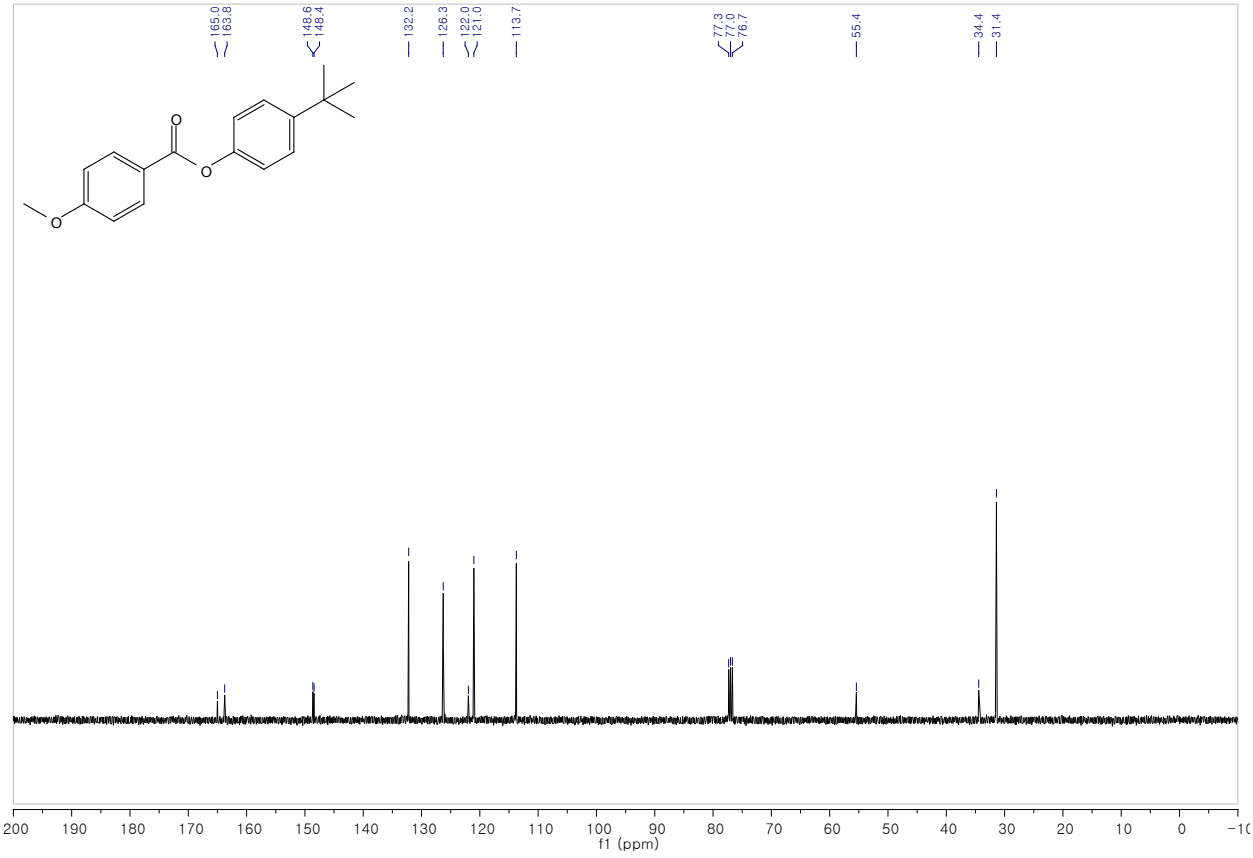

8.05
8.03
7.03
7.01
6.88
6.86
6.84
6.81
3.77
3.70
0.00
1.89
1.93
3.94
3.00
2.89
f1 (ppm)

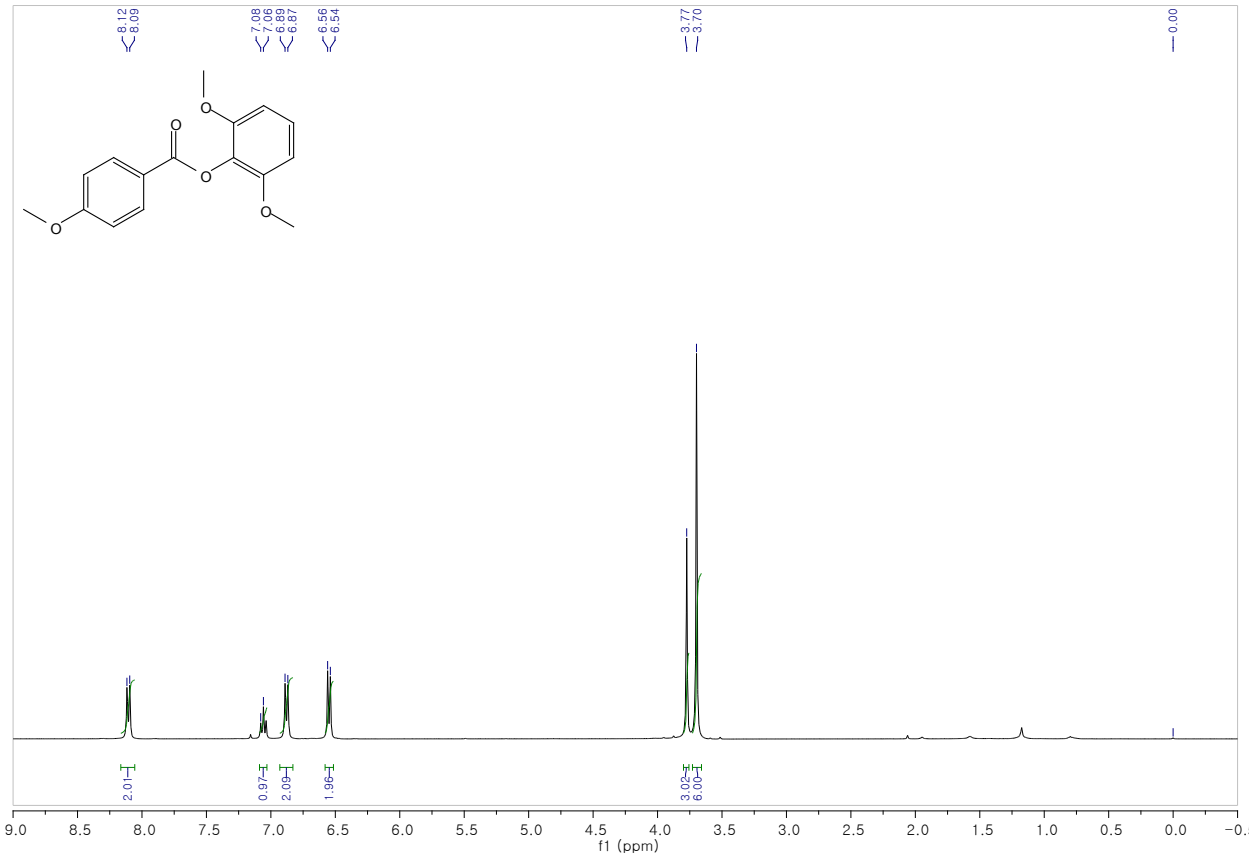

165.1
163.7
157.1
144.4
132.1
122.4
121.8
114.4
113.7
77.3
77.0
76.7
55.5
55.4
f1 (ppm)

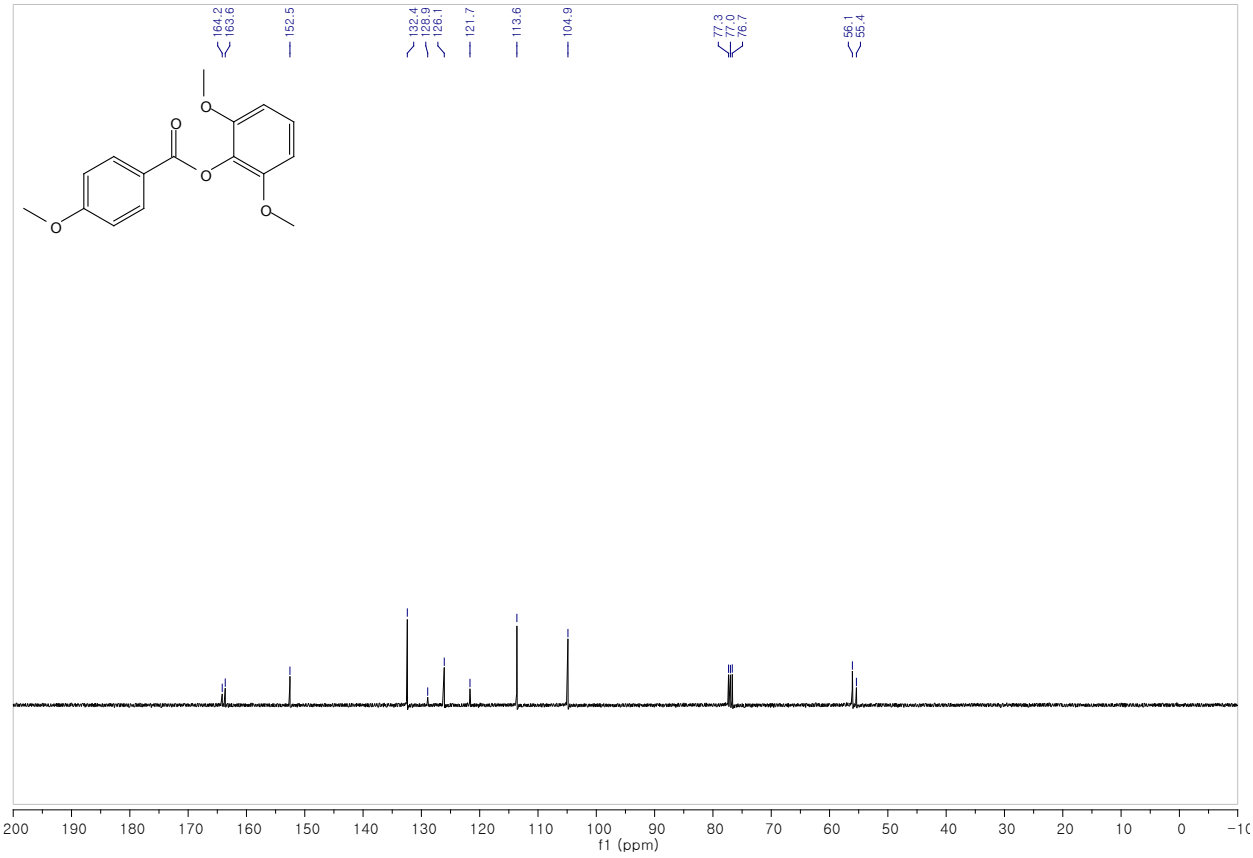

8.24
8.22
8.08
8.06
7.34
7.31
6.94
6.92
3.83
-0.00
1.89
1.85
1.93
2.01
3.00
f1 (ppm)


164.4
163.9
155.9
145.2
132.5
125.2
122.6
120.7
114.0
77.3
77.0
76.7
55.6
f1 (ppm)


8.08
8.06
7.35
7.33
7.05
7.03
6.90
6.88
3.79
1.25
0.00
O
O
O
1.85
1.89
1.95
2.01
3.00
8.86
f1 (ppm)


165.0
163.8
148.6
148.4
132.2
126.3
122.0
121.0
113.7
77.3
77.0
76.7
55.4
34.4
31.4
O
O
O
f1 (ppm)


8.12
8.09
7.08
7.06
6.89
6.87
6.56
6.54
3.77
3.70
0.00
2.01
0.97
2.09
1.96
3.02
6.00
f1 (ppm)


164.2
163.6
152.5
132.4
128.9
126.1
121.7
113.6
104.9
77.3
77.0
76.7
56.1
55.4
f1 (ppm)