SUPPORTING INFORMATION

Sm-Based Grignard Addition of Organohalides into Carbonyls under the Catalysis of CuI

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1. GENERAL

All NMR spectra were measured in $CDCl_3$ or DMSO-d_6, and recorded on a Bruker Avance-500 spectrometer (^{1}H NMR 500 MHz, and ^{13}C NMR 125 MHz) with tetramethylsilane (TMS) or the residual signals of the solvent (δ 7.26 for ^{1}H NMR and δ 77.16 for ^{13}C NMR) as the internal standard. Chemical shifts are expressed in δ values (ppm) and Coupling Constants are given in *J* values (Hz). IR spectra were recorded on a Bruker Tensor-27 spectrometer. Melting points were measured on RY-1 melting point apparatus, and the values are uncorrected. All chemical reagents and solvents were purchased from commercial sources and used without further purification unless otherwise specified. Before use, tetrahydrofuran (THF) was refluxed and redistilled over sodium and benzophenone, and *N,N*-dimethylfromamide (DMF) was dried over 3Å molecule sieve after redistillation. Flash column chromatography was performed over silica gel (100-200 mesh). All reaction mixtures were stirred magnetically and were monitored by thin-layer chromatography using silica gel pre-coated glass plates, which were visualized with an ultraviolet analyzer (black-box type).

2. TYPICAL EXPERIMENTAL PROCEDURES

2.1 Typical procedure for the preparation of tribenzylmethanol from benzyl bromide and dimethyl carbonate

To a mixture of samarium powder (0.3 g, 2 mmol), cuprous iodide (0.038 g, 0.2 mmol) in anhydrous tetrahydrofuran (10 mL) under a nitrogen atmosphere, dimethyl carbonate (0.51 mL, 6 mmol) and benzyl bromide (0.24 mL, 2 mmol) were added while stirring at room temperature. After reaction completion (about 10 h, monitored by TLC), dilute hydrochloric acid (2 mol · L^{-1}, 8 mL) was added and the resulting mixture was extracted with ethyl acetate (3 × 15 mL). The combined organic layer was washed with brine, dried over anhydrous sodium sulfate, and concentrated under reduced pressure. The crude mixture was subjected to flash chromatography on silica gel (petroleum ether/ethyl acetate, 40 : 1 v/v) and recrystalled from ethanol to afford 489.2 mg of tribenzylmethanol (**3a**) in 81 % yield.

2.2 Typical procedure for the preparation of 1-(p-tolyl)cyclohexanol from 1-bromo-4-methylbenzene and cyclohexanone

To a mixture of samarium powder (0.3 g, 2 mmol), cuprous iodide (0.038 g, 0.2 mmol) in anhydrous tetrahydrofuran (10 mL) under a nitrogen atmosphere, cyclohexanone (0.52 mL, 5 mmol) and 1-bromo-4-methylbenzene (0.25 mL, 2 mmol) were added while stirring at room temperature. After reaction completion (about 4 h, monitored by TLC), dilute hydrochloric acid (2 mol · L^{-1}, 8 mL) was added and the resulting mixture was extracted with ethyl acetate (3 × 15 mL). The combined organic layer was washed with brine, dried over anhydrous sodium sulfate, and concentrated under reduced pressure. The crude mixture was subjected to flash chromatography on silica gel (petroleum ether/ethyl acetate, 40 : 1 v/v) and recrystalled from ethanol to afford 338.7 mg of 1-(p-tolyl)cyclohexanol (**3p**) in 89 % yield.

2.3 Typical procedure for the preparation of benzaldehyde from bromobenzene in *N,N*-dimethylfromamide

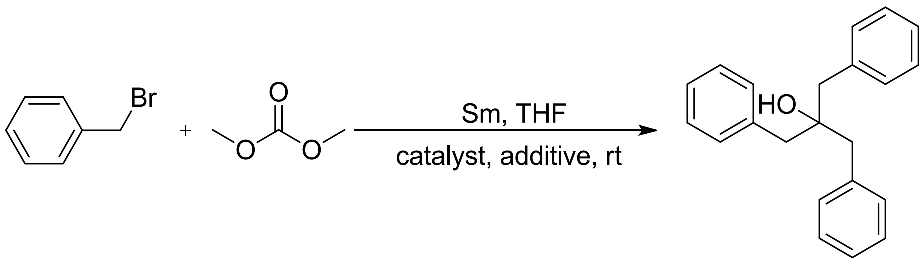
To a mixture of samarium powder (0.3 g, 2 mmol), cuprous iodide (0.038 g, 0.2 mmol) in anhydrous *N,N*-dimethylfromamide (5 mL) under a nitrogen atmosphere, bromobenzene (0.21 mL, 2 mmol) was added while stirring at room temperature. After reaction completion (about 4 h, monitored by TLC), dilute hydrochloric acid (2 mol · L^{-1}, 8 mL) was added and the resulting mixture was extracted with ethyl acetate (3 × 15 mL). The combined organic layer was washed with brine, dried over anhydrous sodium sulfate, and concentrated under reduced pressure. The crude mixture was subjected to flash chromatography on silica gel (petroleum ether/ethyl acetate, 40 : 1 v/v) and recrystalled by ethanol to afford 195.3 mg of benzaldehyde (**4a**) in 92 % yield.

3. SCREEN ON THE REACTION CONDITIONS

A series of control experiments were performed to screen the optimal reaction conditions such as the catalysts, feed ratio, additives, reaction time and temperature. The results are listed in Table S1 (by taking the addition of benzyl bromide into dimethyl carbonate as an example) and Table S2 (by taking the addition of bromobenzene into *n,n*-dimethylformamide as an example). It is proved that 2 equivalents of Sm is sufficient to the reaction.

Table S1 summarizes the investigations on the reaction conditions under which tribenzylmethanol (**3a**) was prepared from benzyl bromide and dimethyl carbonate.

Table S1. Optimization on the Reaction Conditions



Entry[a]	Catalyst	mol%	Additive	Time (h)	Yield (%)[b]
1		-		10	-[c]
2	$NiCl_2$	10		10	-[c]
3	$CoCl_2$	10		10	-[c]
4	$FeCl_3$	10		10	-[c]
5	$InCl_3$	10		10	-[c]
6	$CuBr_2$	10		10	23
7	CuO	10		10	51
8	CuCl	10		10	45
9	CuBr	10		10	67
10	CuI	1		48	50
11	CuI	5		24	78

12	CuI	10		10	81
13	CuI	30		8	83
14	CuI	100		3	83
15	CuI	10		10	74[d]
16	CuI	10		5	55[e]
17	CuI	10	1,10-phen	10	42
18	CuI	10	bipy	10	21
19	CuI	10	PPh_3	10	33
20	CuI	10	TMSCl	10	66
21		10	I_2	10	-[c]
22	CuI	10	I_2	10	57
23	CuI	10	KI	10	32
24	CuI	10	HMPA	10	43

[a] Reaction conditions: benzyl bromide (2 mmol), samarium powder (2 mmol), dimethyl carbonate (0.5 mL), THF (10 mL), room temperature and N_2 atmosphere. [b] Isolated yields based upon benzyl bromide. [c] No desired product detected. [d] In air. [e] Under reflux.

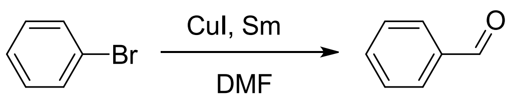
Firstly, a brief screen of the catalysts showed that the copper catalysts were critical to the reaction while no product was detected at all when the reaction was performed for 10 h at room temperature if no any catalyst was added (table S1, entry 1). Similar results were also observed when the reaction was catalyzed by nickel dichloride, cobalt dichloride, iron trichloride, indium trichloride or iodine (Table S1, entries 2-5, 21) in respective. In the presence of 10 mol % divalent copper catalyst, tribenzylmethanol (**3a**) was obtained in a relatively lower yield (23 %, Table S1, entry 6), while moderate to good yields were afforded respectively when cuprous salts (CuO, CuCl, CuBr) were used as the catalysts (Table S1, entries 7-9). Among the salts used here, cuprous iodide was proved to be the most efficient catalyst to afford the desired product in more than 80 % yield (Table S1, entries 11-14). The investigation showed 10 mol % cuprous iodide was sufficient to catalyze the addition in good efficiency (Table S1, entry 12).

Nevertheless, excess amount of cuprous iodide (100 mol %) has very limited effect on the increase of the addition product yield (Table S1, entry 14), although the reaction time was considerably shorten.

It is interesting that the reaction can been carried out in air with a very slight decrease of the product yield (Table S1, entry 15). Subsequent investigation revealed that the reaction temperature influenced the coupling efficiency obviously. Under reflux temperature, the product yield decreased accordingly in the shorter reaction times (Table S1, entries 16). Further, neither ligands (Table S1, entries 17-19) nor activating agents (Table S1, entries 20-22) were needed for the catalyst and samarium metal. Besides, the addition reaction was actually proved to be additive-free (Table S1, entries 23-24).

Table S2 summarizes the investigations on the reaction conditions under which benzaldehyde (**4a**) was prepared from bromobenzene and *N,N*-dimethylformamide.

Table S2. Optimization of the Reaction Conditions



Entry[a]	CuI(mol%)	Additive	*T*(°C)	Time (h)	Yield(%)[b]
1	100		25	2	93
2	30		25	4	93
3	10		25	4	92
4	5		25	12	77
5	1		25	24	54
6			25	12	--[c]
7		$InCl_3$	25	12	--[c]
8		I_2	25	12	--[c]
9	10	I_2	25	8	74
10	10	KI	25	8	83
11	10	TMSCl	25	8	67

12	10	60	4	68
13	10	100	4	51
14	10	150	4	32
15	10	25	4	80[d]
16	10	25	4	71[e]

[a] Reaction conditions: bromobenzene (2 mmol), samarium powder (2 mmol), DMF (5 mL), and N_2 atmosphere. [b] Isolated yields based upon bromobenzene. [c] No reactions occurred. [d] In air. [e] DMF (0.3 mL) in THF under the conditions.

By comparison with Table S1, the investigations described in Table S2 were undergone under the conditions that *N,N*-dimethylformamide was used as both the substrate and the solvent. The results listed in Table S2 showed that 10 mol % amount of cuprous iodide was sufficient to catalyze the addition in excellent yield (Table S1, entry 3), while almost no obvious increase of the product yield can be observed when 100 mol % amount of cuprous iodide was used (Table S2, entry 1), although the reaction time was shorter. However, no reactions can be observed at all in the absence of CuI under the conditions (Table S2, entries 6-8). Similar to the results shown in Table S1, the investigation revealed that neither additives used here (Table S2, entries 9-11) nor high temperature (Table S2, entries 12-14) was favorable to the reaction efficiency. Besides, the reaction can also been carried out in air with a slight decrease of the product yield (Table S2, entry 15). In comparison, the reaction can occur in THF by the use of DMF as a single substrate with relative lower yield (Table S2, entry 16).

4. CHARACTERIZATION DATA FOR ALL PRODUCTS

Tribenzylmethanol (3a): CAS Number: 6712-97-6; white solid; m.p. 116-118°C (lit. 116°C);[1] ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.49 (s, 1 H), 2.76 (m, 6 H), 7.20-7.232 (m, 9 H), 7.27-7.31 (m, 6 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.3, 130.8, 128.1, 126.4, 73.9, 45.8 ppm.

2-methyl-1,3-diphenylpropan-2-ol (3b): CAS Number: 42117-23-7;[2] faint yellow liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.06 (s, 3 H), 1.43 (s, 1 H), 2.84 (m, 4 H), 7.26 (m, 10 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ137.7, 130.8, 128.2, 126.6, 72.6, 48.5, 26.41, 26.36 ppm.

***α*-Phenyl-*α*-(phenylmethyl)benzeneethanol** (**3c**): CAS Number: 5472-27-5; white solid; m.p. 86-88°C (lit. 83.5-85°C);[3] ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.89 (s, 1 H), 3.10-3.13 (d, 2 H, J = 8.5 Hz), 3.29-3.12 (d, 2 H, J = 8.5 Hz), 6.94-9.96 (m, 4 H), 7.15-7.27 (m, 11 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 145.3, 136.4, 130.7, 127.9, 127.8, 126.5, 125.8, 48.7 ppm.

***α*-(4-Methylphenyl)-*α*-(phenylmethyl)-benzeneethanol** (**3d**): CAS Number: 81392-99-6; white solid; m.p. 70-71°C (lit. 72-73°C);[4] ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.85 (s, 1 H), 2.34 (s, 3 H), 3.07-3.10 (d, 2 H, J = 13 Hz), 3.25-3.28 (d, 2 H, J = 13 Hz), 6.95-9.97 (m, 4 H), 7.05-7.07 (m, 2 H), 7.13-7.16 (m, 8 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.3, 136.5, 135.9, 130.8, 128.5, 127.9, 126.4, 125.7, 48.7, 21.0 ppm.

3-Benzylpentan-3-ol (**3e**): CAS Number: 34577-40-7;[5] obtained as a colorless liquid ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.32-7.21 (m, 5 H), 2.74 (s, 2 H), 1.46 (q, J = 7.5 Hz, 4 H), 1.19 (s, 1 H), 0.93 (t, J = 7.5 Hz, 6 H) ppm;^{13}C NMR (125 MHz, $CDCl_3$): δ 137.5, 130.6, 128.4, 126.4, 44.8, 30.5, 8.0 ppm.

1-Benzylcyclopentanol (**3f**): CAS Number: 2015-57-8; white solid; m.p. 56-58 °C (lit. 58-60°C);[6] ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.33-7.21 (m, 5 H), 2.89 (s, 2 H), 1.85-1.79 (m, 2 H), 1.70-1.57 (m, 6 H), 1.27 (s, 1 H) ppm;^{13}C NMR (125 MHz, $CDCl_3$): δ 138.3, 130.2, 128.3, 126.5, 82.1, 47.1, 39.4, 23.5 ppm.

1-(Phenylmethyl)cyclohexanol (**3g**): CAS Number: 1944-01-0;[7] faint yellow liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.23-1.27 (m, 2 H), 1.42-1.62 (m, 10 H), 2.75 (s, 2 H), 7.20-7.24 (m, 3 H), 7.29-7.32 (m, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.2, 130.6, 128.1, 126.4, 71.1, 48.7, 37.3, 25.8, 22.1 ppm.

4-Phenyl-butan-2-ol (3h): CAS Number: 2344-70-9; colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.25-1.26 (m, 3 H), 1.75-1.81 (m, 3 H), 2.65-2.71 (m, 1 H), 2.74-2.79 (m, 1 H), 3.81-3.85 (m, 1 H), 7.18-7.22 (m, 3 H), 7.25-7.30 (m, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.1, 128.4, 125.8, 67.5, 40.8, 32.1, 23.6 ppm.

2-(4-Methyl-benzyl)-1,3-di-p-tolyl-propan-2-ol (**3i**): white solid; m.p. 104-106°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.48 (s, 1 H), 2.34 (s, 9 H), 2.72 (s, 6 H), 7.11 (m, 12 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 135.8, 134.3, 130.7, 128.8, 73.9, 45.2, 21.0 ppm. Anal.

$C_{25}H_{28}O$. Calcd. C, 87.16; H, 8.19. Found C, 87.10; H, 8.21%.

2-(4-Chloro-benzyl)-1,3-bis-(4-chloro-phenyl)-propan-2-ol (**3j**): white solid; m.p. 145-147°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.35 (s, 1 H), 2.68 (s, 6 H), 7.11-7.13 (d, 6 H, J = 8 Hz), 7.26-7.28 (d, 6 H, J = 8 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 135.3, 132.6, 132.0, 128.4, 73.7, 45.1 ppm. Anal. $C_{22}H_{19}Cl_3O$. Calcd. C, 65.12; H, 4.72. Found C, 65.07; H, 4.75%.

2-(2-Chloro-benzyl)-1,3-bis-(2-chloro-phenyl)-propan-2-ol (**3k**): white solid; m.p. 115-117°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.01 (s, 1 H), 3.08 (m, 6 H), 7.16-7.20 (m, 6 H), 7.29-7.31 (m, 3 H), 7.36-7.38 (m, 3 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 135.3, 135.2, 132.9, 129.6, 127.9, 126.4, 76.4, 41.8 ppm. Anal. $C_{22}H_{19}Cl_3O$. Calcd. C, 65.12; H, 4.72. Found C, 65.11; H, 4.71%.

2-(3-Fluoro-benzyl)-1,3-bis-(3-fluoro-phenyl)-propan-2-ol (**3l**): white solid; m.p. 53-55°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.49 (s, 1 H), 2.73 (m, 6 H), 6.93-6.97 (m, 9 H), 7.23-7.28 (m, 3 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.7-161.7 ($J_{C\text{-}F}$ = 250.0 Hz), 139.5-139.4 ($J_{C\text{-}F}$ = 12.5 Hz), 129.64-129.58 ($J_{C\text{-}F}$ = 7.5 Hz), 126.4, 117.6-117.5 ($J_{C\text{-}F}$ = 12.5 Hz), 113.7-113.5 ($J_{C\text{-}F}$ = 25.0 Hz), 73.8, 45.6 ppm. Anal. $C_{22}H_{19}F_3O$. Calcd. C, 74.14; H, 5.37. Found C, 74.10; H, 5.41%.

Bis(2-methylbenzyl)ketone (**3m**): CAS Number: 23592-92-9; white solid; m.p. 53-55°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.17 (s, 6 H), 3.73 (s, 4 H), 7.07-7.09 (m, 2 H), 7.15-7.19 (m, 6 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 205.6, 136.9, 132.9, 130.5, 130.4, 127.4, 126.2, 47.3, 19.6 ppm.

1,3-Di-naphthalen-1-yl-2-naphthalen-1-ylmethyl-propan-2-ol (**3n**): white solid; m.p. 149-151°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.51 (s, 1 H), 3.44 (s, 6 H), 7.33-7.36 (m, 3 H), 7.38-7.43 (m, 9 H), 7.76-7.78 (m, 6 H), 7.80-7.83 (m, 3 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 133.9, 133.7, 133.5, 129.4, 128.7, 127.4, 125.8, 125.3, 125.1, 124.6, 76.1, 41.9 ppm. Anal. $C_{34}H_{28}O$. Calcd. C, 90.23; H, 6.24. Found C, 90.16; H, 6.27%.

3-Phenethyl-1,5-diphenyl-pentan-3-ol (**3o**): CAS Number: 92825-27-9; white solid; m.p. 68-69°C (lit. 68.8-70°C);[8] ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.31 (s, 1 H), 1.89-1.93 (m, 6 H), 2.70-2.74 (m, 6 H), 7.19-7.22 (m, 9 H), 7.29-7.32 (m, 6 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.3, 128.5, 128.4, 125.9, 74.3, 41.3, 30.1 ppm.

1,7-Diphenyl-4-(3-phenyl-propyl)-heptan-4-ol (**3p**): CAS Number: 103281-80-7; faint yellow liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ1.37 (s, 1 H), 1.43-1.46 (m, 6 H), 1.53-1.57 (m, 6 H), 2.56-2.59 (m, 6 H), 7.15-7.21 (m, 9 H), 7.25-7.30 (m, 6 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.3, 128.4, 128.3, 125.8, 74.3, 38.7, 36.3, 25.3 ppm.

2-Methyl-1,3-di-naphthalen-1-yl-propan-2-ol (**3q**): white solid; m.p. 68-69°C; ^1H NMR (500 MHz, $CDCl_3$) δ 1.13 (s, 3 H), 1.51 (s, 1 H), 3.44-3.48 (m, 4 H), 7.43-7.49 (m, 8 H), 7.76-7.78 (m, 2 H), 7.84-7.85 (m, 2 H), 8.11 (m, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 134.1, 133.5, 129.4, 128.8, 127.5, 125.8, 125.5, 125.3, 125.2, 74.3, 44.4, 27.5 ppm.

1-(2-Phenylethyl)cyclohexanol (**3r**): CAS Number: 124620-30-0; white solid; m.p. 55-56°C (lit. 55-56°C);[9] ^1H NMR (500 MHz, $CDCl_3$) δ 1.20-1.23 (m, 1 H), 1.27-1.33 (m, 1 H), 1.47-1.71 (m, 9 H), 1.75-1.82 (m, 2 H), 2.69-2.76 (m, 2 H), 7.14-7.21 (m, 3 H), 7.26-7.32 (m, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.9, 128.4, 125.7, 71.5, 44.4, 37.6, 29.6, 25.9, 22.3 ppm.

1-Cinnamylcyclohexanol (**3s**): CAS Number: 105273-48-1;[10] faint yellow liquid; ^1H NMR (500 MHz, $CDCl_3$): δ 7.40-7.30 (m, 4 H), 7.23 (m, 1 H), 6.47 (d, J = 16 Hz, 1 H), 6.36-6.26 (m, 1 H), 2.39 (d, J = 7.5 Hz, 2 H), 1.65-1.48 (m, 10 H) ppm;^{13}C NMR (125 MHz, $CDCl_3$): δ 137.3, 133.6, 128.5, 127.2, 126.1, 125.4, 71.5, 45.9, 37.5, 25.7, 22.5 ppm.

1-(4-Methylphenyl)cyclohexanol (**3t**): CAS Number: 1821-24-5; white solid; m.p. 50-51°C (lit. 57-58°C);[11] ^1H NMR (500 MHz, $CDCl_3$) δ 1.28-1.30 (m, 1 H), 1.53-1.84 (m, 10 H), 2.34 (s, 3 H), 7.15-7.17 (d, 2 H, J = 8 Hz), 7.39-7.41 (d, 2 H, J = 8 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 146.6, 136.3, 128.9, 124.6, 73.0, 38.9, 25.6, 22.3, 21.0 ppm.

Triphenylmethanol (**3u**): CAS Number: 200-988-5; white solid; m.p. 165-167°C; ^1H NMR (500 MHz, $CDCl_3$) δ2.80 (s, 1 H), 7.24-7.32 (m, 15 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.8, 127.8, 127.2, 82.0 ppm.

Diphenylmethanol (**3v**): CAS Number: 91-01-0; white solid; m.p. 64-65°C (lit. 62-63°C);[12]; ^1H NMR (500 MHz, $CDCl_3$): δ 7.35 (m, 8 H), 7.27 (m, 2 H), 5.8 (s, 1 H), 2.25 (s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.8, 127.5, 127.6, 126.5, 76.3 ppm.

Benzaldehyde (**4a**): CAS Number: 100-52-7;[13] colorless liquid; ^1H NMR (500 MHz, $CDCl_3$) δ7.52-7.55 (m, 2H), 7.62-7.65 (m, 1 H), 7.87-7.89 (m, 2 H), 10.02(s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.4, 136.4, 134.4, 129.7, 129.0 ppm.

4-Methylbenzaldehyde (**4b**):CAS Number: 104-87-0;[14] colorless liquid; ^1H NMR (500 MHz, $CDCl_3$) δ 2.45 (s, 3 H), 7.33 (d, 2 H, J = 7.5 Hz) 7.78 (d, 2 H, J = 7.5 Hz), 9.97 (s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 192.0, 145.5, 134.2, 129.8, 129.7, 21.9 ppm.

4-Methoxybenzaldehyde (**4c**): CAS Number: 123-11-5;[14] colorless liquid; ^1H NMR (500 MHz, $CDCl_3$) δ 3.89 (s, 3 H), 7.01 (d, 2 H, J = 9 Hz) 7.84 (d, 2 H, J = 9 Hz), 9.89 (s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.8, 164.6, 132.0, 130.0, 114.3, 55.6 ppm.

4-Ethylbenzaldehyde (**4d**): CAS Number: 4748-78-1;[15] colorless liquid; ^1H NMR (500 MHz, $CDCl_3$) δ 1.27 (s, 3 H), 2.71-2.75 (m, 2 H), 7.36 (d, 2 H, J = 8 Hz) 7.81 (d, 2 H, J = 8 Hz), 9.97 (s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ192.0, 151.7, 134.4, 130.0, 128.5, 29.1, 15.1 ppm.

4-Biphenylcarboxaldehyde (**4e**): CAS Number: 3218-36-8; white solid; m.p. 55-58°C (lit. 59-60°C);[16] ^1H NMR (500 MHz, $CDCl_3$) δ 7.43-7346 (m, 1 H), 7.49-7.52 (m, 2 H), 7.65-7.67 (m, 2 H), 7.77-7.78 (m, 2 H), 7.97-7.99 (m, 2 H); 10.08 (s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.9, 147.2, 139.7, 135.2, 130.3, 129.0, 128.5, 127.7, 127.4 ppm.

Veratraldehyde (**4f**): CAS Number: 120-14-9; white solid; m.p. 40-43°C (lit. 45°C);[17] ^1H NMR (500 MHz, $CDCl_3$) δ 3.90-3.93 (m, 6 H), 6.94-6.96 (d, 2 H, J = 8 Hz) 7.37 (s, 1 H), 7.41-7.43 (d, 1 H, J = 5 Hz), 9.81 (s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.8, 154.4, 149.6, 130.1, 126.8, 110.4, 108.9, 56.1, 55.9 ppm.

2-Chlorobenzaldehyde (**4g**): CAS Number: 89-98-5;[18] colorless liquid; ^1H NMR (500 MHz, $CDCl_3$) δ 7.34-7.38 (m, 1 H), 7.38-7.42 (m, 1 H), 7.49-7.53 (m, 1 H), 7.88-7.90 (m, 1 H), 10.43 (s, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 189.8, 138.0, 135.3, 132.5, 130.6, 129.4, 127.3 ppm.

3-Chlorobenzaldehyde (**4h**): CAS Number: 587-04-2; white solid; m.p. 16-18°C (lit. 17-18°C);[19] ^1H NMR (500 MHz, $CDCl_3$) δ 7.47-7.51 (m, 1 H), 7.60-7.62 (d, 1 H, J = 8 Hz),7.76-7.78 (d, 1 H, J = 8 Hz) 7.86 (s, 1 H), 9.98 (s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.8, 137.8, 135.5, 134.4, 130.4, 129.3, 128.0 ppm.

4-Bromobenzaldehyde (**4i**): CAS Number:214-365-0; white solid; m.p. 55-58°C (lit. 56-58°C);[20] ^1H NMR (500 MHz, $CDCl_3$) δ 7.68-7.70 (d, 2 H, J = 8 Hz), 7.74-7.76 (d, 2 H, J = 8 Hz), 9.98 (s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.0, 135.1, 132.4, 131.0, 129.8 ppm.

1,4-Phthalaldehyde (**4j**): CAS Number: 623-27-8; white solid; m.p. 115-116°C (lit. 114-116°C);[21] ^1H NMR (500 MHz, $CDCl_3$) δ 8.06 (s, 4 H), 10.14 (s, 2 H); ^{13}C NMR

(125 MHz, $CDCl_3$) δ 191.5, 140.0, 130.1 ppm.

2,4-Dichlorobenzaldehyde (**4k**): CAS Number: 874-42-0; white solid; m.p. 73-74°C (lit. 73-74°C);[22] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.37 (m, 1 H), 7.41 (d, 1 H, J = 5 Hz), 7.45 (d, 1 H, J = 5 Hz), 10.40 (s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.4, 141.1, 138.5, 130.9, 130.4, 130.3, 127.9 ppm.

2-Chloro-6-fluorobenzaldehyde (**4l**): CAS Number: 206-860-500; white solid; m.p. 34-37°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.06-7.10 (m, 1 H), 7.26 (m, 1 H), 7.44-7.49 (m, 1 H), 10.43 (s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 186.8, 164.3-162.2 ($J_{C\text{-}F}$ = 262.5 Hz), 137.0, 135.2-135.1 ($J_{C\text{-}F}$ = 12.5 Hz), 126.8, 121.8-121.7 ($J_{C\text{-}F}$ = 12.5 Hz), 115.7-115.5 ($J_{C\text{-}F}$ = 25.0 Hz) ppm.

Pyridine-4-carboxaldehyde (**4m**): CAS Number: 212-832-3;[23] colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72-7.73 (d, 2 H, J = 5 Hz), 8.90-8.91 (d, 2 H, J = 5 Hz), 10.10 (s, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 191.5, 151.1, 141.2, 122.0 ppm.

Furfural (**4n**): CAS Number:202-627-7;[24] colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.61-7.62 (m, 1 H), 7.27-7.28 (m, 1 H), 7.70 (s, 1H), 9.98 (s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.9, 152.9, 148.1, 121.1, 112.6 ppm.

2-Thenaldehyde (**4o**):CAS Number: 98-03-3;[25] colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21-7.23 (m, 1 H), 7.77-7.79 (m, 2 H), 9.95 (s, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 183.0, 144.0, 136.4, 135.1, 128.3 ppm.

2-Naphthaldehyde (**4p**): CAS Number: 66-99-9; white solid; m.p. 58-60°C (lit. 57-58°C);[26] ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.20 (s, 1 H), 8.36 (s, 1 H), 8.05-7.92 (m, 4 H), 7.69-7.62 (m, 2 H) ppm;^{13}C NMR (125 MHz, $CDCl_3$): δ 192.168, 136.376, 134.461, 134.043, 132.569, 129.456, 129.033, 128.006, 127.020, 122.684 ppm.

1-Naphthaldehyde (**4q**): CAS Number: 66-77-3;[27] colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.41 (s, 1 H), 9.30 (d, J = 8.5 Hz, 1 H), 8.09 (d, J = 8.0 Hz, 1 H), 7.97 (d, J = 7.0 Hz, 1 H), 7.93 (d, J = 8.0 Hz, 1 H), 7.72 (t, J = 7.0 Hz, 1 H), 7.61 (t, J = 7.5 Hz, 2 H) ppm;^{13}C NMR (125 MHz, $CDCl_3$): δ 191.4, 136.6, 135.2, 133.4, 131.3, 130.4, 129.0, 128.4, 126.9, 124.8 ppm.

Cinnamaldehyde (**4r**): CAS Number: 104-55-2;[28] colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.71 (d, J = 8.0 Hz, 1 H), 7.51 (m, 6 H), 6.724 (dd, J = 7.5 Hz, J = 8.0 Hz, 1 H) ;^{13}C NMR (125 MHz, $CDCl_3$): δ 193.7, 152.8, 134.0, 131.3, 129.1, 128.6, 128.5 ppm.

2-Phenylacetaldehyde (**4s**): CAS Number: 122-78-1;[29] colorless liquid;^{1}H NMR (500 MHz, $CDCl_3$): δ 9.75 (t, J = 2.5 Hz, 1 H), 7.39-7.22 (m, 5 H), 3.69 (d, J = 2.5 Hz, 2 H) ppm;^{13}C NMR (125 MHz, $CDCl_3$): δ 199.5, 131.8, 129.6, 129.0, 127.4, 50.6 ppm.

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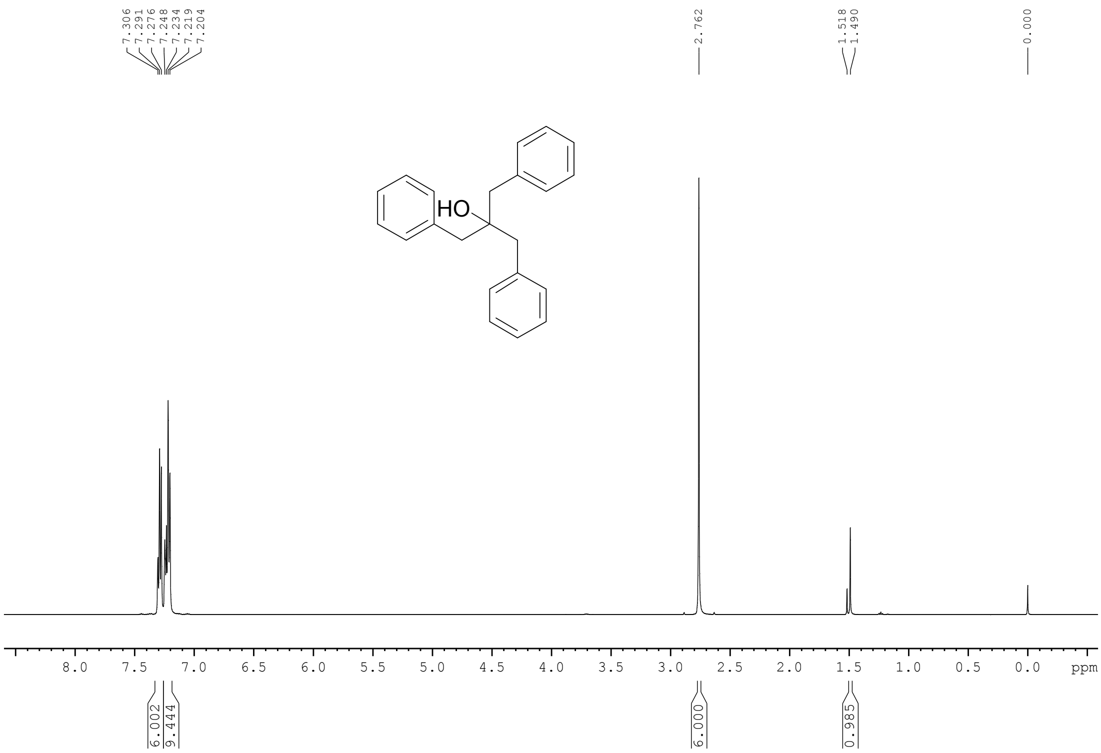
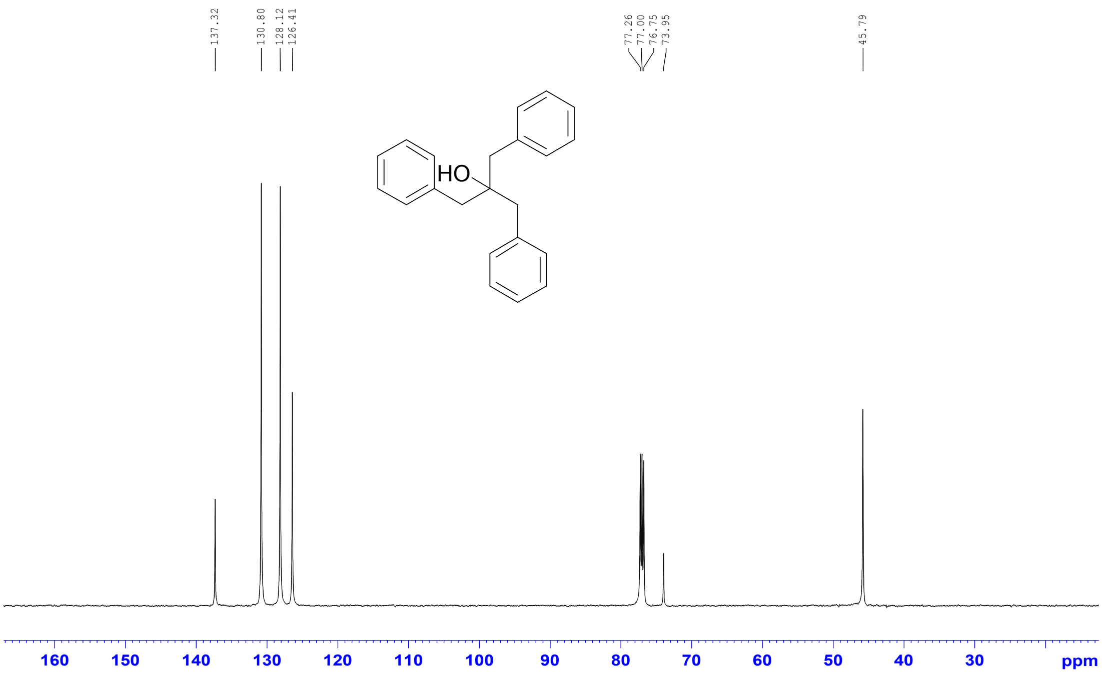
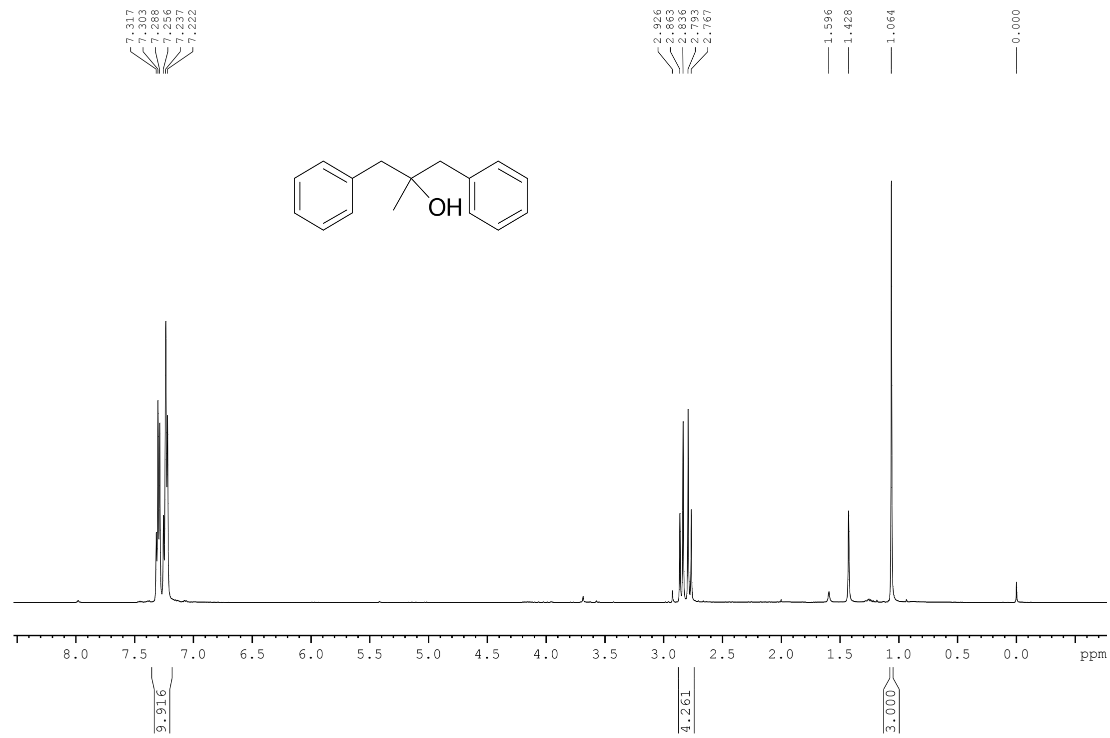
6. COPIES OF ^{1}H NMR AND ^{13}C NMR SPECTRA



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7.288
7.256
7.237
7.222
2.926
2.863
2.836
2.793
2.767
1.596
1.428
1.064
0.000
OH
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 ppm
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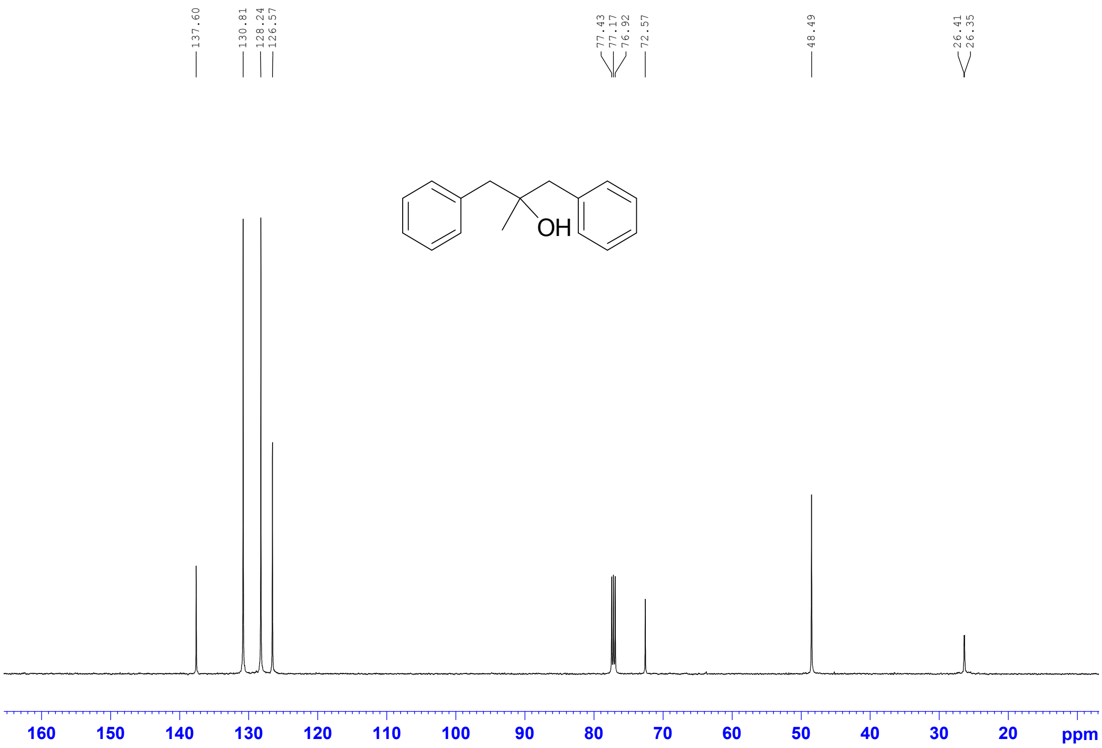
4.261
3.000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128.24
126.57
77.43
77.17
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72.57
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26.41
26.35
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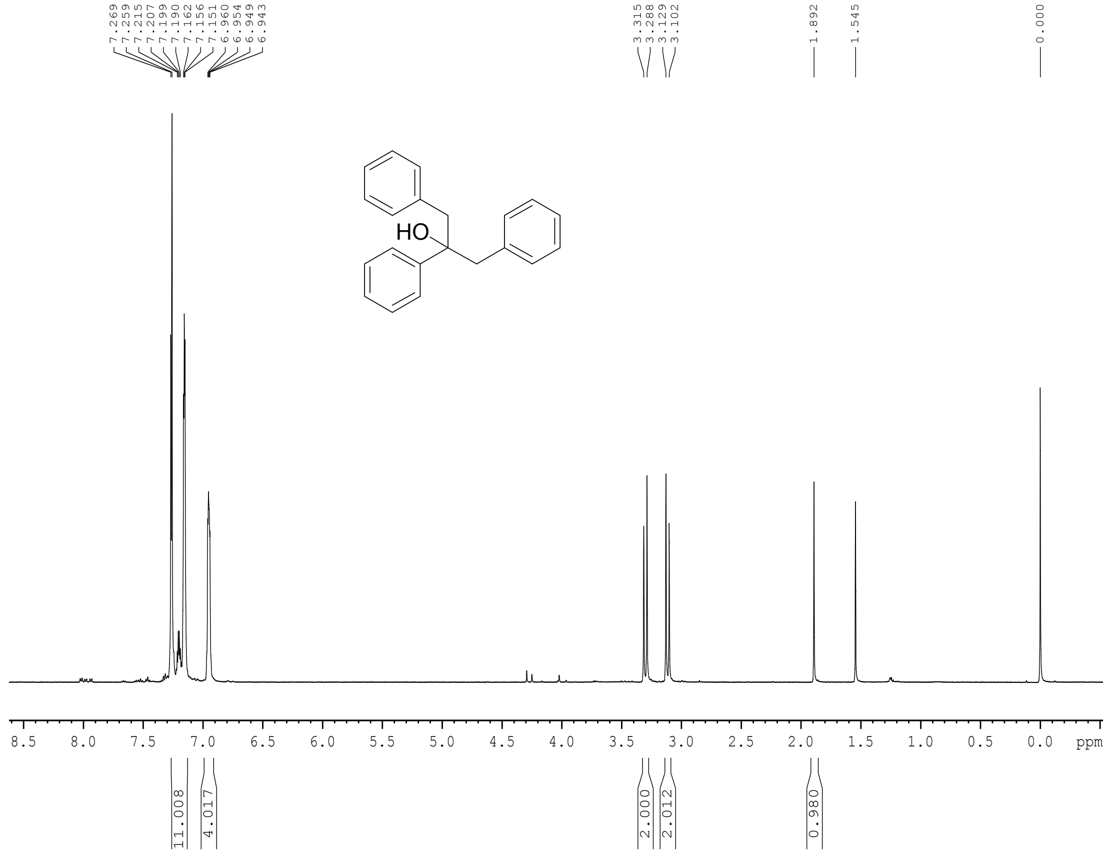
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7.215
7.207
7.199
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7.162
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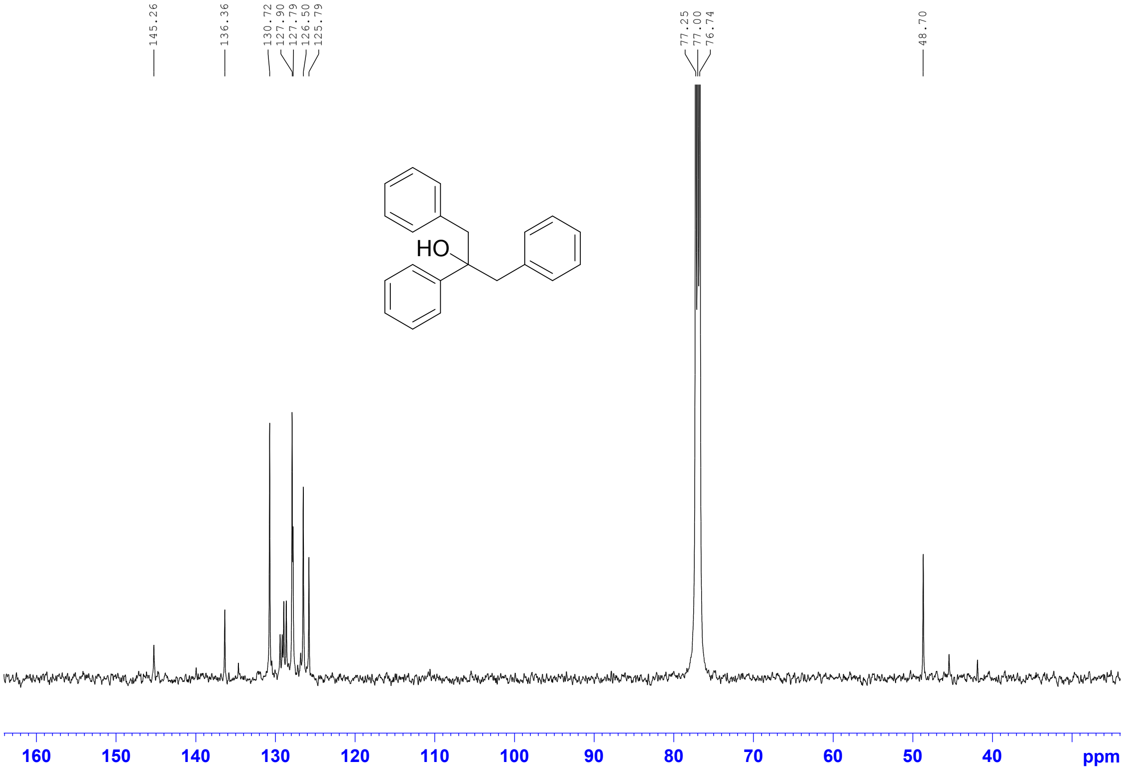
7.151
6.960
6.954
6.949
6.943
3.315
3.288
3.129
3.102
1.892
1.545
0.000
HO
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
11.008
4.017
2.000
2.012
0.980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125.79
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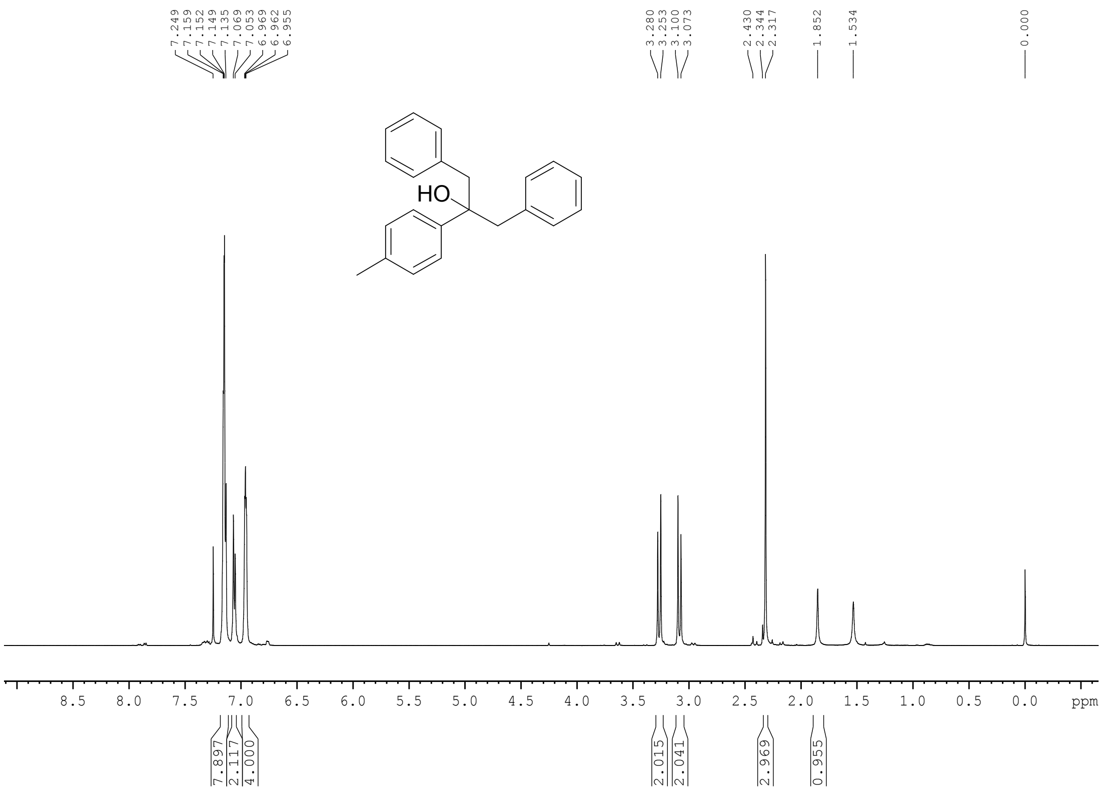
160 150 140 130 120 110 100 90 80 70 60 50 40 ppm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7.135
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6.962
6.955
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3.253
3.100
3.073
2.430
2.344
2.317
1.852
1.534
0.000
HO
8.5 8.0 7.5 7.0 6.5 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 ppm
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2.041
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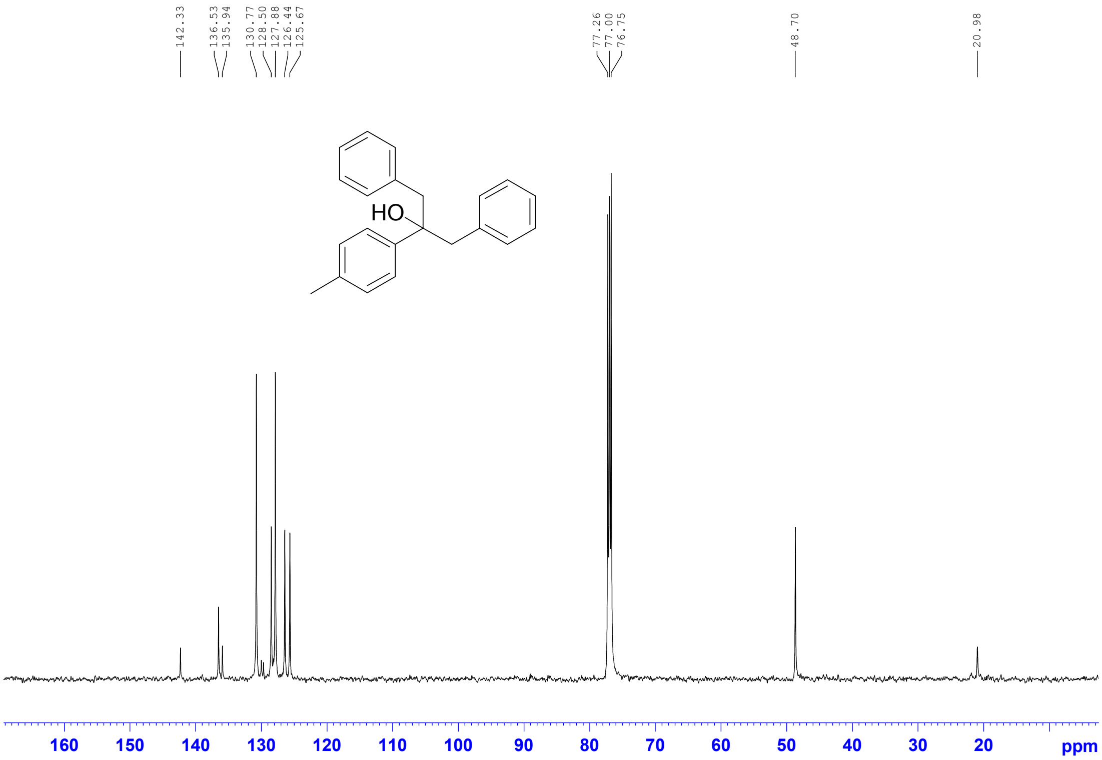
0.955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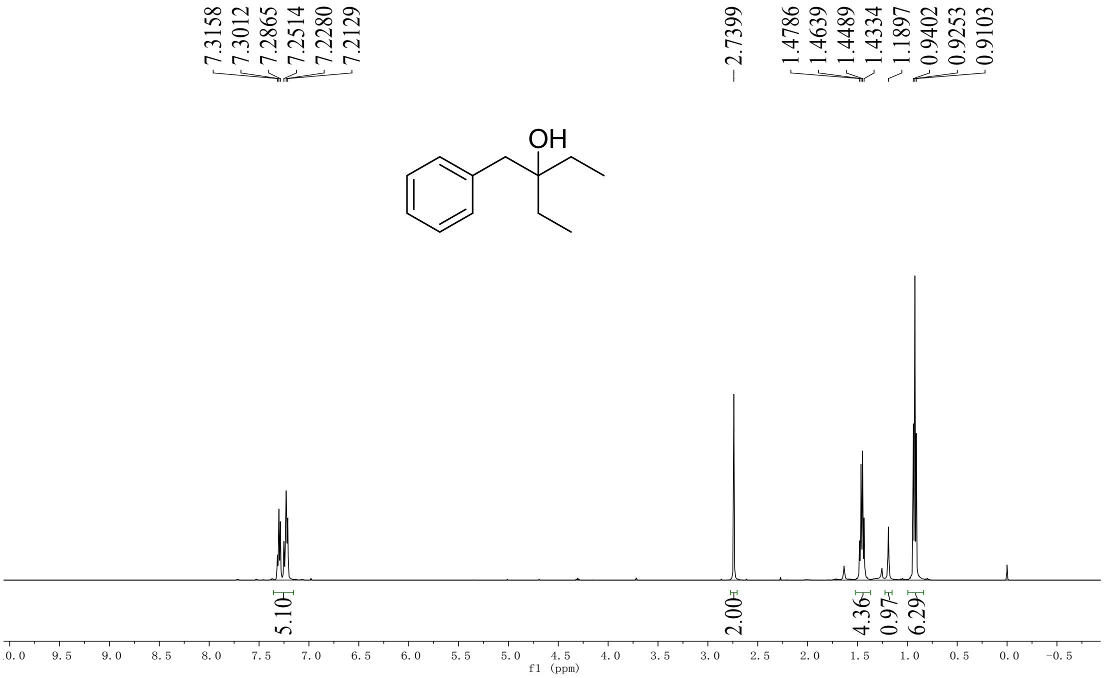
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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1.4489
1.4334
1.1897
0.9402
0.9253
0.9103
OH
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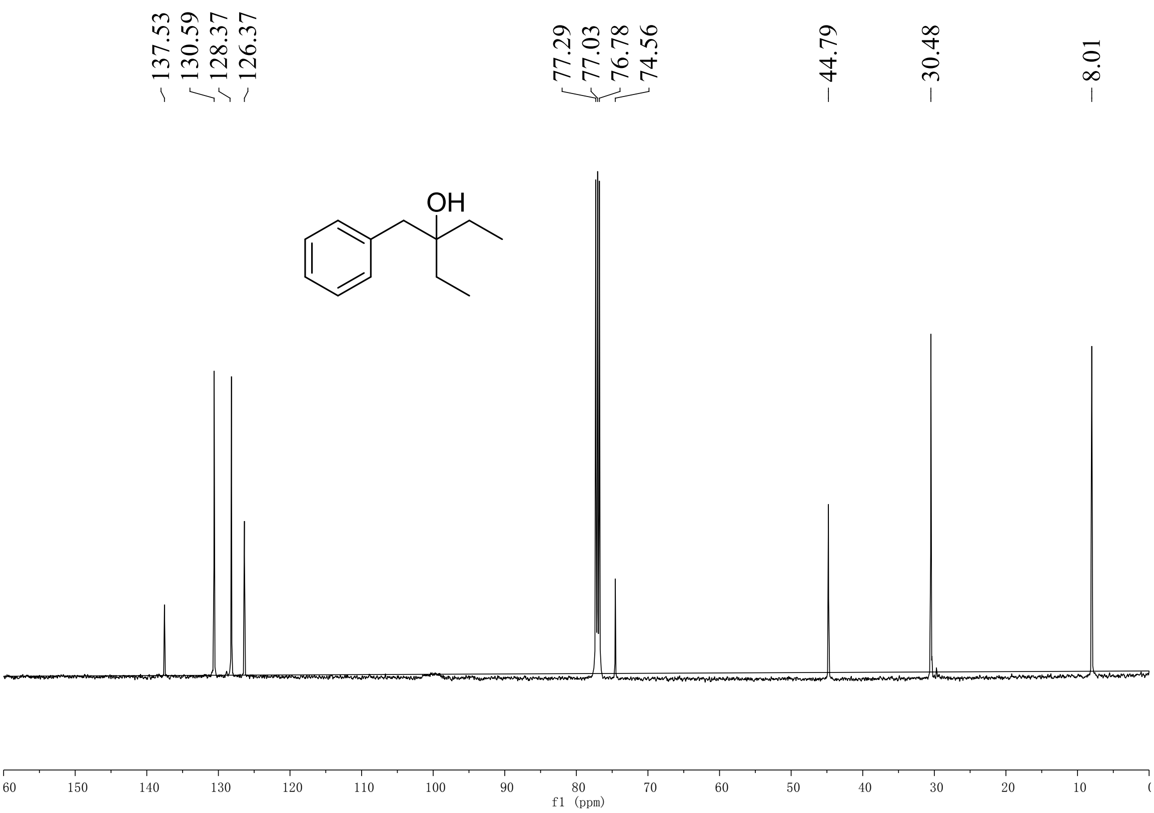
4.36
0.97
6.29
f1 (ppm)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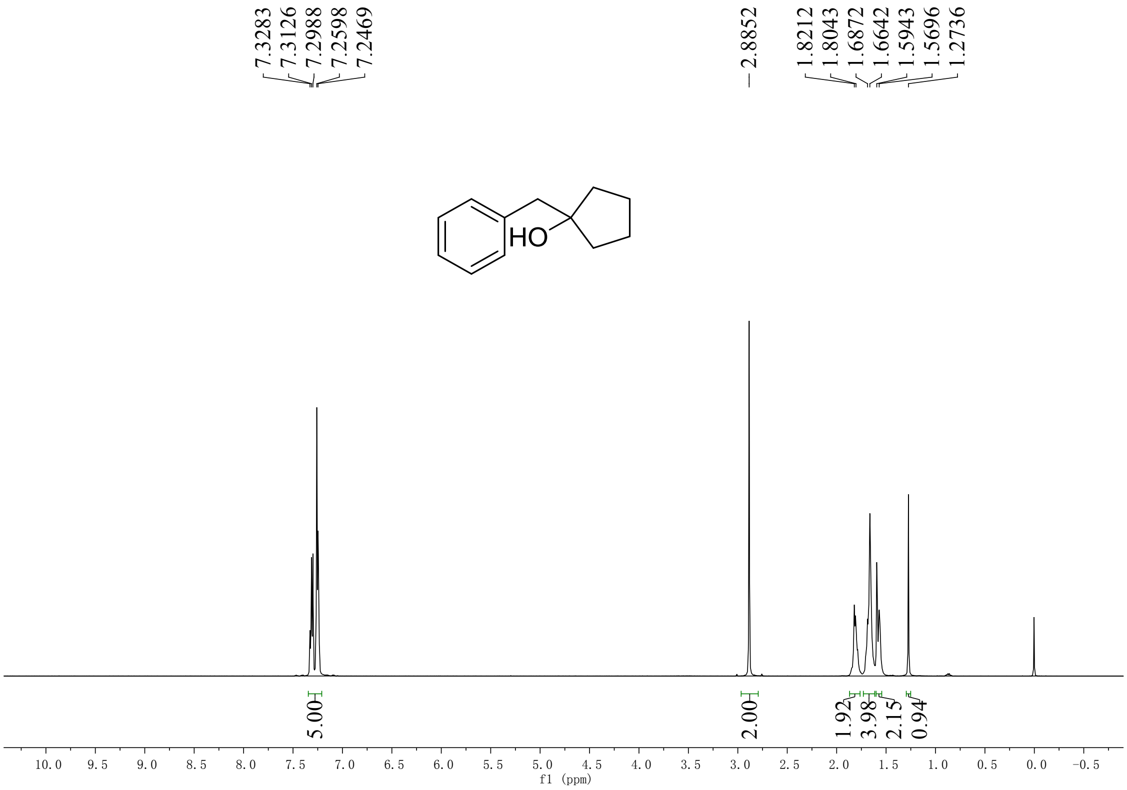
OH
f1 (ppm)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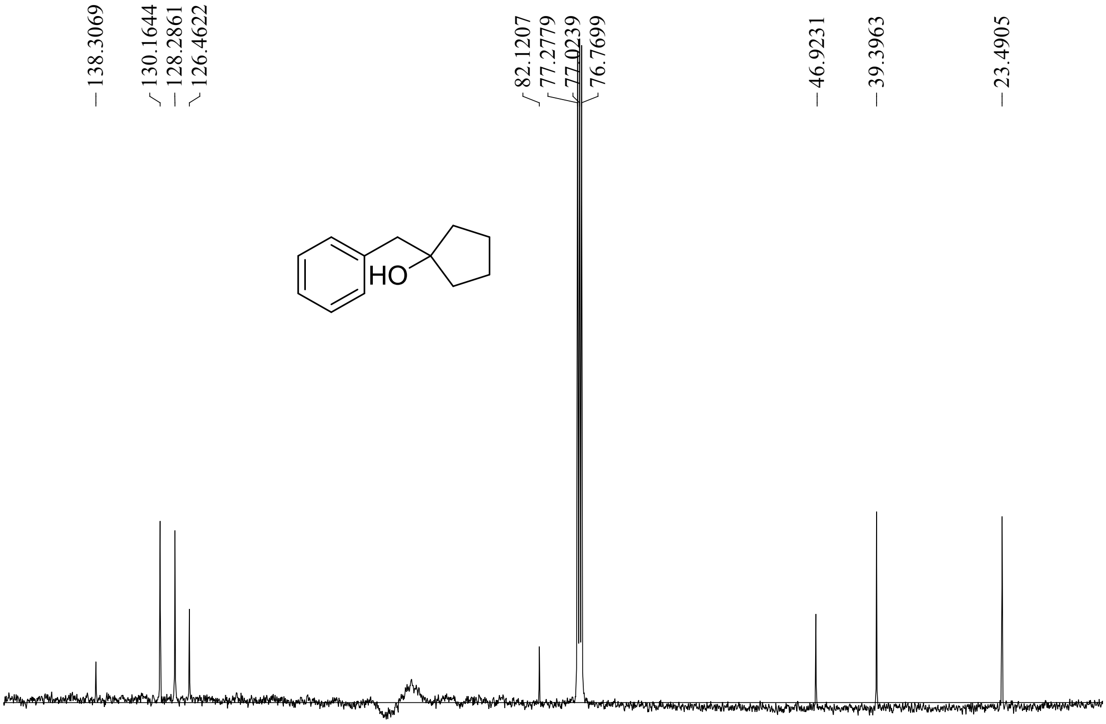
2.15
0.94
f1 (ppm)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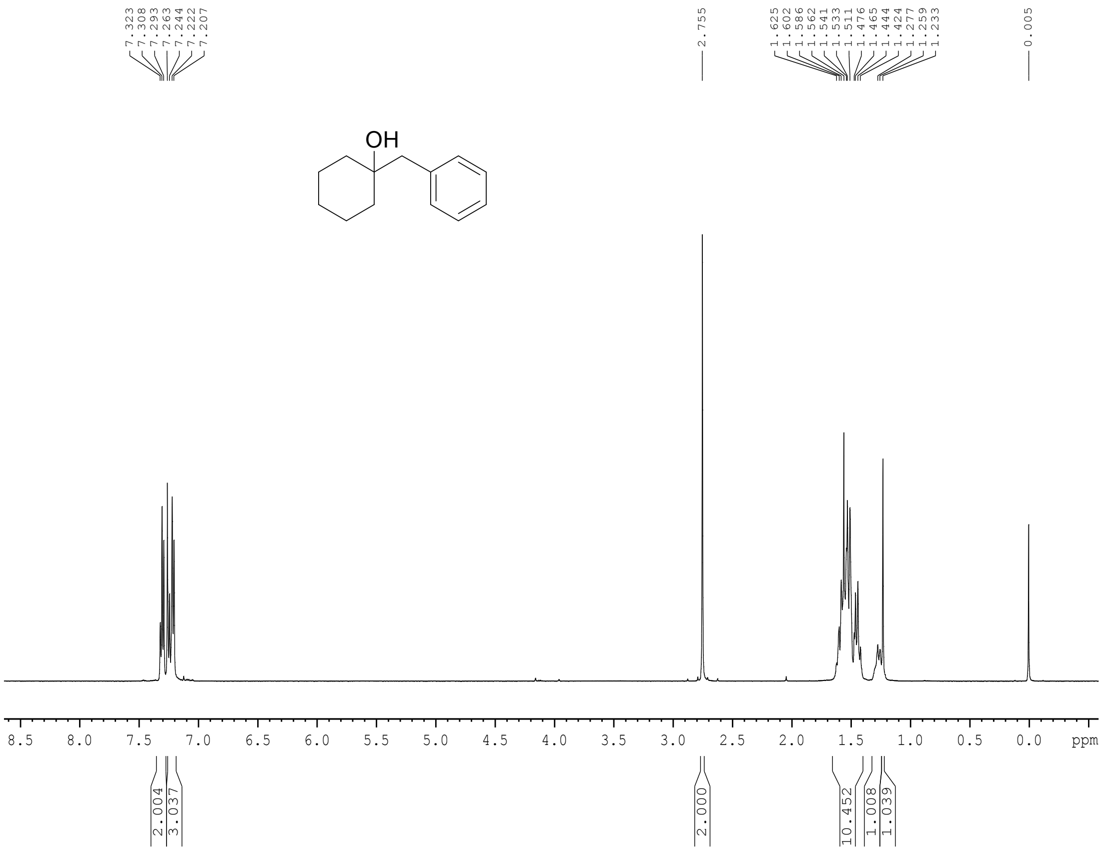
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1.562
1.541
1.533
1.511
1.476
1.465
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2.000
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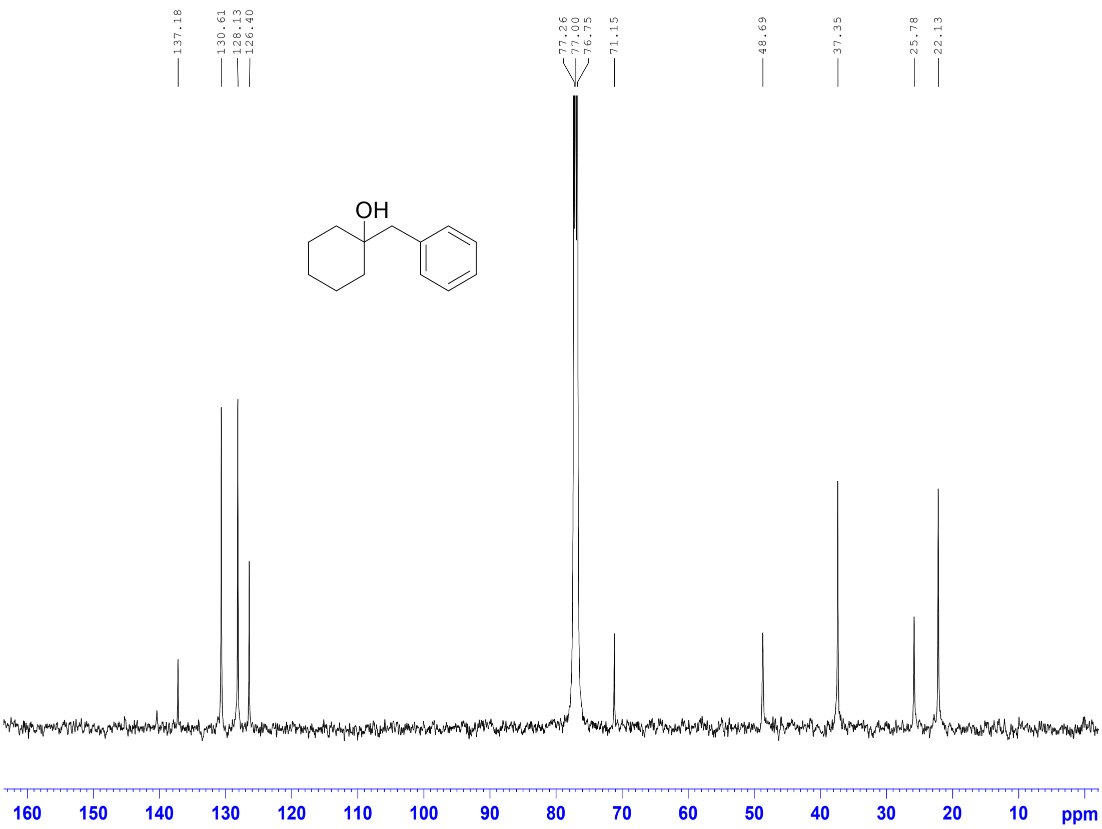
1.039
ppm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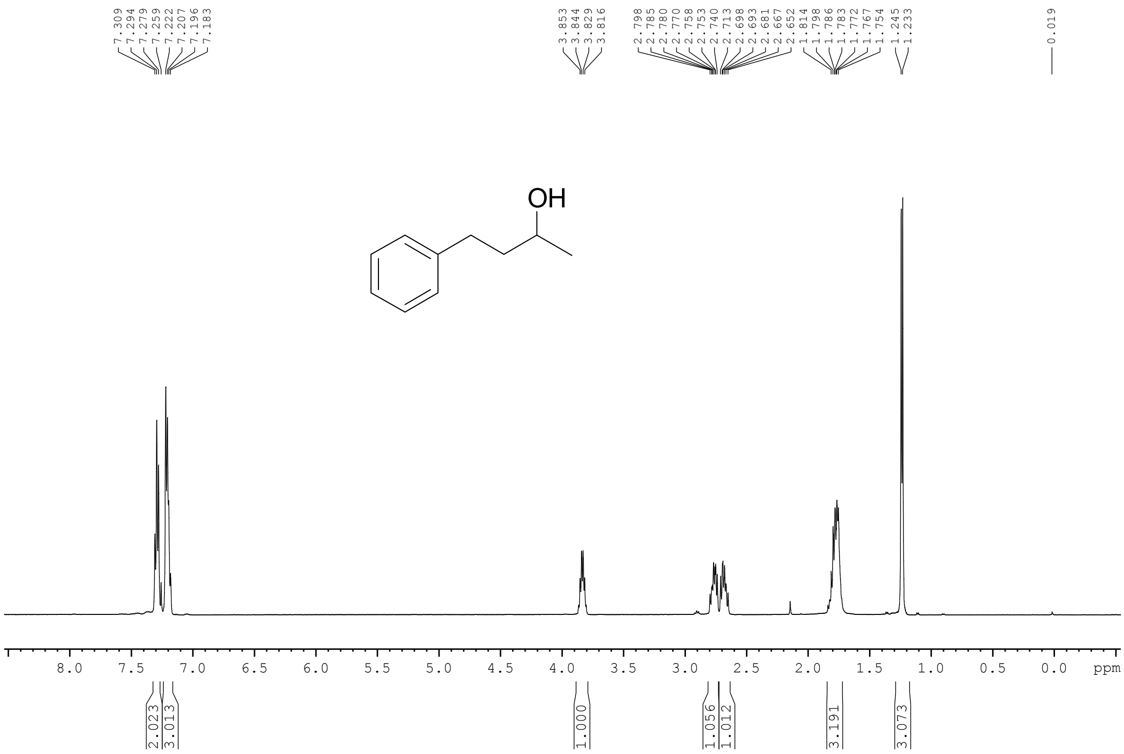
ppm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2.770
2.758
2.753
2.740
2.713
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2.693
2.681
2.667
2.652
1.814
1.798
1.786
1.783
1.772
1.767
1.754
1.245
1.233
0.019
OH
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
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1.012
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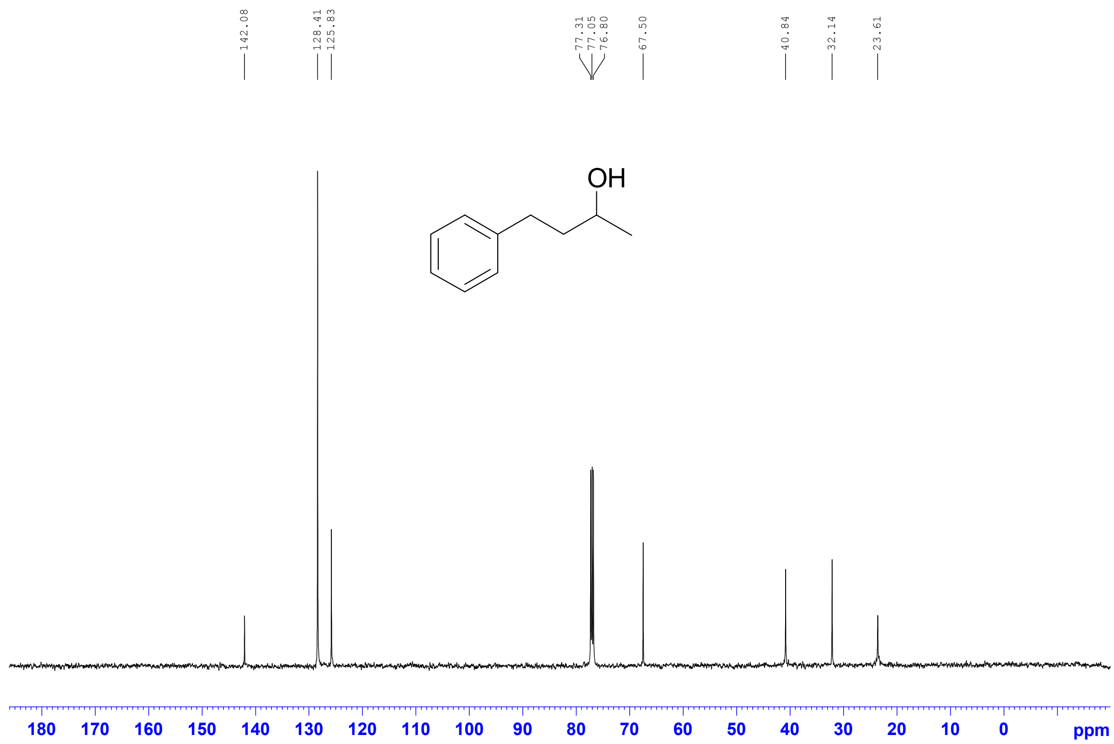
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76.80
67.50
40.84
32.14
23.61
OH
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

7.263
7.112
7.106
2.722
2.341
1.550
1.480
0.018
HO
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 ppm
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9.000
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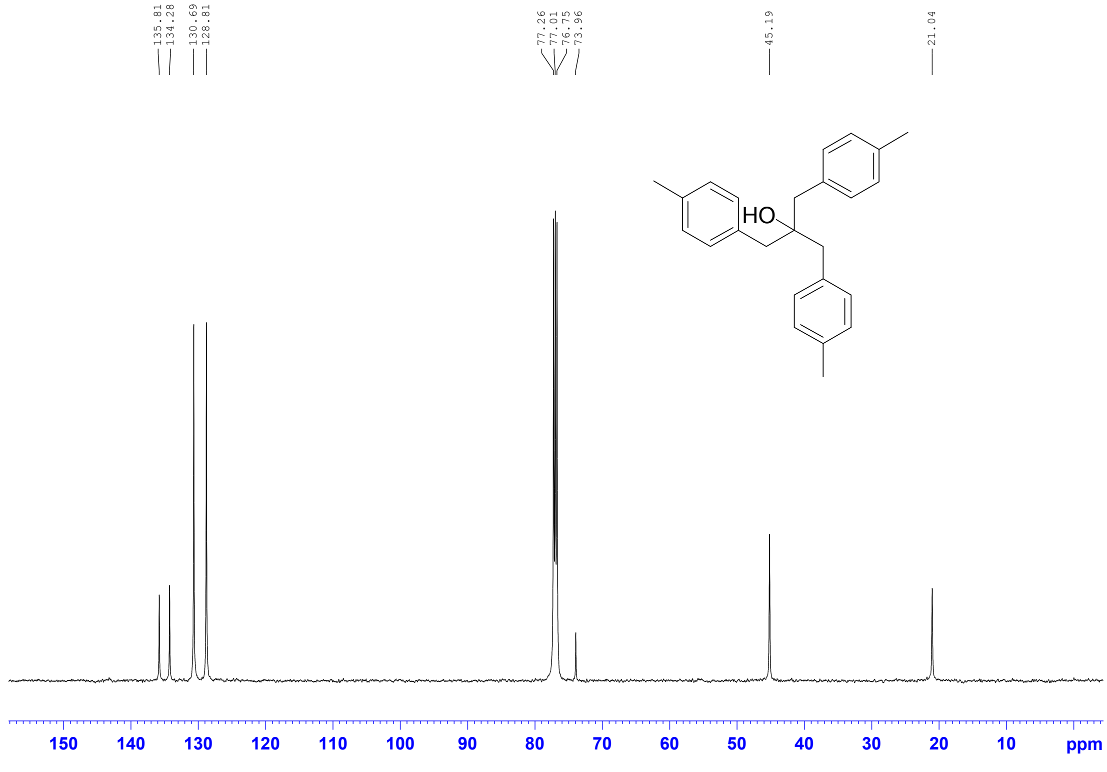

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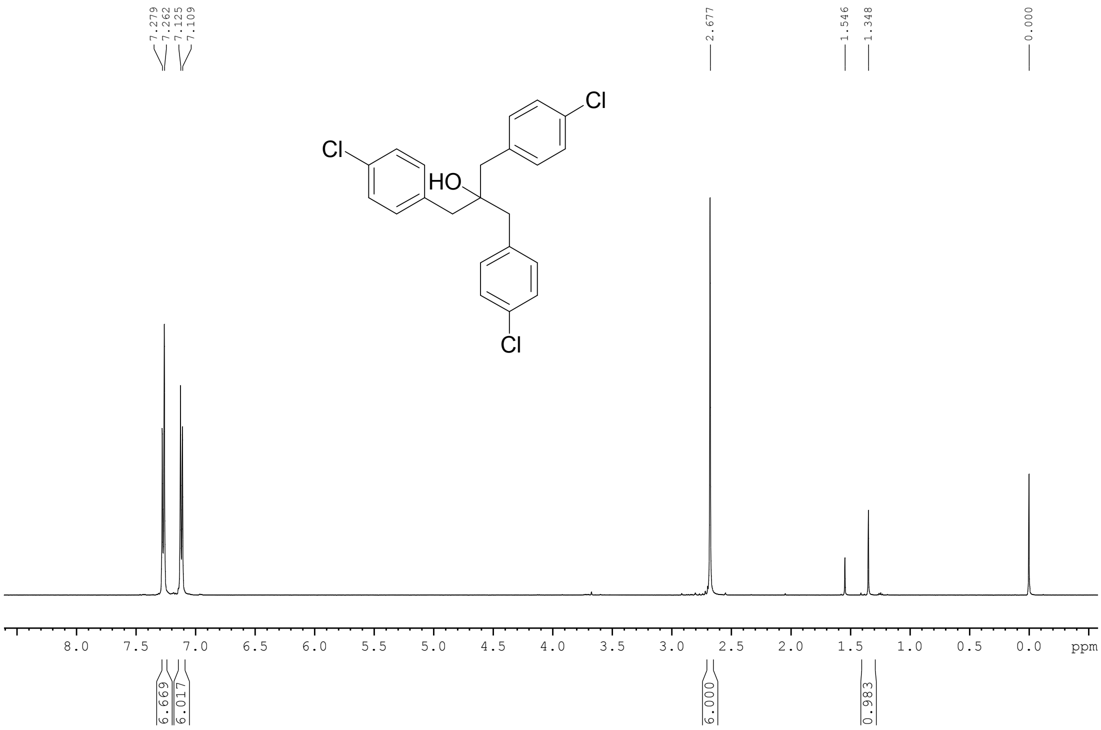
45.19
21.04
HO
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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0.000
Cl
Cl
HO
Cl
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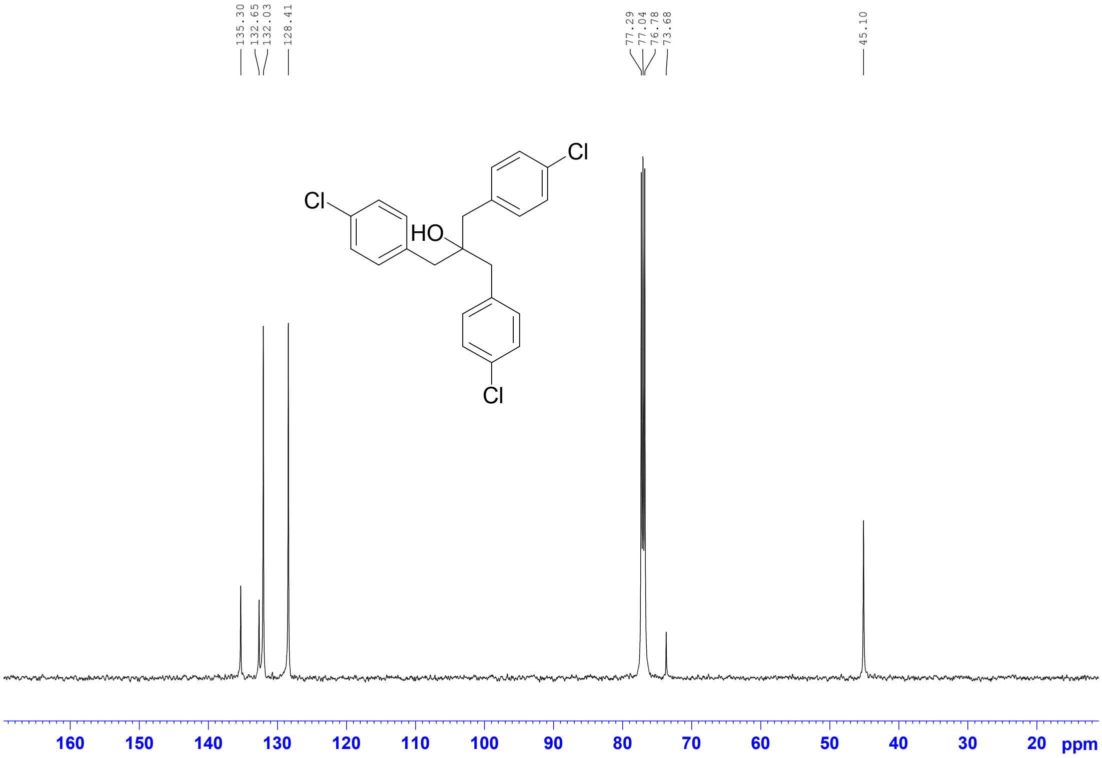
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132.65
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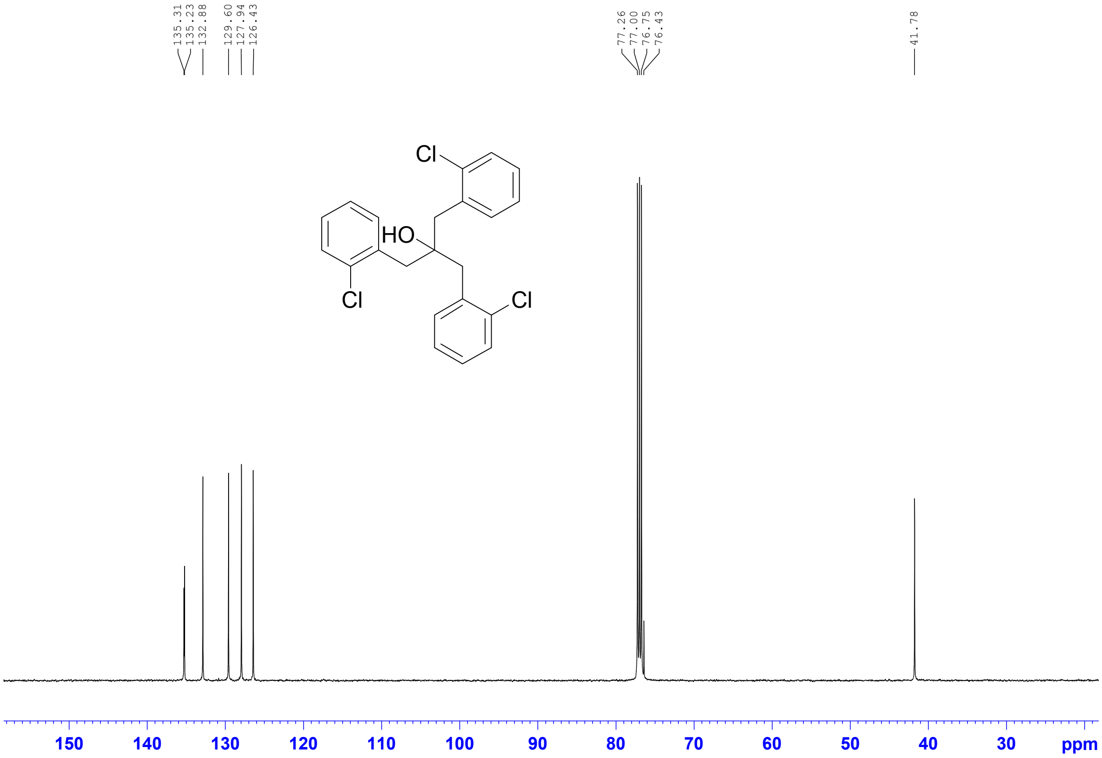
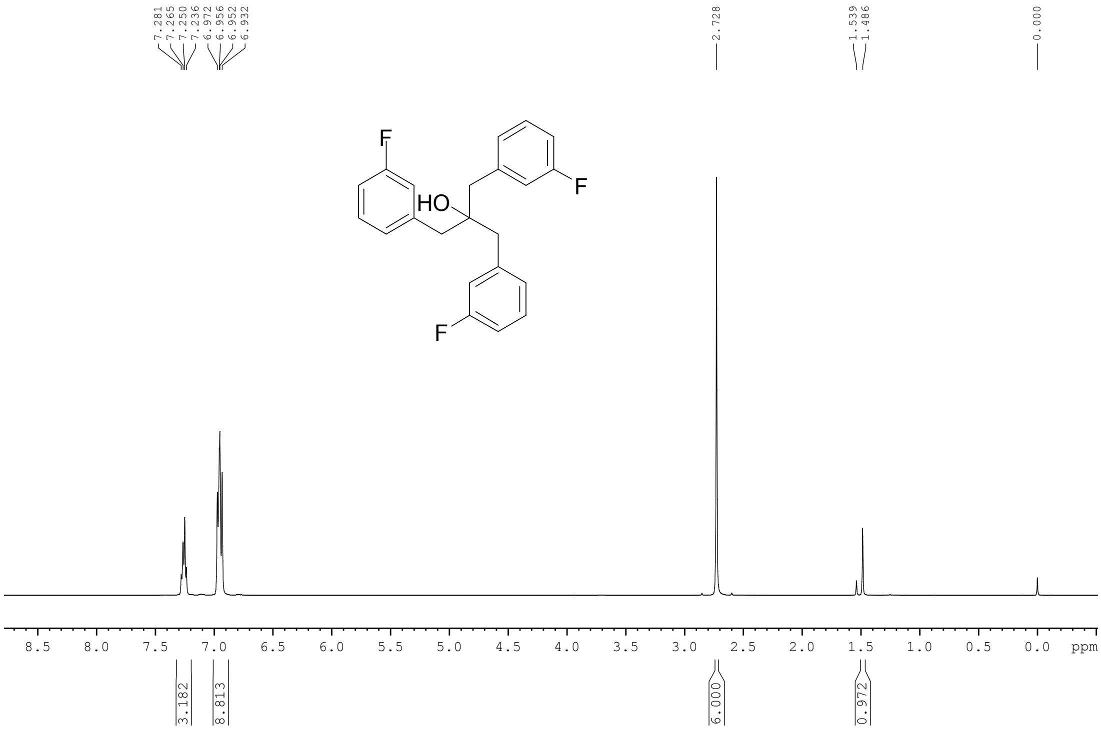
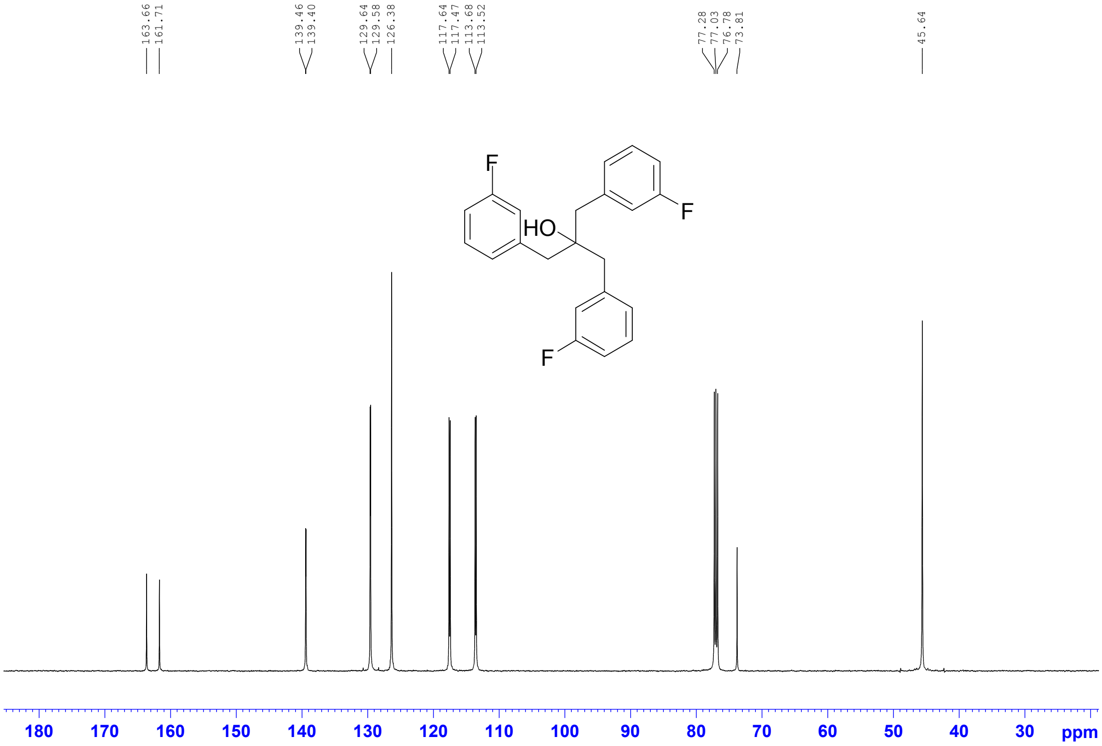
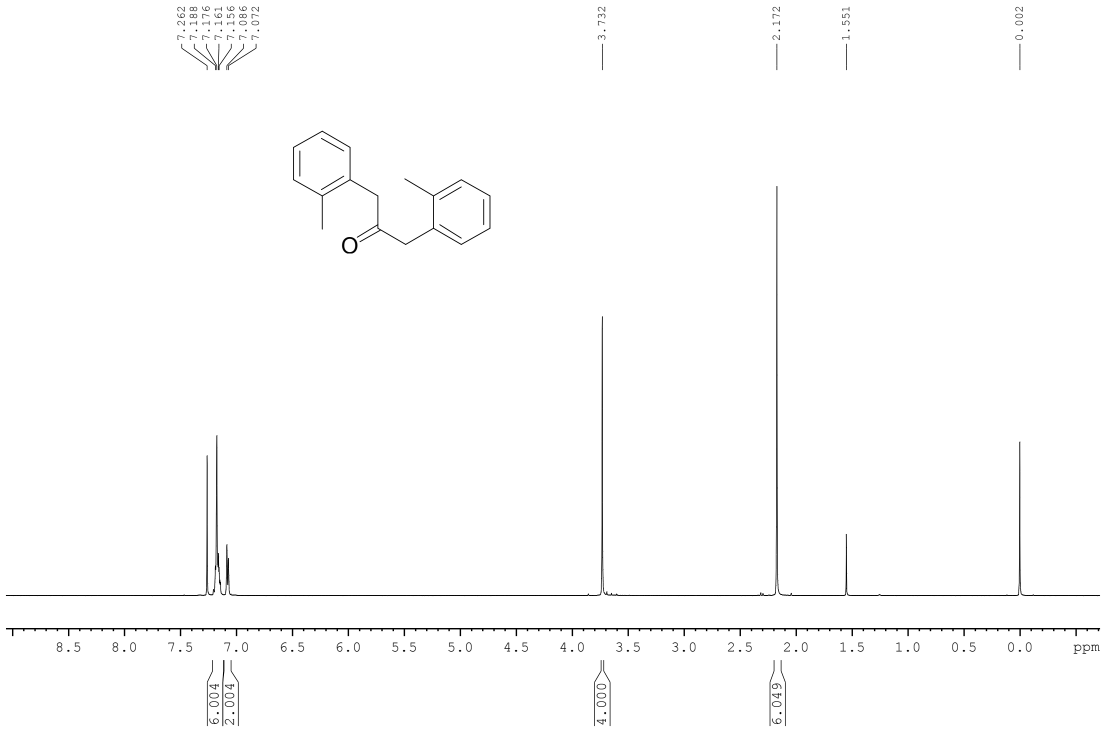
77.29
77.04
76.78
73.68
45.10
Cl
Cl
HO
Cl
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

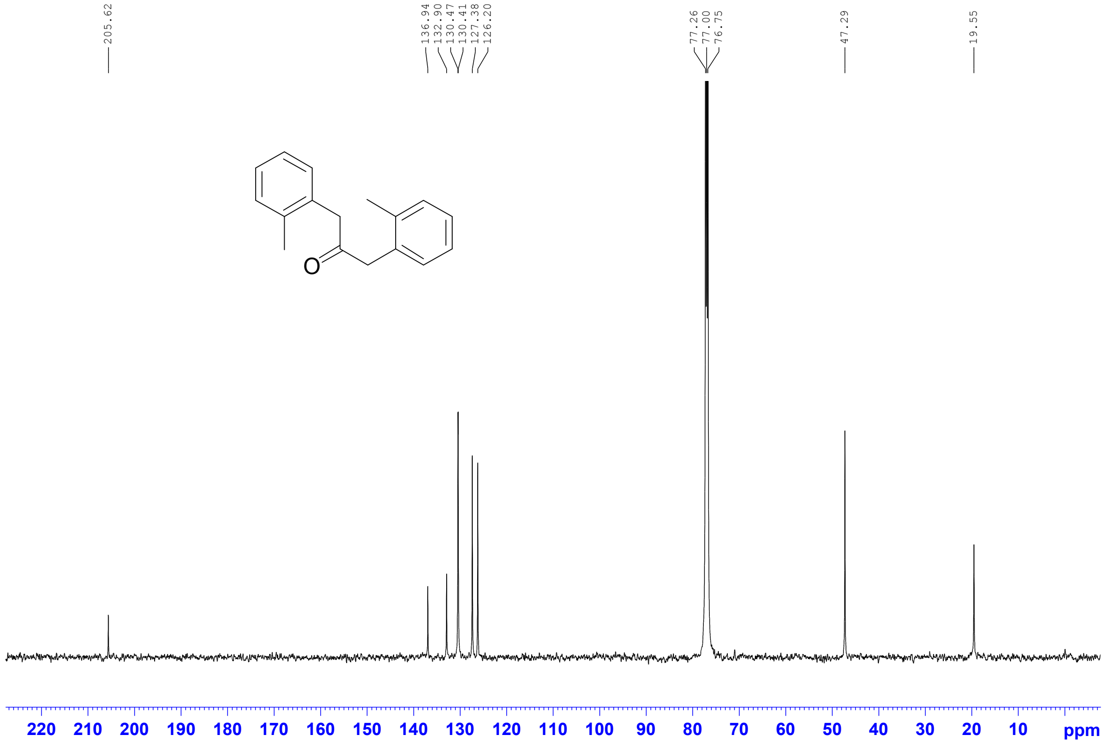

7.380
7.377
7.367
7.362
7.314
7.307
7.300
7.296
7.257
7.200
7.187
7.180
7.173
7.159
3.078
2.008
1.542
0.000
Cl
HO
Cl
Cl
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.938
3.034
6.032
6.000
0.986

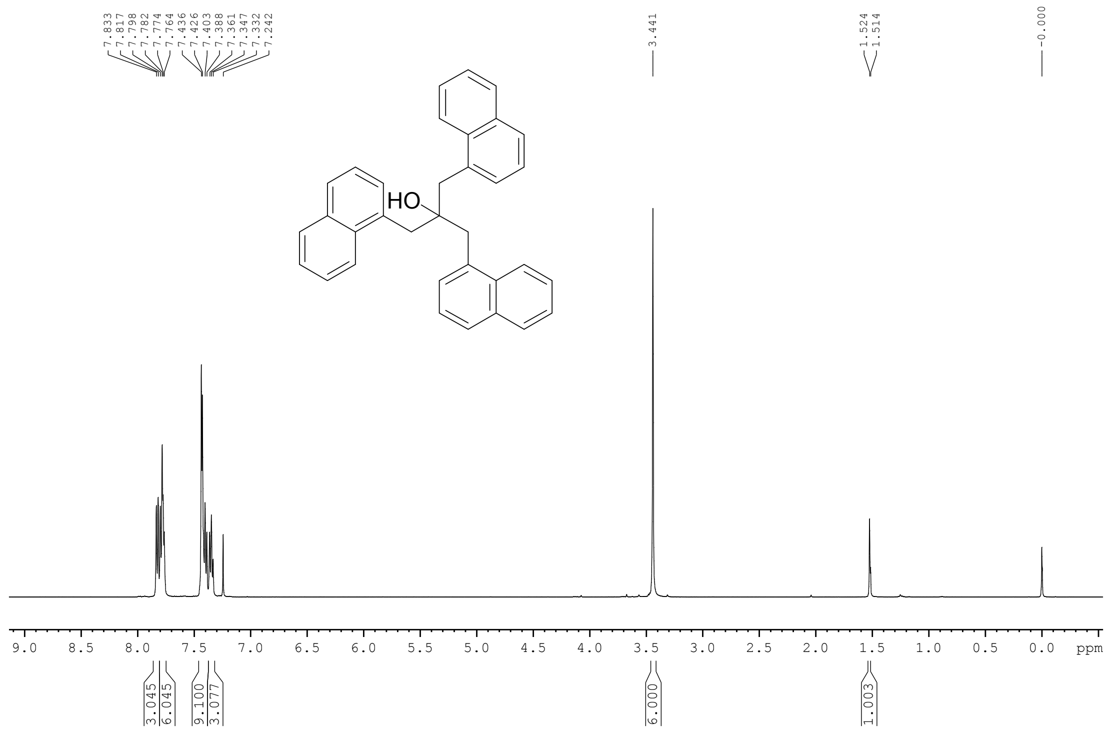

135.31
135.23
132.88
129.60
127.94
126.43
77.26
77.00
76.75
76.43
41.78
Cl
HO
Cl
Cl
150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

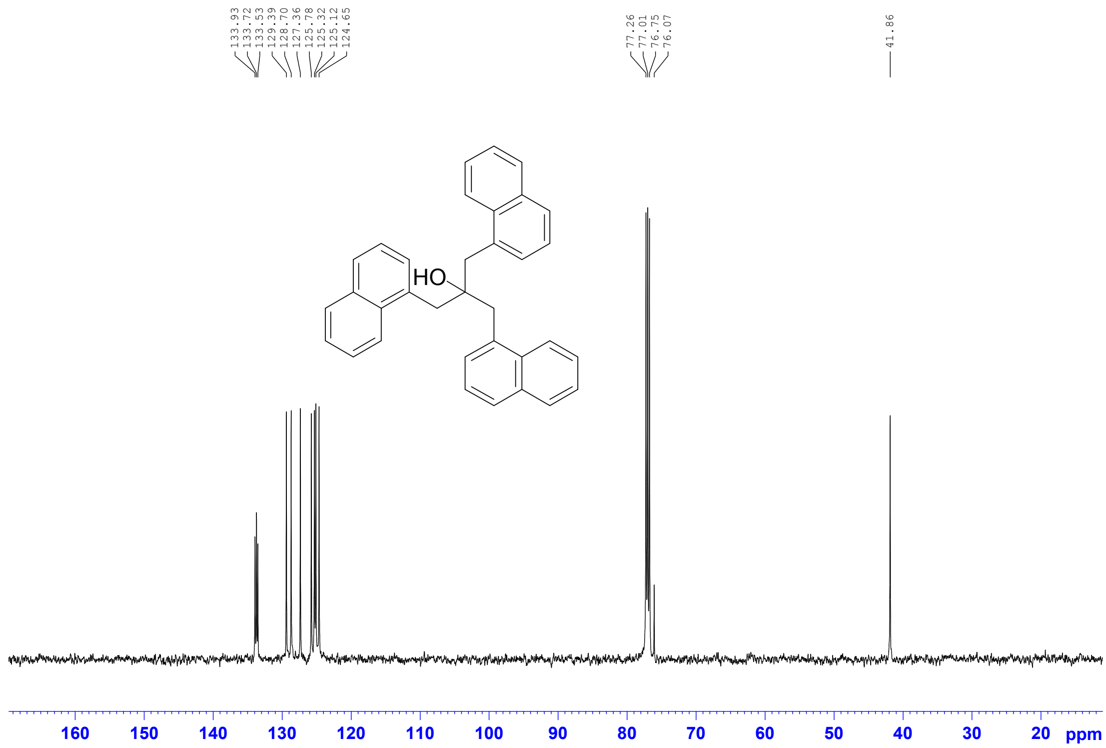

7.281
7.265
7.250
7.236
6.972
6.956
6.952
6.932
2.728
1.539
1.486
0.000
F
HO
F
F
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
3.182
8.813
6.000
0.972

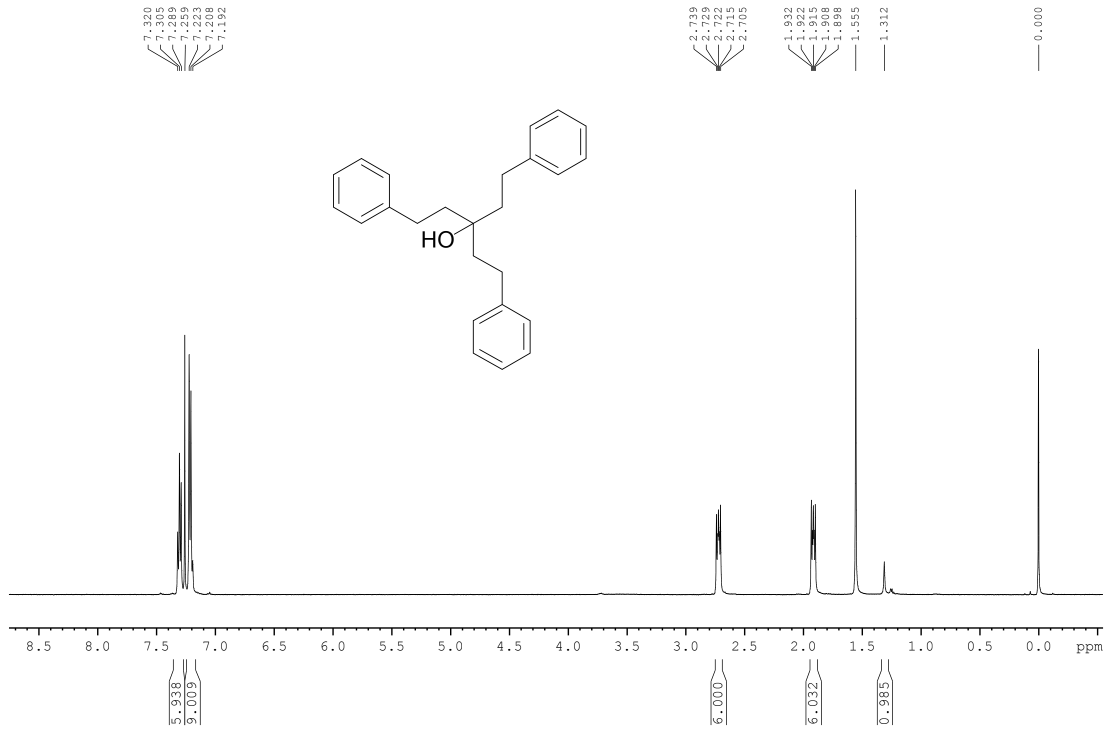

163.66
161.71
139.46
139.40
129.64
129.58
126.38
117.64
117.47
113.68
113.52
77.28
77.03
76.78
73.81
45.64
F
HO
F
F
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

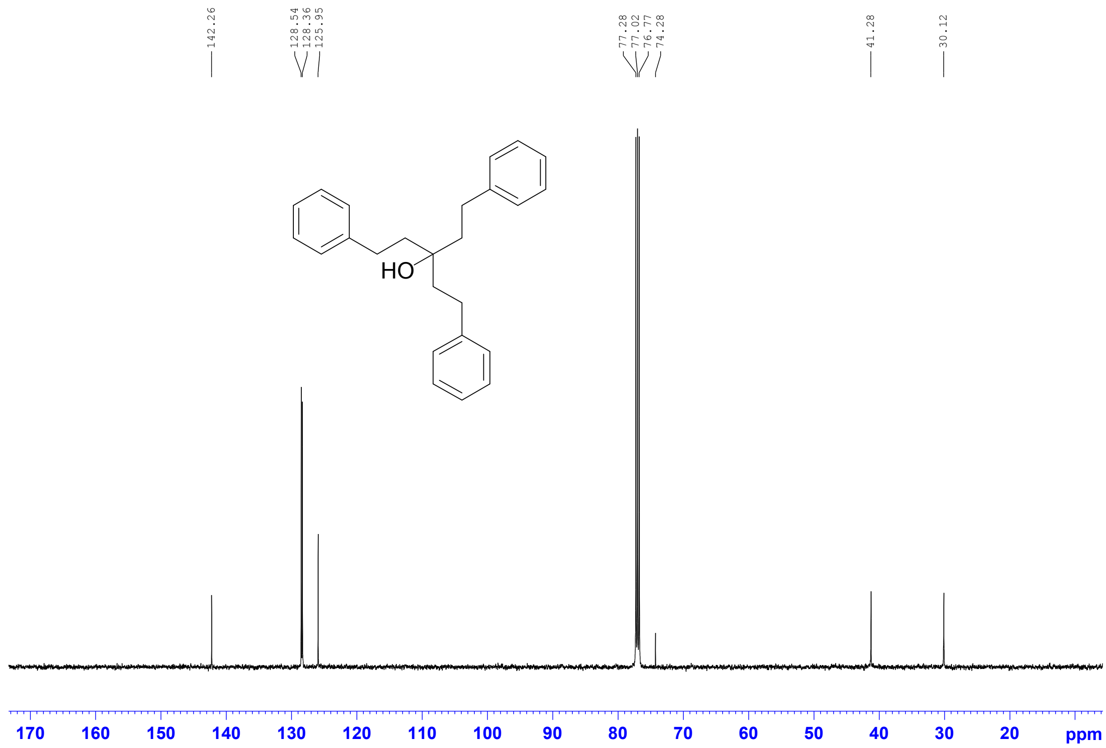

7.262
7.188
7.176
7.161
7.156
7.086
7.072
3.732
2.172
1.551
0.002
O
6.004
2.004
4.000
6.049
ppm

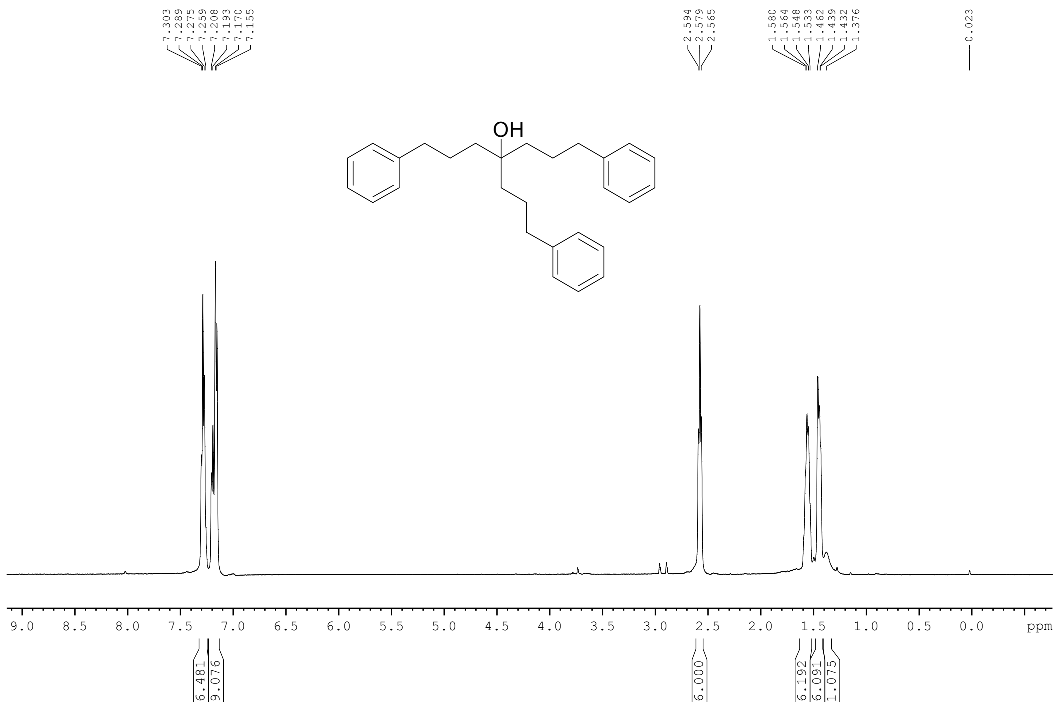

205.62
136.94
132.90
130.47
130.41
127.38
126.20
77.26
77.00
76.75
47.29
19.55
O
ppm

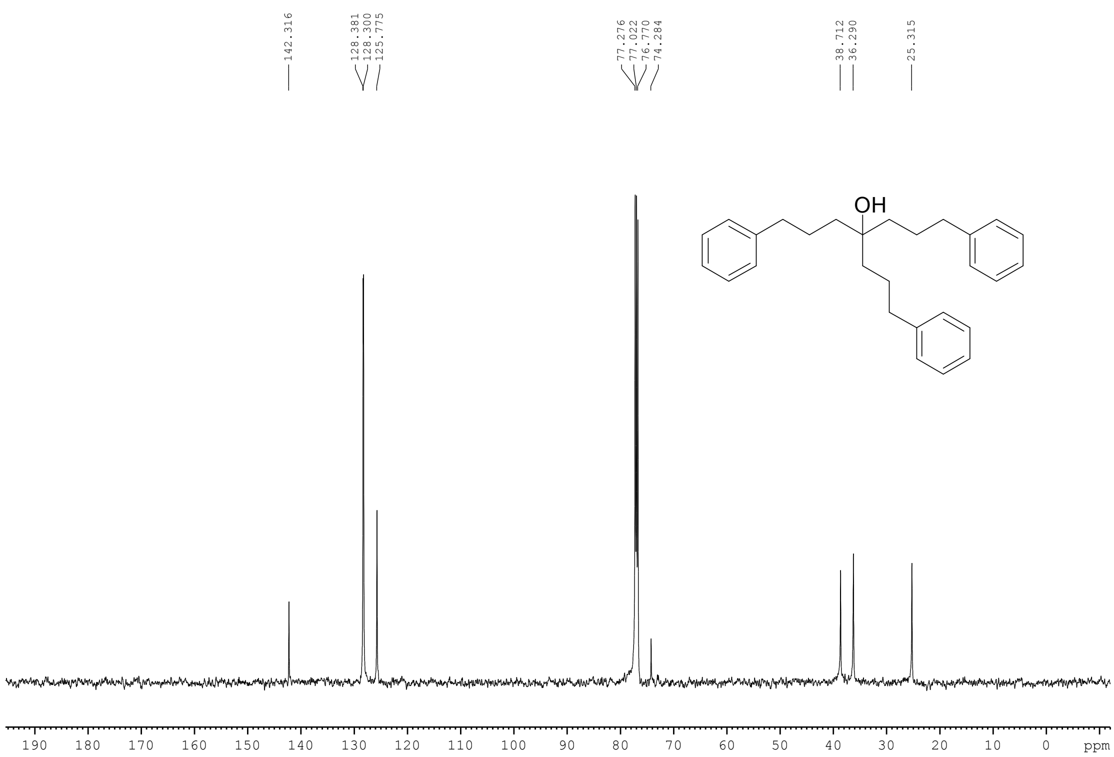


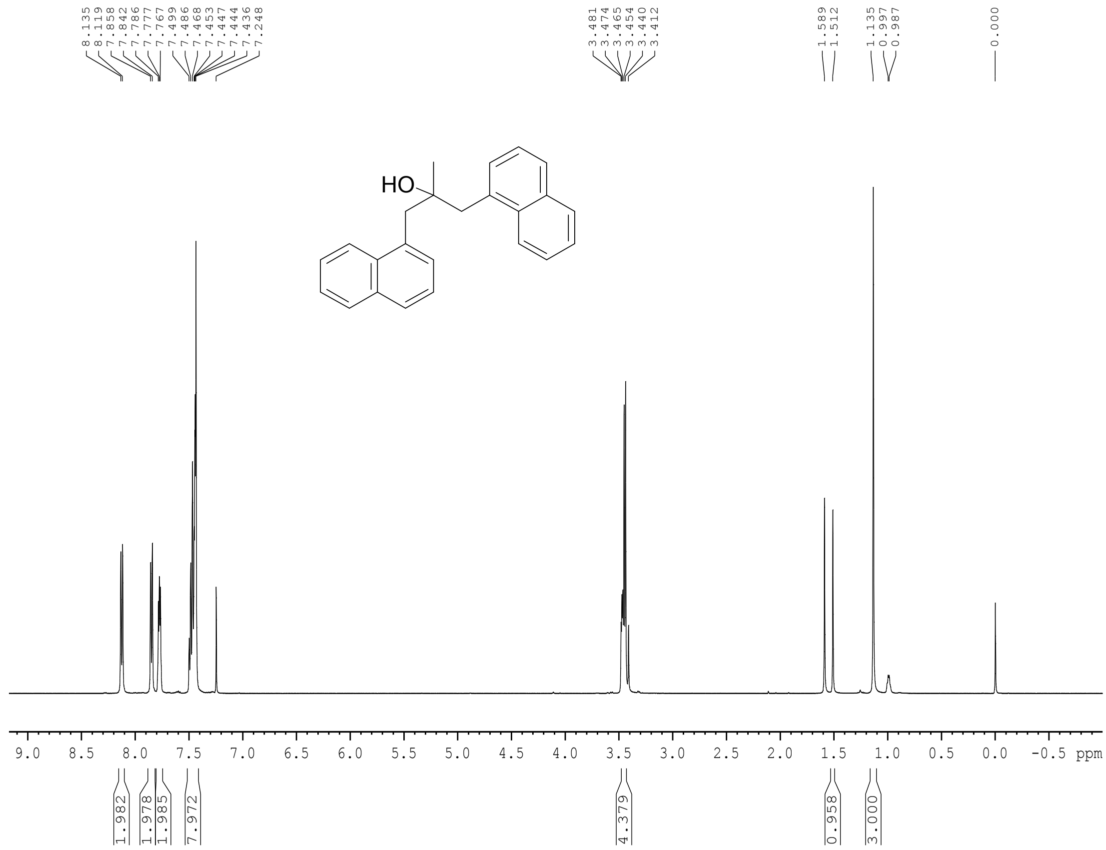


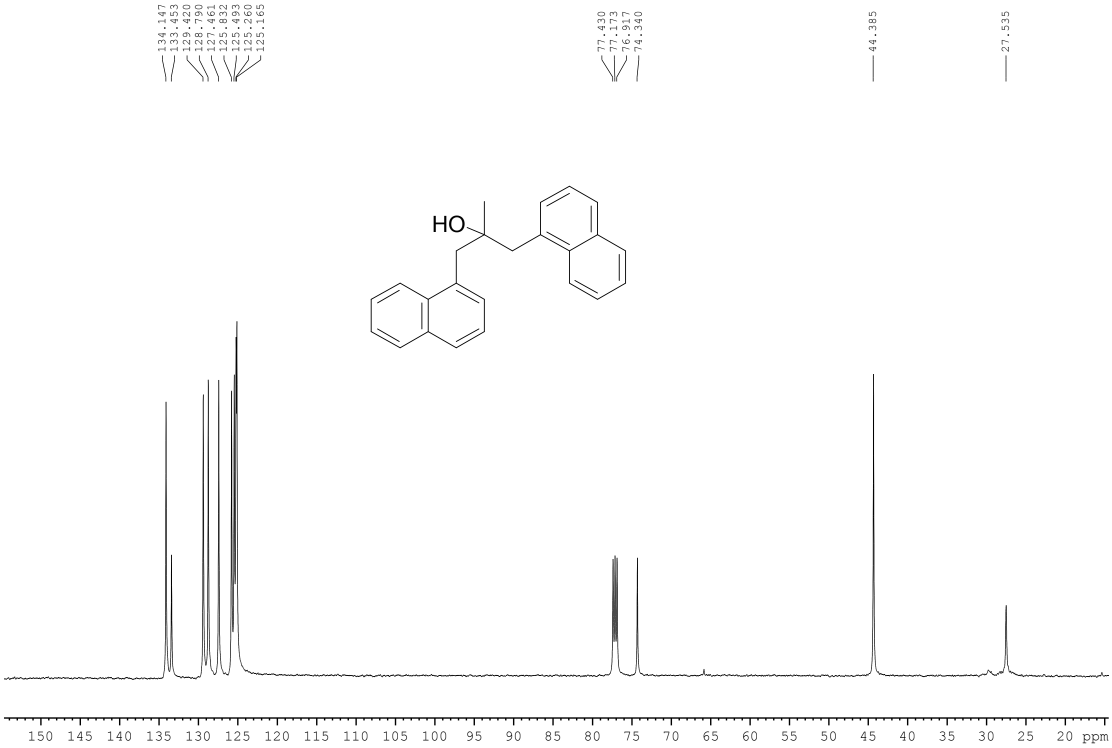

7.320
7.305
7.289
7.259
7.223
7.208
7.192
2.739
2.729
2.722
2.715
2.705
1.932
1.922
1.915
1.908
1.898
1.555
1.312
0.000
HO
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
5.938
9.009
6.000
6.032
0.985

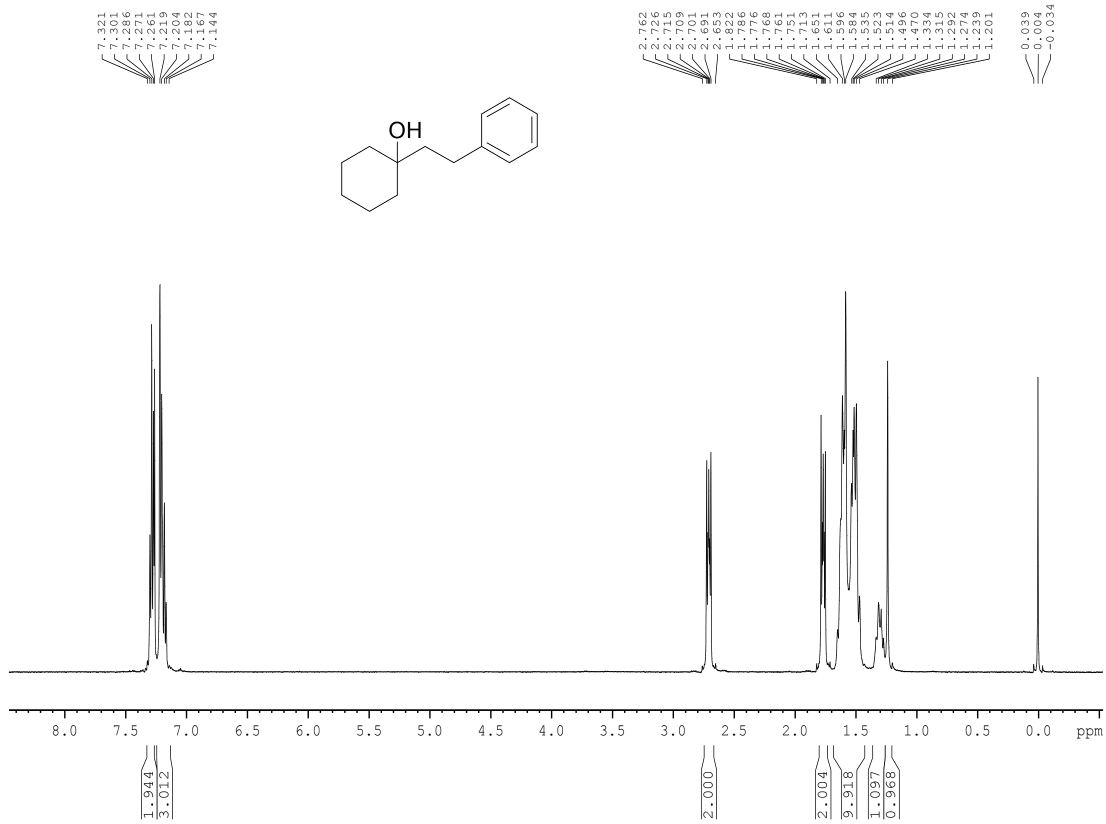

142.26
128.54
128.36
125.95
77.28
77.02
76.77
74.28
41.28
30.12
HO
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

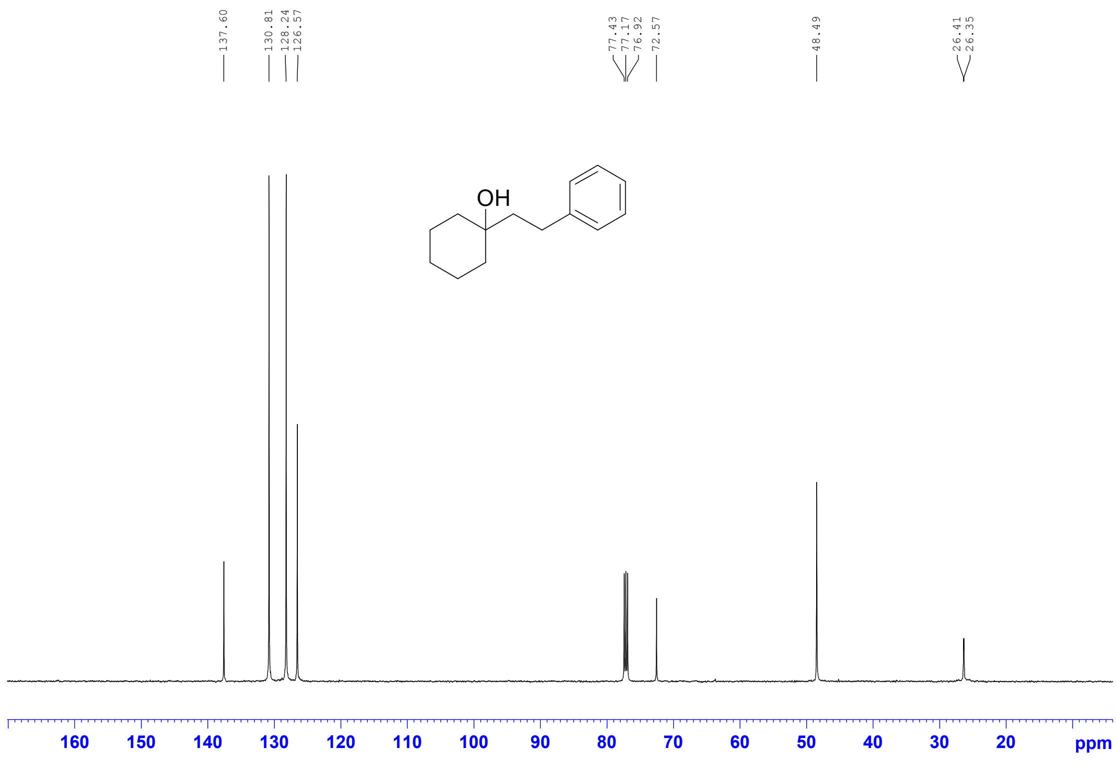

7.303
7.289
7.275
7.259
7.208
7.193
7.170
7.155
2.594
2.579
2.565
1.580
1.564
1.548
1.533
1.462
1.439
1.432
1.376
0.023
OH
6.481
9.076
6.000
6.192
6.091
1.075
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

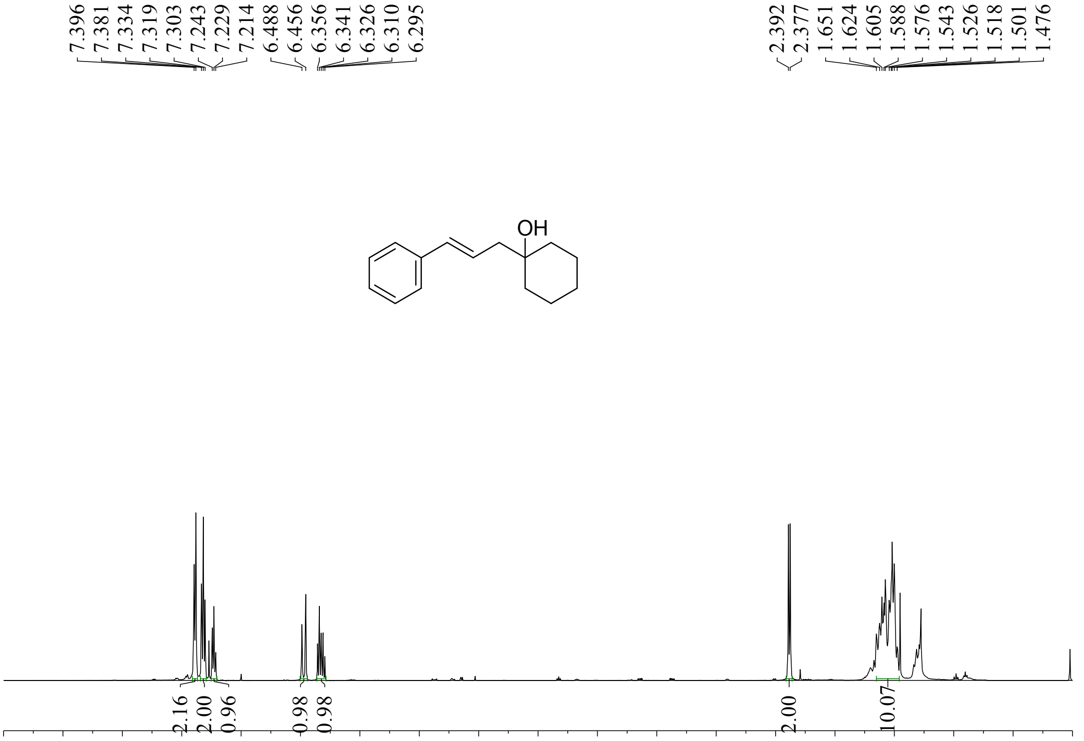

142.316
128.381
128.300
125.775
77.276
77.022
76.770
74.284
38.712
36.290
25.315
OH
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

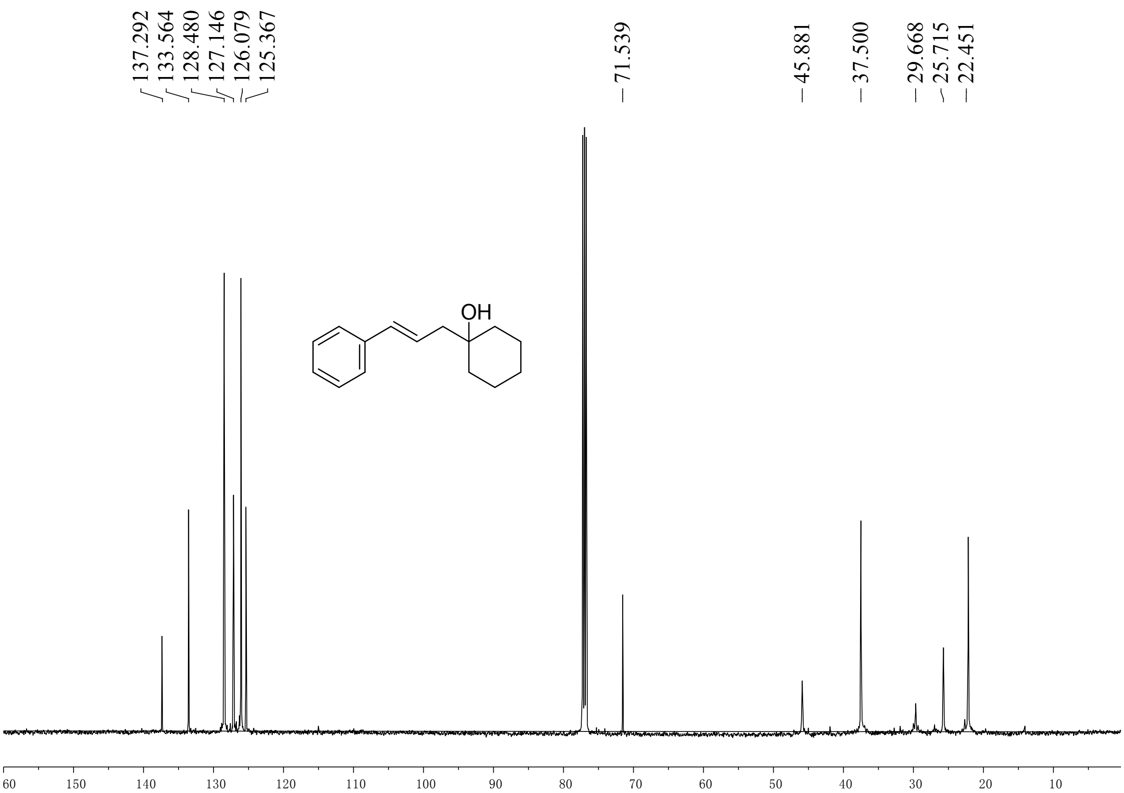

8.135 8.119 7.858 7.842 7.786 7.777 7.767 7.499 7.486 7.468 7.453 7.447 7.444 7.436 7.248
3.481 3.474 3.465 3.454 3.440 3.412
1.589 1.512
1.135 0.997 0.987
0.000
HO
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 ppm
1.982 1.978 1.985 7.972
4.379
0.958 3.000

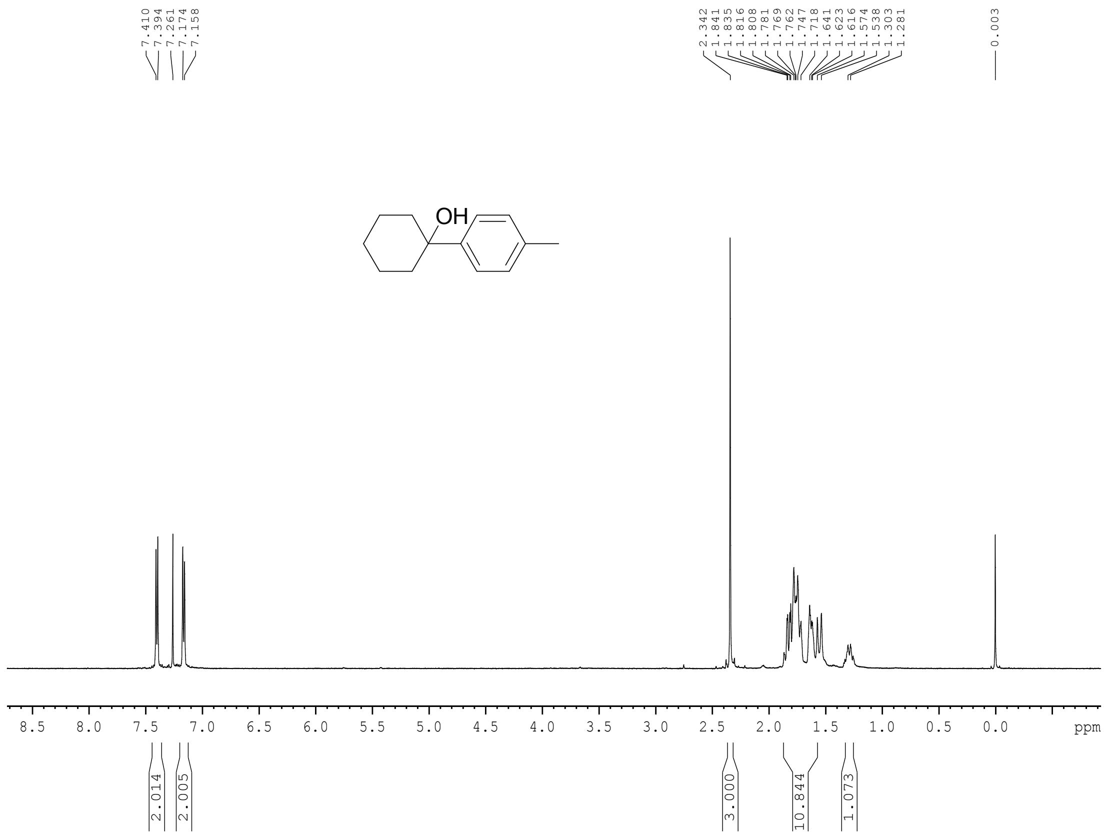

134.147 133.453 129.420 128.790 127.461 125.832 125.493 125.260 125.165
77.430 77.173 76.917 74.340
44.385
27.535
HO
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 ppm

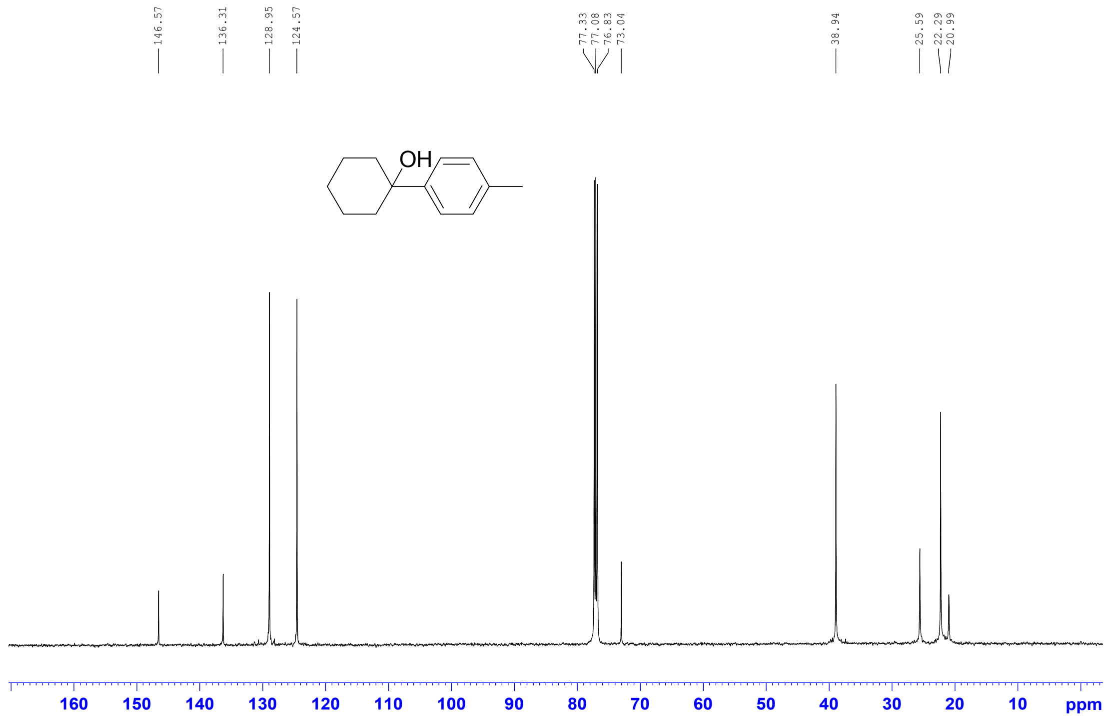

7.321
7.301
7.286
7.271
7.261
7.219
7.204
7.182
7.167
7.144
2.762
2.726
2.715
2.709
2.701
2.691
2.653
1.822
1.786
1.776
1.768
1.761
1.751
1.713
1.651
1.611
1.596
1.584
1.535
1.523
1.514
1.496
1.470
1.334
1.315
1.292
1.274
1.239
1.201
0.039
0.004
-0.034
OH
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.944
3.012
2.000
2.004
9.918
1.097
0.968

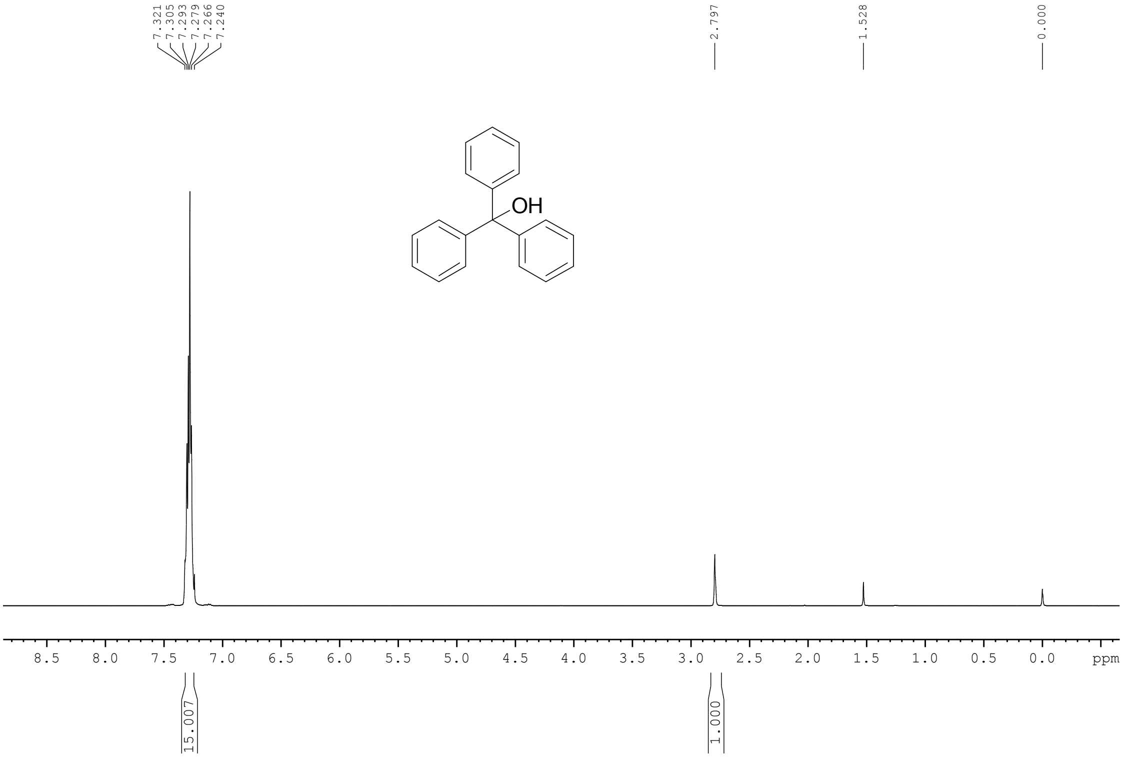

137.60
130.81
128.24
126.57
77.43
77.17
76.92
72.57
48.49
26.41
26.35
OH
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

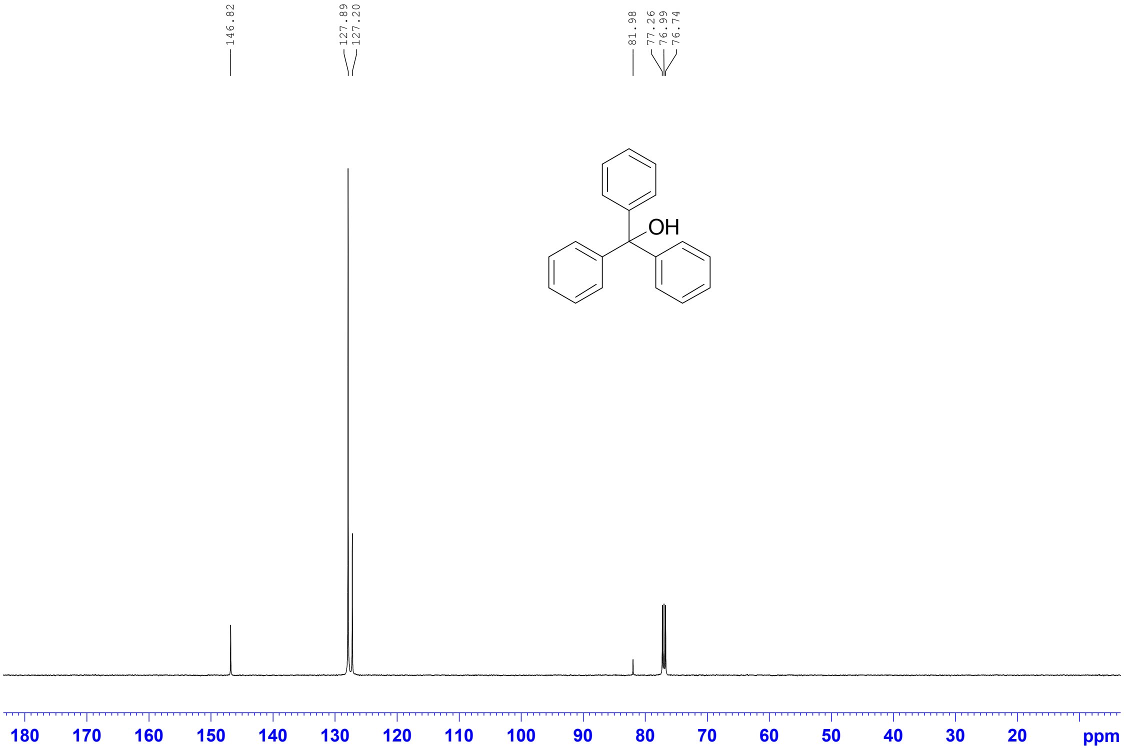

7.396
7.381
7.334
7.319
7.303
7.243
7.229
7.214
6.488
6.456
6.356
6.341
6.326
6.310
6.295
2.392
2.377
1.651
1.624
1.605
1.588
1.576
1.543
1.526
1.518
1.501
1.476
OH
2.16
2.00
0.96
0.98
0.98
2.00
10.07
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

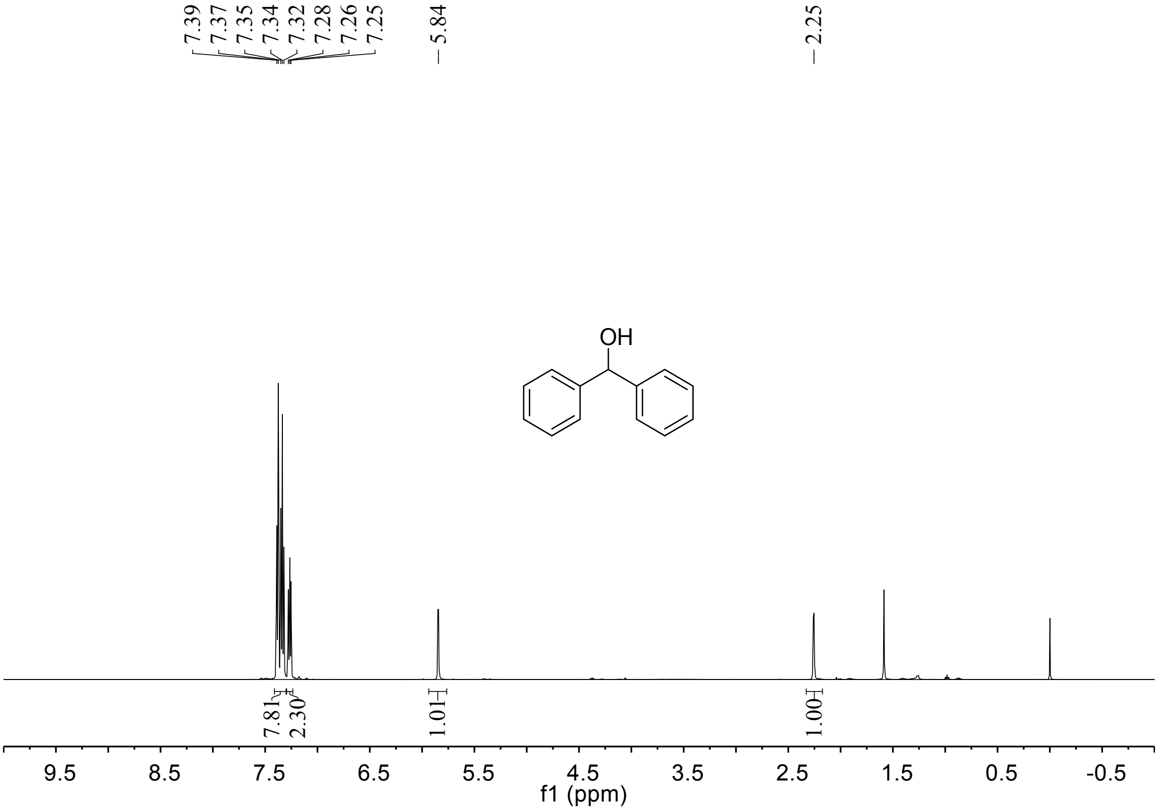

137.292
133.564
128.480
127.146
126.079
125.367
71.539
45.881
37.500
29.668
25.715
22.451
OH
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

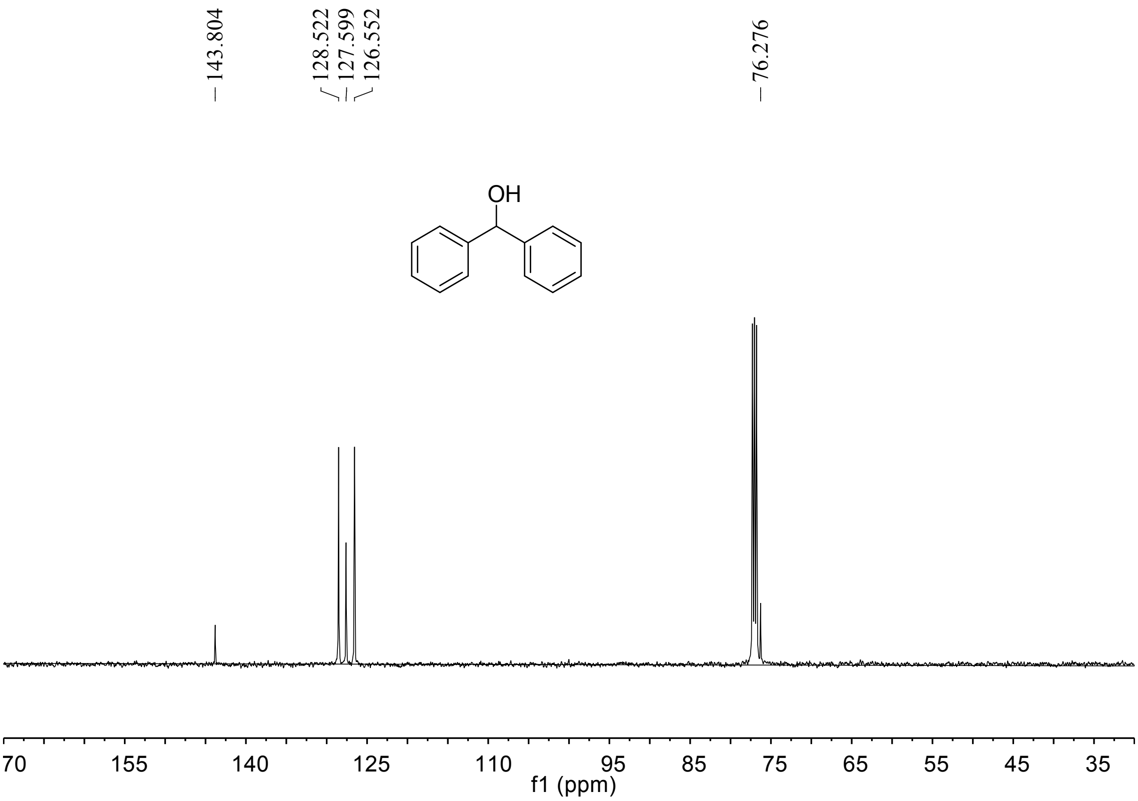

7.410
7.394
7.261
7.174
7.158
2.342
1.841
1.835
1.816
1.808
1.781
1.769
1.762
1.747
1.718
1.641
1.623
1.616
1.574
1.538
1.303
1.281
0.003
OH
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.014
2.005
3.000
10.844
1.073

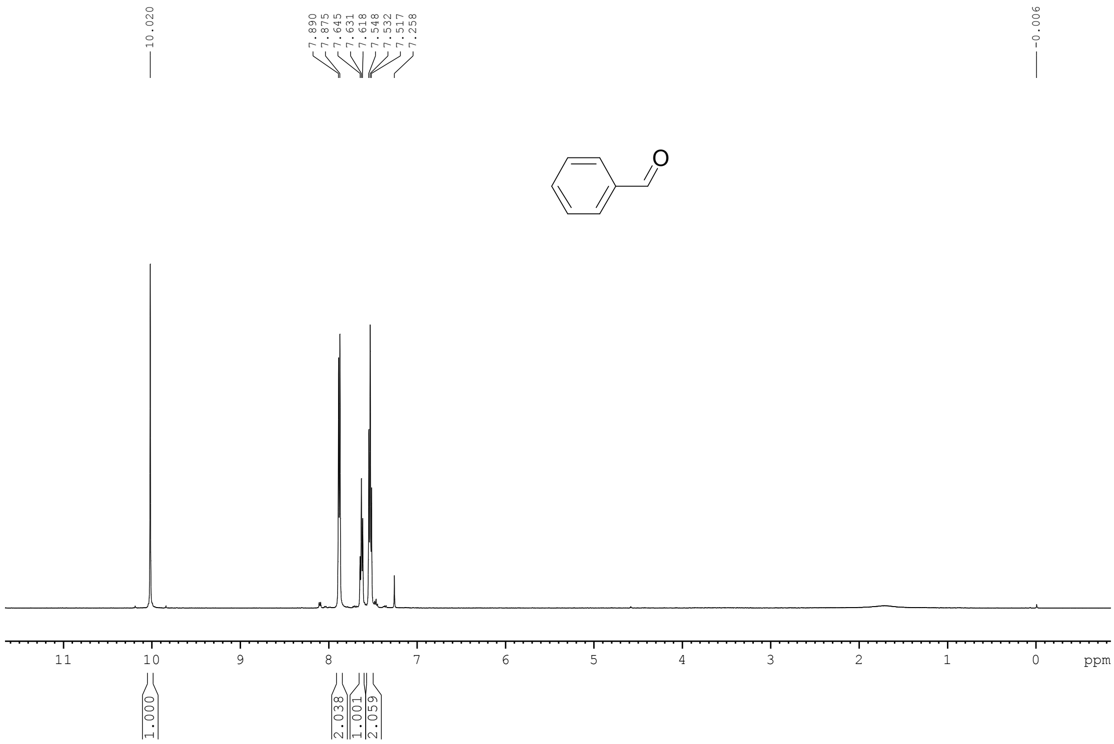

146.57
136.31
128.95
124.57
77.33
77.08
76.83
73.04
38.94
25.59
22.29
20.99
OH
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

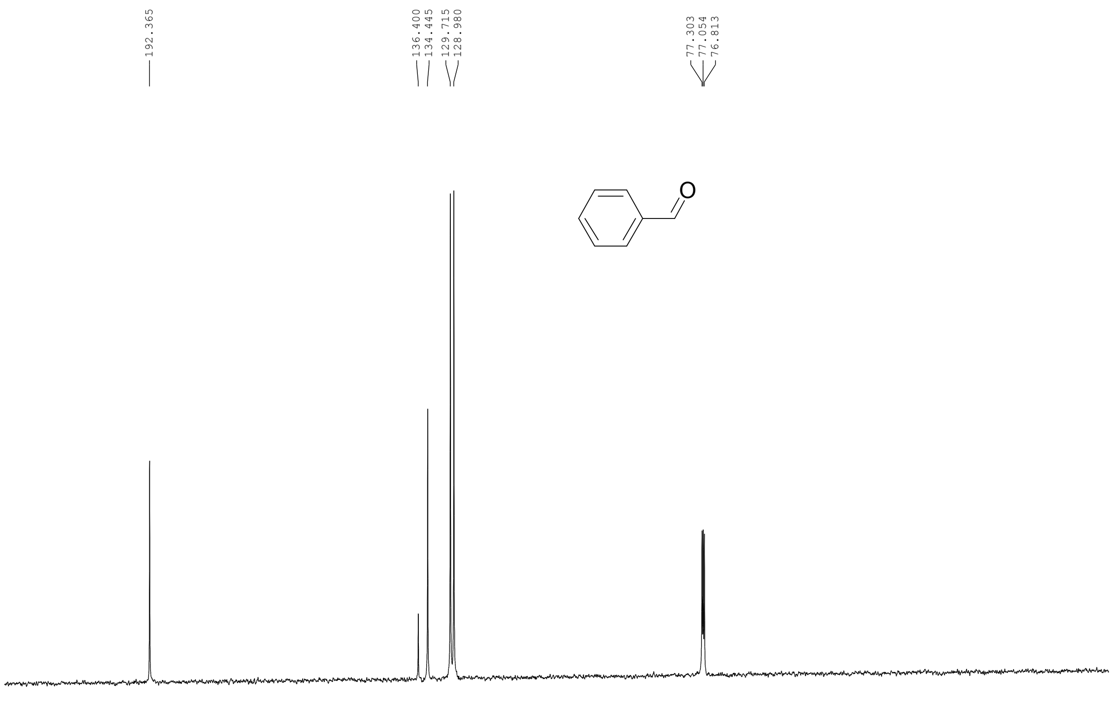

7.321
7.305
7.293
7.279
7.266
7.240
2.797
1.528
0.000
OH
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
15.007
1.000

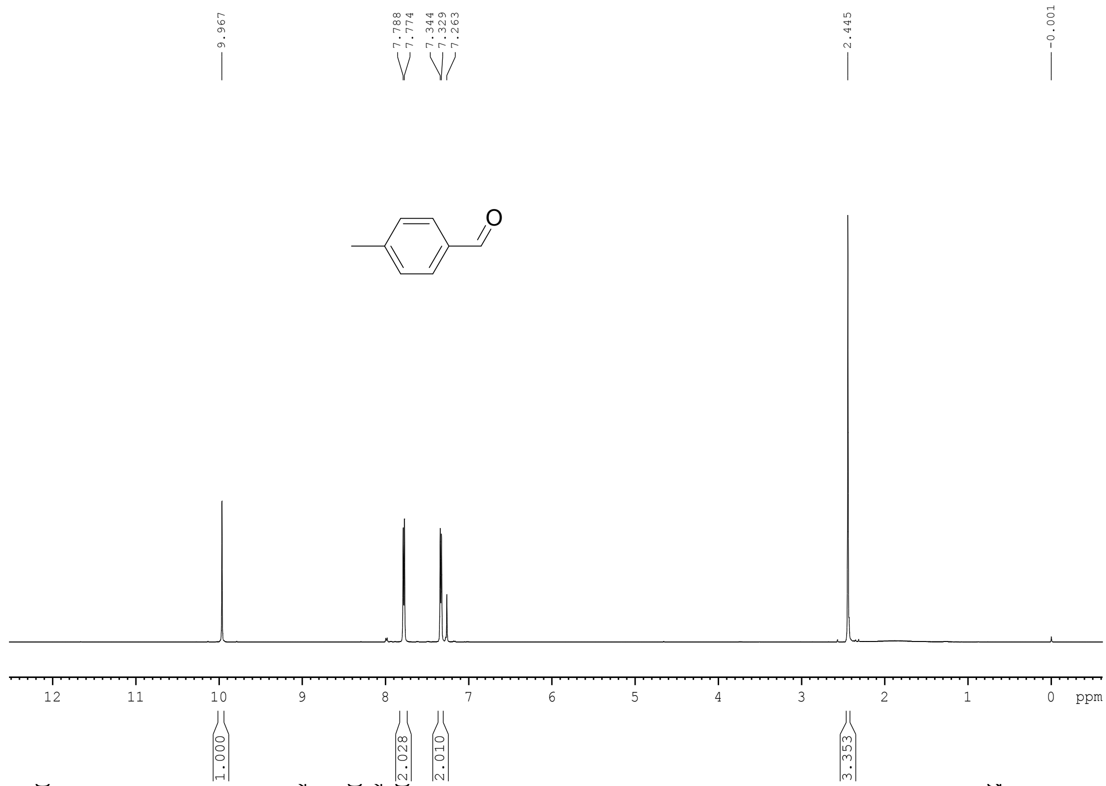

146.82
127.89
127.20
81.98
77.26
76.99
76.74
OH
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

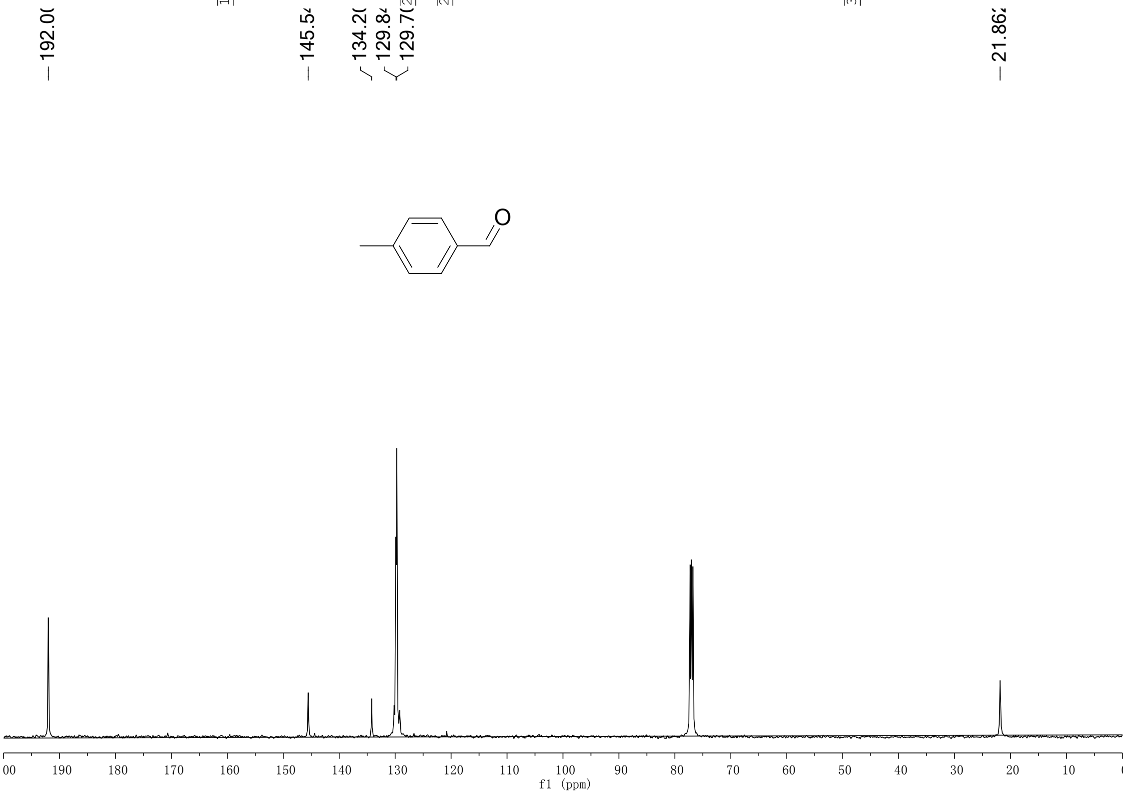

7.39
7.37
7.35
7.34
7.32
7.28
7.26
7.25
5.84
2.25
OH
7.81
2.30
1.01
1.00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

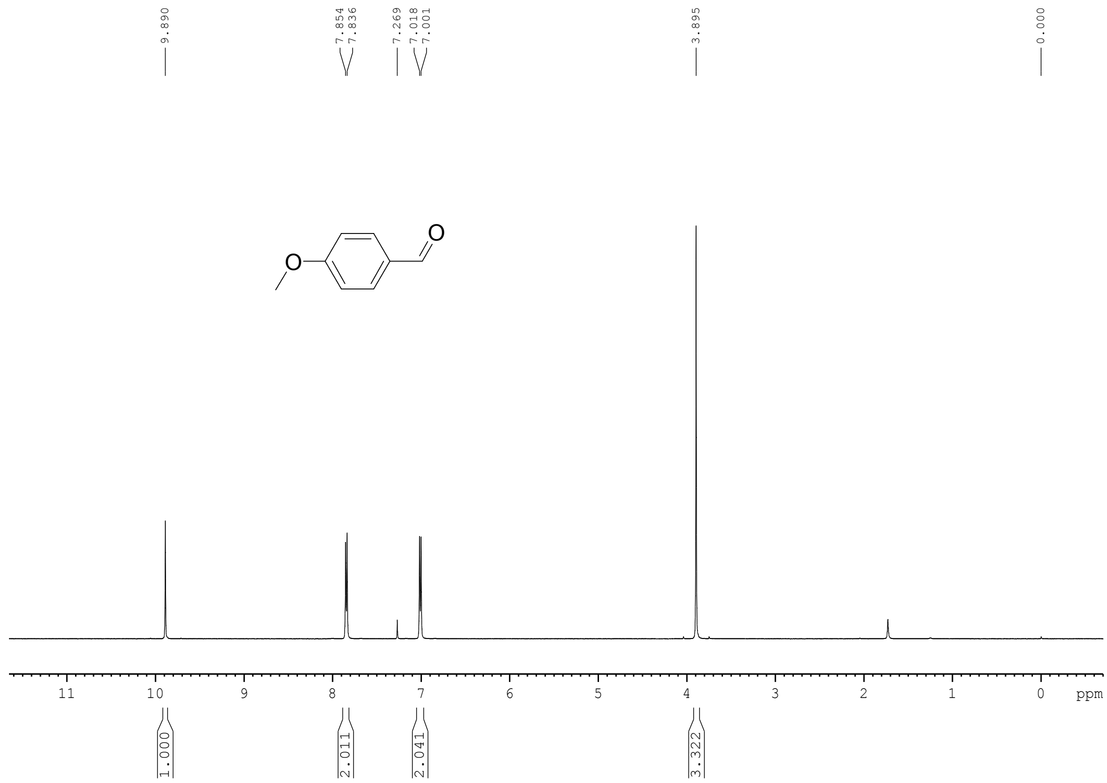

143.804
128.522
127.599
126.552
76.276
OH
70
155
140
125
110
95
85
75
65
55
45
35
f1 (ppm)

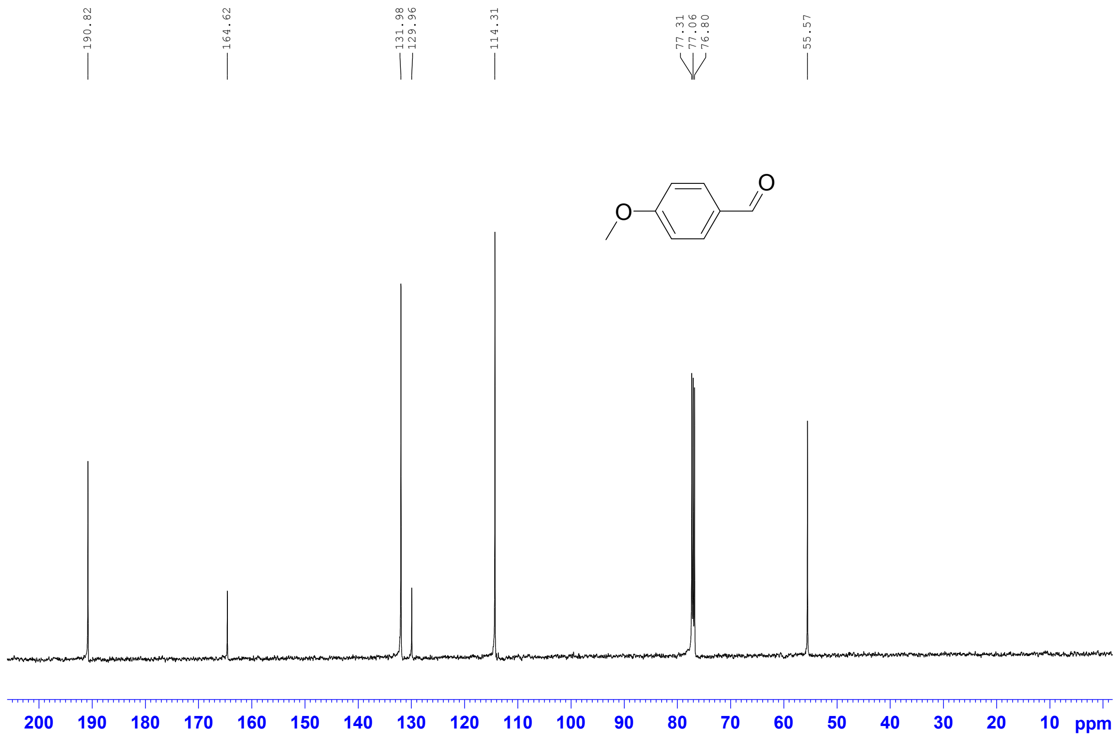

10.020
7.890
7.875
7.645
7.631
7.618
7.548
7.532
7.517
7.258
-0.006
O
ppm
1.000
2.038
1.001
2.059

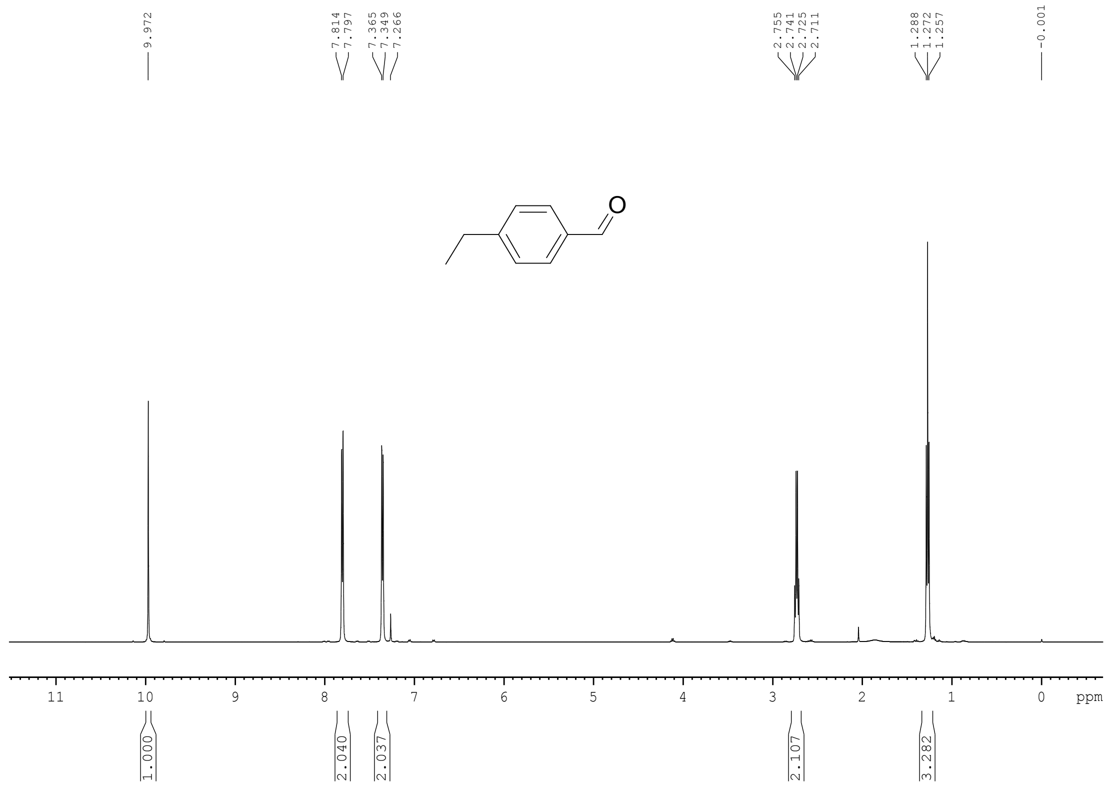

192.365
136.400
134.445
129.715
128.980
77.303
77.054
76.813
O
ppm

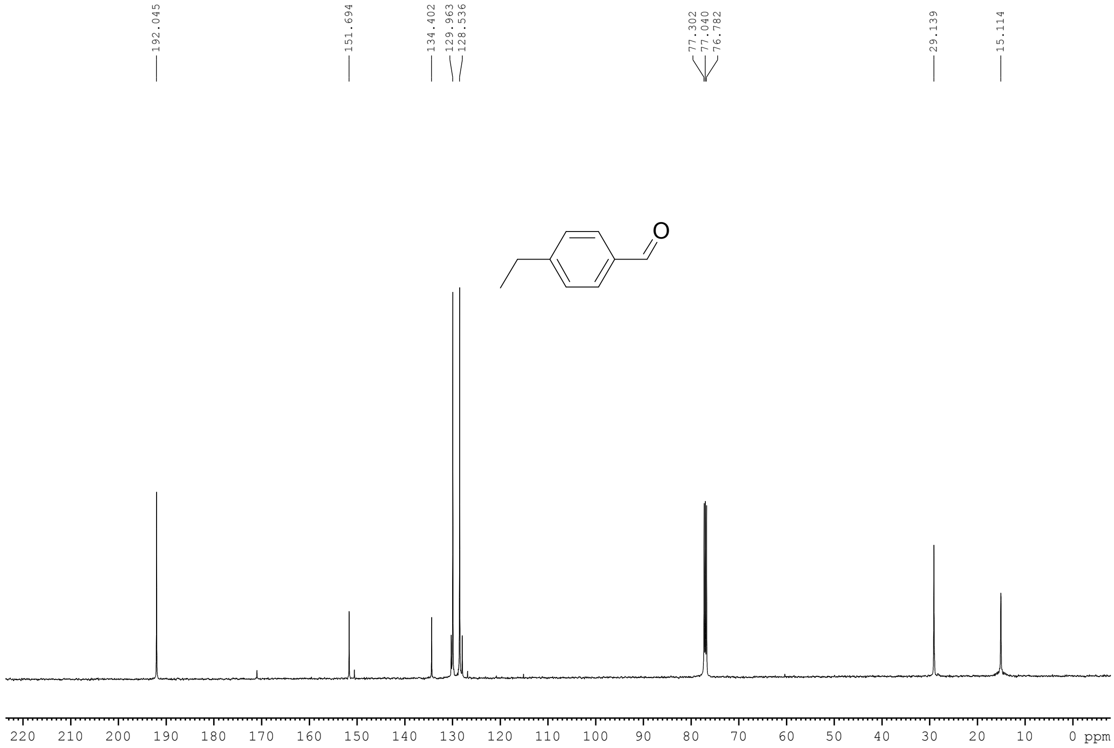

9.967
7.788
7.774
7.344
7.329
7.263
2.445
-0.001
O
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
2.028
2.010
3.353

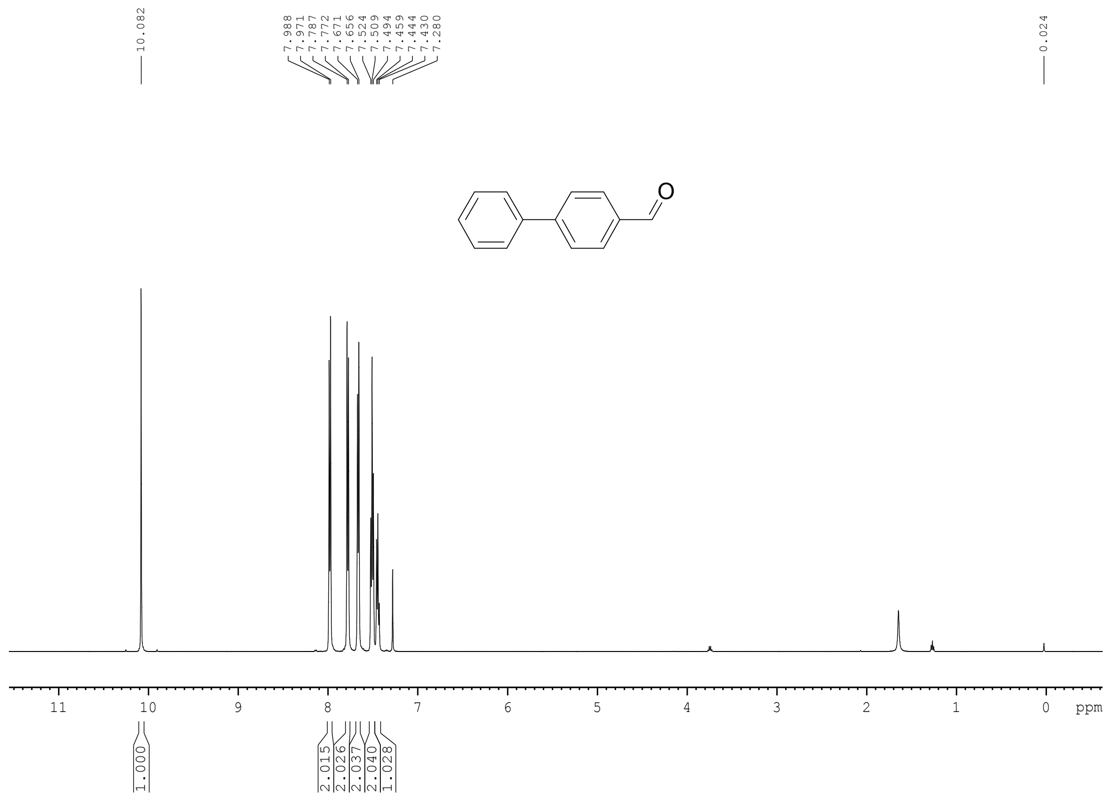

192.0
145.5
134.2
129.8
129.7
21.86
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

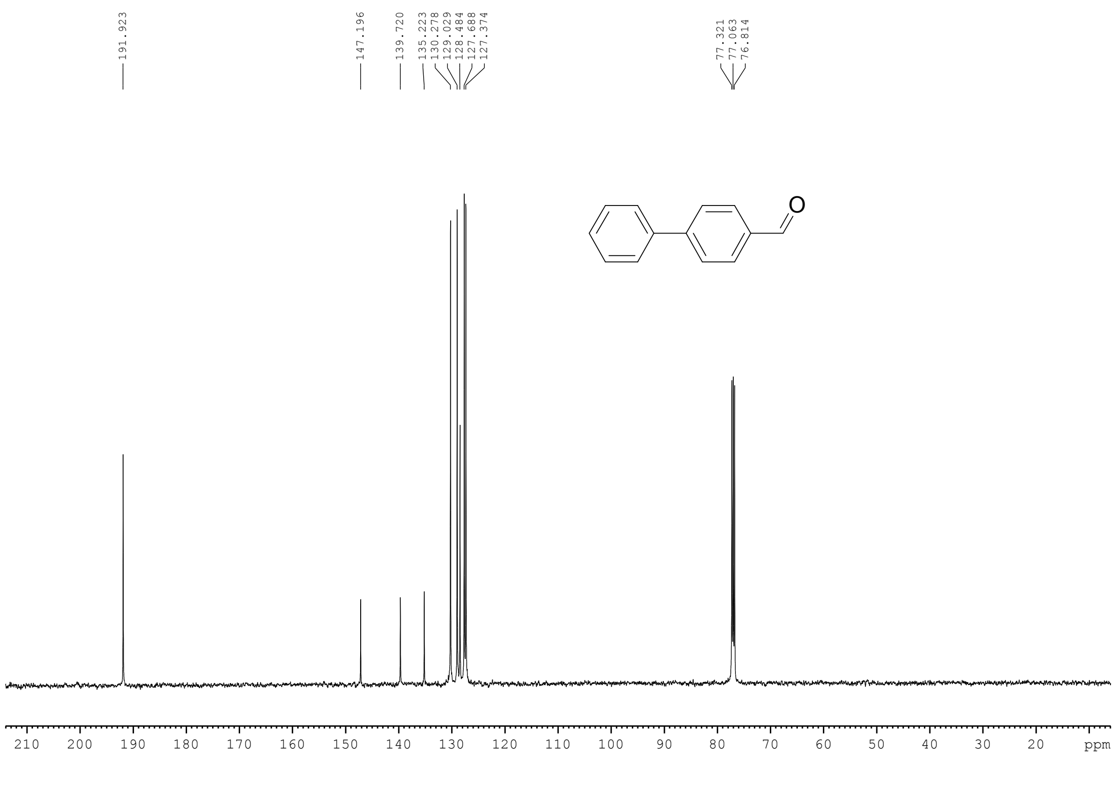

9.890
7.854
7.836
7.269
7.018
7.001
3.895
0.000
O
O
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
2.011
2.041
3.322

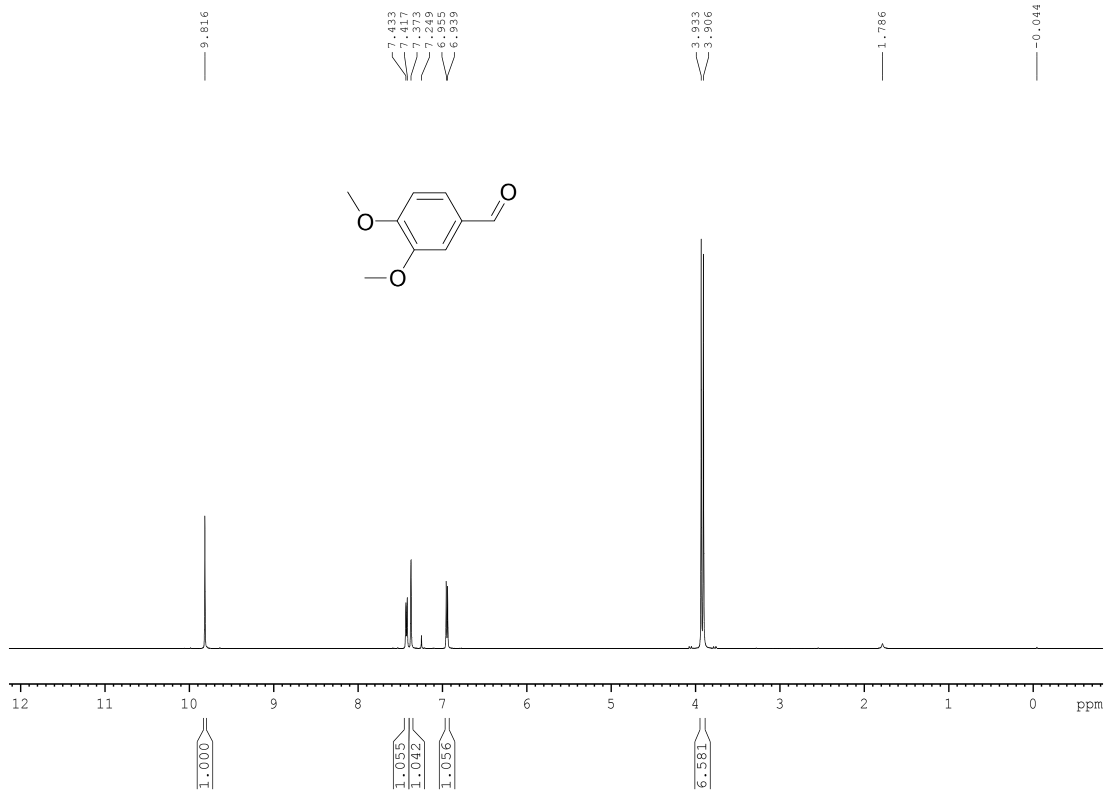

190.82
164.62
131.98
129.96
114.31
77.31
77.06
76.80
55.57
O
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


9.972
7.814
7.797
7.365
7.349
7.266
2.755
2.741
2.725
2.711
1.288
1.272
1.257
-0.001
O
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
2.040
2.037
2.107
3.282

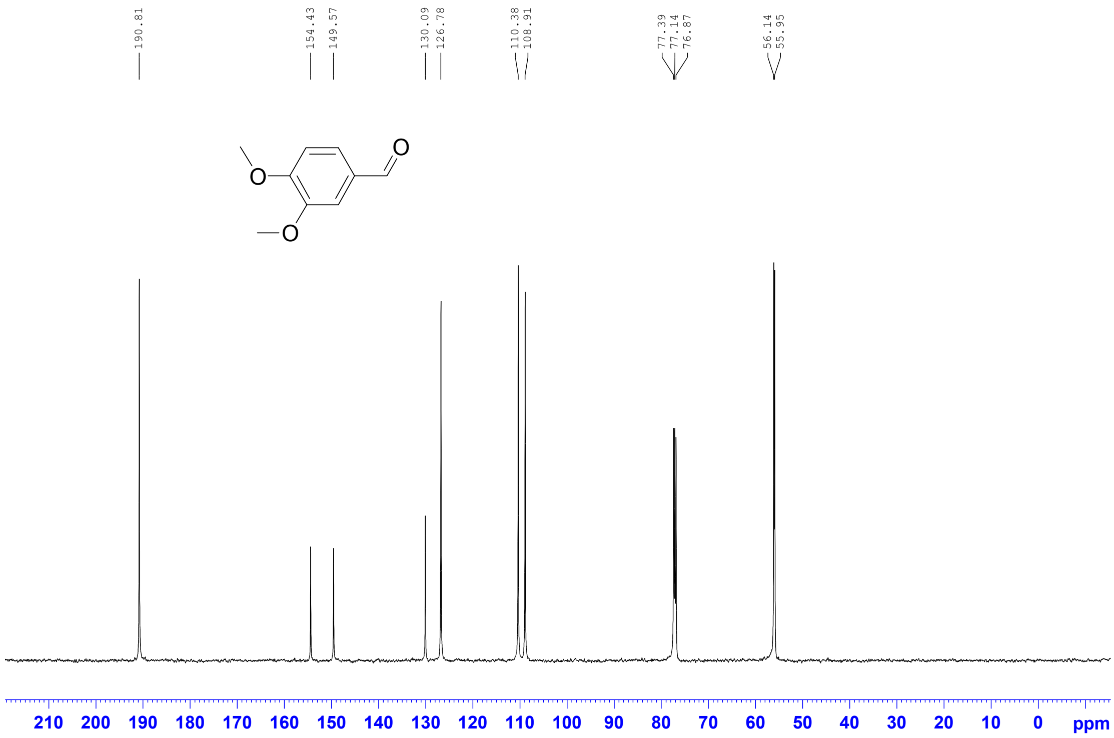

192.045
151.694
134.402
129.963
128.536
77.302
77.040
76.782
29.139
15.114
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


10.082
7.988
7.971
7.787
7.772
7.671
7.656
7.524
7.509
7.494
7.459
7.444
7.430
7.280
0.024
O
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
2.015
2.026
2.037
2.040
1.028

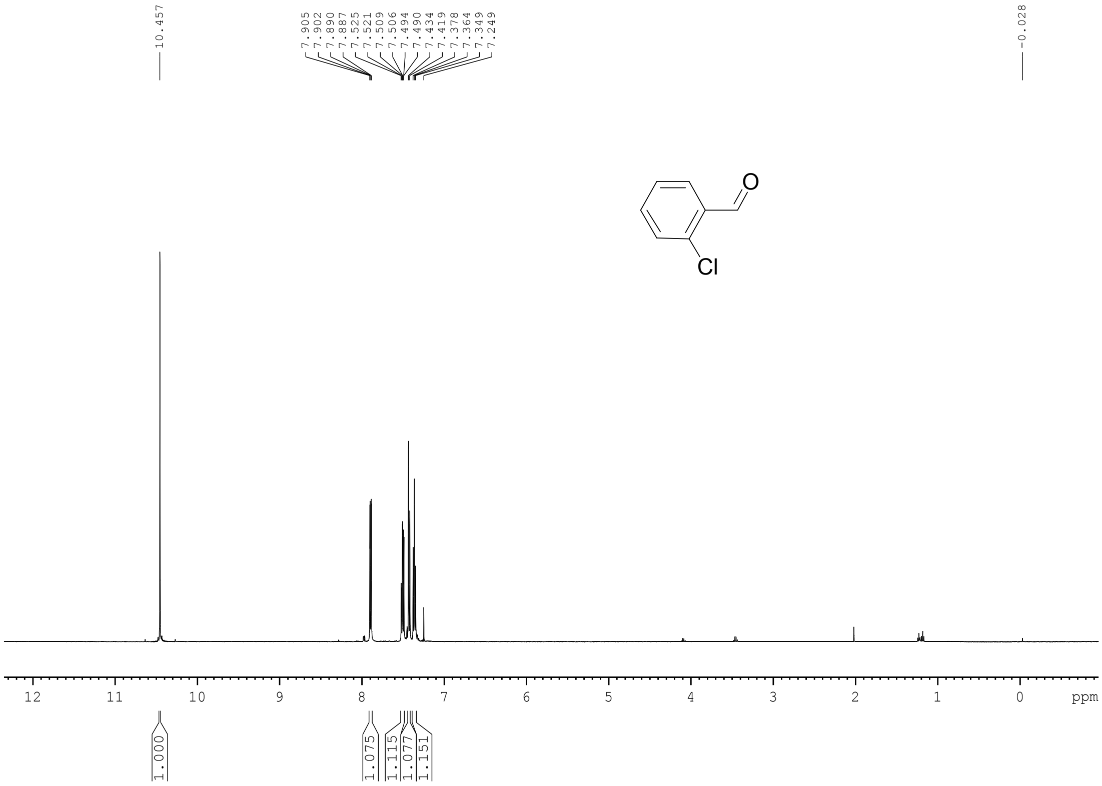

191.923
147.196
139.720
135.223
130.278
129.029
128.484
127.688
127.374
77.321
77.063
76.814
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

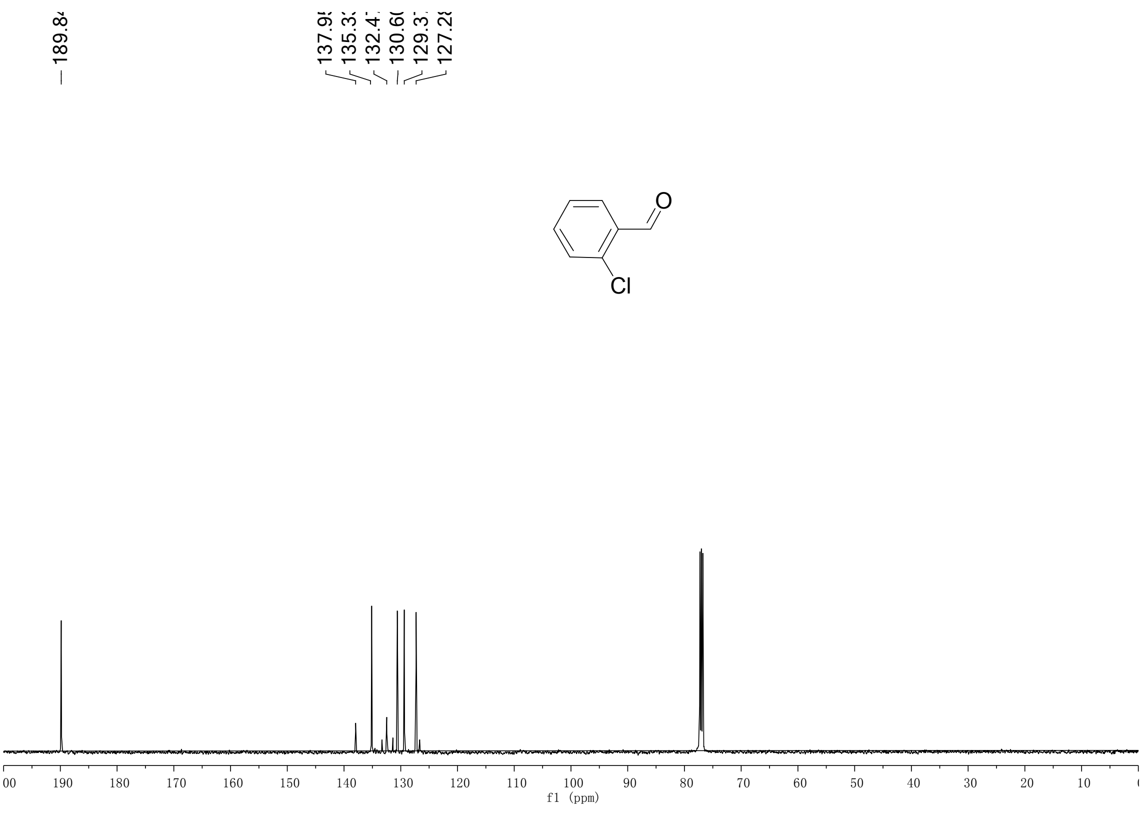


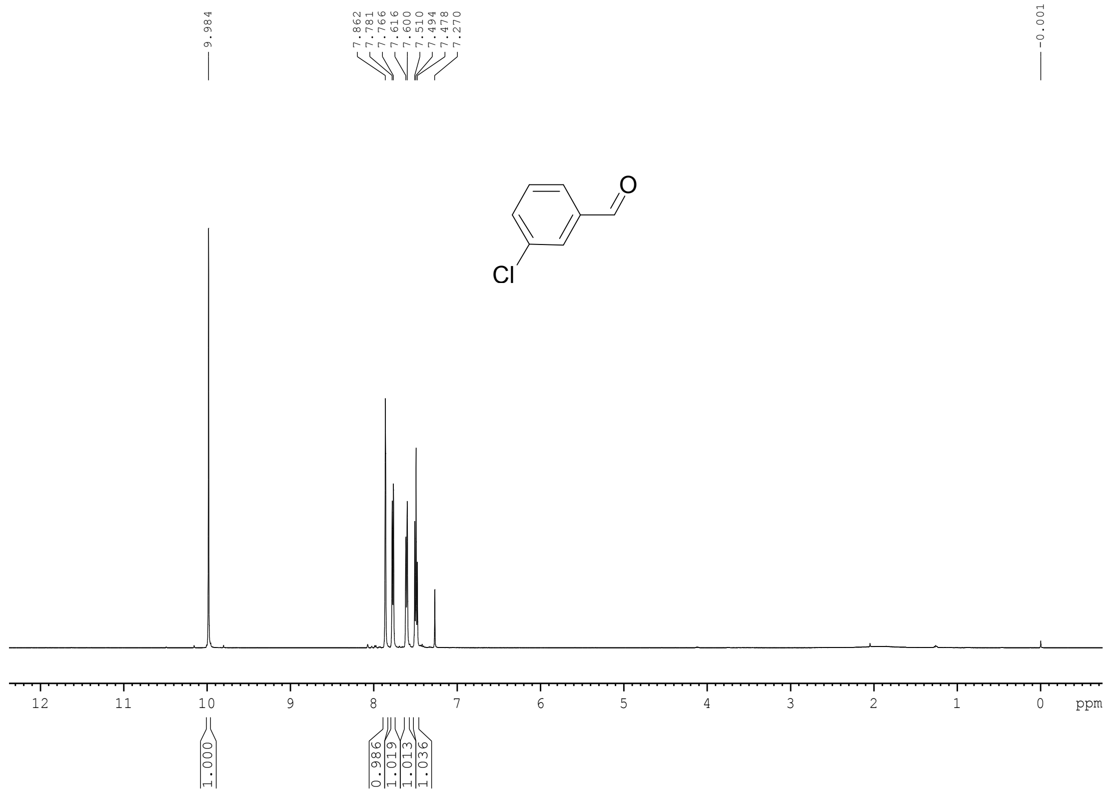
9.816
7.433
7.417
7.373
7.249
6.955
6.939
3.933
3.906
1.786
-0.044
O
O
O
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.055
1.042
1.056
6.581

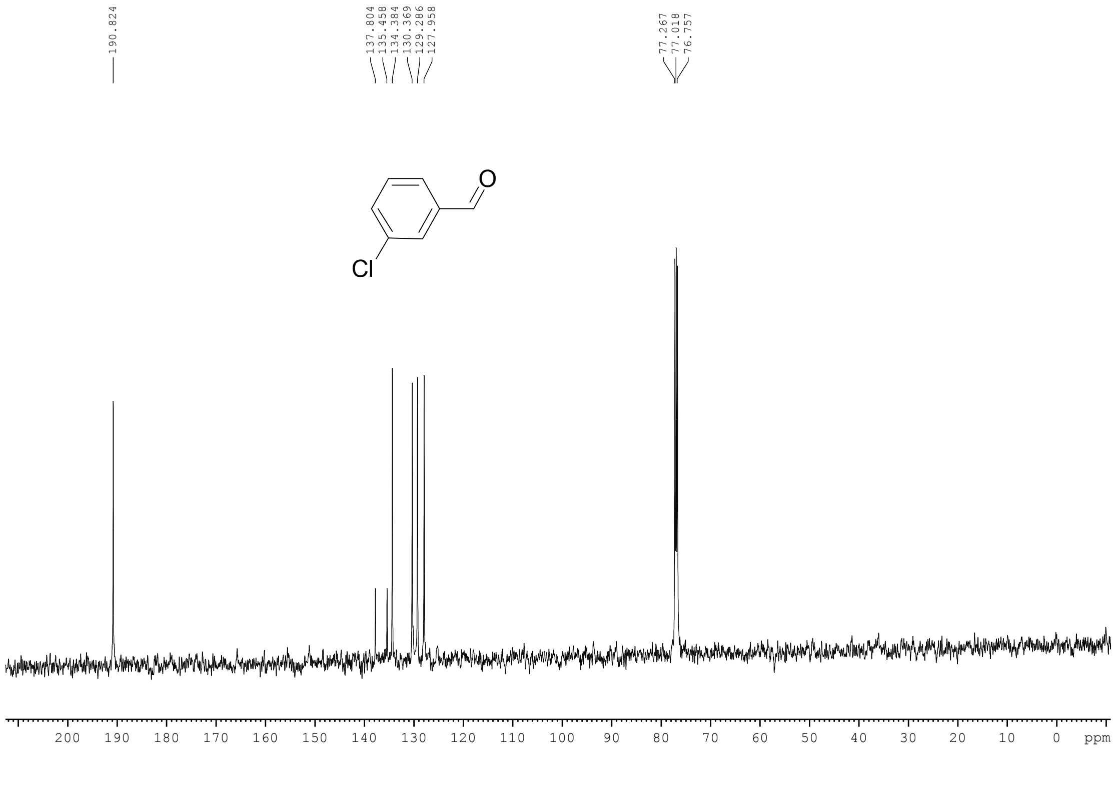


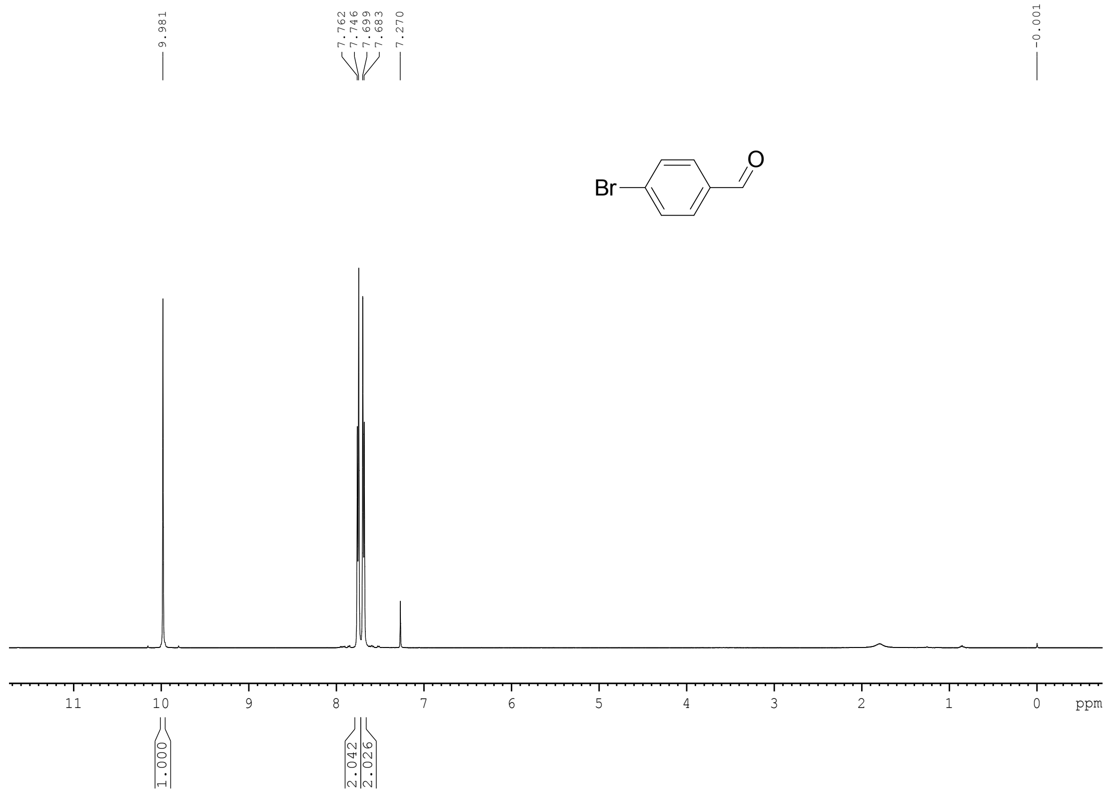
190.81
154.43
149.57
130.09
126.78
110.38
108.91
77.39
77.14
76.87
56.14
55.95
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

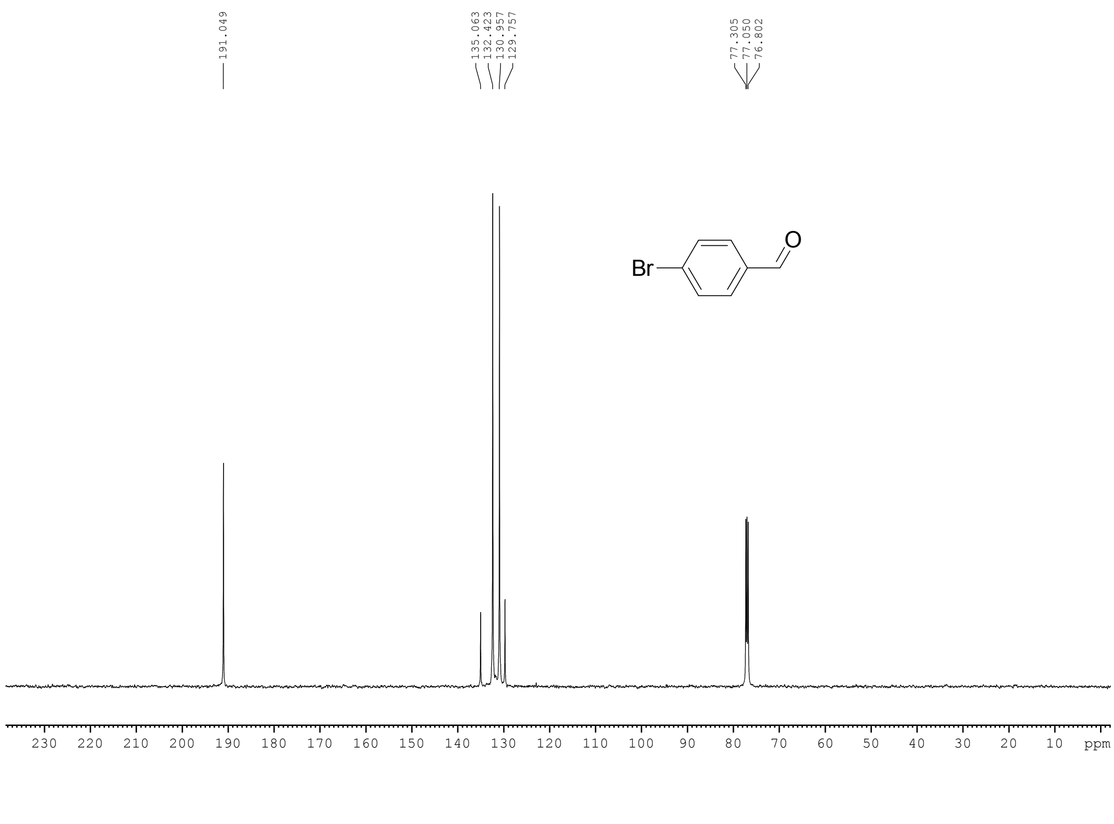

10.457
7.905
7.902
7.890
7.887
7.525
7.521
7.509
7.506
7.494
7.490
7.434
7.419
7.378
7.364
7.349
7.249
-0.028
O
Cl
ppm
1.000
1.075
1.115
1.077
1.151

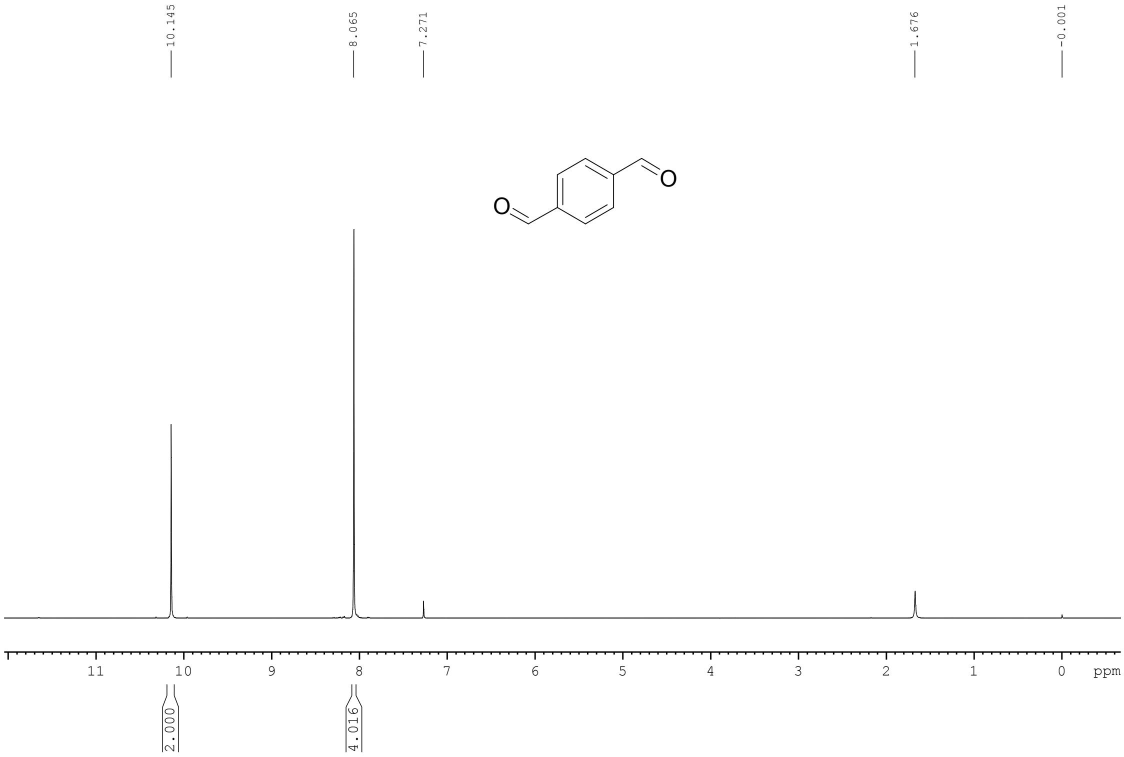

O
Cl
f1 (ppm)

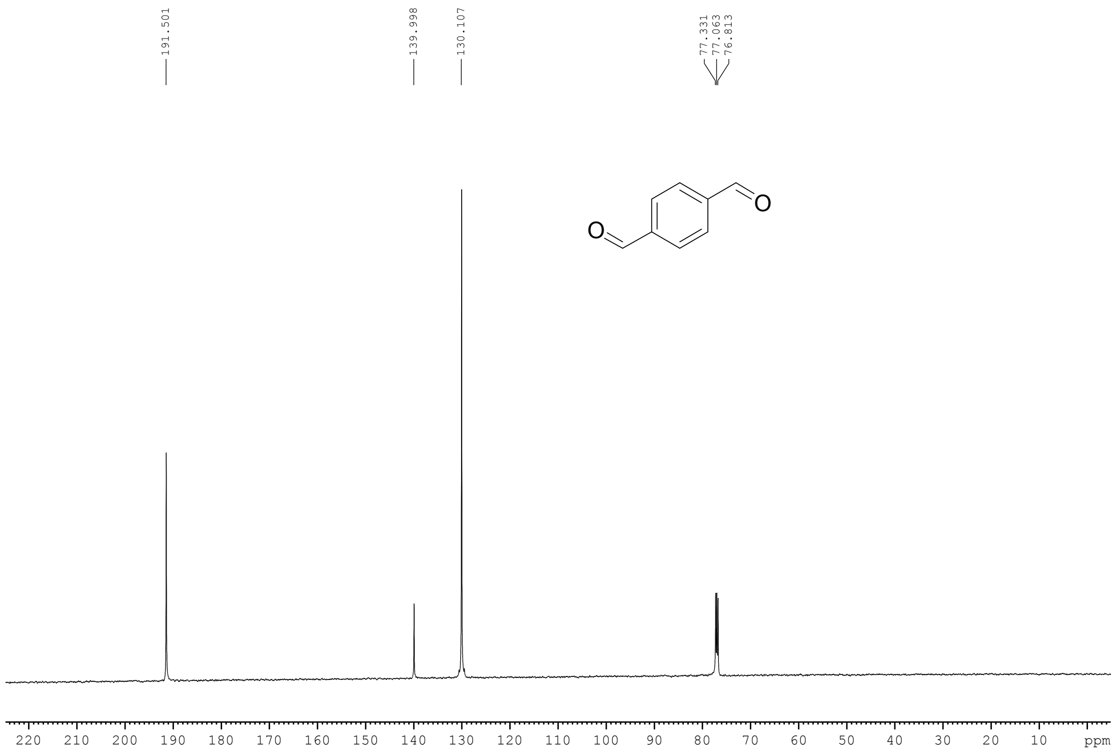

9.984
7.862
7.781
7.766
7.616
7.600
7.510
7.494
7.478
7.270
-0.001
O
Cl
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
0.986
1.019
1.013
1.036

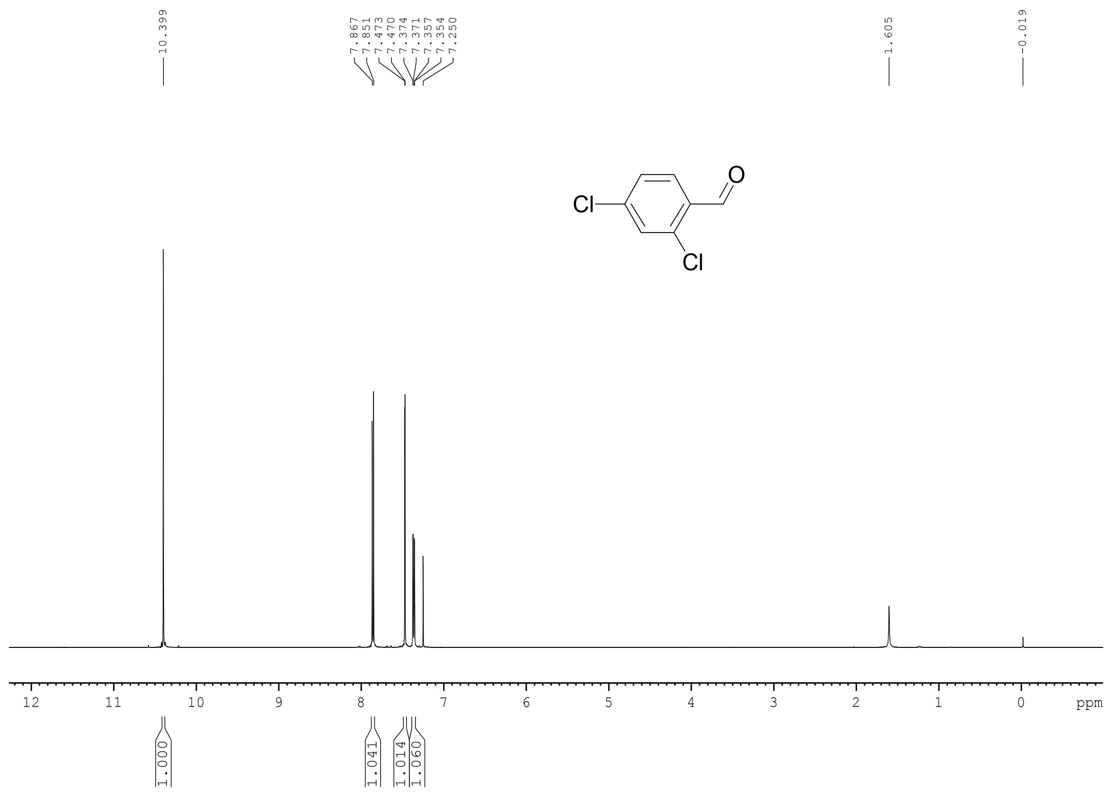

190.824
137.804
135.458
134.384
130.369
129.286
127.958
77.267
77.018
76.757
O
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

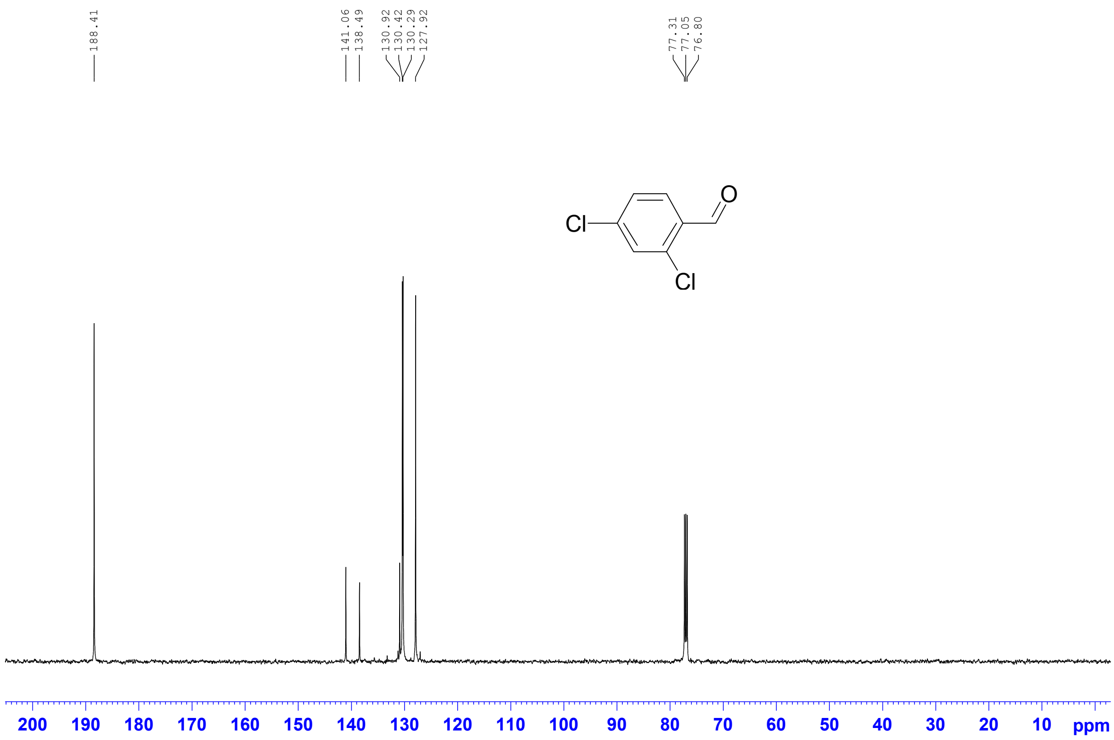

9.981
7.762
7.746
7.699
7.683
7.270
-0.001
Br
O
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
2.042
2.026

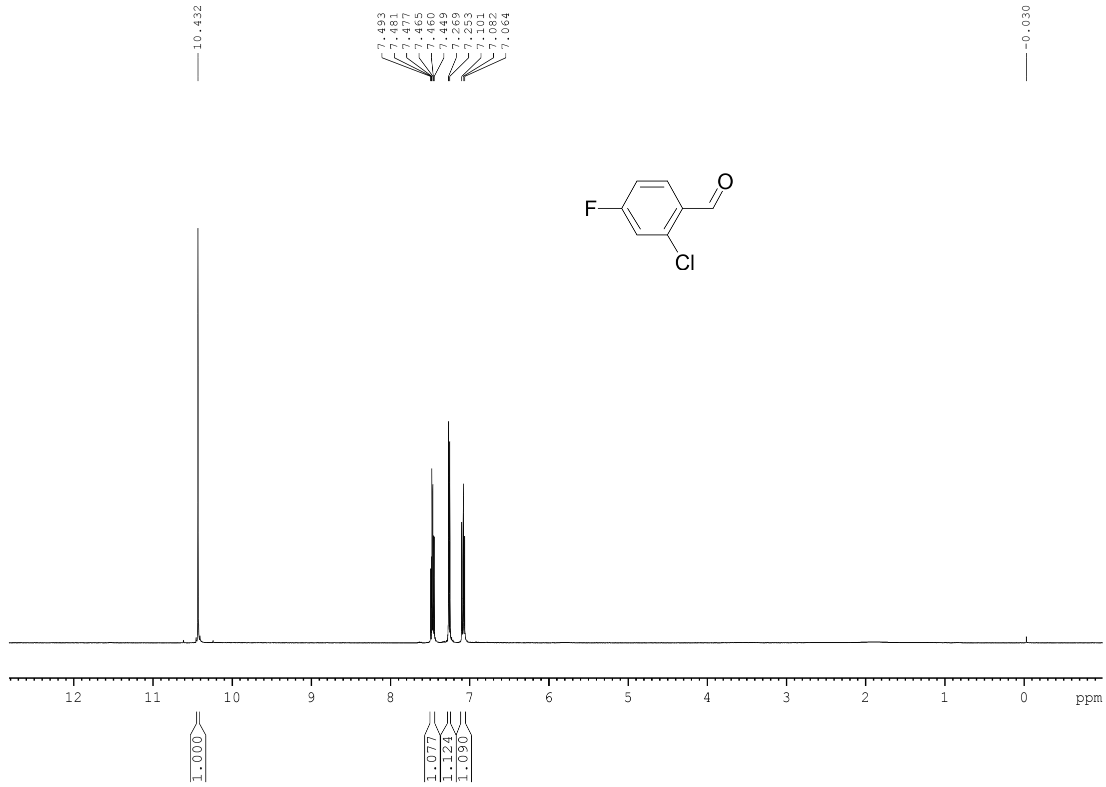

191.049
135.063
132.423
130.957
129.757
77.305
77.050
76.802
Br
O
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

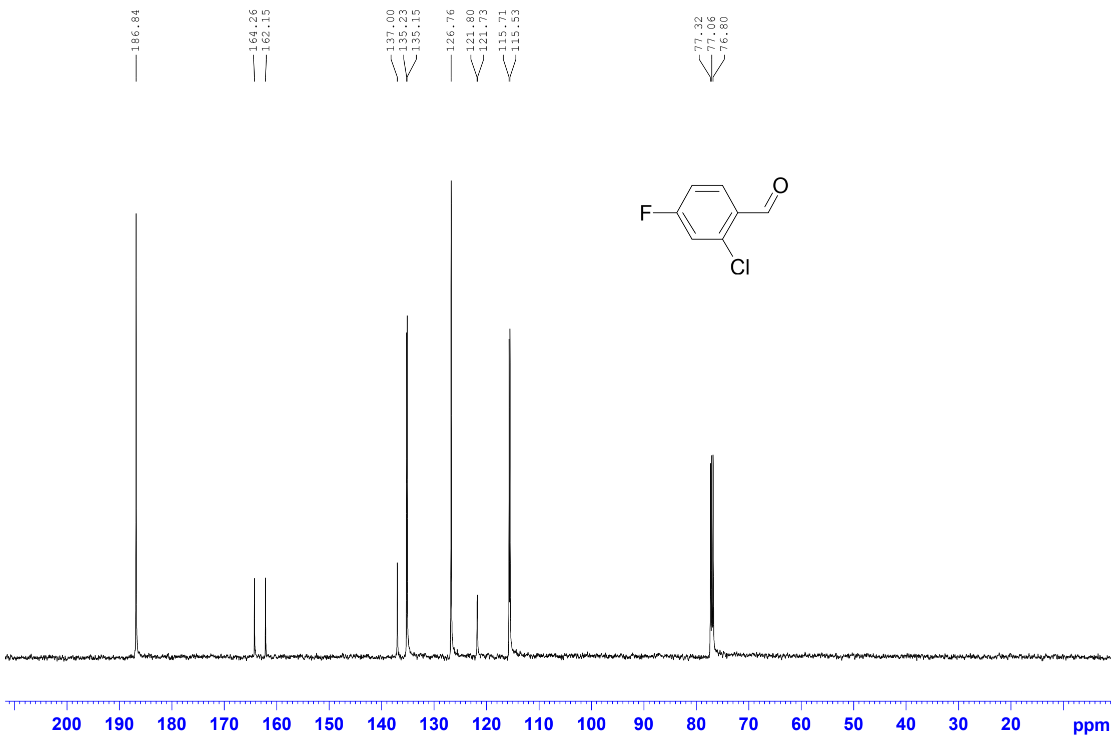

10.145
8.065
7.271
1.676
-0.001
O
O
2.000
4.016
ppm

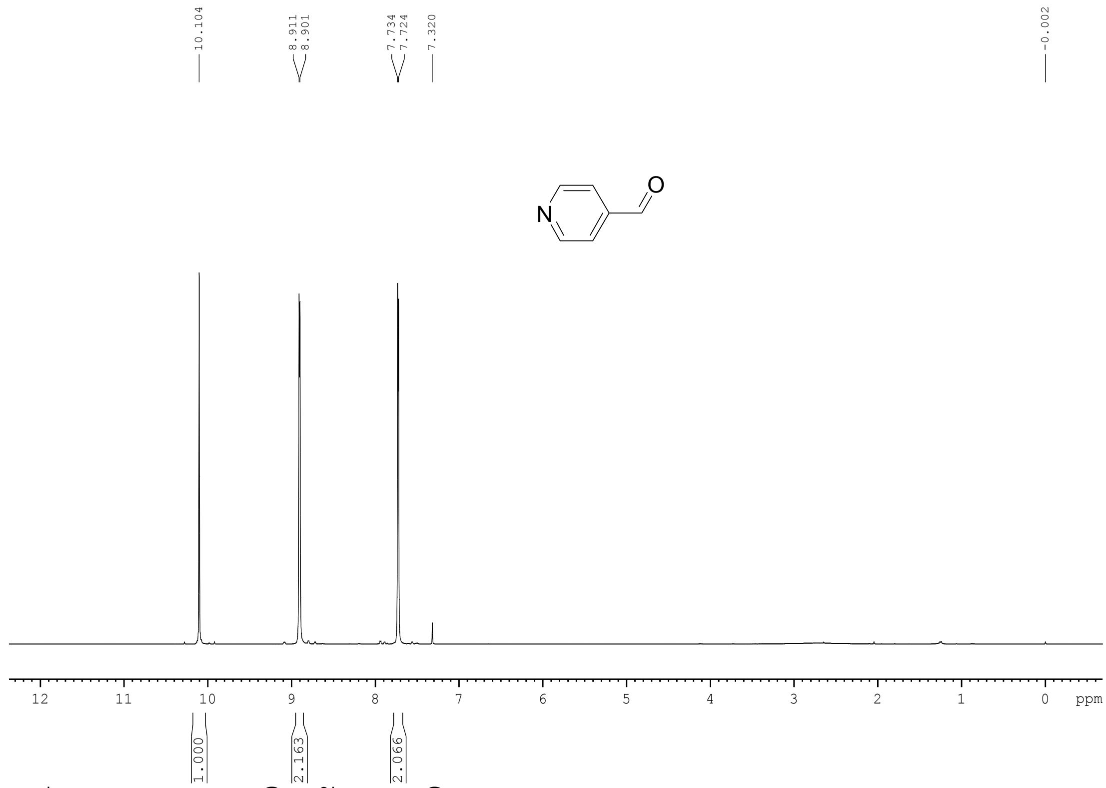

191.501
139.998
130.107
77.331
77.063
76.813
O
O
ppm

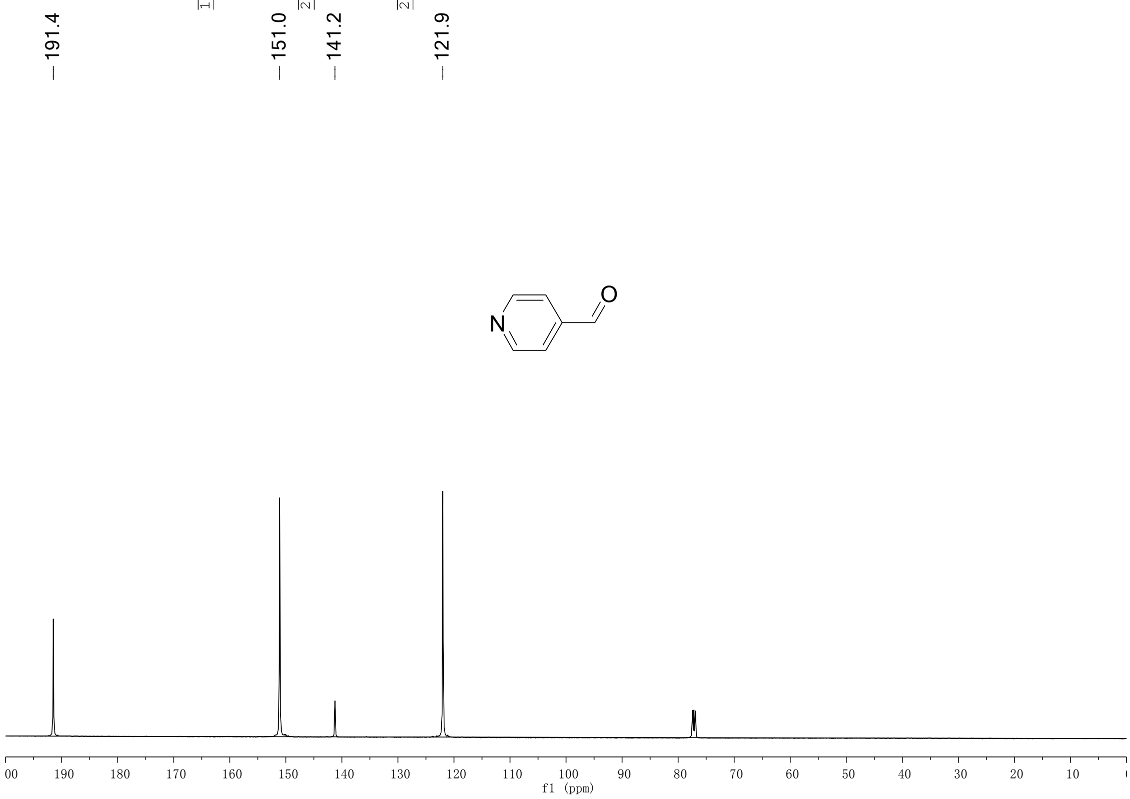

10.399
7.867
7.851
7.473
7.470
7.374
7.371
7.357
7.354
7.250
1.605
-0.019
O
Cl
Cl
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.041
1.014
1.060

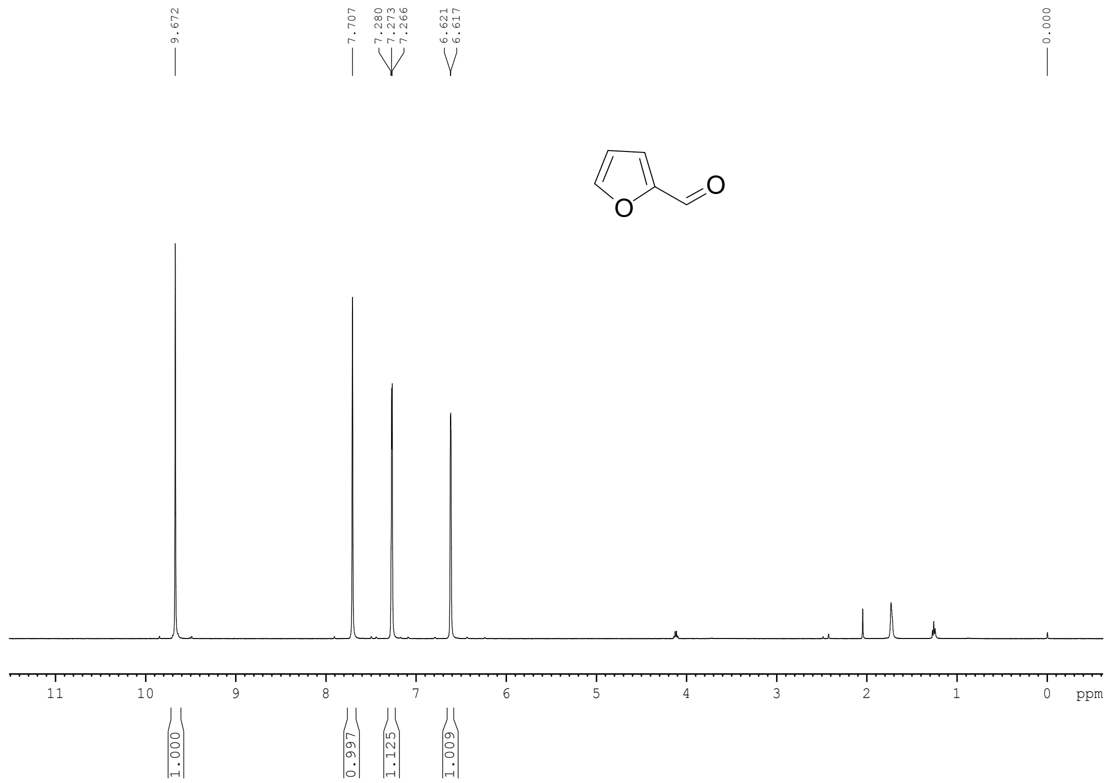

188.41
141.06
138.49
130.92
130.42
130.29
127.92
77.31
77.05
76.80
O
Cl
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

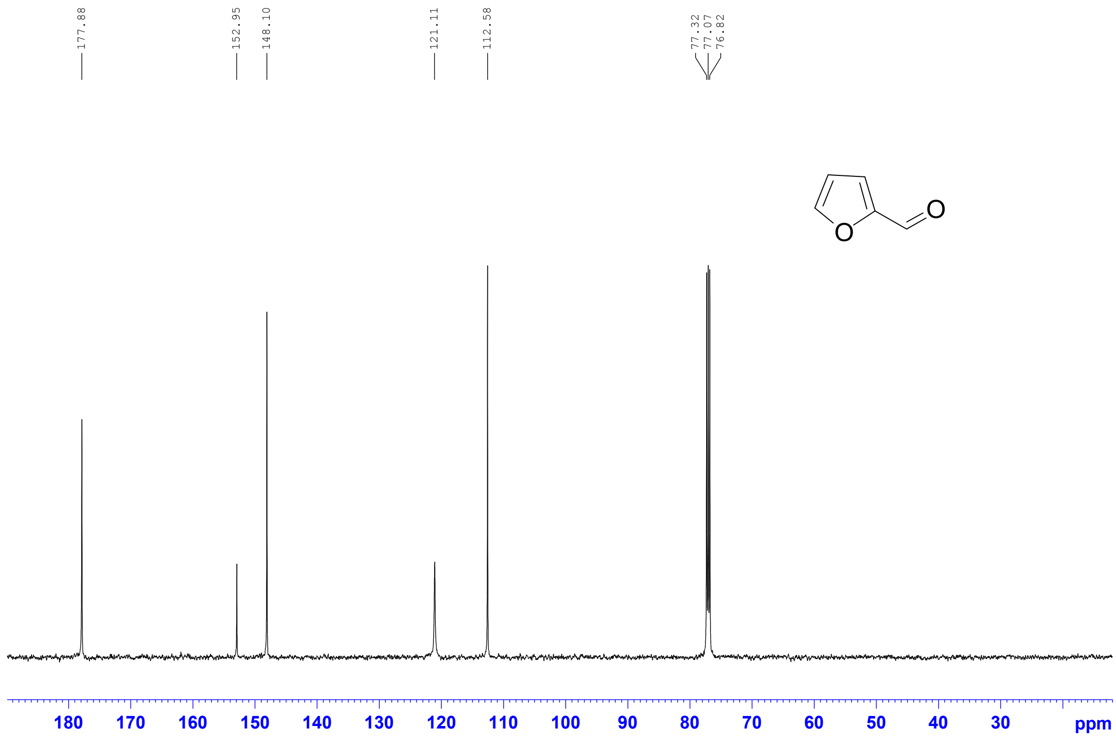

10.432
7.493
7.481
7.477
7.465
7.460
7.449
7.269
7.253
7.101
7.082
7.064
-0.030
F
O
Cl
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.077
1.124
1.090

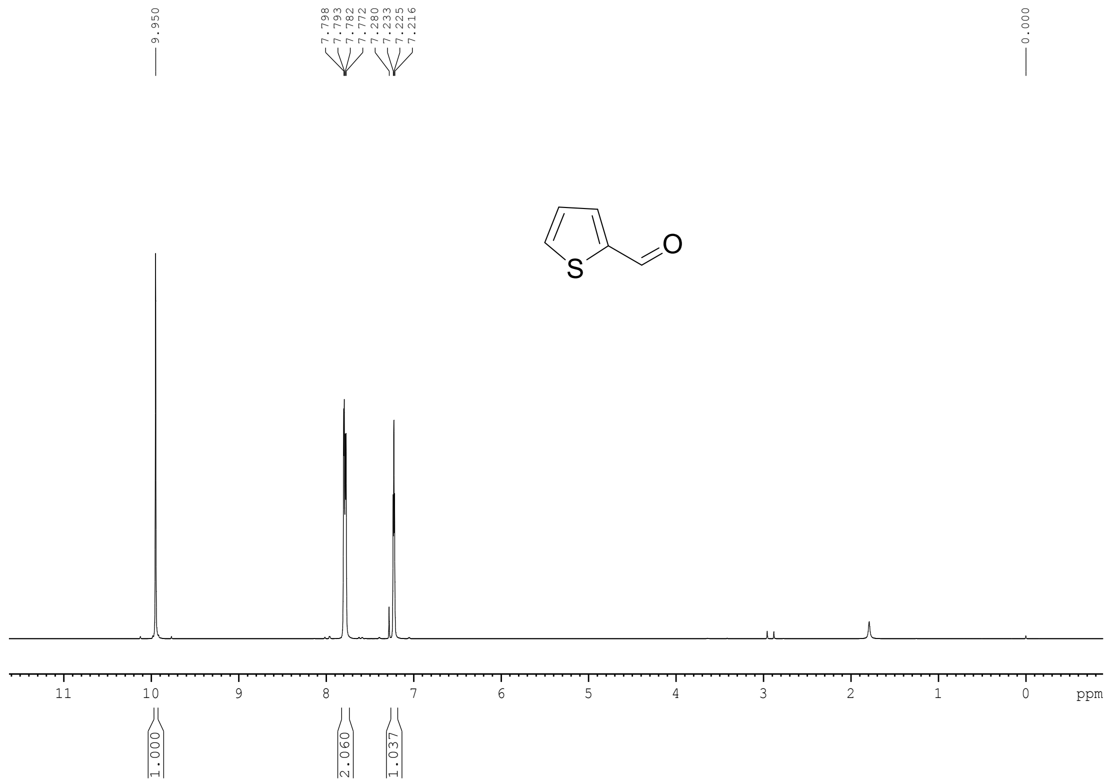

186.84
164.26
162.15
137.00
135.23
135.15
126.76
121.80
121.73
115.71
115.53
77.32
77.06
76.80
F
O
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

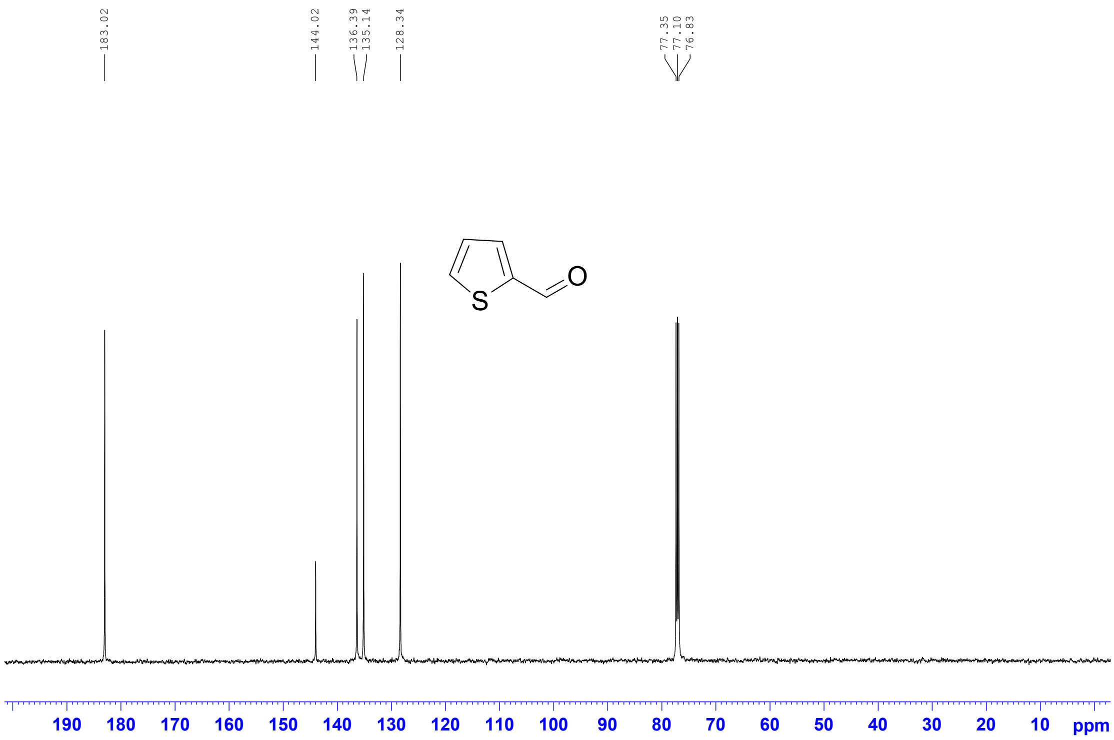

10.104
8.911
8.901
7.734
7.724
7.320
-0.002
N
O
1.000
2.163
2.066
ppm

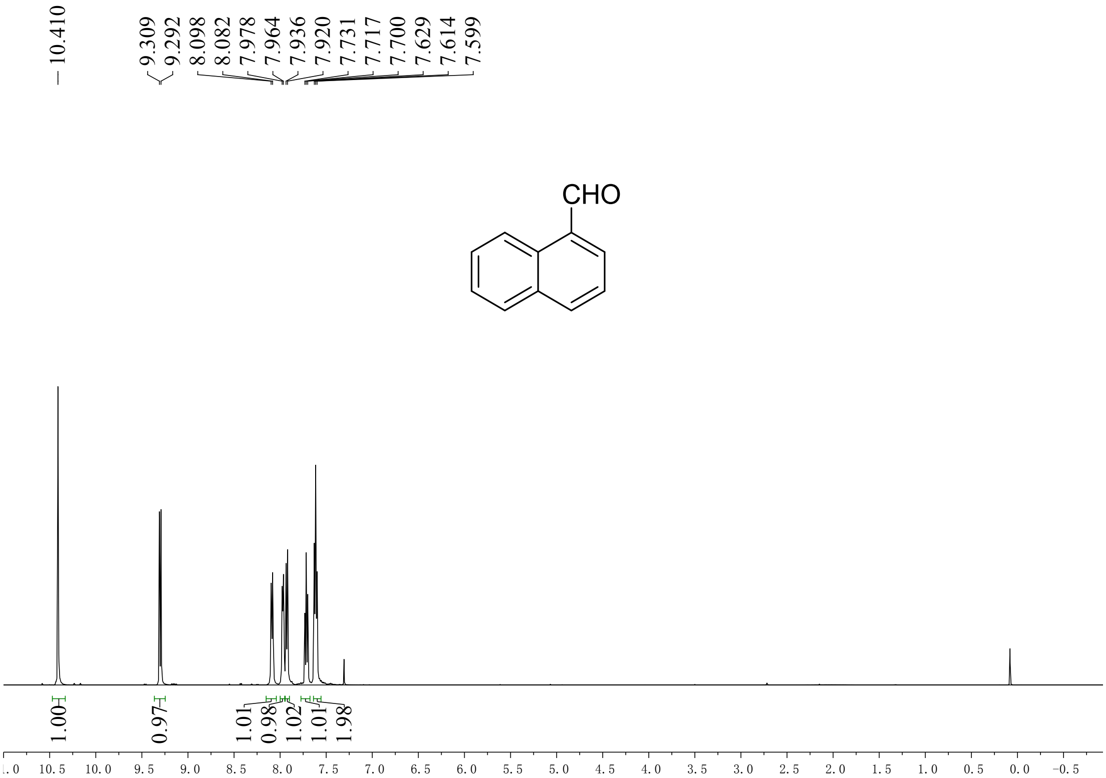

191.4
151.0
141.2
121.9
N
O
f1 (ppm)

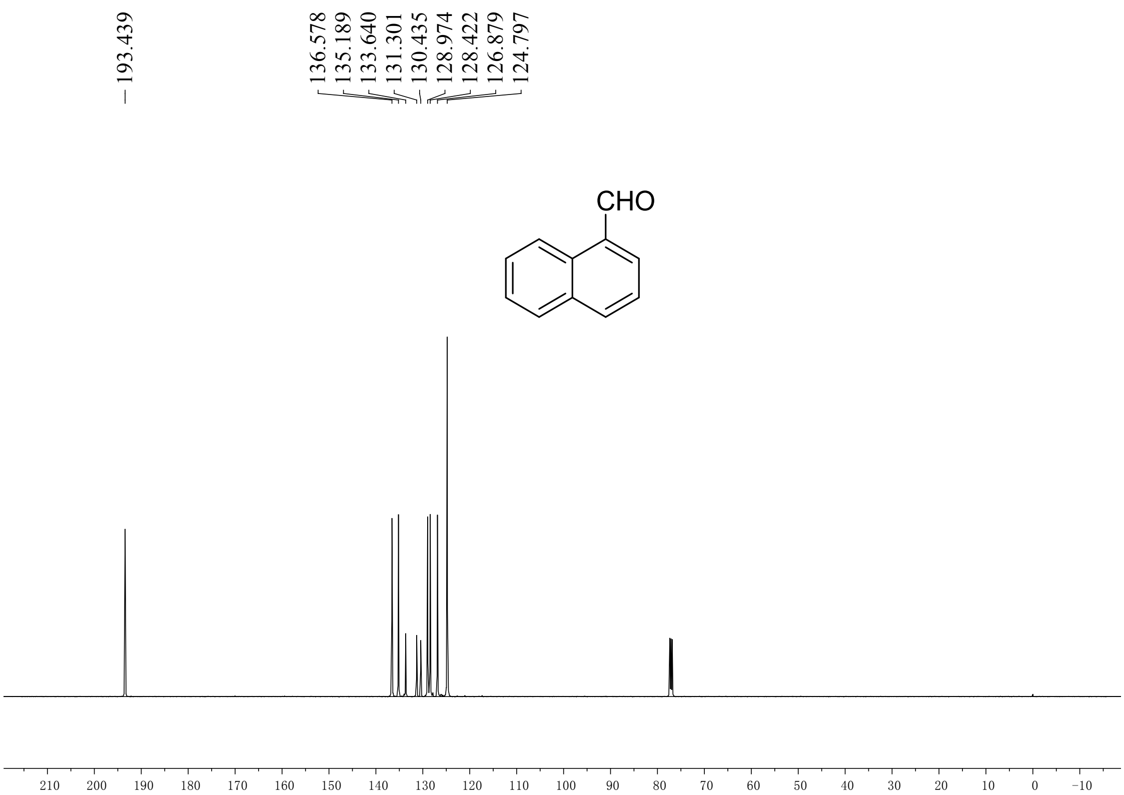

9.672
7.707
7.280
7.273
7.266
6.621
6.617
0.000
O
O
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
0.997
1.125
1.009

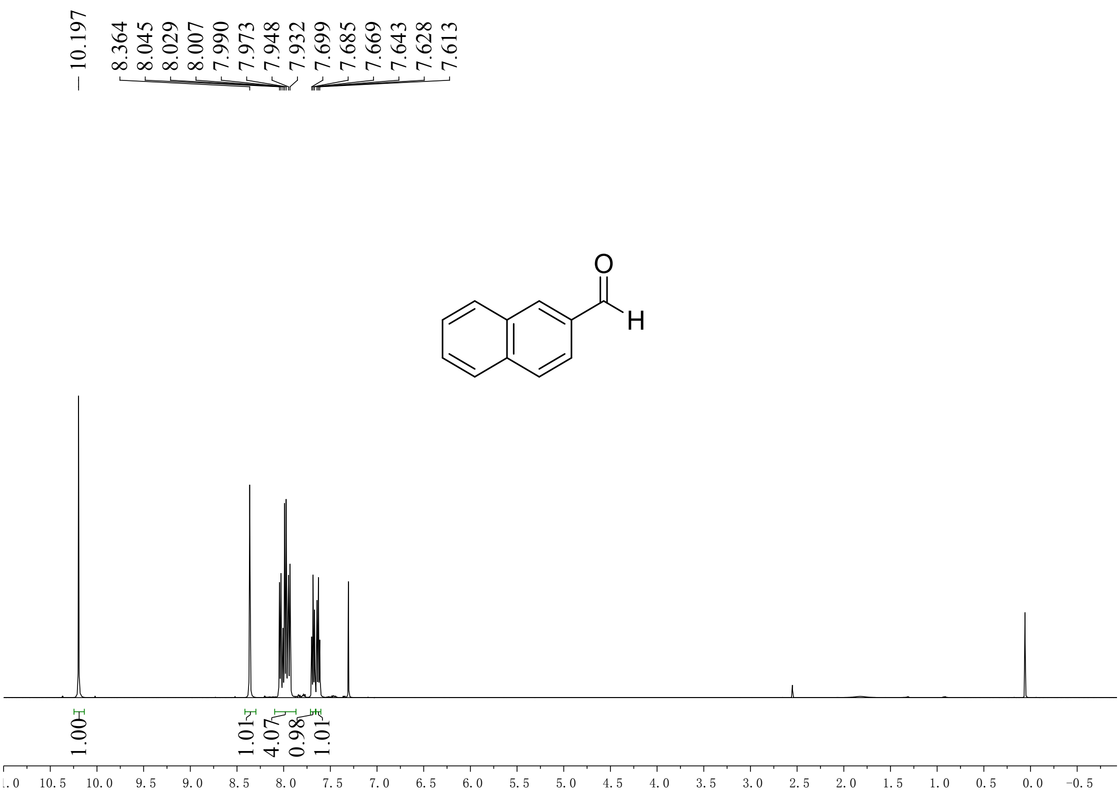

177.88
152.95
148.10
121.11
112.58
77.32
77.07
76.82
O
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

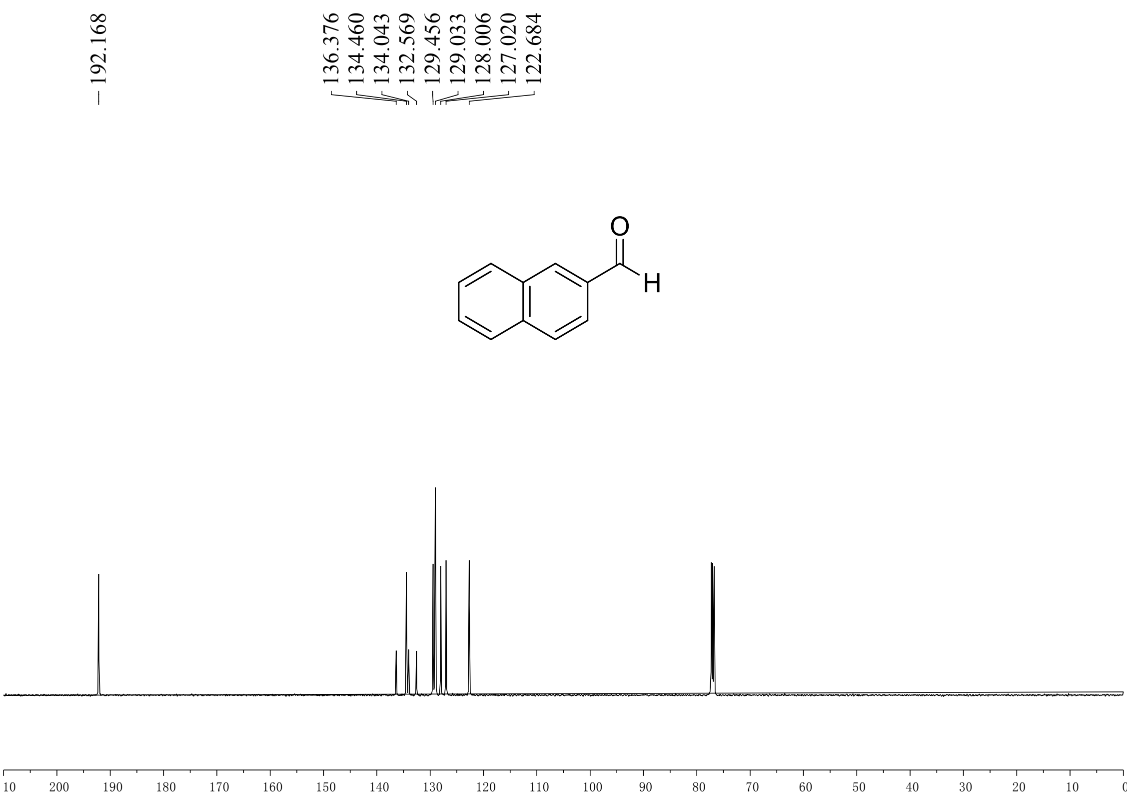

9.950
7.798
7.793
7.782
7.772
7.280
7.233
7.225
7.216
0.000
S
O
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
2.060
1.037

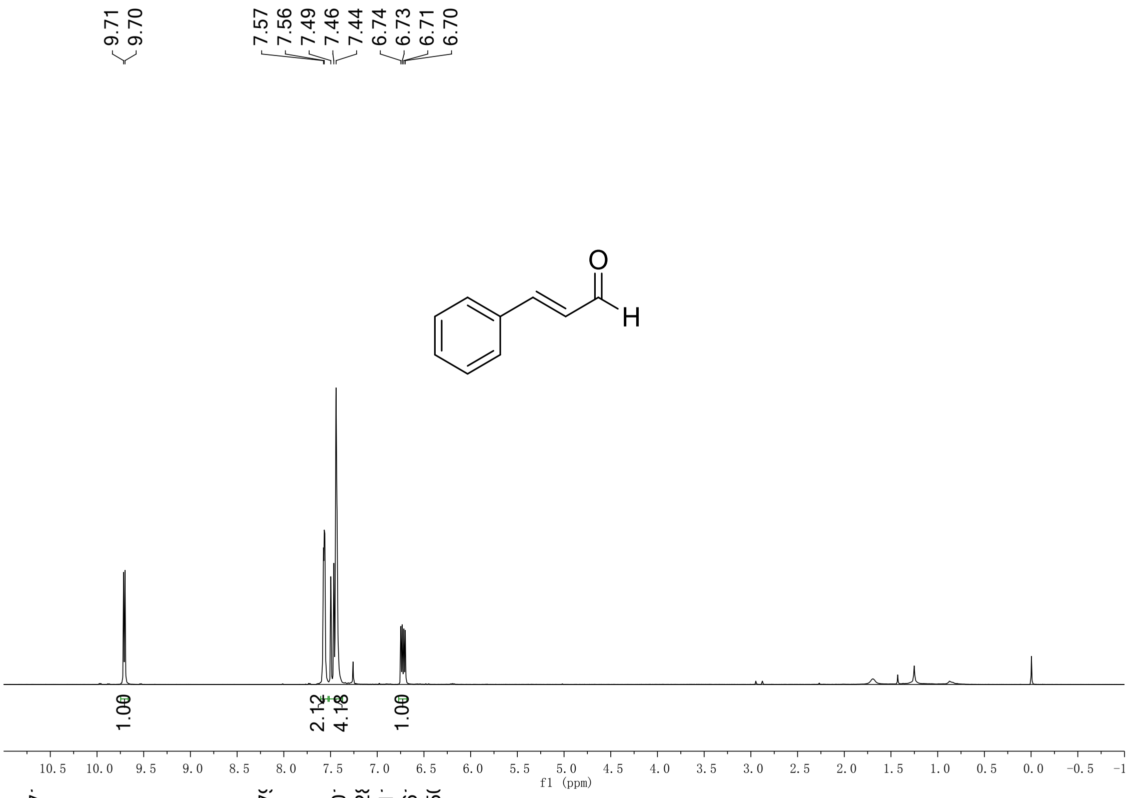

183.02
144.02
136.39
135.14
128.34
77.35
77.10
76.83
S
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

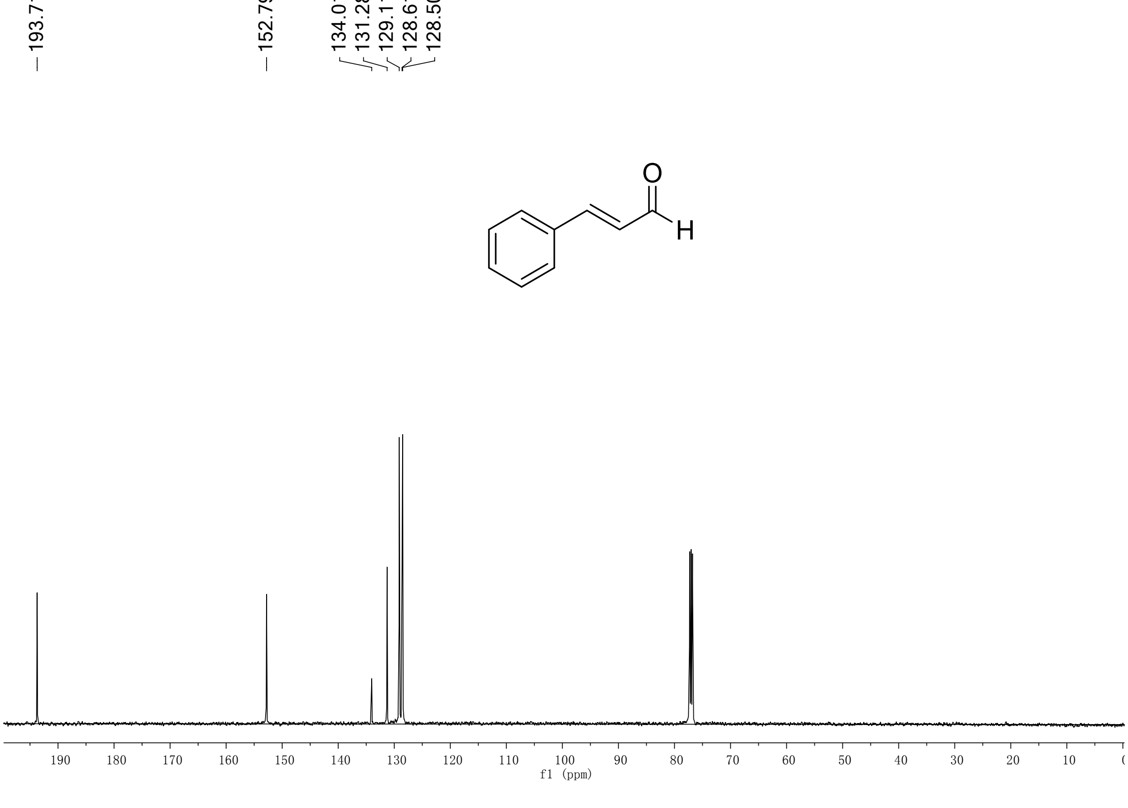

10.410
9.309
9.292
8.098
8.082
7.978
7.964
7.936
7.920
7.731
7.717
7.700
7.629
7.614
7.599
CHO
1.00
0.97
1.01
0.98
1.02
1.01
1.98
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

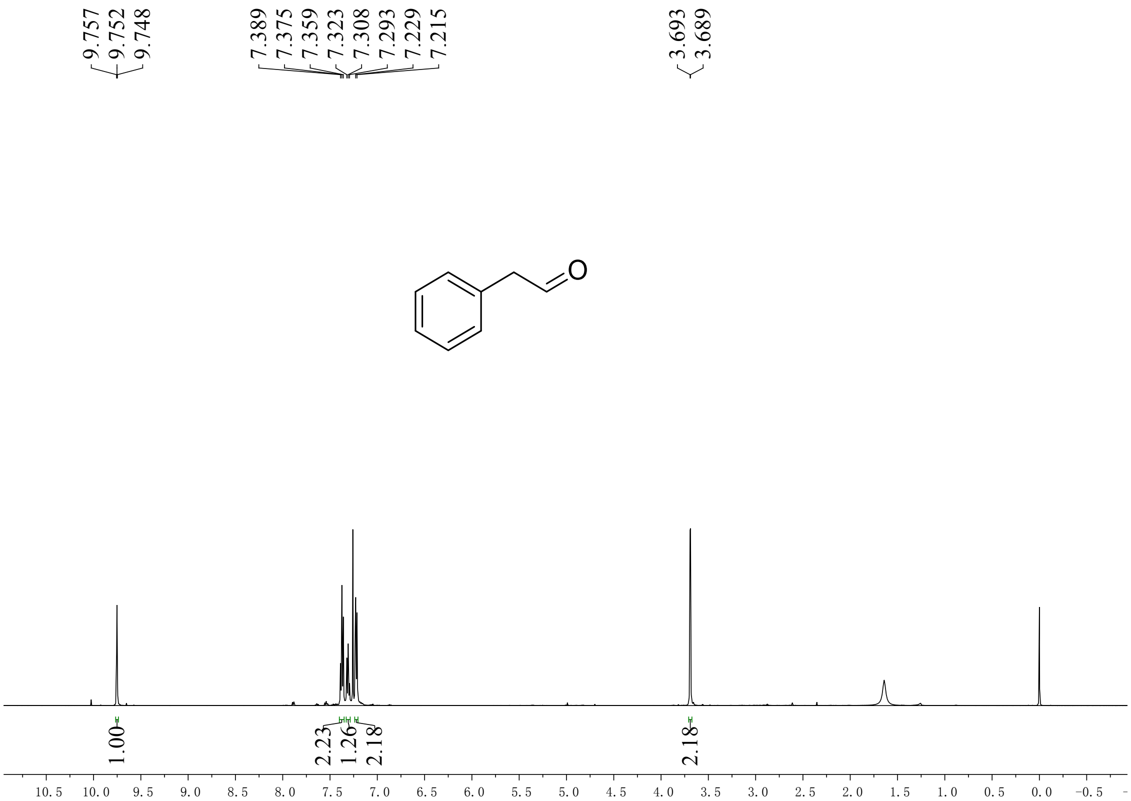

193.439
136.578
135.189
133.640
131.301
130.435
128.974
128.422
126.879
124.797
CHO
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

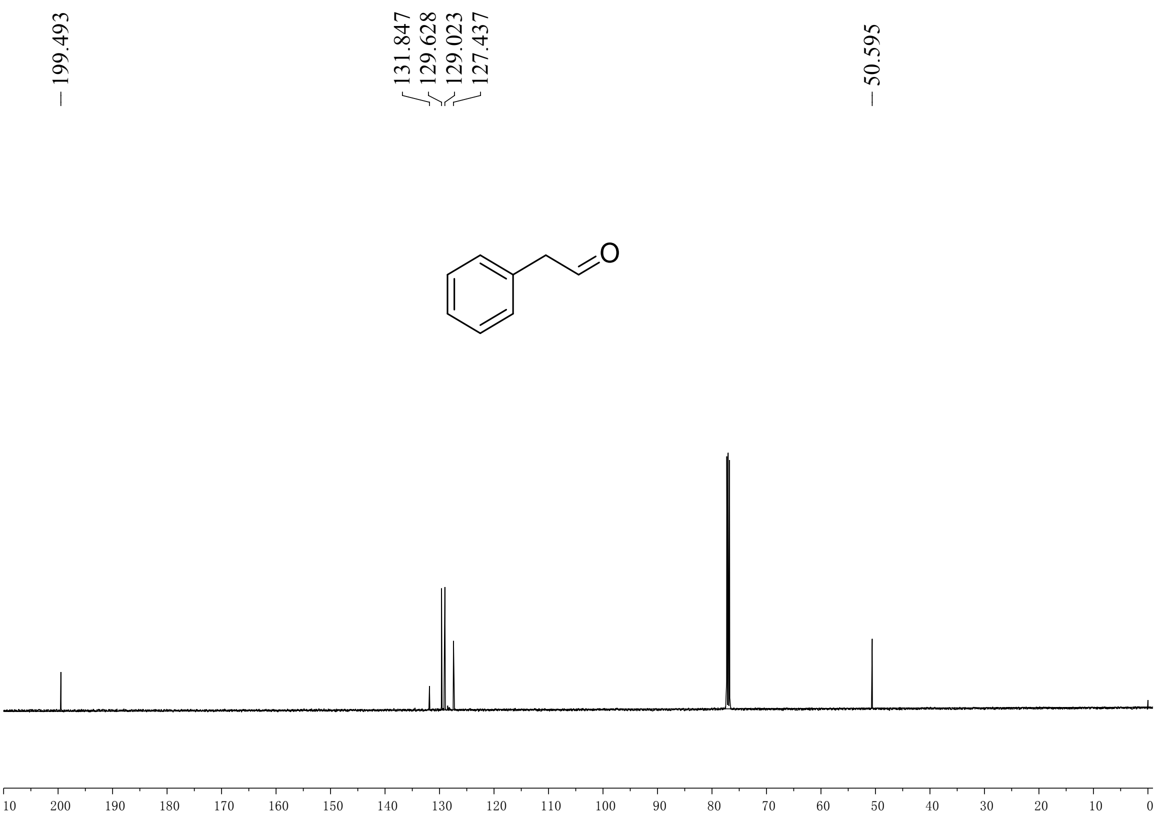

10.197
8.364
8.045
8.029
8.007
7.990
7.973
7.948
7.932
7.699
7.685
7.669
7.643
7.628
7.613
O
H
1.00
1.01
4.07
0.98
1.01


192.168
136.376
134.460
134.043
132.569
129.456
129.033
128.006
127.020
122.684
O
H


9.71
9.70
7.57
7.56
7.49
7.46
7.44
6.74
6.73
6.71
6.70
O
H
1.00
2.12
4.18
1.00
f1 (ppm)


193.7
152.7
134.0
131.2
129.1
128.6
128.5
O
H
f1 (ppm)


9.757
9.752
9.748
7.389
7.375
7.359
7.323
7.308
7.293
7.229
7.215
3.693
3.689
O
1.00
2.23
1.26
2.18
2.18
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


199.493
131.847
129.628
129.023
127.437
50.595
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0