Remarkable Improvement Achieved by Imidazole Derivatives in Ruthenium-Catalyzed Hydroesterification of Alkenes Using Formates

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Supporting Information 1
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1. General method and materials

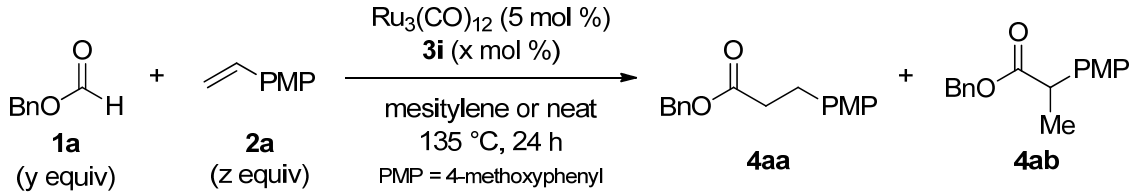
General. All reactions were performed in oven-dried or flame-dried glassware under argon atmosphere. Reactions were monitored by TLC on Merck silica gel 60 F254 plates visualized by UV lump at 254 nm. Column chromatography was performed on Merck silica gel 60 and preparative TLC was performed on Merck silica gel 60 F254 0.5 mm plates. NMR spectra were measured on a JEOL AL-400 NMR spectrometer at 400 MHz for ^{1}H spectra and 100 MHz for ^{13}C spectra, and for ^{1}H NMR, tetramethylsilane (TMS) ($\delta = 0$) in $CDCl_3$ served as an internal standard. For ^{13}C NMR, $CDCl_3$ ($\delta = 77.0$) served as an internal standard. Infrared spectra were measured on a SHIMADZU IR Prestige-21 spectrometer (ATR). High-resolution mass spectra (HRMS) were measured on a JEOL JMS-T100TD time-of-flight mass spectrometer (DART). Melting point was measured using a YAZAWA MICRO MELTING POINT BY-1.

Materials. $Ru_3(CO)_{12}$ was purchased from Strem and used as received. Mesitylene was purchased from TCI and purified by distillation prior to use. Compounds **2a-g**, and **3a-b** were purchased from TCI and used as received. Alkyl and aryl formates **1a-h** were synthesized according to the literature.[1] Analytical data of compounds **1a**,[2] **1b-c** and **1f-g**,[3] **1e**,[4] **1h**,[5] **3e**,[6] **3g**,[7] and **3h**[8] were identical to those reported in precedent literature.

2. Investigation of reaction conditions

We have further investigated reaction conditions (Table S1). Then we found that ratio of catalyst—imidazole ($Ru_3(CO)_{12}$ and **3i**) and equivalence of reagents (**1a** and **2a**) were important to promote hydroesterification reaction as well as to suppress decarbonylation of **1a**. Other Ru sources did not work at all.

Table S1. Investigation of Reaction Conditions.

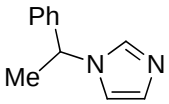


entry	x (mol %)	y (equiv)	z (equiv)	solvent	yield of **4** (%)[a]	**4aa**:**4ab**[b]	yield of BnOH (%)[c]
1	5	1.5	1.0	mesitylene	39	82:18	13
2	15	1.5	1.0	mesitylene	69	37:63	<1
3	30	1.5	1.0	mesitylene	66	43:57	51
4	15	1.5	1.0	neat	74	39:61	57
5	15	1.0	1.5	mesitylene	80	59:41	3
6	15	1.0	1.5	neat	89	54:46	<1
7	15	1.0	1.0	neat	77	44:56	14
8[d]	15	1.5	1.0	mesitylene	N.R.[e]	–	7
9[f]	15	1.5	1.0	mesitylene	trace	–	7

[a]Isolated yield. [b]Ratio determined by ^{1}H NMR analysis of isolated mixture of **4aa** and **4ab**. [c]Yield of BnOH (based on **2a**) determined by crude ^{1}H NMR analysis. [d]$Ru(cod)Cl_2$ and **3g** were used instead of $Ru_3(CO)_{12}$ and **3i**. [e]No reaction. [f]$Ru(PPh_3)HCl$ and **3g** were used instead of $Ru_3(CO)_{12}$ and **3i**.

3. Preparation of compounds

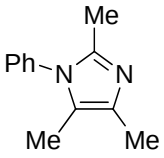
Preparation of imidazole derivatives.



1-(1-Phenylethyl)-1*H*-imidazole (3e)[6]

To a solution of 38% aq. glyoxal (5.04 g, 33.0 mmol, 2.0 equiv) and ammonium acetate (2.54 g, 33.0 mmol, 2.0 equiv) in MeOH (17 mL) was added (±)-1-phenylethylamine (2.00 g, 16.5 mmol) and 35% aq. formaldehyde (2.83 g, 33.0 mmol, 2.0 equiv). The mixture was warmed to 80 °C and stirred for 14 h. The reaction mixture was cooled to RT and diluted with toluene. The solution was washed with 10% aq. NaOH and the aqueous layer was extracted with toluene. The combined organic layer was washed with brine, dried over $MgSO_4$, filtered, and concentrated. The obtained residue was purified by column chromatography on silica gel (EtOAc) to afford the desired product **3e** (0.89 g, 5.18 mmol, 31%) as a pale yellow oil.

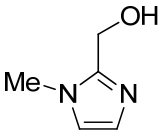
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (s, 1H), 7.28-7.22 (m, 3H), 7.13 (m, 2H), 7.09 (d, 1H, *J* = 2.0 Hz), 5.27 (q, 1H, *J* = 6.9 Hz), 1.78 (d, 3H, *J* = 7.2 Hz).



2,4,5-Trimethyl-1-phenyl-1*H*-imidazole (3f)

To a solution of 2,3-butanedione (3.70 g, 43.0 mmol, 2.0 equiv) and ammonium acetate (3.31 g, 33.0 mmol, 2.0 equiv) in MeOH (17 mL) was added aniline (2.00 g, 21.5 mmol) and 90% aq. acetaldehyde (2.10 g, 43.0 mmol, 2.0 equiv). The mixture was warmed to 80 °C and stirred for 20 h. The reaction mixture was cooled to RT and diluted with toluene. The solution was washed with 10% aq. NaOH and the aqueous layer was extracted with toluene. The combined organic layers were washed with brine, dried over $MgSO_4$, filtered, and concentrated. The obtained residue was purified by column chromatography on silica gel (EtOAc) to afford the desired product **3f** (1.23 g, 6.60 mmol, 31%) as a dark red oil.

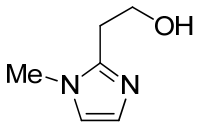
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.41 (m, 3H), 7.19-7.16 (m, 2H), 2.18 (s, 6H), 1.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.8, 137.2, 131.6, 129.4, 128.4, 127.5, 123.0, 13.8, 12.5 and 9.4; IR (ATR) 2920, 1597, 1499, 1404, 1387, 762 and 698 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{12}H_{15}N_2$: 187.1230; found 187.1240.



(1-Methyl-1*H*-imidazol-2-yl)methanol (3g)[8]

This compound was synthesized according to reported procedure. Yield: 73%.

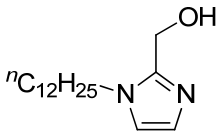
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (s, 1H), 6.90 (s, 1H), 6.84 (s, 1H), 4.66 (s, 2H), 3.72 (s, 3H).



2-(1-Methyl-1*H*-imidazol-2-yl)ethanol (3h)[8]

This compound was synthesized according to reported procedure. Yield: 4%.

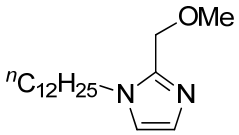
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92 (s, 1H), 6.81 (s, 1H), 4.04 (t, 2H, *J* = 5.6 Hz), 3.64 (s, 1H), 3.58 (s, 3H), 2.83 (t, 2H, *J* = 5.9 Hz).



(1-Dodecyl-1*H*-imidazol-2-yl)methanol (3i)[9]

This compound was synthesized from 1-dodecylimidazole according to reported procedure.[8] Yield: 50%.

^{1}H NMR (400MHz, $CDCl_3$) δ 6.92 (d, 1H, *J* = 1.5 Hz), 6.86 (d, 1H, *J* = 1.0 Hz), 4.66 (s, 2H), 3.96 (t, 2H, *J* = 7.6 Hz), 1.79-1.76 (m, 2H), 1.31-1.25 (m, 18H), 0.88 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.4, 127.1, 120.1, 56.3, 46.2, 32.0, 31.2, 29.7, 29.6, 29.4, 29.3, 26.8, 22.8 and 14.2.



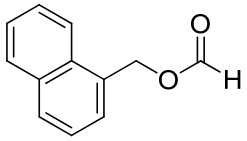
1-Dodecyl-2-(methoxymethyl)-1*H*-imidazole (3j)

To a solution of **3i** (213 mg, 0.800 mmol) in THF (5.0 mL) was added NaH (64.0 mg, 1.60 mmol, 2.0 equiv) at 0 °C. The mixture was warmed to RT and stirred for 45 min. MeI (100 μL, 1.60 mmol, 2.0 equiv) was added to the mixture. After the reaction mixture was stirred at RT for 2 h, EtOAc and H_2O were added carefully. The solution was separated and the aqueous layer was extracted with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$, filtered, and concentrated. The obtained residue was purified by PTLC ($CHCl_3$/MeOH 1/1) to afford the desired product **3j** (172 mg, 0.613 mmol, 77%) as a pale yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (s, 1H), 6.91 (s, 1H), 4.53 (s, 2H), 3.96 (t, 2H, *J* = 7.3 Hz), 3.32 (s, 3H), 1.81-1.72 (m, 2H), 1.35-1.23 (m, 18H), 0.88 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.9, 127.4, 120.3, 66.2, 57.5, 45.9, 31.7, 30.8, 29.50, 29.48, 29.4, 29.3, 29.2, 29.0, 26.5, 22.5 and 13.9; IR (ATR) 2920, 1492, 1462, 1188, 1087, 987 and 732 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{17}H_{33}N_2O$: 281.2593; found 281.2603.

Preparation of formates.

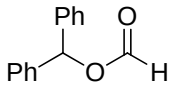
Formates **1a-h** were synthesized by formylation of the corresponding alcohols.[3] ^{1}H NMR spectra of compounds **1a-c**, **1e-f**, and **1g** were exactly identical to the reported data.



Naphthalen-1-ylmethyl formate (**1d**)

1-Naphthylmethanol (1.58 g, 10.0 mmol) was added to formic acid (4.0 mL) and the mixture was stirred at 60 °C for 3.5 h. The reaction mixture was diluted with CH_2Cl_2 and H_2O. The solution was separated and the aqueous layer was extracted with CH_2Cl_2, washed with saturated $NaHCO_3$ aq., dried over $MgSO_4$, filtered, and concentrated. The obtained residue was purified by column chromatography on silica gel (hexane/EtOAc 100/1) to afford **1d** (0.586 g, 3.15 mmol, 32%) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.98 (t, 1H, J = 7.8 Hz), 7.85 (t, 2H, J = 7.8 Hz), 7.56-7.41 (m, 4H), 5.63 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 133.6, 131.4, 130.6, 129.5, 128.7, 127.7, 126.6, 125.9, 125.1, 123.3 and 63.8; IR (ATR) 1716, 1145, and 771 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{12}H_{11}O_2$: 187.0754; found 187.0754.

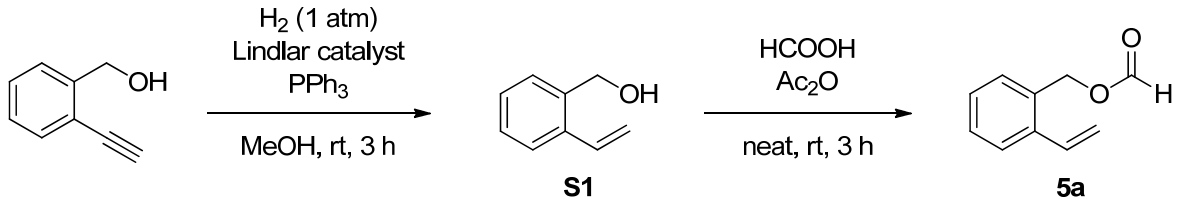


Benzhydryl formate (1h)[10]

Formic acid (1.70 mL, 45.0 mmol, 4.5 equiv) was added to acetic anhydride (4.70 mL, 50.0 mmol, 5.0 equiv) at RT. The resulting mixture was stirred at 60 °C for 1 h and cooled to RT. Benzhydrol (1.21 mL, 10.0 mmol) was added to the solution and the mixture was stirred for 0.5 h. The reaction mixture was diluted with Et_2O, washed with H_2O three times, dried over $MgSO_4$, filtered, and concentrated. The obtained residue was purified by column chromatography on silica gel (hexane/EtOAc 20/1) to afford the desired product **1h** (1.18 g, 7.84 mmol, 78%) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (s, 1H), 7.36-7.29 (m, 10H), 7.00 (s, 1H)

Preparation of substrates for intramolecular hydroesterification.



(2-Vinylphenyl)methanol (S1)

To a solution of 2-ethynylbenzyl alcohol (2.00 g, 15.1 mmol) in MeOH (14 mL) was added triphenylphosphine (150 mg, 0.57 mmol) and 5% palladium on calcium carbonate (30 mg). The mixture was stirred at RT under H_2 atmosphere (1 atm) for 3 h. The reaction mixture was filtered through Celite pad and concentrated. The obtained residue was purified by column chromatography on silica gel (hexane/EtOAc 6/1) to afford the desired product **S1** (2.03 g, 15.1 mmol, 100% yield) as a colorless oil.

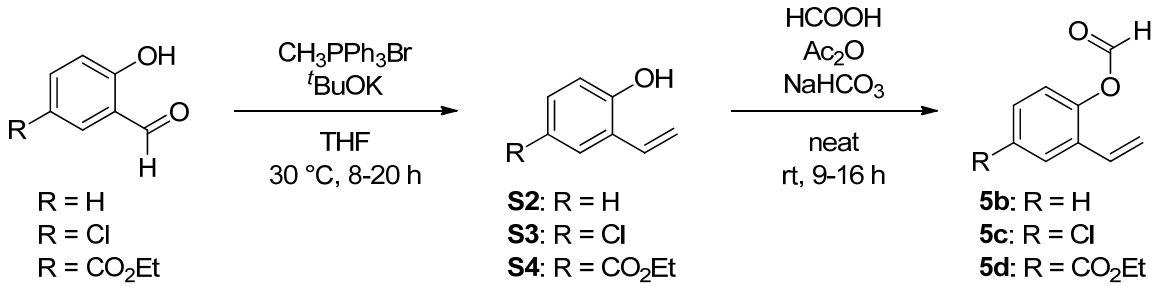
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (dd, 1H, *J* = 6.8, 2.0 Hz), 7.34 (dd, 1H, *J* = 6.8, 2.0 Hz), 7.31-7.23 (m, 2H), 7.03 (dd, 1H, *J* = 17.5, 10.8 Hz), 5.70 (dd, 1H, *J* = 17.5, 1.2 Hz), 5.34 (dd, 1H, *J* = 10.8, 1.2 Hz), 4.72 (s, 2H), 2.11 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.5, 136.6, 133.7, 128.3, 128.1, 127.9, 125.9, 116.4 and 63.3; IR (ATR) 3318, 1483, 1452, 1413, 945, 912, 760 and 729 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_9H_{11}O$: 135.0805; found 135.0810.

2-Vinylbenzyl formate (5a)

Formic acid (5.80 mL, 153 mmol, 10 equiv) was added to acetic anhydride (11.6 mL, 122 mmol, 8.0 equiv) at RT. The resulting mixture was stirred at 60 °C for 1 h and cooled to RT. **S1** (2.03 g, 15.3 mmol) was added to the solution and the mixture was stirred for 3 h. The reaction mixture was diluted with Et_2O, washed with H_2O three times, dried over $MgSO_4$, filtered, and concentrated. The obtained residue was purified by column chromatography on silica gel (hexane/EtOAc 15/1) to afford the desired product **5a** (2.16 g, 13.3 mmol, 87%) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.55 (d, 1H, *J* = 7.2 Hz), 7.38-7.33 (m, 2H), 7.27 (ddd, 1H, *J* = 7.6, 7.2, 1.2 Hz), 6.97 (dd, 1H, *J* = 17.6, 11.2 Hz), 5.70 (dd, 1H, *J* = 17.6, 0.8 Hz), 5.38 (dd, 1H, *J* = 11.2, 0.8 Hz), 5.28 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 137.6, 133.6, 132.2, 130.2, 129.2, 128.0, 126.2, 117.1 and 63.7; IR (ATR) 1717, 1144, 916, 772 and 750 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{10}H_{11}O_2$: 163.0754; found 163.0760.

General procedure of the synthesis of compounds 5b-5d.



Method 1: To a solution of methyltriphenylphosphonium bromide (18.9 mmol, 2.3 equiv) in dry THF (30 mL) was added 1 M ^{t}BuOK solution in THF (18.9 mL, 2.3 equiv). The mixture was stirred at RT for 2 h and cooled to –78 °C. Corresponding aldehyde or ketone (8.20 mmol) was added, warmed to RT slowly and stirred at 30 °C for 8-20 h. The reaction mixture was quenched with 1 M HCl aq., diluted with EtOAc, washed with brine. The obtained solution was dried over $MgSO_4$, filtered, and concentrated. The obtained residue was purified by column chromatography on silica gel.
Method 2: Formic acid (23.6 mmol, 10 equiv) was added to acetic anhydride (18.9 mmol, 8 equiv) at RT. The resulting mixture was stirred at 60 °C for 1 h and cooled to RT. Phenol derivative synthesized above (2.40 mmol) and sodium hydrogen carbonate (4.80 mmol, 2.0 equiv) were added to the solution and the mixture was stirred for 9-16 h. The reaction mixture was diluted with Et_2O, washed with H_2O three times, dried over $MgSO_4$, filtered, and concentrated. The obtained residue was purified by column chromatography on neutral silica gel to afford the desired product.

2-Vinylphenol (S2)[11]
S2 was obtained from *o*-hydroxybenzaldehyde using method 1 as a colorless oil. Yield: 100% yield.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, 1 H, *J* = 7.5 Hz), 7.14-7.10 (m, 1 H), 6.92-6.87 (m, 2 H), 6.77 (d, 1 H, *J* = 7.9 Hz), 5.72 (d, 1 H, *J* = 17.6 Hz), 5.32 (d, 1 H, *J* = 11.4 Hz), 5.14 (s, 1H).

2-Vinylphenyl formate (5b)
5b was obtained from **S2** using method 2 as a colorless oil. Yield: 100% yield.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.60 (dd, 1H, *J* = 7.2, 1.6 Hz), 7.33-7.23 (m, 2H), 7.08 (dd, 1H, *J* = 7.6, 1.2 Hz), 6.80 (dd, 1H, *J* = 17.6, 11.2 Hz), 5.78 (dd, 1H, *J* = 17.6, 0.8 Hz), 5.37 (dd, 1H, *J* = 11.2, 0.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 147.3, 130.2, 130.1, 129.0, 126.8, 126.8, 122.2, 117.1; IR (ATR) 1759, 1736, 1483, 1450, 1211, 1173, 1107, 1086, 918 and 762 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_9H_9O_2$: 149.0598; found 149.0600.

4-Chloro-2-vinylphenol (S3)[12]
S3 was obtained from 3-chlorosalicylaldehyde using method 1 as a colorless oil. Yield: 100% yield.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, 1 H, *J* = 7.5 Hz), 7.14-7.10 (m, 1 H), 6.92-6.87 (m, 1 H), 6.77 (d, 1 H, *J* = 7.9 Hz), 5.72 (d, 1 H, *J* = 17.6 Hz), 5.32 (d, 1 H, *J* = 11.4 Hz), 5.14 (s, 1H).

4-Chloro-2-vinylphenyl formate (5c)
5c was obtained from **S3** using method 2 as a colorless oil. Yield: 42%
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.56 (d, 1H, *J* = 2.4 Hz), 7.26 (dd, 1H, *J* = 8.4, 2.4 Hz), 7.04 (d, 1H, *J* = 8.0 Hz), 6.72 (dd, 1H, *J* = 17.6, 11.2 Hz), 5.78 (d, 1H, *J* = 17.6 Hz), 5.42 (d, 1H, *J* = 11.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 145.3, 132.1, 131.6, 128.9, 128.5, 126.4, 123.4, 118.1; IR (ATR) 1734, 1474, 1408, 1211, 1167, 1111, 1076 and 1042 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_9H_8ClO_2$: 183.0208; found 183.0208.

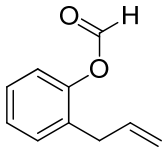
Ethyl 4-hydroxy-3-vinylbenzoate (S4)
S4 was obtained from 5-ethoxycarbonylsalicylaldehyde, which was synthesized according to previous report,[13] using method 1 as white needle (m.p. 105 °C). Yield: 86%.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, 1H, *J* = 2.4 Hz), 7.84 (dd, 1H, *J* = 8.8, 2.4 Hz), 6.93 (dd, 1H, *J* = 17.2, 11.2 Hz), 6.84 (d, 1H, *J* = 8.8 Hz), 5.91 (s, 1H), 5.83 (dd, 1H, *J* = 17.2, 1.2 Hz), 5.42 (dd, 1H, *J* =

11.2, 1.6 Hz), 4.36 (q, 2H, *J* = 7.6 Hz), 1.39 (t, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 157.7, 130.7, 130.6, 129.2, 124.9, 122.3, 116.4, 115.7, 61.2 and 14.3; IR (ATR) 3362, 1686, 1603, 1273, 752 and 635 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{11}H_{13}O_3$:193.0859; found 193.0867.

Ethyl 4-(formyloxy)-3-vinylbenzoate (5d)

5d was obtained from **S4** using method 2 as a colorless oil. Yield: 99%.

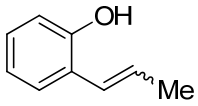
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 8.29 (d, 1H, *J* = 2.0 Hz), 7.98 (dd, 1H, *J* = 8.8, 2.0 Hz), 7.18 (d, 1H, *J* = 8.8 Hz), 6.80 (dd, 1H, *J* = 17.2, 11.2 Hz), 5.90 (dd, 1H, *J* = 17.2, 0.8 Hz), 5.45 (dd, 1H, *J* = 11.2, 0.8 Hz), 4.40 (q, 2H, *J* = 6.8 Hz), 1.41 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 158.3, 150.1, 130.1, 129.8, 129.2, 128.9, 128.2, 122.1, 118.1, 61.2, 14.2; IR (ATR) 1744, 1713, 1287, 1248, 1171, 1105, 1074 and 758 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{12}H_{13}O_4$: 221.0809; found 221.0801.



2-Allylphenyl formate (5e)

5e was obtained from 2-allylphenol by formylation analogous to synthesis of **5b** as a colorless oil. Yield: 93%.

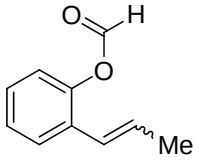
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.30-7.21 (m, 3H), 7.07 (dd, 1H, *J* = 8.0, 2.0 Hz), 5.91 (ddt, 1H, *J* = 17.2, 10.0, 6.4 Hz), 5.09 (dd, 1H, *J* = 10.0, 1.2 Hz), 5.04 (ddt, 1H, *J* = 17.2, 1.6, 1.2 Hz), 3.34 (d, 2H, *J* = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 147.9, 135.4, 131.5, 130.4, 127.3, 126.3, 121.6, 116.2 and 34.1; IR (ATR) 1761, 1736, 1487, 1209, 1167, 1117 and 742 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{10}H_{11}O_2$: 163.0754; found 163.0758.



2-(Prop-1-en-1-yl)phenol (S5)[14]

Compound **S5** was synthesized according to previous report (*E*:*Z* = 80:20).[15]

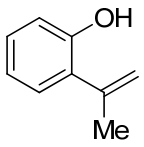
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (dd, 1H, *J* = 8.0, 1.2 Hz), 7.10(dt, 1H, *J* = 8.0, 1.2 Hz), 6.89 (t, 1H, *J* = 8.0 Hz), 6.80 (d, 1H, *J* = 8.0 Hz), 6.61 (dq, 1H, *J* = 15.9, 1.4 Hz, (*E*)), 6.42 (d, 1H, *J* = 11.2 Hz, (*Z*)), 6.21 (dq, 1H, *J* = 15.9, 6.6 Hz, (*E*)), 6.02 (dq, 1H, *J* = 11.2, 7.0 Hz, (*Z*)), 5.02 (s, 1H), 1.92 (dd, 3H, *J* = 6.5, 1.3 Hz, (*E*)), 1.72 (dd, 3H, *J* = 6.5, 1.3 Hz, (*Z*)).



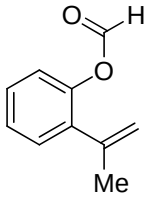
2-(Prop-1-en-1-yl)phenyl formate (5f)

5f (*E*:*Z* = 80:20) was obtained from **S5** (*E*:*Z* = 80:20) by formylation analogous to synthesis of **5b** as a colorless oil. Yield: 85%.

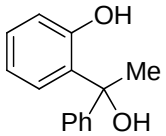
(*E*)-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.51-7.47 (m, 1H), 7.22-7.17 (m, 2H), 7.04-6.99 (m, 1H), 6.44 (dd, 1H, *J* = 16.0, 2.0 Hz), 6.24 (dq, 1H, *J* = 16.0, 6.8 Hz), 1.86 (dd, 3H, *J* = 6.8, 1.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 146.5, 130.2, 128.9, 127.6, 126.6, 126.5, 123.8, 121.8 and 18.7.
(*Z*)-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.33 (dd, 1H, *J* = 7.2, 1.6 Hz), 7.27-7.16 (m, 2H), 7.08 (dd, 1H, *J* = 7.6, 1.6 Hz), 6.33 (dd, 1H, *J* = 11.6, 1.2 Hz), 5.86 (dq, 1H, *J* = 11.6, 6.8 Hz), 1.75 (dd, 3H, *J* = 6.8, 2.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 147.5, 130.5, 129.9, 129.4, 127.9, 126.0, 123.8, 121.7 and 14.4.
(*E*)/(*Z*)-mixture: IR (ATR) 1759, 1736, 1483, 1445, 1215, 1173, 1113, 962 and 740 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{10}H_{11}O_2$: 163.0754; found 163.0763.



2-(Prop-1-en-2-yl)phenol (S6)[16]
S6 was obtained from *o*-hydroxyacetophenone by Wittig reaction analogous to synthesis of **S2** as a colorless oil. Yield: 87%.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17-7.14 (m, 2H), 6.95-6.88 (m, 2H), 5.69 (s, 1H), 5.42 (t, 1H, *J* = 1.7 Hz), 5.16 (s, 1H), 2.13 (s, 3H).

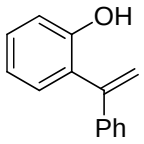


2-(Prop-1-en-2-yl)phenyl formate (5g)
5g was obtained from **S6** by formylation analogous to synthesis of **5b** as a colorless oil. Yield: 88%.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (s, 1H), 7.31-7.21 (m, 3H), 7.06 (dd, 1H, *J* = 7.6, 1.6 Hz), 5.21 (q, 1H, *J* = 1.2 Hz), 5.04 (s, 1H), 2.06 (t, 3H, *J* = 1.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 146.6, 141.2, 136.4, 129.5, 128.3, 126.5, 122.1, 116.8 and 23.3; IR (ATR) 1761, 1738, 1487, 1445, 1186, 1103, 905 and 762 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{10}H_{11}O_2$: 163.0754; found 163.0757.



2-(1-Hydroxy-1-phenylethyl)phenol (S7)[17]
To a solution of *o*-hydroxyacetophenone (2.0 g, 14.7 mmol) in dry THF (20 mL) was added 1 M PhMgBr solution (32.3 mL, 32.3 mmol, 2.2 equiv) at 0 °C. The mixture was warmed to reflux temperature and stirred for 8 h. The reaction mixture was cooled to 0 °C and then 15% AcOH aq. and toluene were added. The aqueous layer was extracted with toluene three times and the combined organic layers were washed with brine, dried over $MgSO_4$, filtered, and concentrated. The obtained residue was purified by column chromatography on silica gel to afford the desired product **S7** (2.2 g, 10.3 mmol, 70%) as a yellow solid (m.p. 110 °C).

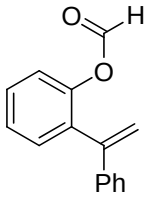
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H), 7.36-7.13 (m, 6H), 6.98 (d, 1H, *J* = 7.2 Hz), 6.82 (d, 2H, *J* = 7.5 Hz), 3.18 (s, 1H), 1.94 (s, 3H).



2-(1-phenylvinyl)phenol (S8)[18]

To a solution of **S7** (1.60 g, 7.50 mmol) in benzene (10 mL) was added I_2 (10.0 mg). The mixture was stirred at reflux temperature for 13 h. The reaction mixture was cooled to RT, washed with $Na_2S_2O_3$ aq. and brine, dried over $MgSO_4$, filtered, and concentrated. The obtained residue was purified by column chromatography on silica gel (hexane/EtOAc 9/1) to afford the desired product **S8** (1.40 g, 7.20 mmol, 96%) as a colorless oil.

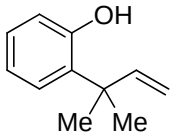
.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.30 (m, 5H), 7.28-7.21 (m, 1H), 7.13 (dd, 1H, *J* = 7.5, 1.6 Hz), 6.96-6.90 (m, 2H), 5.86 (d, 1H, *J* = 1.2 Hz), 5.41 (d, 1H, *J* = 1.2 Hz), 5.17 (s, 1H).



2-(1-Phenylvinyl)phenyl formate (5h)

5h was obtained from **S8** by formylation analogous to synthesis of **5b** as a colorless oil. Yield: 100% yield.

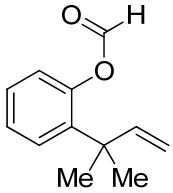
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.41-7.24 (m, 8H), 7.11 (d, 1H, *J* = 8.4 Hz), 5.72 (d, 1H, *J* = 1.2 Hz), 5.33 (d, 1H, *J* = 1.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 147.3, 145.3, 140.2, 134.7, 131.4, 129.0, 128.3, 127.9, 126.7, 126.6, 122.4 and 116.9; IR (ATR) 1736, 1485, 1447, 1188, 1115, 1090, 907, 760 and 700 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{15}H_{13}O_2$: 225.0910; found 225.0903.



2-(2-Methylbut-3-en-2-yl)phenol (S9)[19]

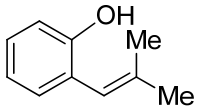
Compound **S9** was synthesized according to previous report.[20]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22-7.03 (m, 2H), 6.84-6.73 (m, 2H), 6.12 (dd, 1H, *J* = 17.6, 10.6 Hz), 5.78 (s, 1H), 5.26 (d, 1H, *J* = 17.6 Hz), 5.21 (d, 1H, *J* = 10.6 Hz), 1.36 (s, 6H).

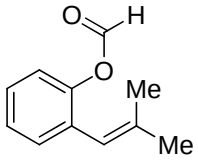


2-(2-Methylbut-3-en-2-yl)phenyl formate (5i)

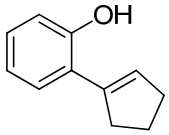
5i was obtained from **S9** by formylation analogous to synthesis of **5b** as a colorless oil. Yield: 71%.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.44 (dd, 1H, *J* = 8.0, 2.4 Hz), 7.30-7.20 (m, 2H), 6.99 (dd, 1H, *J* = 7.6, 2.0 Hz), 6.01-5.94 (m, 1H), 5.02-4.94 (m, 2H), 1.47 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 148.5, 147.0, 139.2, 127.7, 127.5, 126.4, 123.3, 111.2, 40.4 and 27.7; IR (ATR) 1761, 1740, 1485, 1443, 1184, 1099 and 752 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{12}H_{15}O_2$: 191.1067; found 191.1072.



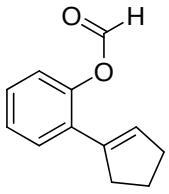
2-(2-Methylprop-1-en-1-yl)phenol (S10)
S10 was obtained from *o*-hydroxyacetophenone by Wittig reaction using isopropyltriphenylphosphonium iodide analogous to synthesis of **S2** as a colorless oil. Yield: 71%.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (ddd, 1H, *J* = 7.2, 6.8, 2.0 Hz), 7.04 (dd, 1H, *J* = 7.2, 1.6 Hz), 6.90-6.84 (m, 2H), 6.12 (s, 1H), 5.08 (s, 1H), 1.94 (d, 3H, *J* = 0.8 Hz), 1.68 (d, 3H, *J* = 1.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 140.5, 129.8, 128.2, 124.6, 120.1, 118.7, 114.8, 25.8 and 19.4; IR (ATR) 3422, 2970, 2911, 1576, 1485, 1445, 1215, 1171, 1096 and 748 cm^{-1}; HRMS (ESI) $[M+H]^+$ calcd for $C_{10}H_{13}O$: 149.0961; found 149.0965.



2-(2-Methylprop-1-en-1-yl)phenyl formate (5j)
5j was obtained from **S10** by formylation analogous to synthesis of **5b** as a colorless oil. Yield: 100%.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.30-7.21 (m, 3H), 7.07 (dd, 1H, *J* = 7.2, 1.6 Hz), 6.10 (s, 1H), 1.89 (d, 1H, *J* = 1.2 Hz), 1.74 (d, 3H, *J* = 1.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 147.6, 138.4, 131.3, 131.0, 127.5, 126.1, 121.5, 119.0, 26.2 and 19.4; IR (ATR) 2913, 1738, 1483, 1445, 1188, 1171, 1111 and 760 cm^{-1}; HRMS (ESI) $[M+H]^+$ calcd for $C_{11}H_{13}O_2$: 177.0910; found 177.0914.

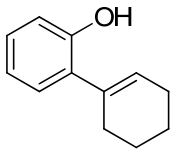


2-(Cyclopent-1-en-1-yl)phenol (S11)
Compound **S11** was synthesized according to previous report.[21]
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (dd, 1H, *J* = 7.8, 1.4 Hz), 7.13 (ddd, 1H, *J* = 7.8, 6.8, 1.4 Hz), 6.90-6.86 (m, 2H), 6.10 (m, 1H), 5.57 (s, 1H), 2.75-2.69 (m, 2H), 2.62-2.56 (m, 2H), 2.04-1.97 (m, 2H).

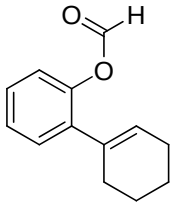


2-(Cyclopent-1-en-1-yl)phenyl formate (5k)

5k was obtained from **S11** by formylation analogous to synthesis of **5b** as a colorless oil. Yield: 96%.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (s, 1H), 7.39-7.36 (m, 1H), 7.28-7.21 (m, 2H), 7.08-7.04 (m, 1H), 6.19-6.14 (m, 1H), 2.73-2.65 (m, 2H), 2.56-2.48 (m, 2H), 2.00-1.91 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 147.3, 134.0, 131.8, 130.6, 129.3, 127.8, 126.7, 122.4, 35.4, 33.8 and 23.3; IR (ATR) 2949, 2843, 1759, 1738, 1487, 1445, 1175, 1115, 1090 and 746 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{12}H_{13}O_2$:189.0910; found 189.0917.



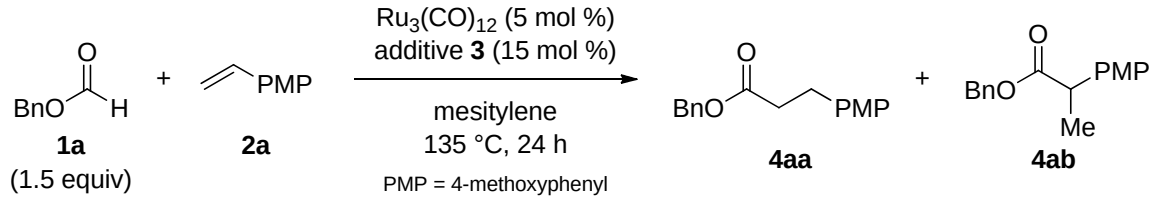
2-(Cyclohex-1-en-1-yl)phenol (S12)
Compound **S12** was synthesized according to previous report.[23]
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (ddd, 1H, *J* = 8.1, 7.8, 1.5 Hz), 7.07 (dd, 1H, *J* = 7.8, 1.5 Hz), 6.91 (dd, 1H, *J* = 8.3, 1.0 Hz), 6.87 (ddd, 1H, *J* = 8.3, 8.1, 1.0 Hz), 5.87 (m, 1H), 5.64 (s, 1H), 2.29-2.25 (m, 2H), 2.23-2.19 (m, 2H), 1.80-1.76 (m, 2H), 1.74-1.68 (m, 2H).



2-(Cyclohex-1-en-1-yl)phenyl formate (5l)
5l was obtained from **S12** by formylation analogous to synthesis of **5b** as a colorless oil. Yield: 92%.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.28-7.21 (m, 3H), 7.07-7.03 (m, 1H), 5.77-5.74 (m, 1H), 2.28-2.22 (m, 2H), 2.18-2.11 (m, 2H), 1.77-1.69 (m, 2H), 1.67-1.61 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 147.1, 137.4, 134.7, 129.9, 128.6, 127.9, 126.7, 122.1, 29.2, 25.7, 23.0 and 22.0; IR (ATR) 2928, 1761, 1740, 1483, 1443, 1177, 1115, 1092 and 750 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{13}H_{15}O_2$ 203.1067; found 203.1065.

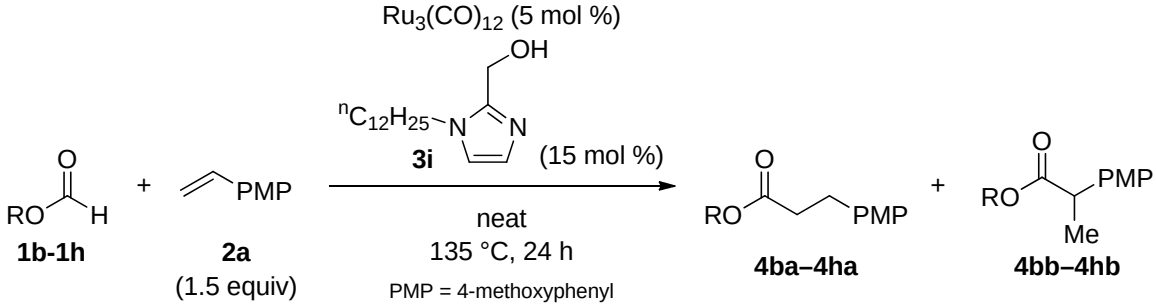
4. General experimental procedure

General experimental procedure of investigations for effect of additives (Table 1).



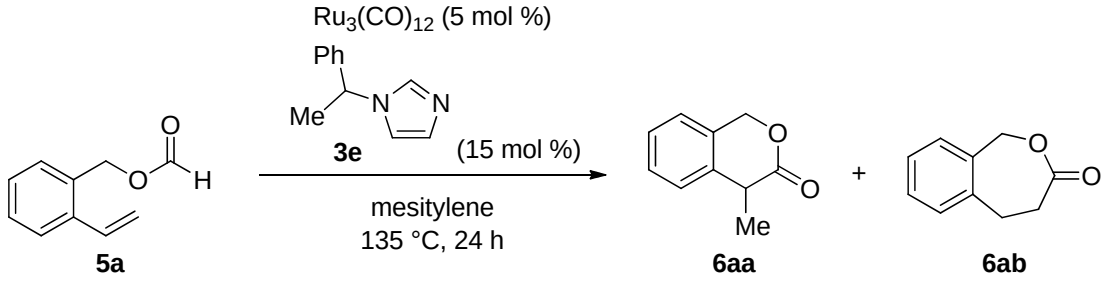
Benzyl formate (**1a**, 77.0 μL, 0.600 mmol, 1.5 equiv), imidazole derivative as additive **3** (0.0600 mmol, 15 mol %), $Ru_3(CO)_{12}$ (12.8 mg, 0.0200 mmol, 5 mol %), and mesitylene (0.20 mL) were added to a 2-mL vial equipped with a silicon septum cap under flowing Ar. 4-Methoxystyrene (**2a**, 53.2 μL, 0.400 mmol) was added to the vial and then sealed by a new silicon septum cap. The mixture was warmed to 135 °C (bath temperature) and stirred for 24 h. The reaction mixture was cooled to RT and was diluted with EtOAc, washed with H_2O three times, dried over Na_2SO_4, filtered, and concentrated. The obtained residue was purified by column chromatography on silica gel (hexane/EtOAc 5/1) to afford mixture of the desired product **4aa** and **4ab** as a colorless oil.

General experimental procedure of intermolecular hydroesterification (Tables 2 and 3).



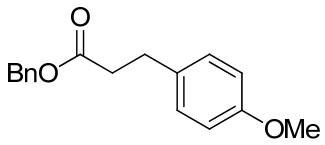
Formate (0.400 mmol), **3i** (16.0 mg, 0.0600 mmol, 15 mol %), and $Ru_3(CO)_{12}$ (12.8 mg, 0.0200 mmol, 5 mol %) were added to a 2-mL vial equipped with a silicon septum cap under flowing Ar. Alkene (0.600 mmol, 1.5 equiv) was added to the vial and then sealed by a new silicon septum cap. The mixture was warmed to 135 °C (bath temperature) and stirred for 24 h. The reaction mixture was cooled to RT and was diluted with EtOAc, washed with H_2O three times, dried over Na_2SO_4, filtered, and concentrated. The obtained residue was purified by column chromatography on silica gel (hexane/EtOAc 5/1) to afford mixture of the desired linear and branched product as colorless oil.

Representative experimental procedure of intramolecular hydroesterification (Table 4, entry 2).



5a (100 mg, 0.620 mmol), **3e** (16.0 mg, 0.0930 mmol, 15 mol %), and mesitylene (0.30 mL) were added to a 2-mL vial equipped with a silicon septum cap under flowing Ar. $Ru_3(CO)_{12}$ (20.0 mg, 0.0310 mmol, 5 mol %) was added to the vial and then sealed by a new silicon septum cap. The mixture was warmed to 135 °C (bath temperature) and stirred for 24 h. The reaction mixture was cooled to RT and directly purified by PTLC on silica gel (hexanes/EtOAc 4/1) to afford *exo* product **6aa** (68 mg, 0.422 mmol, 68%) as a colorless oil and *endo* product **6ab** (8 mg, 0.050 mmol, 8%) as a colorless oil.

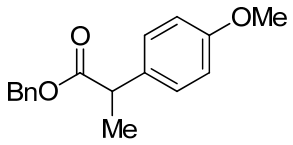
5. Analytical data of hydroesterification products



Benzyl 3-(4-methoxyphenyl)propanoate (4aa)[22]

4aa was obtained from **1a** and **2a** as a colorless oil. Yield: 48%.

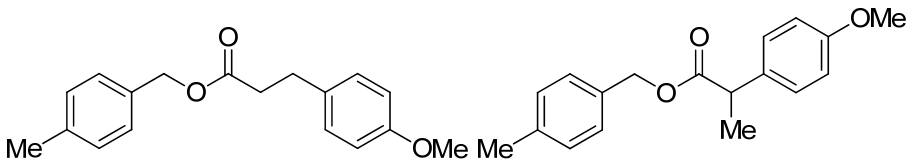
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.27 (m, 5H), 7.10 (d, 2H, *J* = 8.3 Hz), 6.81 (d, 2H, *J* = 8.3 Hz), 5.10 (s, 2H), 3.78 (s, 3H), 2.91 (t, 2H, *J* = 7.6 Hz), 2.65 (t, 2H, *J* = 7.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 158.1, 136.0, 132.5, 129.2, 128.5, 128.2, 113.9, 66.2, 55.2, 36.2 and 30.1; IR (ATR) 2934, 1732, 1512, 1244, 1148, 1034, 826, 735, 696 and 519 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{17}H_{19}O_3$: 271.1329; found 271.1323.



Benzyl 2-(4-methoxyphenyl)propanoate (4ab)

4ab was obtained from **1a** and **2a** as a colorless oil. Yield: 41%.

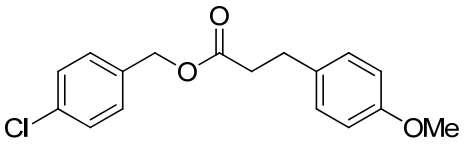
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.25 (m, 7H), 6.85 (d, 2H, *J* = 8.8 Hz), 5.12 (d, 1H, *J* = 12.7 Hz) 5.06 (d, 1H, *J* = 12.7 Hz), 3.78 (s, 3H), 3.73 (q, 1H, *J* = 7.1 Hz), 1.49 (d, 3H, *J* = 7.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.6, 158.7, 136.0, 132.5, 128.5, 128.4, 128.0, 127.8, 113.9, 66.3, 55.2, 44.6 and 18.5; IR (ATR) 2934, 1732, 1510, 1244, 1153, 1034, 833, 737 and 696 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{17}H_{19}O_3$: 271.1329; found 271.1323.



4-Methylbenzyl 3-(4-methoxyphenyl)propanoate (4ba) and **4-methylbenzyl 2-(4-methoxyphenyl)propanoate (4bb)**

Mixture of **4ba** and **4bb** was obtained from **1b** and **2a** as a colorless oil. Yield: 83% (**4ba**:**4bb** = 53:47).

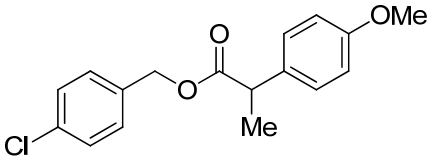
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22-7.18 (m, 2H), 7.15-7.12 (m, 2H), 7.08 (d, 2H, *J* = 11.0 Hz), 6.84 (d, 2H, *J* = 11.0 Hz), 6.79 (d, 2H, *J* = 11.0 Hz), 5.07 (d, 1H, *J* = 15.9 Hz, **4bb**), 5.05 (s, 2H, **4ba**), 5.00 (d, 1H, *J* = 15.9 Hz, **4bb**), 3.77 (s, 3H), 3.76 (s, 3H), 3.70 (q, 1H, *J* = 8.6 Hz, **4bb**), 2.89 (t, 2H, *J* = 9.8 Hz, **4ba**), 2.62 (t, 2H, *J* = 9.8 Hz, **4ba**), 2.34 (s, 3H), 2.32 (s, 3H), 1.47 (d, 3H, *J* = 8.6 Hz, **4bb**); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 172.7, 158.6, 158.0, 137.9, 137.8, 133.0, 132.9, 132.5, 132.4, 129.2, 129.13, 129.06, 128.5, 128.3, 128.0, 113.9, 113.8, 66.3, 66.1, 55.2, 55.1, 44.6, 36.1, 30.0, 21.11, 21.10 and 18.5; IR (ATR) 1730, 1512, 1244, 1151, 1033 and 806 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{18}H_{20}O_3$: 285.1485; found 285.1483.



4-Chlorobenzyl 3-(4-methoxyphenyl)propanoate (4ca)

4ca was obtained from **1c** and **2a** as a colorless oil. Yield: 31%.

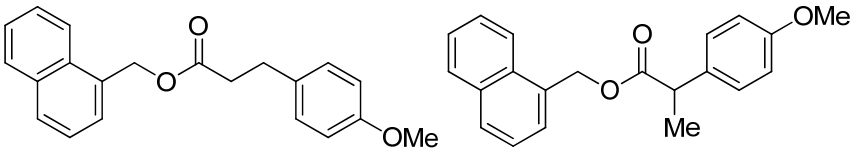
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, 2H, *J* = 11.0 Hz), 7.21 (d, 2H, *J* = 11.0 Hz), 7.08 (d, 2H, *J* = 11.0 Hz), 6.80 (d, 2H, *J* = 11.0 Hz), 5.05 (s, 2H), 3.78 (s, 3H), 2.90 (t, 2H, *J* = 9.8 Hz), 2.64 (t, 2H, *J* = 9.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 158.1, 134.4, 132.3, 129.5, 129.2, 128.7, 113.8, 65.3, 55.2, 36.1 and 30.0 (one aromatic carbon signal is missing); IR (ATR) 1732, 1512, 1244, 1149, 1033 and 825 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{17}H_{17}ClO_3$: 305.0939; found 305.0934.



4-Chlorobenzyl 2-(4-methoxyphenyl)propanoate (4cb)

4cb was obtained from **1c** and **2a** as a colorless oil. Yield: 30%.

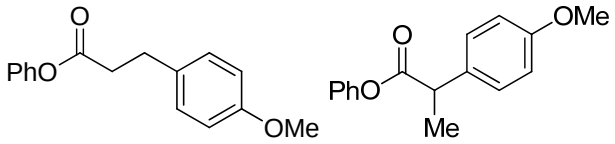
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, 2H, *J* = 11.0 Hz), 7.20 (d, 2H, *J* = 11.0 Hz), 7.15 (d, 2H, *J* = 11.0 Hz), 6.85 (d, 2H, *J* = 11.0 Hz), 5.04 (s, 2H), 3.79 (s, 3H), 3.71 (q, 1H, *J* = 9.2 Hz), 1.48 (d, 3H, *J* = 9.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.4, 158.7, 134.5, 133.9, 132.3, 129.2, 128.6, 128.5, 114.0, 65.5, 55.2, 44.6 and 18.4; IR (ATR) 11732, 1510, 1246, 1155, 1085 and 804 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{17}H_{17}ClO_3$: 305.0939; found 305.0931.



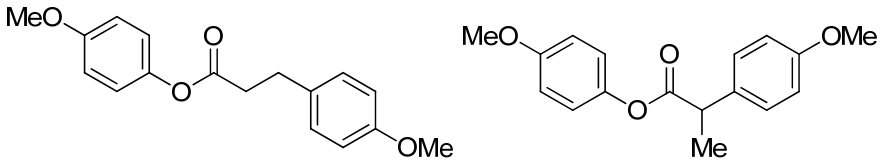
Naphthalen-1-ylmethyl 3-(4-methoxyphenyl)propanoate (4da) and **naphthalen-1-ylmethyl 2-(4-methoxyphenyl)propanoate (4db)**

Mixture of **4da** and **4db** was obtained from **1d** and **2a** as a colorless oil. Yield: 79% (**4da**:**4db** = 44:56).

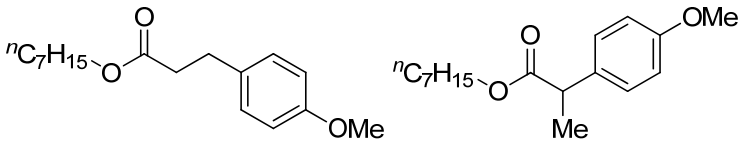
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91-7.79 (m, 2H), 7.51-7.37 (m, 4H), 7.21 (d, 2H, *J* = 11.0 Hz, **4db**), 7.06 (d, 2H, *J* = 11.0 Hz, **4da**), 6.80 (d, 2H, *J* = 11.0 Hz, **4da**), 6.77 (d, 2H, *J* = 11.0 Hz, **4db**), 5.55 (s, 2H, **4da**), 5.54 (d, 1H, *J* = 15.9 Hz, **4db**), 5.50 (d, 1H, *J* = 15.9 Hz, **4db**), 3.77 (s, 3H), 3.75 (s, 3H), 3.71 (q, 1H, *J* = 9.2 Hz, **4db**), 2.90 (t, 2H, *J* = 9.8 Hz, **4da**), 2.62 (t, 2H, *J* = 9.8 Hz, **4da**), 1.48 (d, 3H, *J* = 9.2 Hz, **4db**); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 172.8, 158.6, 158.0, 133.61, 133.56, 132.31, 132.29, 131.5, 131.44, 131.36, 131.3, 129.2, 129.14, 129.06, 128.6, 128.50, 128.47, 127.4, 127.1, 126.4, 126.3, 125.84, 125.76, 125.2, 125.1, 123.53, 123.47, 113.9, 113.8, 64.9, 64.4, 55.12, 55.08, 44.6, 36.1, 30.0 and 18.5; IR (ATR) 1728, 1510, 1244, 1151, 1033 and 790 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{21}H_{20}O_3$: 321.1485; found 321.1493.



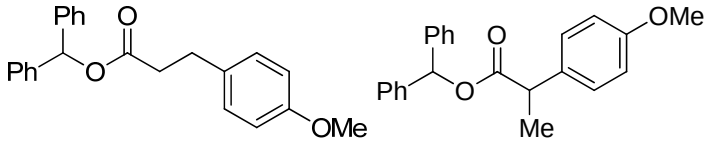
Phenyl 3-(4-methoxyphenyl)propanoate (4ea) and **phenyl 2-(4-methoxyphenyl)propanoate (4eb)**
Mixture of **4ea** and **4eb** was obtained from **1e** and **2a** as a colorless oil. Yield: 43% (**4ea**:**4eb** = 68:32).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.30 (m, 2H), 7.24-7.16 (m, 3H), 7.01-6.98 (m, 2H), 6.91-6.84 (m, 2H), 3.91 (q, 1H, *J* = 7.2 Hz, **4eb**), 3.77 (s, 3H), 3.01 (t, 2H, *J* = 7.6 Hz, **4ea**), 2.84 (t, 2H, *J* = 16.1 Hz, **4ea**), 1.58 (d, 3H, *J* = 5.9 Hz, **4eb**); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.4, 171.6, 158.9, 158.3, 150.9, 150.7, 132.3, 132.2, 129.5, 129.4, 128.7, 125.9, 125.8, 121.7, 121.5, 114.3, 114.1, 114.0, 55.4, 44.9, 36.4, 30.2 and 18.7; IR (ATR) 2934, 1753, 1611, 1512, 1246, 1194, 1128, 1032, 827 and 689 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{16}H_{17}O_3$: 257.1172; found 257.1180.



4-Methoxyphenyl 3-(4-methoxyphenyl)propanoate (4fa) and **4-methoxyphenyl 2-(4-methoxyphenyl)propanoate (4fb)**
Mixture of **4fa** and **4fb** was obtained from **1f** and **2a** as a colorless oil. Yield: 57% (**4fa**:**4fb** = 48:52).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, 2H, *J* = 11.0 Hz, **4fb**), 7.17 (d, 2H, *J* = 11.0 Hz, **4fa**), 6.93-6.81 (m, 6H), 3.88 (q, 1H, *J* = 9.2 Hz, **4fb**), 3.79 (s, 3H), 3.78 (s, 3H), 3.77 (s, 3H), 3.75 (s, 3H), 3.00 (t, 2H, *J* = 9.8 Hz, **4fa**), 2.81 (t, 2H, *J* = 9.8 Hz, **4fa**), 1.57 (d, 3H, *J* = 9.2 Hz, **4fb**); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.6, 171.8, 158.8, 158.1, 157.2, 157.1, 144.3, 144.1, 132.18, 132.16, 129.3, 128.5, 122.2, 122.1, 114.4, 114.3, 114.1, 113.9, 55.5, 55.2, 44.7, 36.2, 30.1 and 18.5; IR (ATR) 1749, 1504, 1238, 1184, 1099, 1029 and 813 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{17}H_{18}O_4$: 287.1278; found 287.1283.

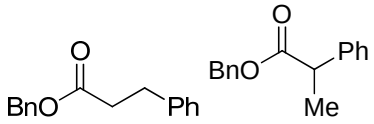


Heptyl 3-(4-methoxyphenyl)propanoate (4ga) and **heptyl 2-(4-methoxyphenyl)propanoate (4gb)**
Mixture of **4ga** and **4gb** was obtained from **1g** and **2a** as a yellow oil. Yield: 76% (**4ga**:**4gb** = 61:39).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (1H, d,), 7.11 (d, 1H, *J* = 8.8 Hz), 6.83 (dd, 2H, *J* = 10.7, 8.8 Hz), 4.04 (td, 2H, *J* = 6.8, 3.9 Hz), 3.77 (d, 3H, *J* = 2.9 Hz), 3.74 (s, 3H), 3.65 (q, 1H, *J* = 7.2 Hz, **4gb**), 2.88 (t, 2H, *J* = 7.8 Hz, **4ga**), 2.58 (t, 2H, *J* = 7.8 Hz, **4ga**), 1.57 (m, 2H), 1.47 (d, 3H, *J* = 7.3 Hz, **4gb**), 1.26 (m, 8H), 0.87 (q, 3H, *J* = 6.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 173.0, 158.5, 158.0, 132.7, 132.5, 129.1, 128.4, 113.8, 64.7, 64.5, 55.1, 44.6, 36.1, 31.6, 30.1, 28.8, 28.5, 25.8, 25.7, 22.5, 18.4 and 14.0; IR (ATR) 2928, 1732, 1612, 1512, 1458, 1246, 1204, 1167, 1036 and 827 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{17}H_{27}O_3$: 279.1955; found 279.1953.



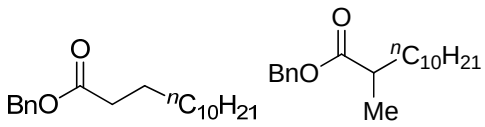
Benzhydryl 3-(4-methoxyphenyl)propanoate (4ha) and **benzhydryl 2-(4-methoxyphenyl)propanoate (4hb)**

Mixture of **4ha** and **4hb** was obtained from **1h** and **2a** as a colorless oil. Yield: 73% (**4ha**:**4hb** = 83:17). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, 2H, *J* = 7.3 Hz), 7.55 (t, 1H, *J* = 8.3 Hz), 7.45 (t, 2H, *J* = 7.6 Hz), 7.34-7.19 (m, 5H), 7.10-7.04 (m, 2H), 6.88-6.77 (m, 3H), 3.80-3.72 (m, 1H, **4hb**), 3.75 (s, 3H, **4ha**), 3.74 (s, 3H, **4hb**), 2.91 (t, 2H, *J* = 7.6 Hz, **4ha**), 2.70 (t, 2H, *J* = 7.6 Hz, **4ha**), 1.49 (d, 3H, *J* = 7.3 Hz, **4hb**); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.6, 171.9, 158.0, 140.1, 137.5, 132.3, 123.0, 129.2, 128.6, 128.5, 128.4, 128.3, 128.2, 128.1, 127.8, 127.5, 127.2, 127.1, 127.0, 126.6, 113.9, 113.8, 55.2, 55.1, 44.8, 36.3, 30.0 and 18.2; IR (ATR) 1734, 1659, 1512, 1246, 1150, 1032, 829, 745, 700 and 638 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{23}H_{23}O_3$: 347.1642; found 347.1633.



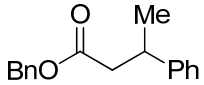
Benzyl 3-phenylpropanoate (4ia)[23] and **benzyl 2-phenylpropanoate (4ib)**[24]

Mixture of **4ia** and **4ib** was obtained from **1a** and **2b** as a colorless oil. Yield: >99% (**4ia**:**4ib** = 55:45). ^{1}H NMR ($CDCl_3$) δ 7.35-7.17 (m, 10H), 5.13 (d, 1H, *J* = 12.7 Hz), 5.11 (s, 2H), 5.07 (d, 1H, *J* = 12.2 Hz), 3.78 (q, 1H, *J* = 7.2 Hz, **4ib**), 2.97 (t, 2H, *J* = 7.8 Hz, **4ia**), 2.69 (t, 2H, *J* = 7.8 Hz, **4ia**), 1.52 (d, 3H, *J* = 7.2 Hz, **4ib**); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.2, 172.6, 140.4, 136.0, 135.9, 128.6, 128.5, 128.4, 128.2, 128.1, 128.0, 127.8, 127.5, 127.1, 126.2, 66.3, 66.2, 45.5, 35.8, 30.9 and 18.4; IR (ATR) 3030, 1732, 1497, 1454, 1200, 1152, 1030, 733 and 694 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{17}H_{19}O_2$: 241.1223; found 241.1214.



Benzyl tridecanoate (4ja) and **benzyl 2-methyltridecanoate (4jb)**

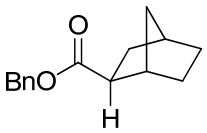
Mixture of **4ja** and **4jb** was obtained from **1a** and **2c** as a gray oil. Yield: 75% (**4ja**:**4jb** = 76:24). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.28 (m, 5H), 5.10 (s, 2H), 2.48 (q, 1H, *J* = 7.0 Hz, **4jb**), 2.35 (t, 2H, *J* = 7.6 Hz, **4ja**), 1.63 (m, 2H), 1.25-1.28 (m, 18H), 1.16 (d, 3H, *J* = 6.8 Hz, **4jb**), 0.86 (t, 3H, *J* = 8.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.8, 176.5, 176.4, 173.8, 136.4, 136.3, 128.6, 128.3, 66.1, 66.0, 65.9, 47.5, 45.8, 45.6, 39.7, 34.4, 33.9, 32.0, 29.8, 29.7, 29.6, 29.5, 29.4, 29.3, 27.3, 25.1, 22.8, 17.2 and 14.3; IR (ATR) 2922, 2853, 1736, 1456, 1213, 1155, 1115, 748, 733 and 696 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{20}H_{33}O_2$: 305.2475; found 305.2476.



Benzyl 3-phenylbutanoate (4k)[25]

4k was obtained from **1a** and **2d** as a colorless oil. Yield: 50%.

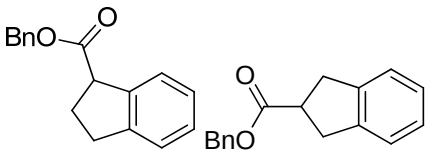
^{1}H NMR (400MHz, $CDCl_3$) δ 7.33-7.18 (m, 10H), 5.05 (s, 2H), 3.30 (q, 1H, *J* = 7.3 Hz), 2.64 (dq, 2H, *J* = 7.6, 7.5 Hz), 1.30 (d, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.1, 145.5, 135.9, 128.5, 128.4, 128.1, 126.7, 126.4, 66.1, 42.9, 36.5 and 21.8; IR (ATR) 2963, 1730, 1495, 1454, 1265, 1152, 1020, 976, 750 and 696 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{17}H_{19}O_2$: 255.1380; found 255.1385.



(1*S*,2*S*,4*R*)-Benzyl bicyclo[2.2.1]heptane-2-carboxylate (4l)[26]

4l was obtained from **1a** and **1e** as a colorless oil. Yield: 83%.

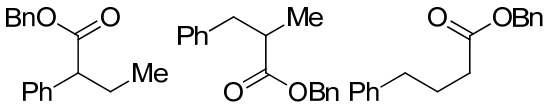
^{1}H NMR (400MHz, $CDCl_3$) δ 7.37-7.33 (m, 5H), 5.10 (s, 2H), 2.52 (br s, 1H), 2.37 (q, 1H, *J* = 4.6 Hz), 2.30 (br s, 1H), 1.89-1.83 (m, 1H), 1.54-1.49 (m, 4H), 1.23-1.19 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.8, 136.4, 128.5, 128.0, 66.0, 46.5, 40.9, 36.5, 36.0, 34.1, 29.4 and 28.6; IR (ATR) 2953, 1728, 1310, 1213, 1155, 1065, 1024, 735 and 696 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{15}H_{19}O_2$: 232.1380; found 232.1380.



Benzyl 2,3-dihydro-1*H*-indene-1-carboxylate (4ma) and **benzyl 2,3-dihydro-1*H*-indene-2-carboxylate (4mb)**

Mixture of **4ma** and **4mb** was obtained from **1a** and **2f** as a colorless oil. Yield: 88% (**4ma**:**4mb** = 76:24).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.34 (m, 4H), 7.21-7.16 (m, 5H), 5.16 (s, 2H), 4.09 (t, 1H, *J* = 7.3 Hz, **4ma**), 3.40-3.31 (m, 1H, **4mb**), 3.29-3.18 (m, 4H, **4mb**), 3.14-3.06 (m, 1H, **4ma**), 2.94-2.87 (m, 1H, **4ma**), 2.51-2.42 (m, 1H, **4ma**), 2.37-2.28 (m, 1H, **4ma**); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.2, 173.9, 144.3, 141.7, 140.7, 136.2, 128.7, 128.3, 128.2, 127.7, 126.8, 126.6, 125.0, 124.8, 124.5, 66.7, 66.6, 50.3, 43.8, 36.3, 31.9 and 28.8; IR (ATR) 2947, 1730, 1603, 1456, 1258, 1153, 1016, 970, 745 and 696 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{17}H_{17}O_2$: 253.1223; found 253.1231.

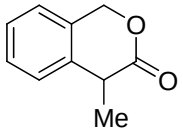


Benzyl 2-phenylbutanoate (4na),[27] **benzyl 2-methyl-3-phenylpropanoate (4nb)**,[24] and **benzyl 4-phenylbutanoate (4nc)**[29]

Mixture of **4na**, **4nb** and **4nc** was obtained from **1a** and **2g** as a colorless oil. Yield: 69% (**4na**:**4nb**:**4nc** = 51:20:29).

^{1}H NMR (400MHz, $CDCl_3$) δ 7.56-7.13 (m, 10H), 5.14 (d, 1H, *J* = 12.7 Hz), 5.11 (s, 2H), 5.07 (s, 2H), 5.06 (d, 1H, *J* = 12.7 Hz), 3.51 (t, 1H, *J* = 7.8 Hz, **4na**), 3.04 (q, 1H, *J* = 6.7 Hz, **4nb**), 2.80 (q, 1H, *J* = 7.0 Hz, **4nb**), 2.70 (t, 1H, *J* = 6.6 Hz, **4nb**), 2.64 (t, 2H, *J* = 7.8 Hz, **4nc**), 2.38 (t, 2H, *J* = 7.6 Hz, **4nc**), 2.18-2.07 (m, 1H, **4na**), 2.01-1.94 (m, 2H, **4nc**), 1.87-1.77 (m, 1H, **4na**), 1.18 (d, 3H, *J* = 6.8 Hz, **4nb**), 0.88 (t, 3H, *J* = 7.3 Hz, **4na**); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.9, 173.3, 141.3, 139.2, 136.1, 129.0, 128.5, 128.4, 128.3, 128.2, 128.1, 128.0, 127.9, 126.3, 126.0, 66.3, 66.1, 41.5, 39.7, 35.1, 33.6, 26.6, 26.5 and

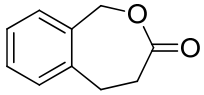
16.8; IR (ATR) 3028, 1732, 1497, 1454, 1153, 1028, 743, 696 and 509 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{17}H_{19}O_2$: 255.1380; found 255.1389.



4-Methylisochroman-3-one (6aa)[28]

6aa was obtained from **5a** as a colorless oil. Yield: 67%.

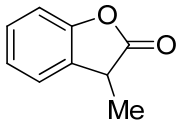
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.24 (m, 4H), 5.34 (d, 1H, *J* = 13.6 Hz), 5.28 (d, 1H, *J* = 13.6 Hz), 3.64 (q, 1H, *J* = 6.8 Hz), 1.64 (d, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.4, 135.4, 131.8, 128.7, 126.9, 124.5, 124.4, 69.0, 39.2, and 12.7; IR (ATR) 1736, 1462, 1381, 1240, 1150, 1123, 1043, 1022, 793, 752, and 733 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{10}H_{11}O_2$: 163.0754; found 163.0763.



4,5-Dihydrobenzo[*c*]oxepin-3(1*H*)-one (6ab)[29]

6ab was obtained from **5a** as a colorless oil. Yield: 8%.

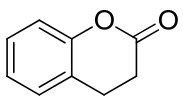
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.25 (m, 1H), 7.23-7.15 (m, 3H), 5.28 (s, 2H), 3.28-3.24 (m, 2H), 3.11-3.07 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.0, 137.0, 133.1, 129.9, 129.20, 129.17, 126.6, 70.2, 31.5, and 28.3; IR (ATR) 1726, 1452, 1381, 1236, 1152, 1016, and 754 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{10}H_{11}O_2$: 163.0754; found 163.0749.



3-Methylbenzofuran-2(3*H*)-one (6ba)[30]

6ba was obtained from **5b** as a colorless oil. Yield: 71%.

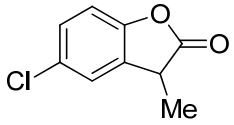
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.24 (m, 2H), 7.15 (t, 1H, *J* = 7.5 Hz), 7.09 (d, 1H, *J* = 8.0 Hz), 3.72 (q, 1H, *J* = 7.6 Hz), 1.56 (d, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.8, 153.4, 128.72, 128.66, 124.1, 123.8, 110.6, 38.2, and 15.7; IR (ATR) 1800, 1618, 1477, 1464, 1292, 1231, 1202, 1125, 1086, 1030, 989, 878, 748, and 727 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_9H_9O_2$: 149.0597; found 149.0597.



Chroman-2-one (6bb)[31]

6bb was obtained from **5b** as a colorless oil. Yield: 11%.

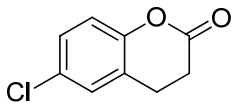
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-7.10 (m, 2H), 7.10-6.95 (m, 2H), 3.01-2.89 (m, 2H), 2.78-2.69 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 152.0, 128.3, 128.0, 124.4, 122.6, 117.0, 29.3, and 23.7; IR (ATR) 1768, 1751, 1489, 1458, 1244, 1225, 1138, 1107, 1024, 897, and 754 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_9H_9O_2$: 149.0597; found 149.0589.



5-Chloro-3-methylbenzofuran-2(3*H*)-one (6ca)

6ca was obtained from **5c** as a colorless oil. Yield: 67%.

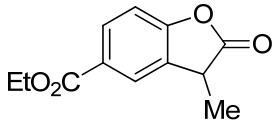
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.24 (m, 2H), 7.03 (d, 1H, *J* = 8.4 Hz), 3.74 (q, 1H, *J* = 7.6 Hz), 1.57 (d, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.1, 151.8, 130.4, 129.4, 128.8, 128.4, 124.2, 111.8, 38.5 and 15.7; IR (ATR) 1803, 1471, 1231, 1132, 1094, 1026, 849 and 812 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_9H_8ClO_2$: 183.0207; found 183.0214.



6-Chlorochroman-2-one (6cb)[33]

6cb was obtained from **5d** as a white solid (m.p. 107 °C). Yield: 13%.

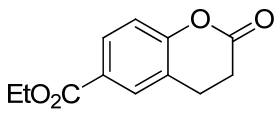
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.17 (m, 2H), 6.99 (d, 1H, *J* = 8.5 Hz), 3.05-2.94 (m, 2H), 2.84-2.74 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 150.5, 129.4, 128.3, 127.9, 124.2, 118.3, 28.8, and 23.6; IR (ATR) 1734, 1479, 1414, 1341, 1280, 1225, 1179, 1163, 1153, 1115, 1082, 899, and 818 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_9H_8ClO_2$: 183.0207; found 183.0211.



Ethyl 3-methyl-2-oxo-2,3-dihydrobenzofuran-5-carboxylate (6da)

6da was obtained from **5d** as a white solid (m.p. 97 °C). Yield: 59%.

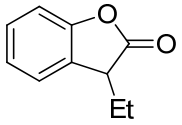
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (ddd, 1H, *J* = 8.0, 1.2, 0.8 Hz), 7.97 (dd, 1H, *J* = 1.2, 0.8 Hz), 7.15 (d, 1H, *J* = 8.0 Hz), 4.38 (qdd, 2H, *J* = 7.6, 0.8, 0.8 Hz), 3.78 (q, 1H, *J* = 7.2 Hz), 1.62 (d, 3H, *J* = 7.2 Hz), 1.41 (t, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.2, 165.8, 156.8, 131.2, 128.9, 126.7, 125.5, 110.5, 61.2, 38.1, 15.7, 14.3; IR (ATR) 1802, 1709, 1620, 1242, 1022, 993 and 768 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{12}H_{13}O_4$: 221.0808; found 221.0808.



Ethyl 2-oxochroman-6-carboxylate (6db)

6db was obtained from **5d** as a colorless oil. Yield: 14%.

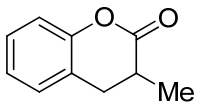
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, 1H, *J* = 8.4, 1.2 Hz), 7.93 (d, 1H, *J* = 1.2 Hz), 7.09 (d, 1H, *J* = 8.4 Hz), 4.38 (q, 2H, *J* = 7.6 Hz), 3.07 (t, 2H, *J* = 8.0 Hz), 2.82 (t, 2H, *J* = 8.0 Hz), 1.40 (t, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 165.7, 155.2, 130.0, 129.7, 126.7, 122.5, 117.0, 61.1, 28.9, 23.6 and 14.3; IR (ATR) 1775, 1709, 1285, 1265, 1115, 1098, 1026, 897 and 770 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{12}H_{13}O_4$: 221.0808; found 221.0810.



3-Ethylbenzofuran-2(3*H*)-one (6ea)[32]

6ea was obtained from **5e** or **5f** as a colorless oil. Yield: 90% from **5e**, 82% from **5f**.

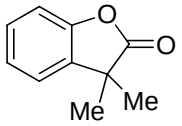
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.26 (m, 2H), 7.17-7.13 (m, 1H), 7.10 (d, 1H, *J* = 8.0 Hz), 3.70 (t, 1H, *J* = 5.6 Hz), 2.11-2.01 (m, 2H), 0.97 (t, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.0, 153.8, 128.6, 127.1, 124.1, 123.9, 110.5, 44.4, 24.2, and 10.0; IR (ATR) 1800, 1618, 1477, 1462, 1229, 1126, 1047, 908, 878, and 750 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{10}H_{11}O_2$: 163.0754; found 163.0756.



3-Methylchroman-2-one (6eb)[33]

6eb was obtained from **5d** or **5f** as a white solid (m.p. 61 °C). Yield: 10% from **5e**, 13% from **5f**.

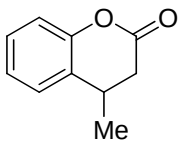
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.12 (m, 2H), 7.10-6.98 (m, 2H), 3.06-2.85 (m, 1H), 2.83-2.61 (m, 2H), 1.37 (d, 3H, *J* = 6.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 151.8, 128.1, 127.9, 124.2, 122.8, 116.5, 34.2, 31.6, and 15.3; IR (ATR) 1746, 1489, 1458, 1358, 1225, 1150, 1113, 937, and 756 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{10}H_{11}O_2$: 163.0754; found 163.0751.



3,3-Dimethylbenzofuran-2(3*H*)-one (6ga)[34]

Following the general procedure except for using **3f** in place of **3e**, **6ga** was obtained from **5g** as a colorless oil. Yield: 28%.

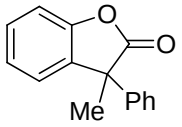
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (ddd, 1H, *J* = 7.6, 7.2, 1.6 Hz), 7.22 (dd, 1H, *J* = 7.6, 1.6 Hz), 7.15 (ddd, 1H, *J* = 8.0 7.2, 0.8 Hz), 7.11 (dd, 1H, *J* = 8.0, 0.8 Hz), 1.50 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.8, 152.2, 133.6, 128.5, 124.2, 122.7, 110.7, 42.8, and 25.2; IR (ATR) 1798, 1618, 1477, 1458, 1290, 1233, 1188, 1119, 1103, 1034, 935, 876, and 750 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{10}H_{11}O_2$: 163.0754; found 163.0754.



4-Methylchroman-2-one (6gb)[35]

Following the general procedure except for using **3f** in place of **3e**, **6gb** was obtained from **5g** as colorless oil. Yield: 58%.

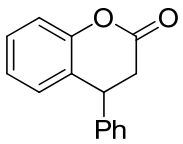
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.06 (m, 4H), 3.24-3.17 (m, 1H), 2.89 (dd, 1H, *J* = 15.8, 5.5 Hz), 2.60 (dd, 1H, *J* = 15.8, 8.6 Hz), 1.36 (d, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.2, 151.2, 128.2, 127.8, 126.5, 124.6, 117.0, 36.8, 28.5, and 19.8; IR (ATR) 1763, 1487, 1449, 1348, 1215, 1146, 1115, 1078, 908, and 756 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{10}H_{11}O_2$: 163.0754; found 163.0747.



3-Methyl-3-phenylbenzofuran-2(3*H*)-one (6ha)[35]

Following the general procedure except for using **3f** in place of **3e**, **6ha** was obtained from **5h** as a colorless oil. Yield: 72%.

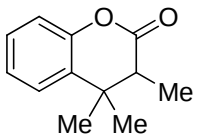
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.15 (m, 9H), 1.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.6, 152.7, 139.5, 132.6, 129.0, 128.8, 127.8, 126.4, 124.52, 124.49, 111.0, 50.8, and 24.8; IR (ATR) 1800, 1477, 1462, 1445, 1227, 1148, 1024, 887, 752, 729, and 694 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{15}H_{13}O_2$: 225.0910; found 225.0904.



4-Phenylchroman-2-one (6hb)[36]

Following the general procedure except for using **3f** in place of **3e**, **6hb** was obtained from **5h** as a white solid (m.p. 82 °C). Yield: 16%.

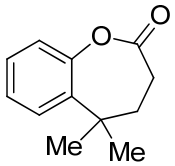
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.29 (m, 4H), 7.18-7.13 (m, 3H), 7.09 (t, 1H, J = 7.5 Hz), 6.98 (d, 1H, J = 7.5 Hz), 4.35 (t, 1H, J = 7.0 Hz), 3.09 (dd, 1H, J = 16.1, 6.2 Hz), 3.03 (dd, 1H, J = 16.1, 7.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 151.7, 140.3, 129.1, 128.8, 128.3, 127.6, 127.5, 125.8, 124.6, 117.1, 40.7, and 37.0; IR (ATR) 1765, 1485, 1454, 1213, 1130, 924, 754, and 698 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{15}H_{13}O_2$: 225.0910; found 225.0911.



3,4,4-Trimethylchroman-2-one (6ia)

6ia was obtained from **5i** as a colorless oil. Yield: 83%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (dd, 1H, J = 7.6, 1.6 Hz), 7.25 (ddd, 1H, J = 7.6, 7.2, 1.6 Hz), 7.14 (ddd, 1H, J = 8.4, 7.2, 1.6 Hz), 7.03 (dd, 1H, J = 8.4, 1.6 Hz), 2.62 (q, 1H, J = 7.6 Hz), 1.37 (s, 3H), 1.21 (d, 3H, J = 7.6 Hz), 1.20 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 150.1, 131.9, 128.1, 124.7, 124.6, 116.7, 45.1, 36.0, 26.4, 22.9 and 10.2; IR (ATR) 2974, 1763, 1447, 1207, 1161, 1065, 1011 and 754 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{12}H_{15}O_2$: 191.1067; found 191.1075.

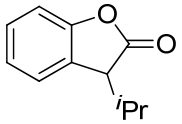


5,5-Dimethyl-4,5-dihydrobenzo[*b*]oxepin-2(3*H*)-one (6ib)

6ib was obtained from **5i** as a colorless oil. Yield: 9%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (dd, 1H, J = 8.0, 2.0 Hz), 7.29 (ddd, 1H, J = 7.6, 7.2, 2.0 Hz), 7.21 (ddd, 1H, J = 8.0, 7.2, 1.6 Hz), 7.10 (dd, 1H, J = 7.6, 1.6 Hz), 2.44 (t, 2H, J = 7.2 Hz), 2.08 (t, 2H, J = 7.2

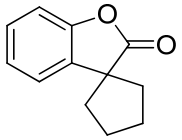
Hz), 1.42 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 151.6, 136.1, 128.2, 126.6, 125.8, 120.8, 41.1, 36.0, 30.7 and 29.4; IR (ATR) 2965, 1753, 1440, 1204, 1132, 1084 and 756 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{12}H_{15}O_2$: 191.1067; found 191.1068.



3-Isopropylbenzofuran-2(3H)-one (6j)[37]

6j was obtained from **5j** as a colorless oil. Yield: 99%.

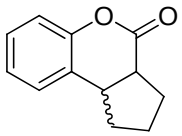
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27-7.18 (m, 2H), 7.00-7.10 (m, 2H), 3.56 (d, 1H, *J* = 3.9 Hz), 2.41 (m, 1H), 1.01 (d, 3H, *J* = 6.9 Hz), 0.89 (d, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.4, 154.1, 128.7, 126.1, 124.5, 123.8, 110.5, 49.7, 31.3, 19.3, and 18.4; IR (ATR) 2965, 1802, 1618, 1477, 1460, 1231, 1126, 1043, 891, 750 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{11}H_{13}O_2$: 177.0910; found 177.0917.



2*H*-Spiro[benzofuran-3,1'-cyclopentan]-2-one (6ka)[38]

Following the general procedure except for using **3f** in place of **3e**, **6ka** was obtained from **5k** as a colorless oil. Yield: 47%.

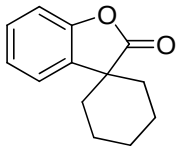
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (ddd, 1H, *J* = 8.0, 7.6, 1.6 Hz), 7.21 (dd, 1H, *J* = 7.6, 1.6 Hz), 7.15 (ddd, 1H, *J* = 8.0, 7.6, 1.2 Hz), 7.09 (dd, 1H, *J* = 7.6, 1.2 Hz), 2.30-2.22 (m, 2H), 2.14-2.06 (m, 2H), 2.06-1.90 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 181.8, 152.4, 134.2, 128.2, 124.3, 122.6, 110.4, 52.0, 39.6 and 26.4, ; IR (ATR) 2957, 1794, 1618, 1476, 1460, 1231, 1119, 1036, 974, 876, and 748 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{12}H_{13}O_2$: 189.0910; found 189.0914.



1,3,3a,9b-Tetrahydrocyclopenta[*c*]chromen-4(2*H*)-one (6kb)

Following the general procedure except for using **3f** in place of **3e**, **6kb** (diastereomer mixture) was obtained from **5k** as a colorless oil. Yield: 28%.

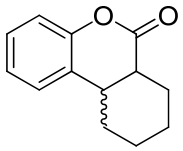
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.01 (m, 8H), 3.30-3.26 (m, 1H), 3.09-3.04 (m, 1H), 3.02-2.92 (m, 1H), 2.46-2.39 (m, 1H), 2.39-2.26 (m, 2H), 2.20-2.09 (m, 3H), 2.04-1.92 (m, 2H), 1.84-1.61 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 170.7, 152.6, 150.6, 128.8, 128.1, 128.1, 128.0, 125.1, 124.4, 124.2, 124.1, 116.8, 116.4, 46.6, 42.9, 41.5, 40.8, 33.7, 28.7, 27.5, 23.4, 22.9 and 22.9; IR (ATR) 2955, 1755, 1487, 1452, 1219, 1144, 1123, 1105 and 752 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{12}H_{13}O_2$: 189.0910; found 189.0919.



2*H*-Spiro[benzofuran-3,1'-cyclohexan]-2-one (6la)

6la was obtained from **5l** as a colorless oil. Yield: 72%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (dd, 1H, *J* = 7.6, 0.8 Hz), 7.28 (ddd, 1H, *J* = 8.0, 7.6, 1.6 Hz), 7.13 (ddd, 1H, *J* = 7.6, 7.6, 0.8 Hz), 7.10 (d, 1H, *J* = 8.0 Hz), 1.99-1.87 (m, 4H), 1.79-1.62 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.5, 152.3, 133.4, 128.2, 123.8, 123.8, 110.6, 46.0, 33.8, 24.9 and 20.7; IR (ATR) 2933, 2855, 1796, 1460, 1231, 1150, 1007 and 752 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{13}H_{15}O_2$: 203.1067; found 203.1063.

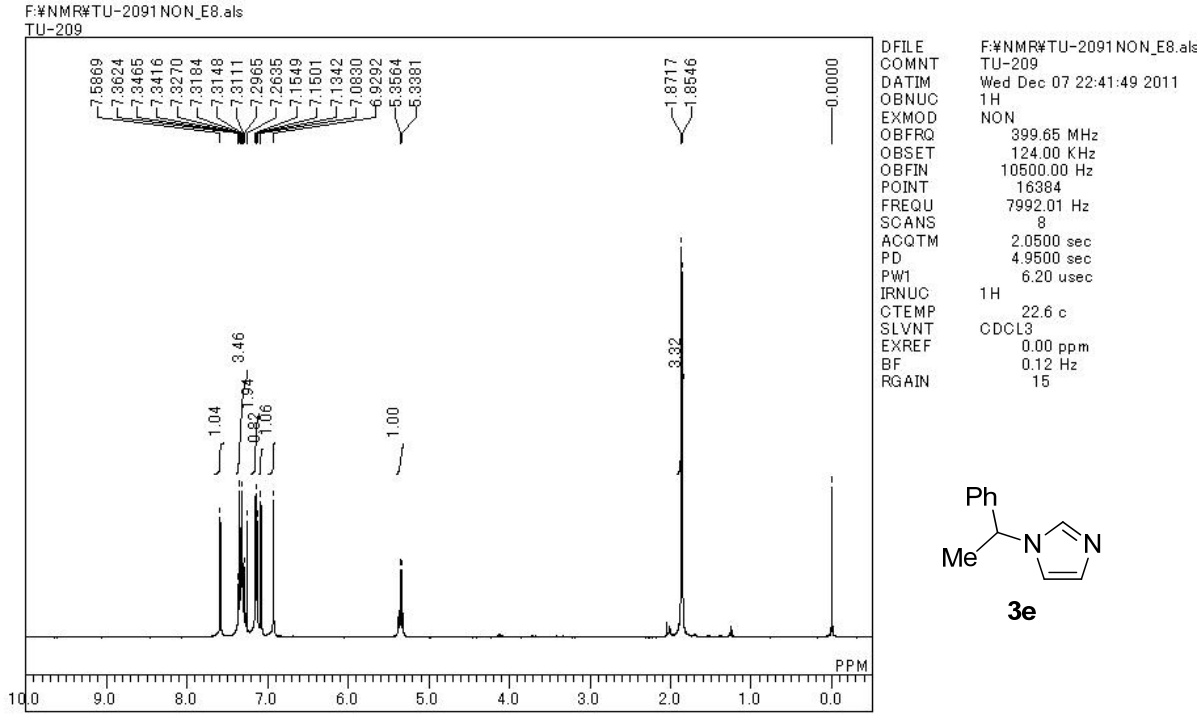


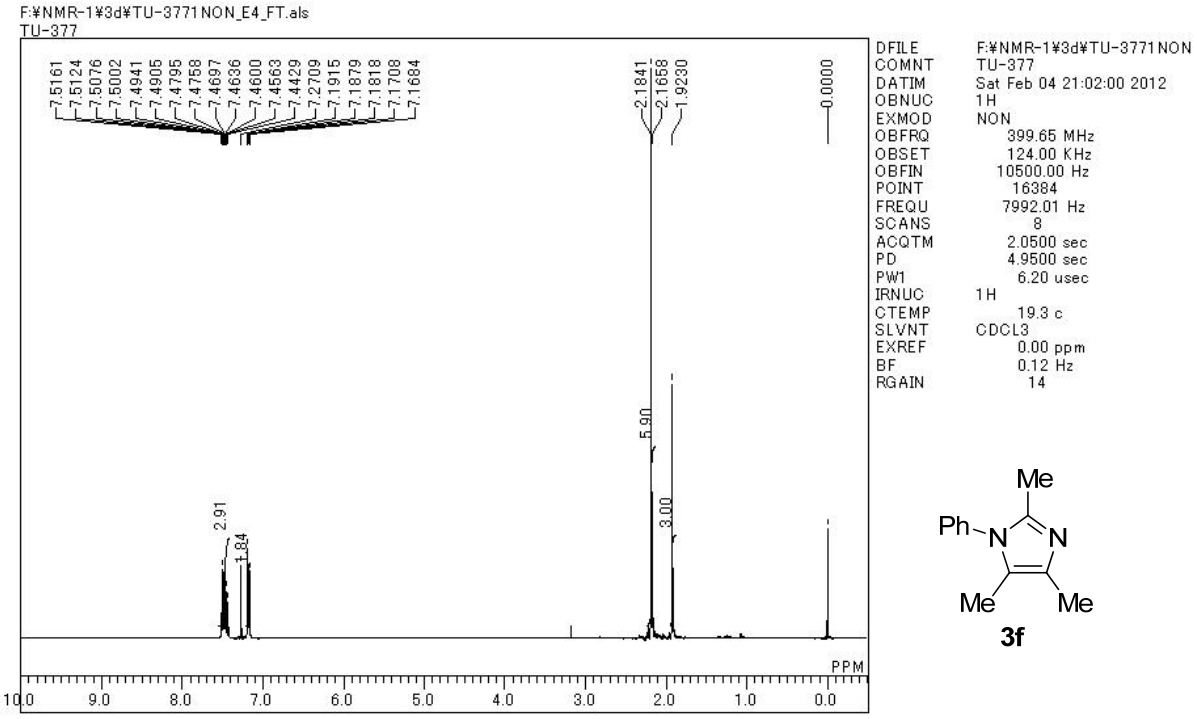
6a,7,8,9,10,10a-Hexahydro-6*H*-benzo[*c*]chromen-6-one (6lb)

6lb (diastereomer mixture) was obtained from **5l** as a colorless oil. Yield: 28%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.00 (m, 8H), 3.00-2.90 (m, 1H), 2.75-2.67 (m, 1H), 2.54-2.48 (m, 1H), 2.40-2.30 (m, 1H), 2.25-2.10 (m, 2H), 2.00-1.89 (m, 4H), 1.85-1.20 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 170.4, 151.0, 150.8, 128.1, 127.5, 127.3, 124.5, 124.4, 124.3, 123.8, 116.7, 116.6, 110.6, 42.5, 39.8, 38.0, 36.0, 33.9, 28.9, 26.3, 25.0, 24.9, 24.7, 21.8 and 20.7; IR (ATR) 2933, 2859, 1751, 1485, 1452, 1217, 1153, 1113 and 760 cm^{-1}; HRMS (DART) $[M+H]^+$ calcd for $C_{13}H_{15}O_2$: 203.1067; found 203.1073.

6. NMR spectra of newly obtained compounds

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7.5076
7.5002
7.4941
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7.4758
7.4697
7.4636
7.4600
7.4563
7.4429
7.2709
7.1915
7.1879
7.1818
7.1708
7.1684
2.1841
2.1658
1.9230
0.0000
5.90
3.00
2.91
1.84
PPM
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9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
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EXMOD NON
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OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
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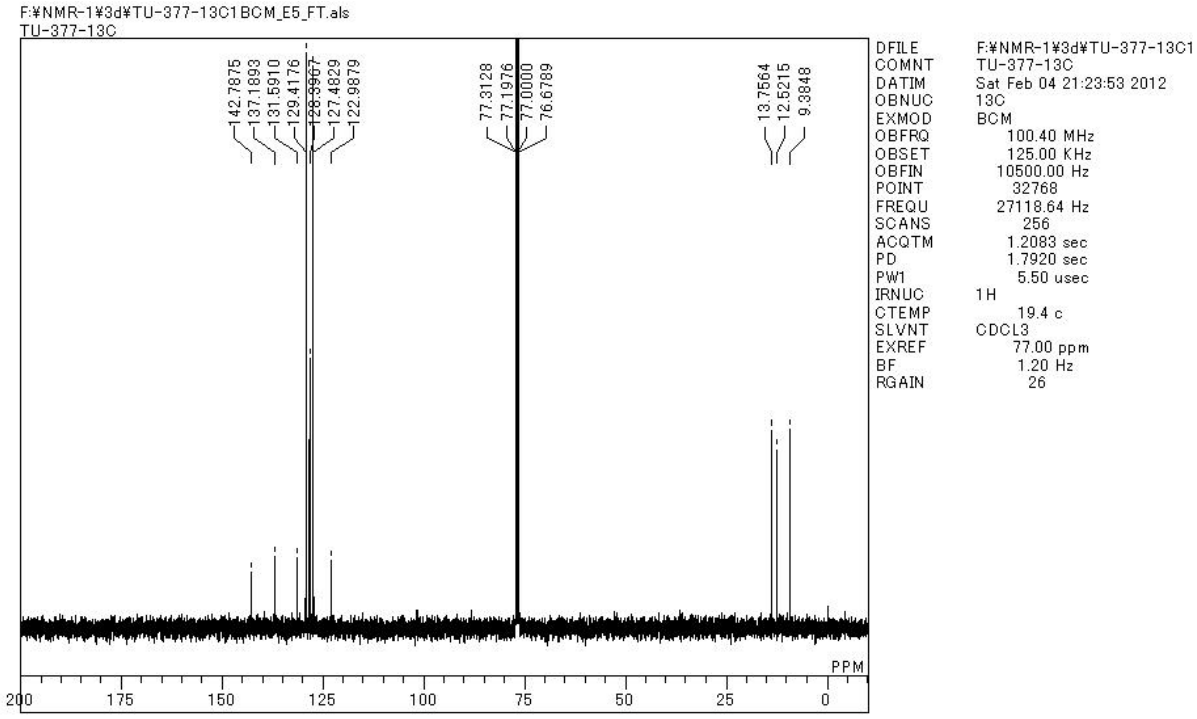
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 19.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 14

Me
Ph
N
N
Me
Me

3f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129.4176
128.3967
127.4829
122.9879
77.3128
77.1976
77.0000
76.6789
13.7564
12.5215
9.3848
PPM
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150
125
100
75
50
25
0
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OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 256
ACQTM 1.2083 sec
PD 1.7920 sec
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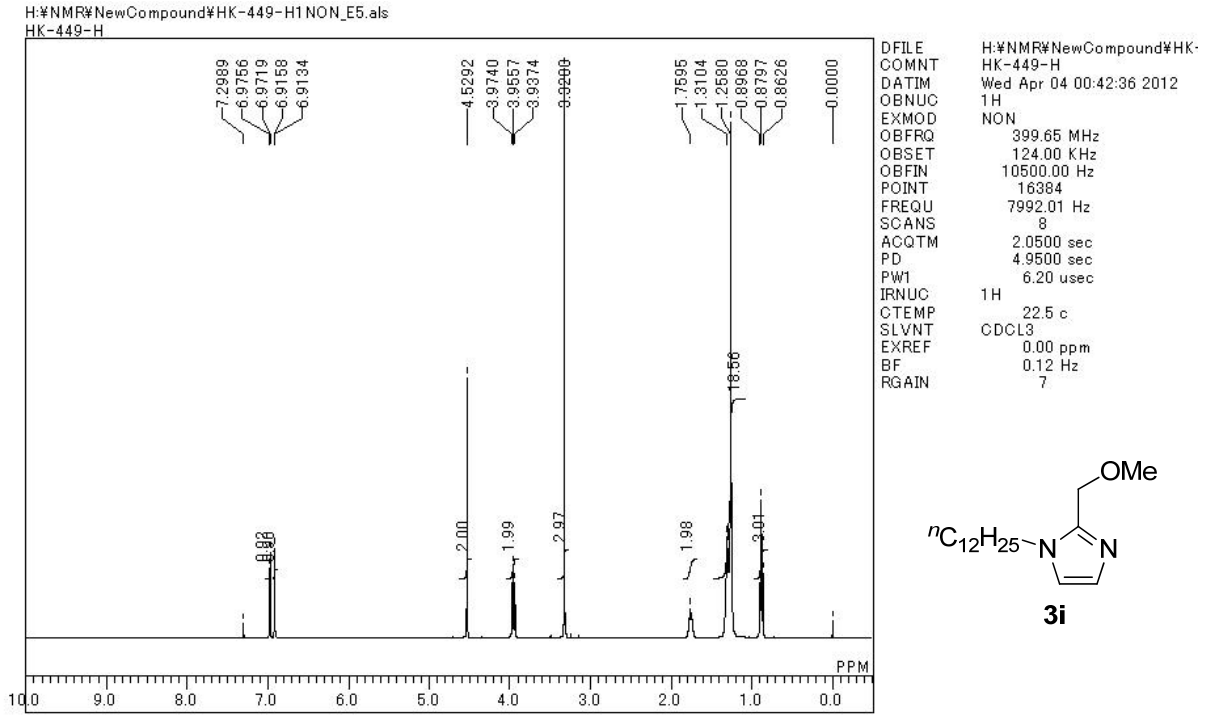
IRNUC 1H
CTEMP 19.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 26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6.9158
6.9134
4.5292
3.9740
3.9557
3.9374
3.0000
1.7595
1.3104
1.2580
0.8968
0.8797
0.8626
0.0000
18.56
2.00
1.99
2.97
1.98
3.01
PPM
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9.0
8.0
7.0
6.0
5.0
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3.0
2.0
1.0
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EXMOD NON
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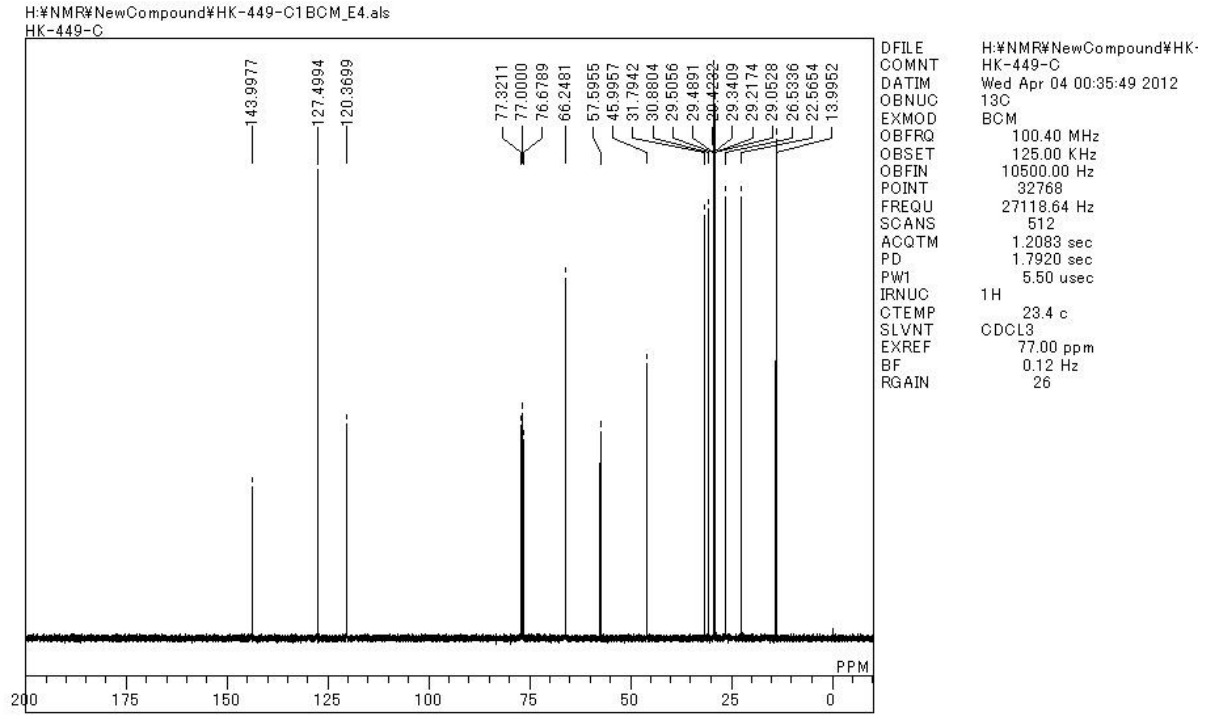
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 7

OMe
$^{n}C_{12}H_{25}$
N
N

3i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77.3211
77.0000
76.6789
66.2481
57.5955
45.9957
31.7942
30.8804
29.5056
29.4891
29.3409
29.2174
29.0528
26.5336
22.5654
13.9952
PPM
200
175
150
125
100
75
50
25
0
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COMNT HK-449-C
DATIM Wed Apr 04 00:35:49 2012
OBNUC 13C
EXMOD BCM
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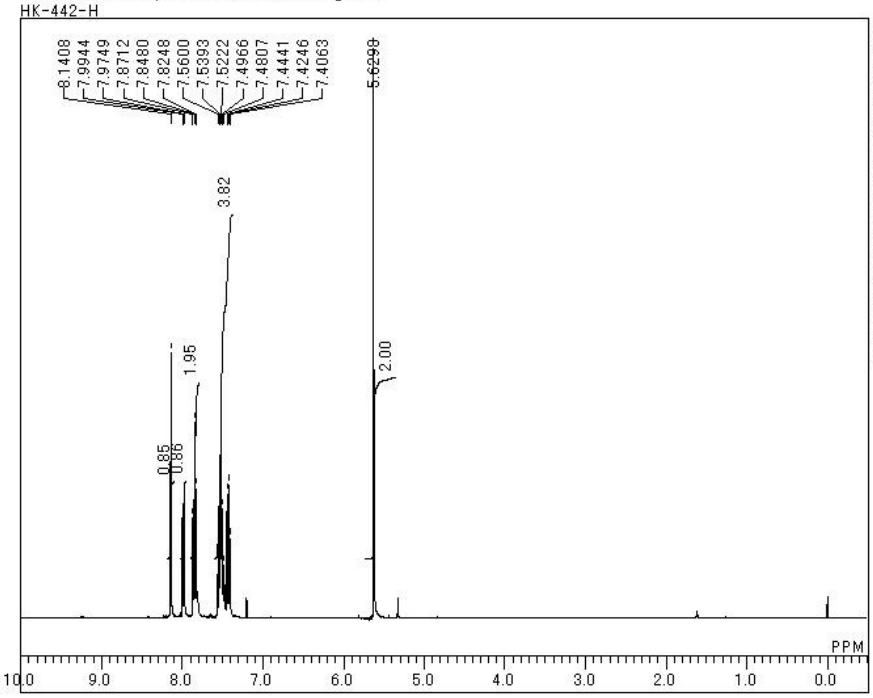
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 512
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 23.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 26

H:¥NMR¥NewCompound¥HK-442-H1NON_E6.als
HK-442-H



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EXMOD	NON
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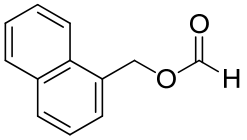
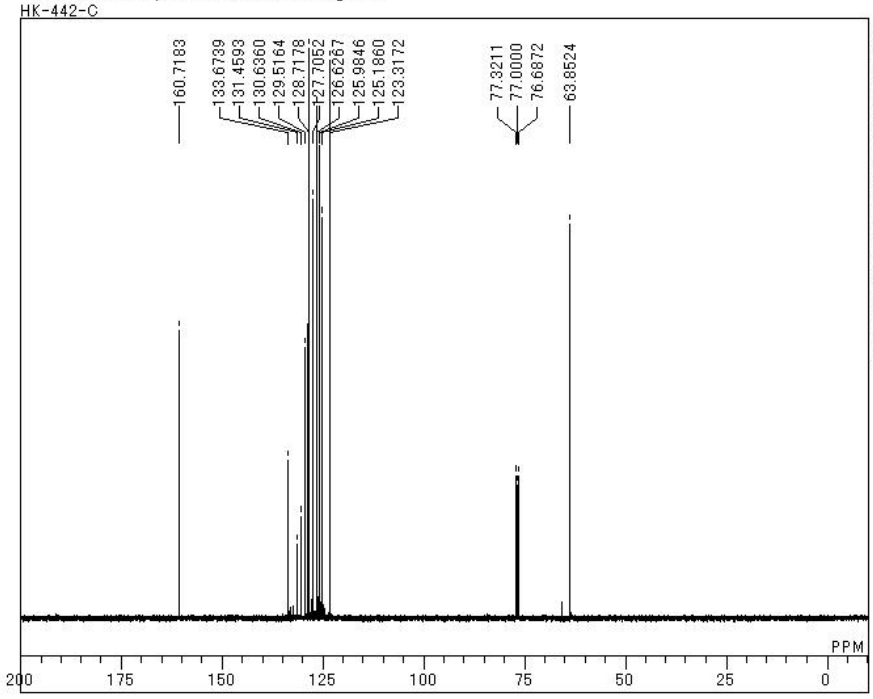
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	22.5 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	9



1d

H:¥NMR¥NewCompound¥HK-442-C1BCM_E3.als
HK-442-C



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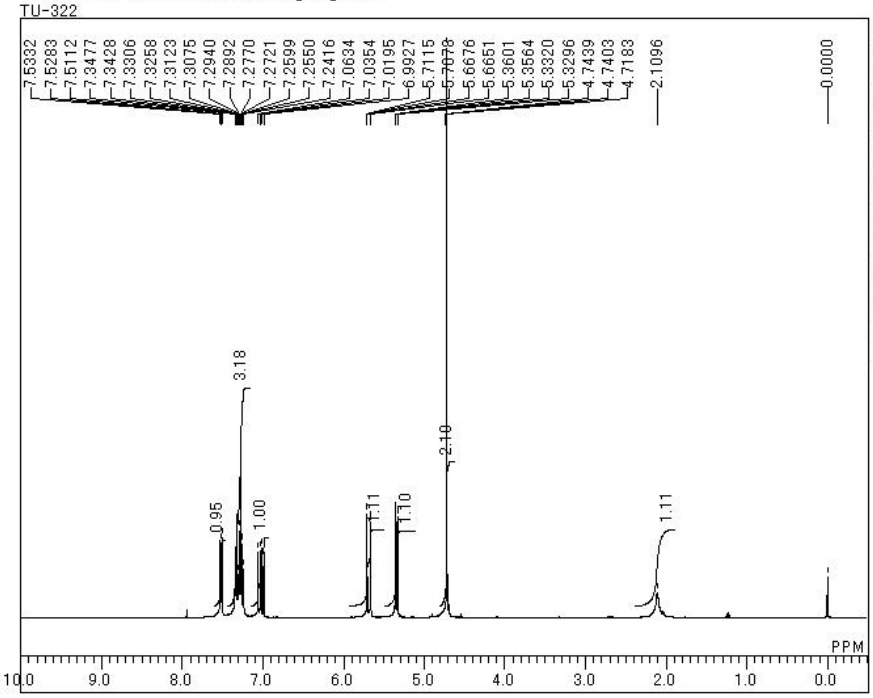
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	512
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	24.1 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	26

F:¥NMR-1¥5a-alcohol¥TU-3221NON_E12_FT.als
TU-322



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EXMOD	NON
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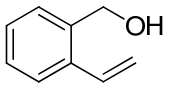
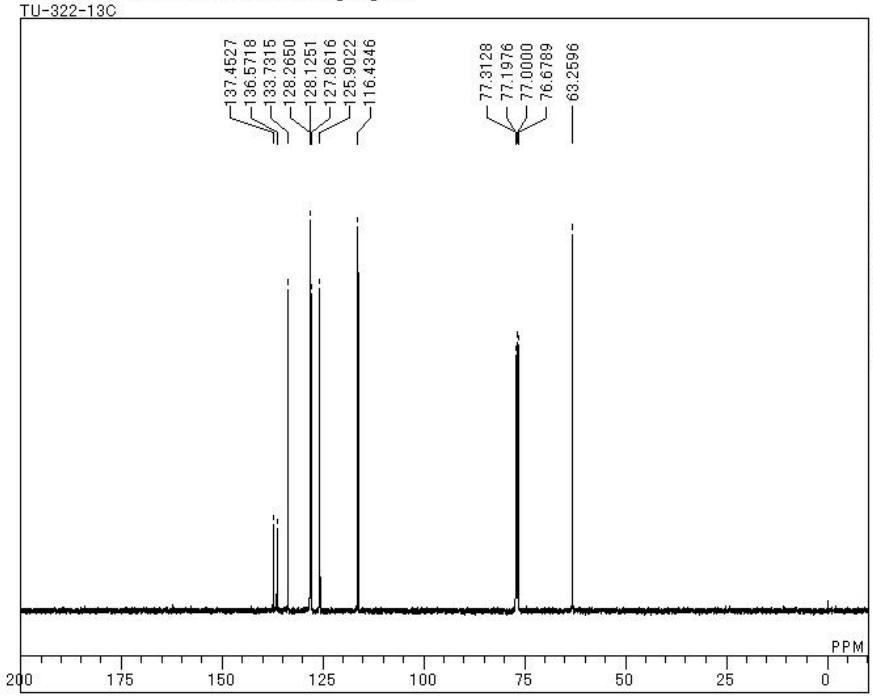
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	22.2 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	11



S1

F:¥NMR-1¥5a-alcohol¥TU-322-13C1BCM_E13_FT.als
TU-322-13C



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FREQU	27118.64 Hz
SCANS	1024
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PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	22.9 c
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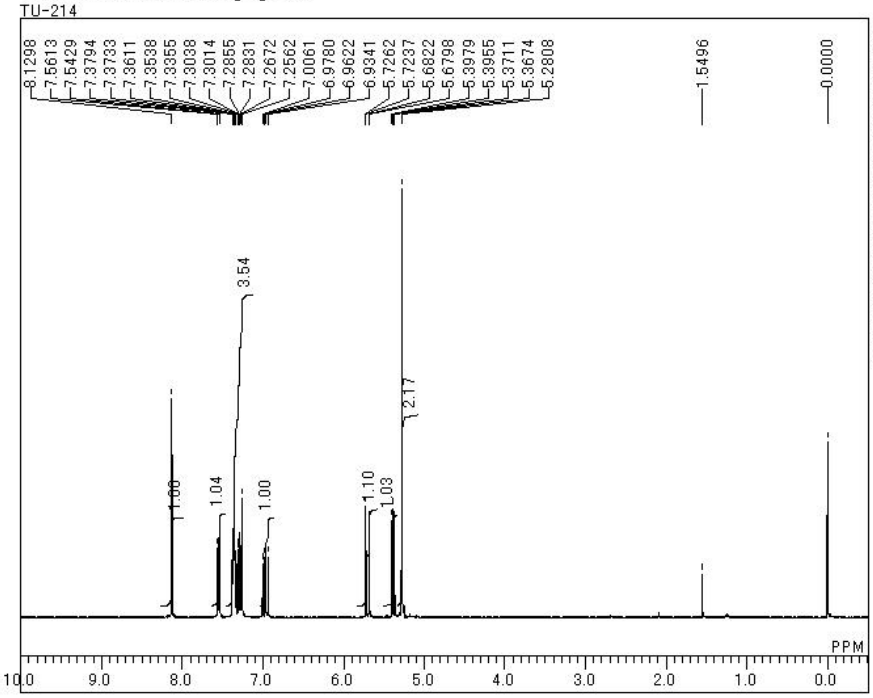
BF	1.20 Hz
RGAIN	26

F:¥NMR-1¥5a¥TU-2141NON_E6_FT.als
TU-214



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OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
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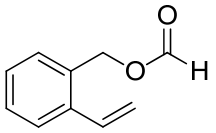
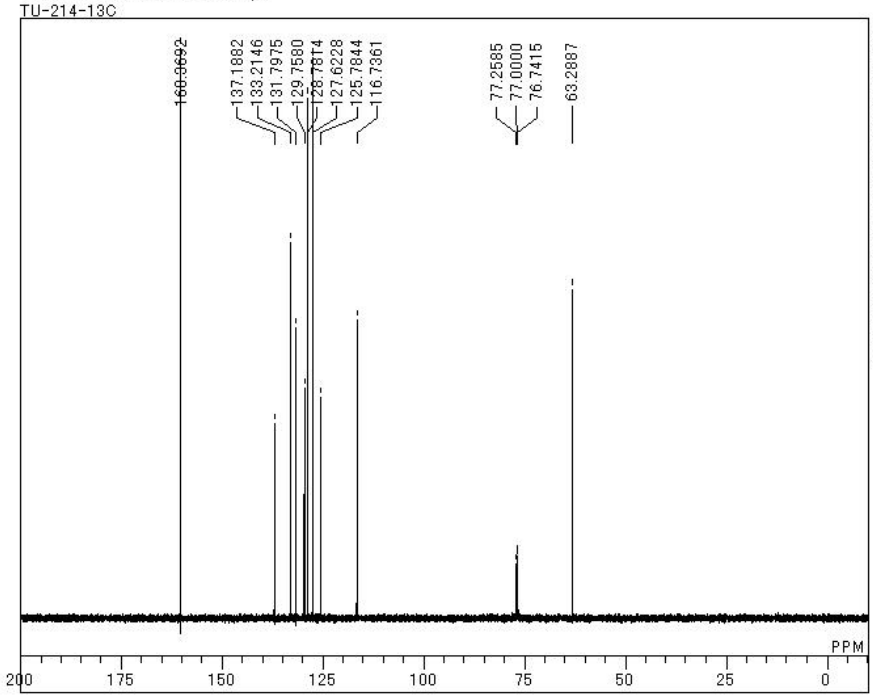
IRNUC	1H
CTEMP	23.7 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	15



5a

F:¥NMR-1¥5a¥TU-214-13C-1.jdf
TU-214-13C



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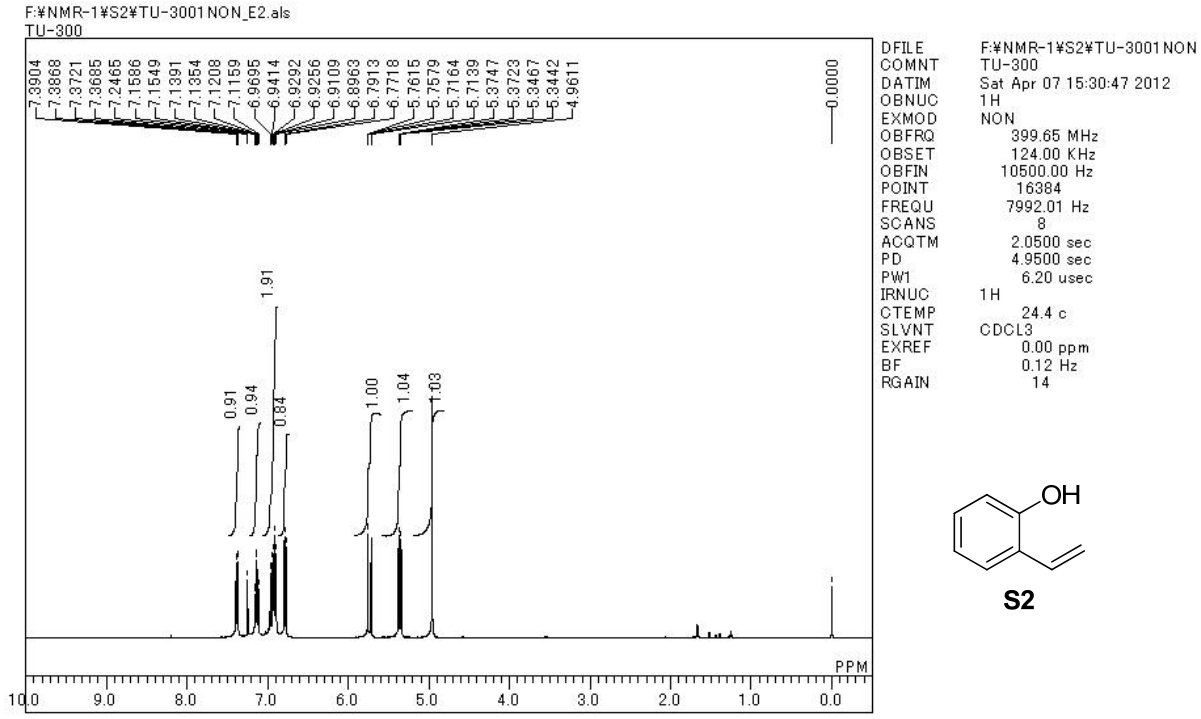
OBSET	3.45 KHz
OBFIN	6.00 Hz
POINT	32768
FREQU	39062.50 Hz
SCANS	128
ACQTM	0.8389 sec
PD	1.5000 sec
PW1	5.57 usec
IRNUC	1H
CTEMP	21.7 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50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6.7718
5.7615
5.7579
5.7164
5.7139
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5.3723
5.3467
5.3442
4.9611
0.0000
1.91
0.91
0.94
0.84
1.00
1.04
1.03
PPM
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9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
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OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
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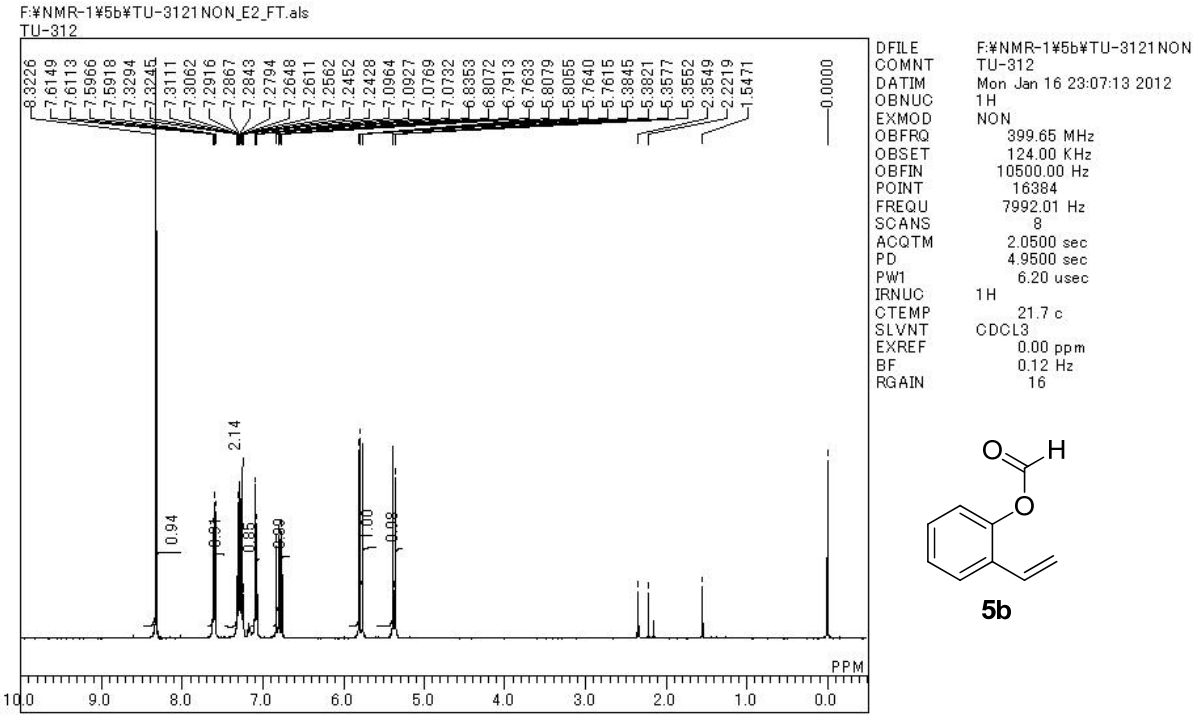
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 24.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 14

OH

S2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7.5918
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7.2611
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7.2452
7.2428
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7.0769
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6.7633
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5.8055
5.7640
5.7615
5.3845
5.3821
5.3577
5.3552
2.3549
2.2219
1.5471
0.0000
2.14
0.94
0.91
0.85
0.89
11.00
0.98
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
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OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
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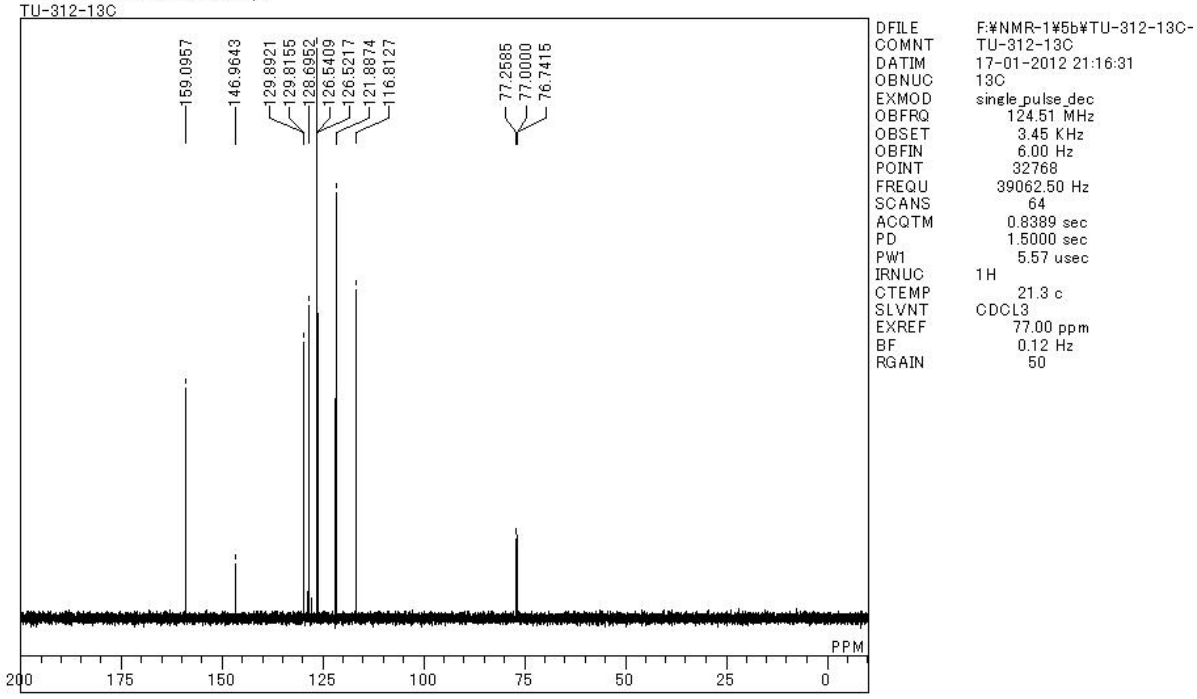
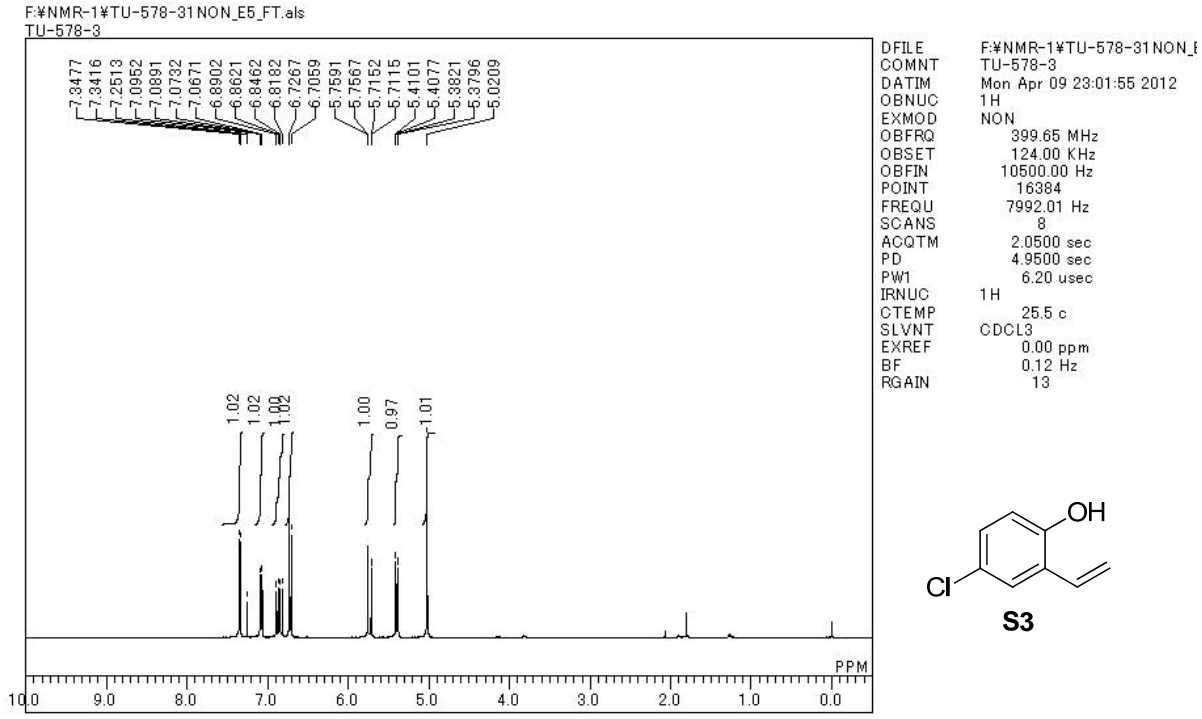
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 21.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16
O
H
O

5b

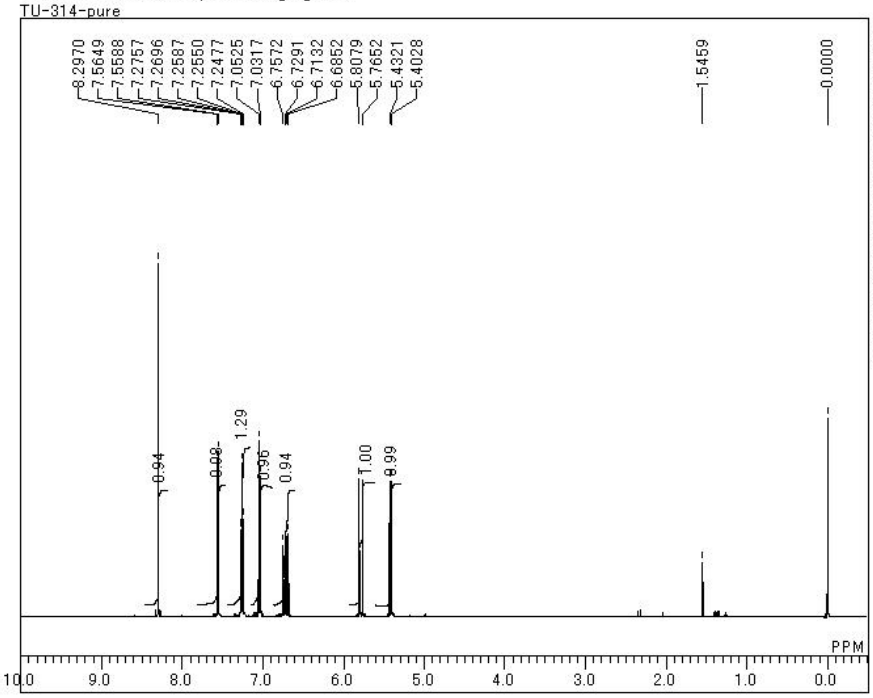

F:¥NMR-1¥5b¥TU-312-13C-1.jdf
TU-312-13C
159.0957
146.9643
129.8921
129.8155
128.6952
126.6409
126.5217
121.8874
116.8127
77.2585
77.0000
76.7415
PPM
200
175
150
125
100
75
50
25
0
DFILE F:¥NMR-1¥5b¥TU-312-13C-
COMNT TU-312-13C
DATIM 17-01-2012 21:16:31
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 124.51 MHz
OBSET 3.45 KHz
OBFIN 6.00 Hz
POINT 32768
FREQU 39062.50 Hz
SCANS 64
ACQTM 0.8389 sec
PD 1.5000 sec
PW1 5.57 usec
IRNUC 1H
CTEMP 21.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50


F:¥NMR-1¥TU-578-31NON_E5_FT.als
TU-578-3
7.3477
7.3416
7.2513
7.0962
7.0891
7.0732
7.0671
6.8902
6.8621
6.8462
6.8182
6.7267
6.7059
5.7591
5.7567
5.7152
5.7115
5.4101
5.4077
5.3821
5.3796
5.0209
1.02
1.02
1.00
1.02
1.00
0.97
1.01
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥NMR-1¥TU-578-31NON_E
COMNT TU-578-3
DATIM Mon Apr 09 23:01:55 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 25.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 13

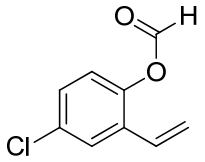
OH
Cl

S3

F:¥NMR-1¥5c¥TU-314-pure1NON_E5_FT.als
TU-314-pure

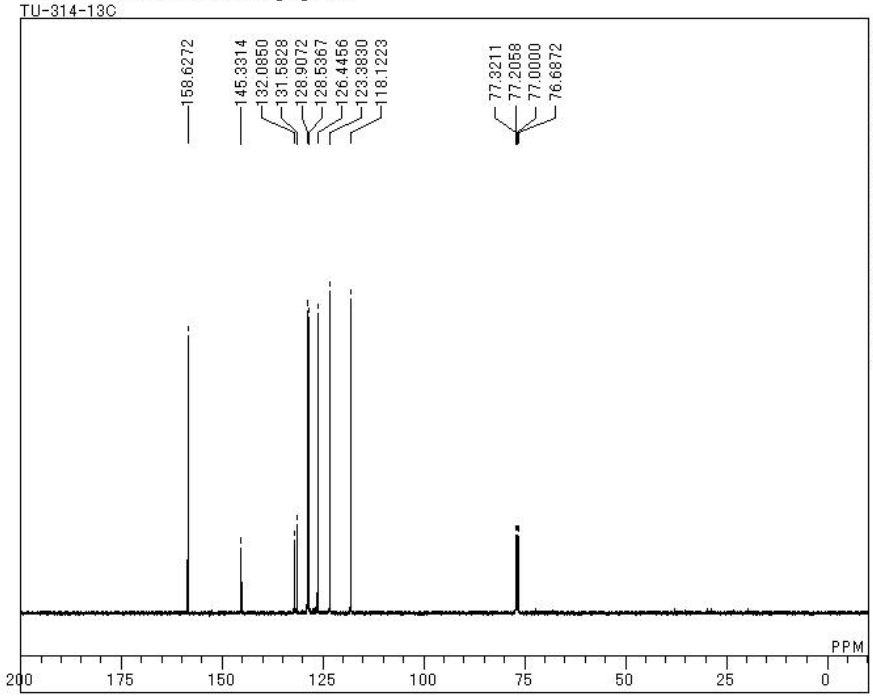


DFILE	F:¥NMR-1¥5c¥TU-314-pure
COMNT	TU-314-pure
DATIM	Wed Jan 18 11:55:33 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	22.5 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	16

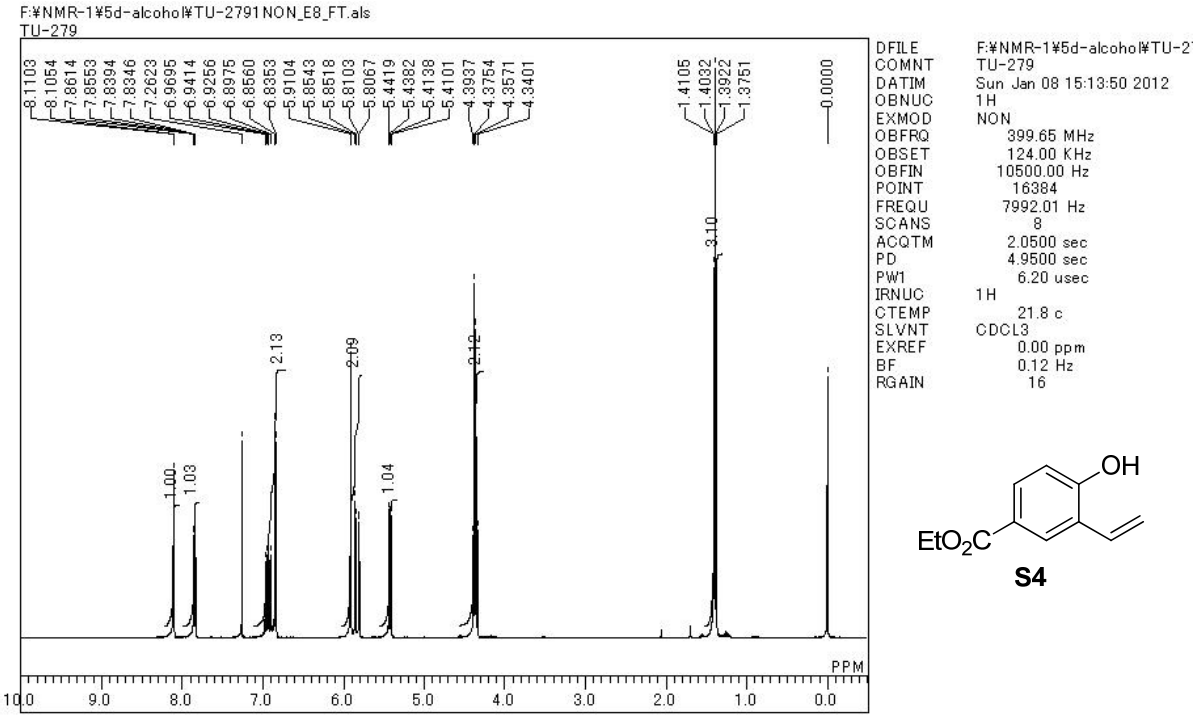


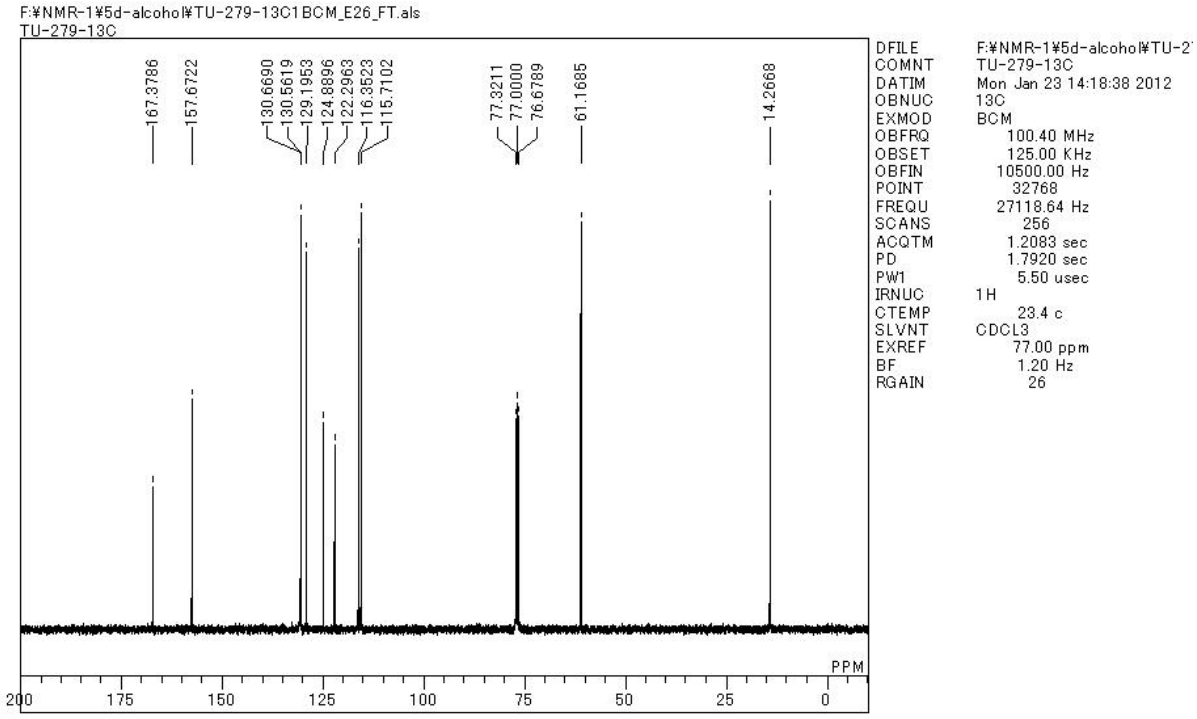
5c

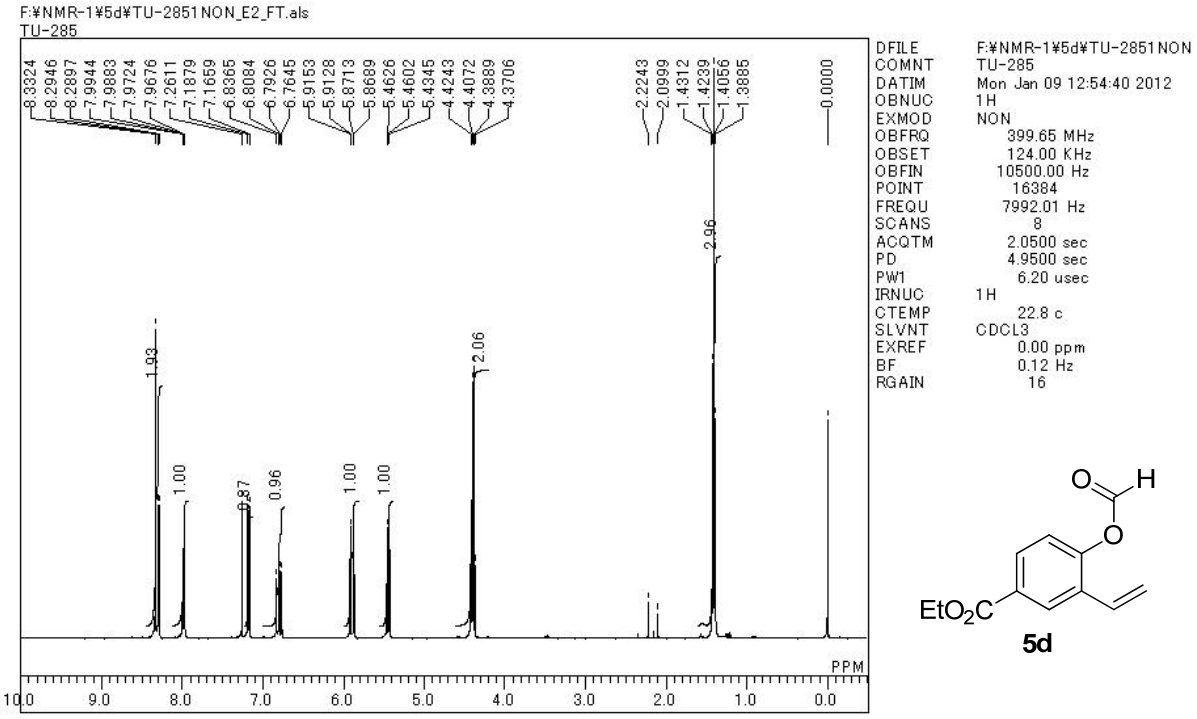
F:¥NMR-1¥5c¥TU-314-13C1BCM_E7_FT.als
TU-314-13C



DFILE	F:¥NMR-1¥5c¥TU-314-13C1
COMNT	TU-314-13C
DATIM	Wed Jan 18 12:27:12 2012
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	256
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	23.1 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	27

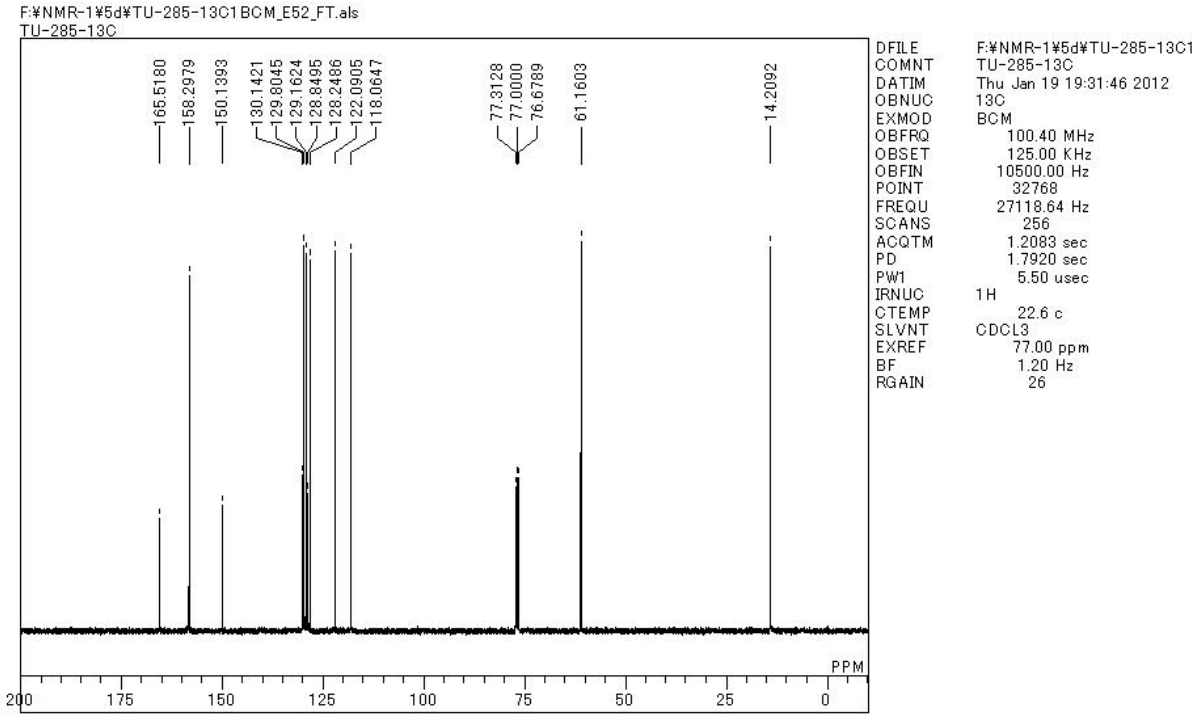

F:¥NMR-1¥5d-alcohol¥TU-2791NON_E8_FT.als
TU-279
8.1103
8.1054
7.8614
7.8553
7.8394
7.8346
7.2623
6.9695
6.9414
6.9256
6.8975
6.8560
6.8353
5.9104
5.8543
5.8518
5.8103
5.8067
5.4419
5.4382
5.4138
5.4101
4.3937
4.3754
4.3571
4.3401
1.4105
1.4032
1.3922
1.3751
0.0000
3.10
2.13
2.09
2.12
1.00
1.03
1.04
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥NMR-1¥5d-alcohol¥TU-2
COMNT TU-279
DATIM Sun Jan 08 15:13:50 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 21.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16
OH
EtO2C
S4


F:¥NMR-1¥5d-alcohol¥TU-279-13C1BCM_E26_FT.als
TU-279-13C
167.3786
157.6722
130.6690
130.5619
129.1953
124.8896
122.2963
116.3523
115.7102
77.3211
77.0000
76.6789
61.1685
14.2668
PPM
200
175
150
125
100
75
50
25
0
DFILE F:¥NMR-1¥5d-alcohol¥TU-2
COMNT TU-279-13C
DATIM Mon Jan 23 14:18:38 2012
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 256
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 23.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 26

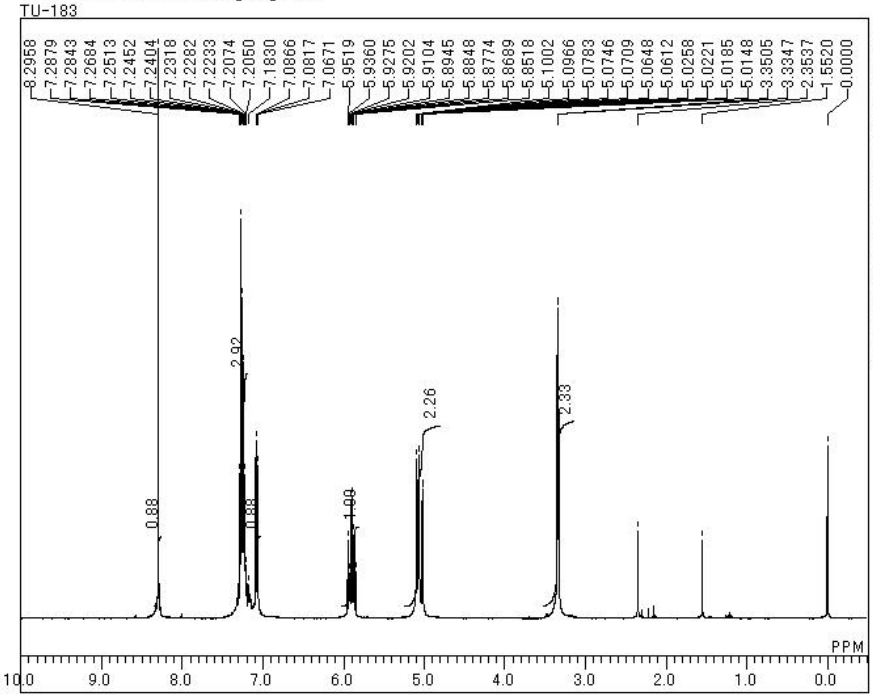

F:¥NMR-1¥5d¥TU-2851NON_E2_FT.als
TU-285
8.3324
8.2946
8.2897
7.9944
7.9883
7.9724
7.9676
7.2611
7.1879
7.1659
6.8365
6.8084
6.7926
6.7645
5.9153
5.9128
5.8713
5.8689
5.4626
5.4602
5.4345
4.4243
4.4072
4.3889
4.3706
2.2243
2.0999
1.4312
1.4239
1.4056
1.3885
0.0000
1.93
1.00
0.97
0.96
1.00
1.00
2.06
2.96
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥NMR-1¥5d¥TU-2851NON
COMNT TU-285
DATIM Mon Jan 09 12:54:40 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 22.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16

O
H
O
EtO2C

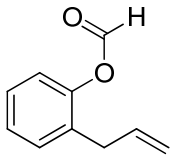
5d


F:¥NMR-1¥5d¥TU-285-13C1BCM_E52_FT.als
TU-285-13C
165.5180
158.2979
150.1393
130.1421
129.8045
129.1624
128.8495
128.2486
122.0905
118.0647
77.3128
77.0000
76.6789
61.1603
14.2092
PPM
200
175
150
125
100
75
50
25
0
DFILE F:¥NMR-1¥5d¥TU-285-13C1
COMNT TU-285-13C
DATIM Thu Jan 19 19:31:46 2012
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 256
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 26

F:¥NMR-1¥5e¥TU-1831NON_E24_FT.als
TU-183

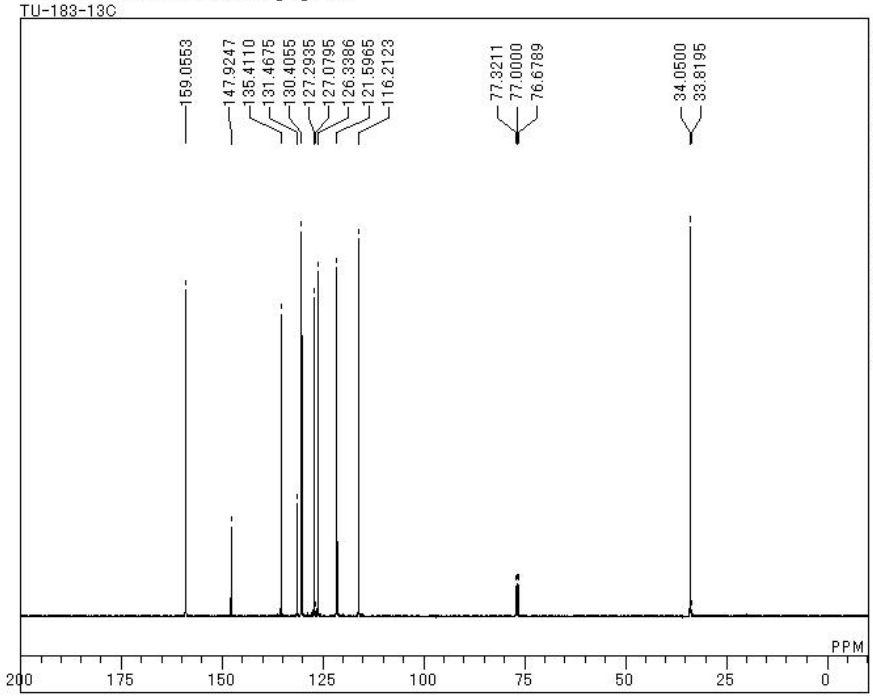


DFILE	F:¥NMR-1¥5e¥TU-1831NON
COMNT	TU-183
DATIM	Tue Nov 29 20:08:28 2011
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	22.5 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	13

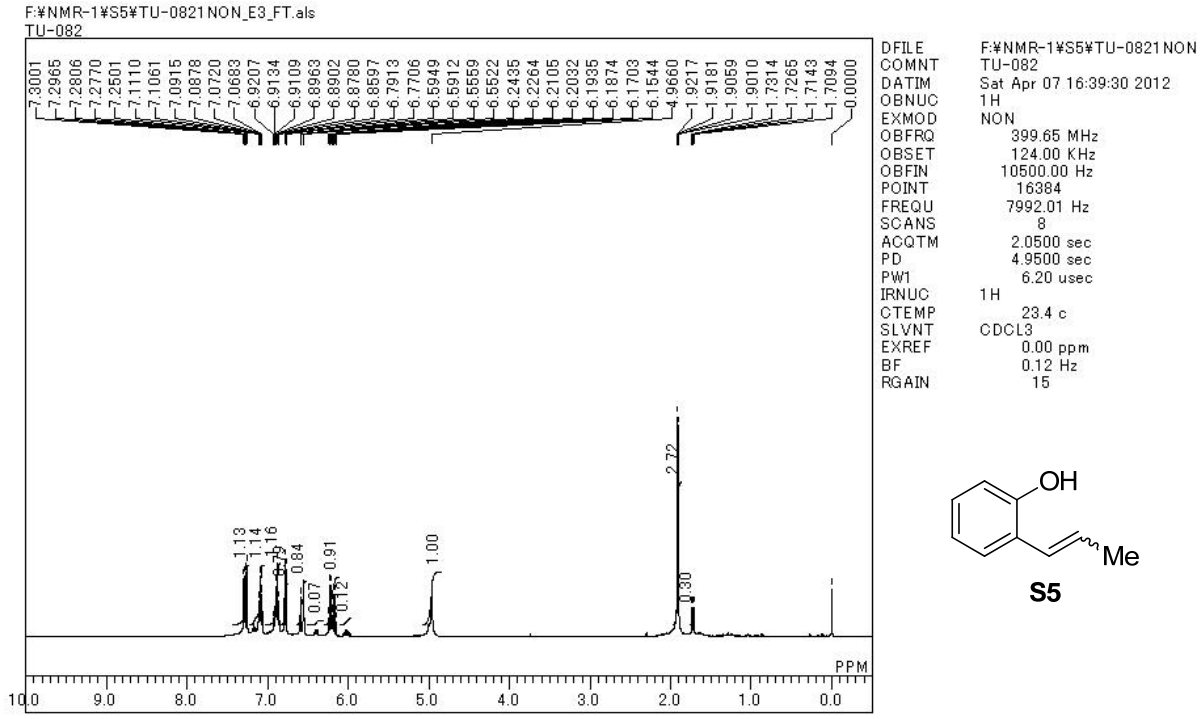


5e

F:¥NMR-1¥5e¥TU-183-13C1BCM_E8_FT.als
TU-183-13C



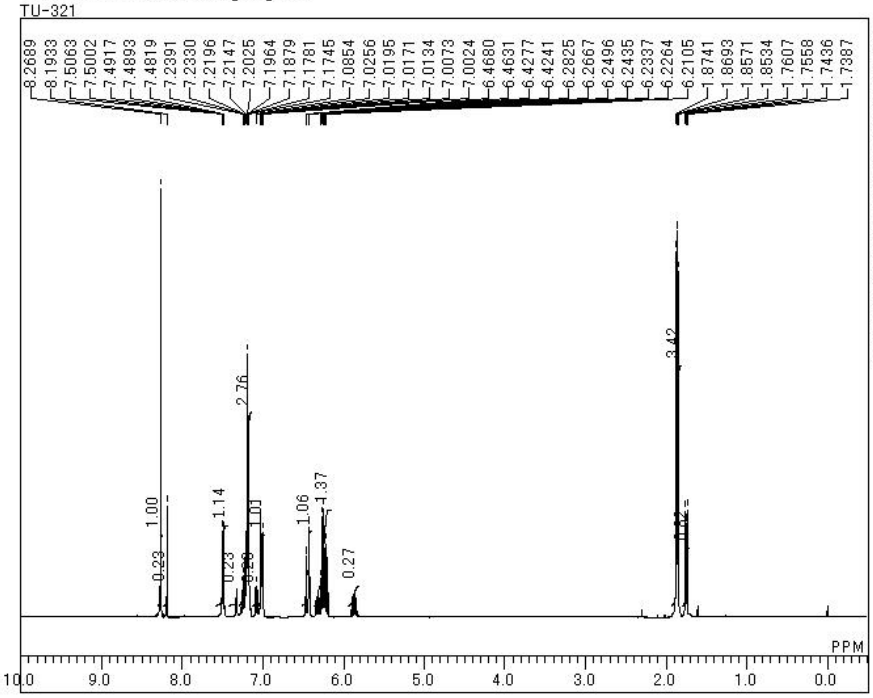
DFILE	F:¥NMR-1¥5e¥TU-183-13C1
COMNT	TU-183-13C
DATIM	Thu Jan 19 12:10:44 2012
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	256
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	22.5 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	25


F:¥NMR-1¥S5¥TU-0821NON_E3_FT.als
TU-082
7.3001
7.2965
7.2806
7.2770
7.2501
7.1110
7.1061
7.0915
7.0878
7.0720
7.0683
6.9207
6.9134
6.9109
6.8963
6.8902
6.8780
6.8597
6.7913
6.7706
6.5949
6.5912
6.5559
6.5522
6.2435
6.2264
6.2105
6.2032
6.1935
6.1874
6.1703
6.1544
4.9660
1.9217
1.9181
1.9059
1.9010
1.7314
1.7265
1.7143
1.7094
0.0000
1.13
1.14
1.16
0.79
0.84
0.91
0.07
0.12
1.00
2.72
0.80
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥NMR-1¥S5¥TU-0821NON
COMNT TU-082
DATIM Sat Apr 07 16:39:30 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 23.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15

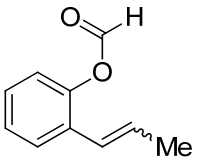
OH
Me

S5

F:¥NMR-1¥5f¥TU-3211NON_E34_FT.als
TU-321



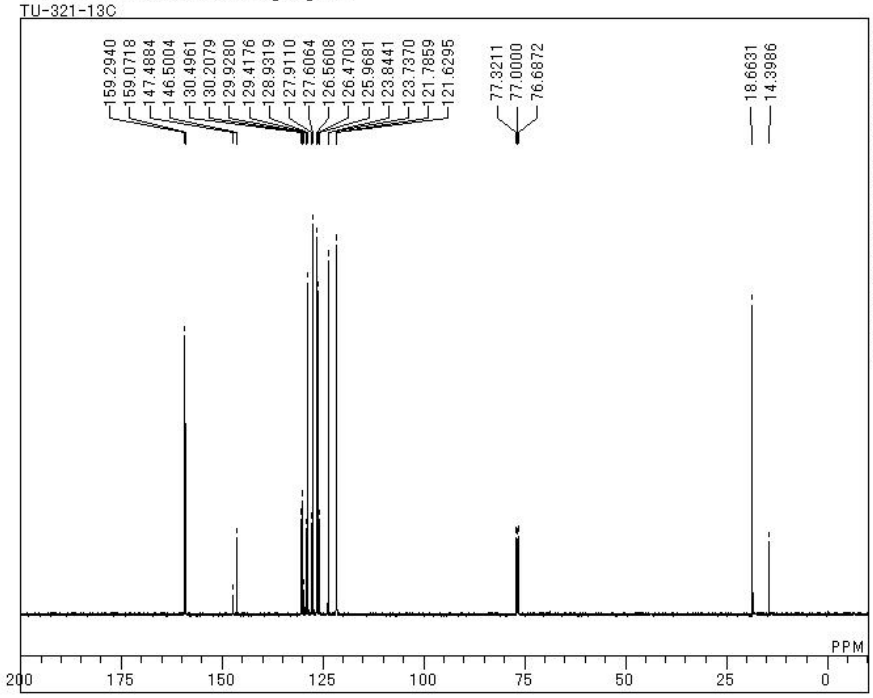
DFILE	F:¥NMR-1¥5f¥TU-3211NON_
COMNT	TU-321
DATIM	Thu Jan 19 16:33:53 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	21.8 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	7



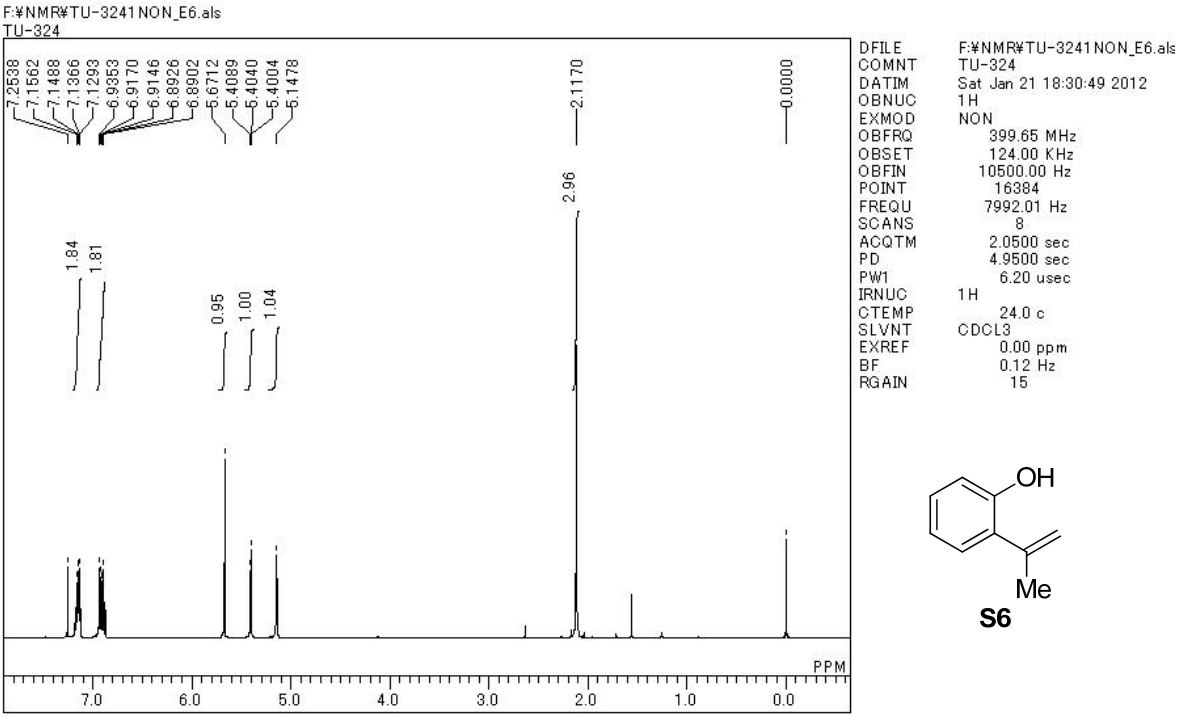
5f

(*E*:*Z* = 80:20)

F:¥NMR-1¥5f¥TU-321-13C1BCM_E35_FT.als
TU-321-13C



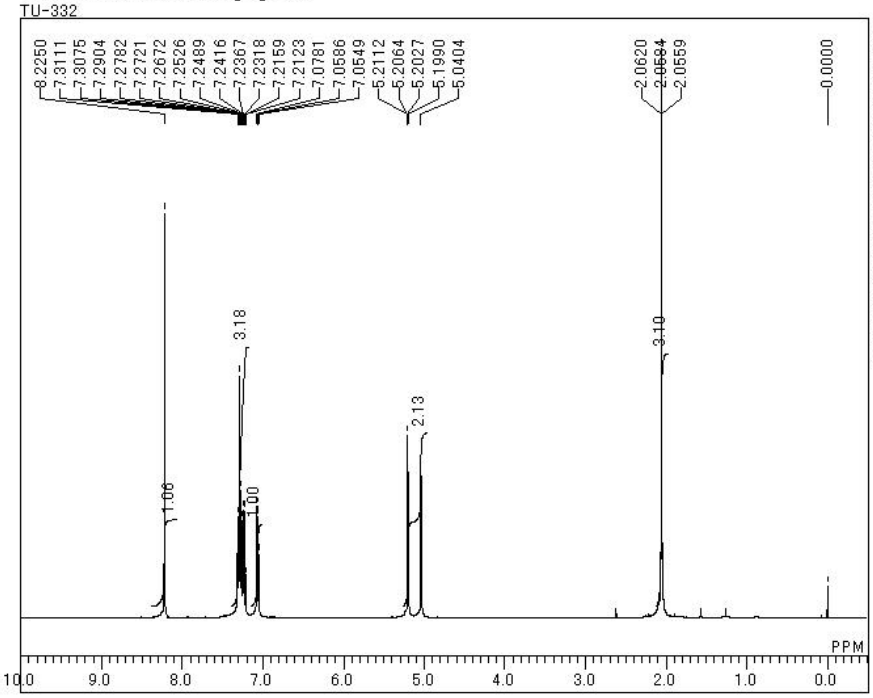
DFILE	F:¥NMR-1¥5f¥TU-321-13C1
COMNT	TU-321-13C
DATIM	Thu Jan 19 16:51:57 2012
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	256
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	22.9 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	26


F:¥NMR¥TU-3241NON_E6.als
TU-324
7.2538
7.1662
7.1488
7.1366
7.1293
6.9353
6.9170
6.9146
6.8926
6.8902
5.6712
5.4089
5.4040
5.4004
5.1478
2.1170
0.0000
2.96
1.84
1.81
0.95
1.00
1.04
PPM
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥NMR¥TU-3241NON_E6.als
COMNT TU-324
DATIM Sat Jan 21 18:30:49 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 24.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15

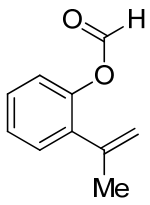
OH
Me

S6

F:¥NMR-1¥5g¥TU-3321NON_E8_FT.als
TU-332

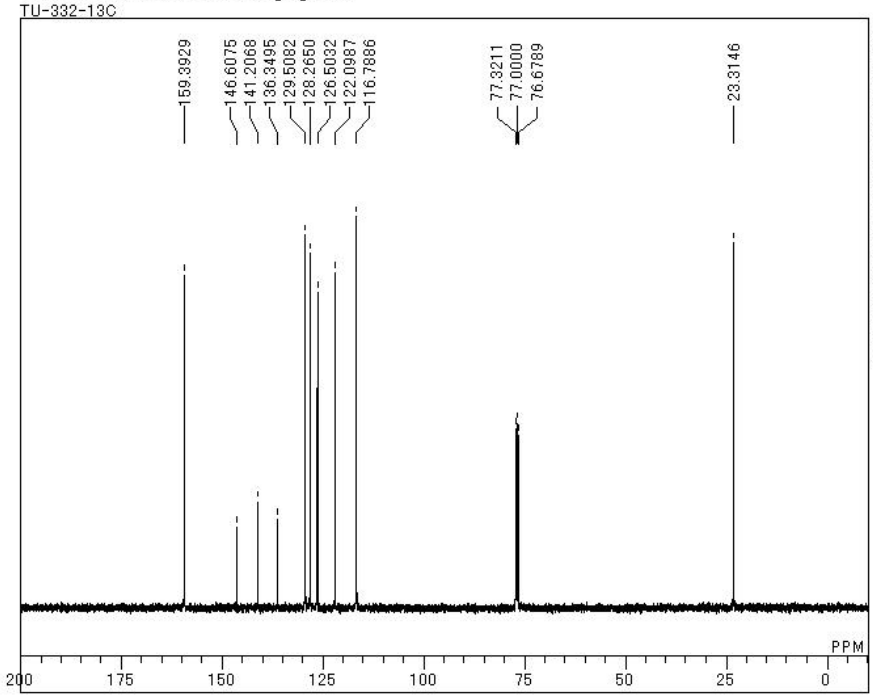


DFILE	F:¥NMR-1¥5g¥TU-3321NON_
COMNT	TU-332
DATIM	Tue Jan 24 13:11:10 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	22.1 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	11

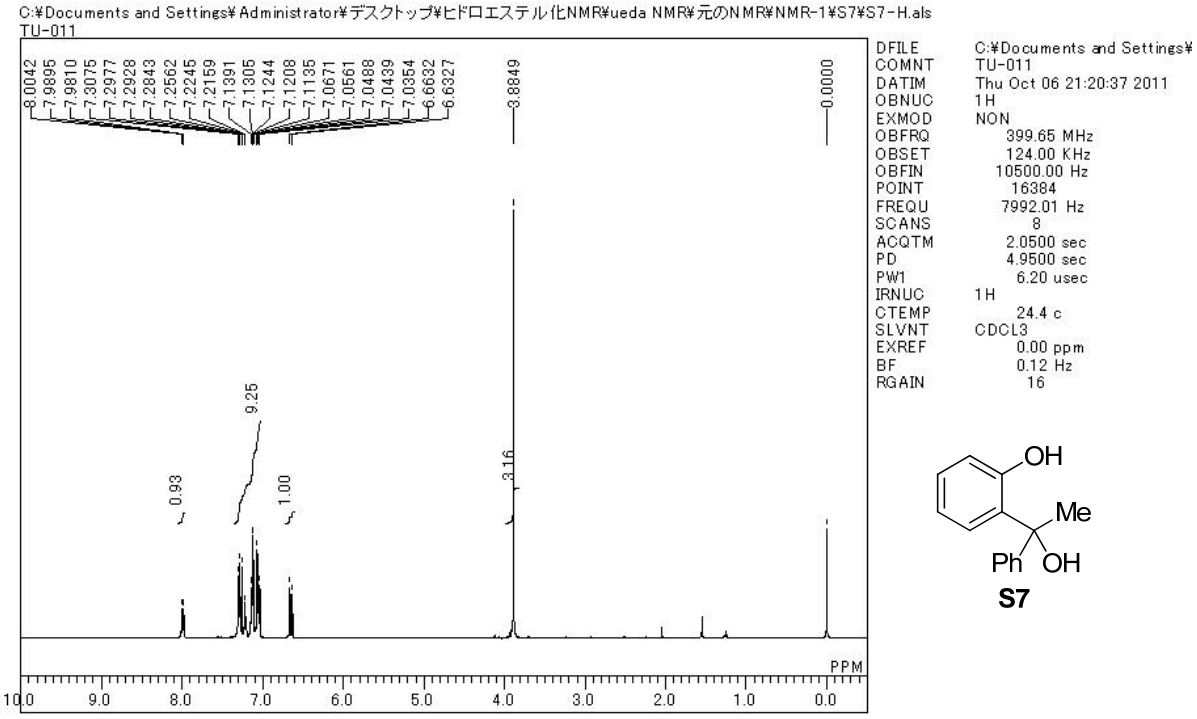


5g

F:¥NMR-1¥5g¥TU-332-13C1BCM_E9_FT.als
TU-332-13C

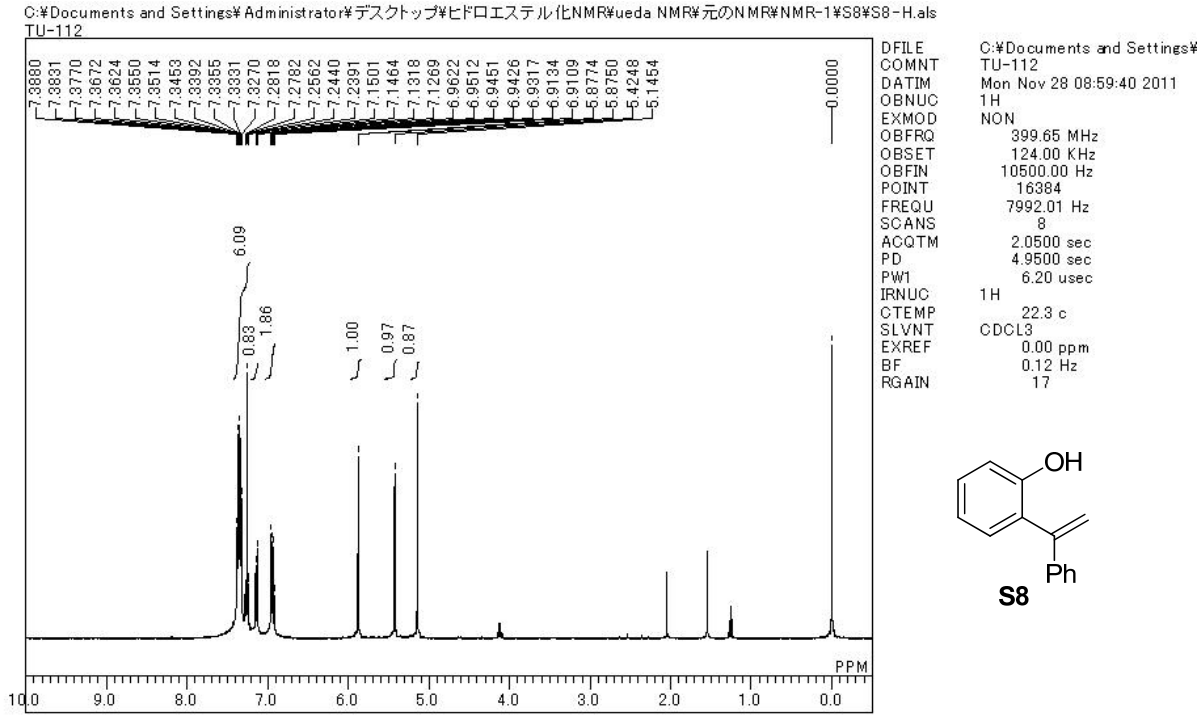


DFILE	F:¥NMR-1¥5g¥TU-332-13C1
COMNT	TU-332-13C
DATIM	Tue Jan 24 13:26:17 2012
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	256
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	22.4 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	26

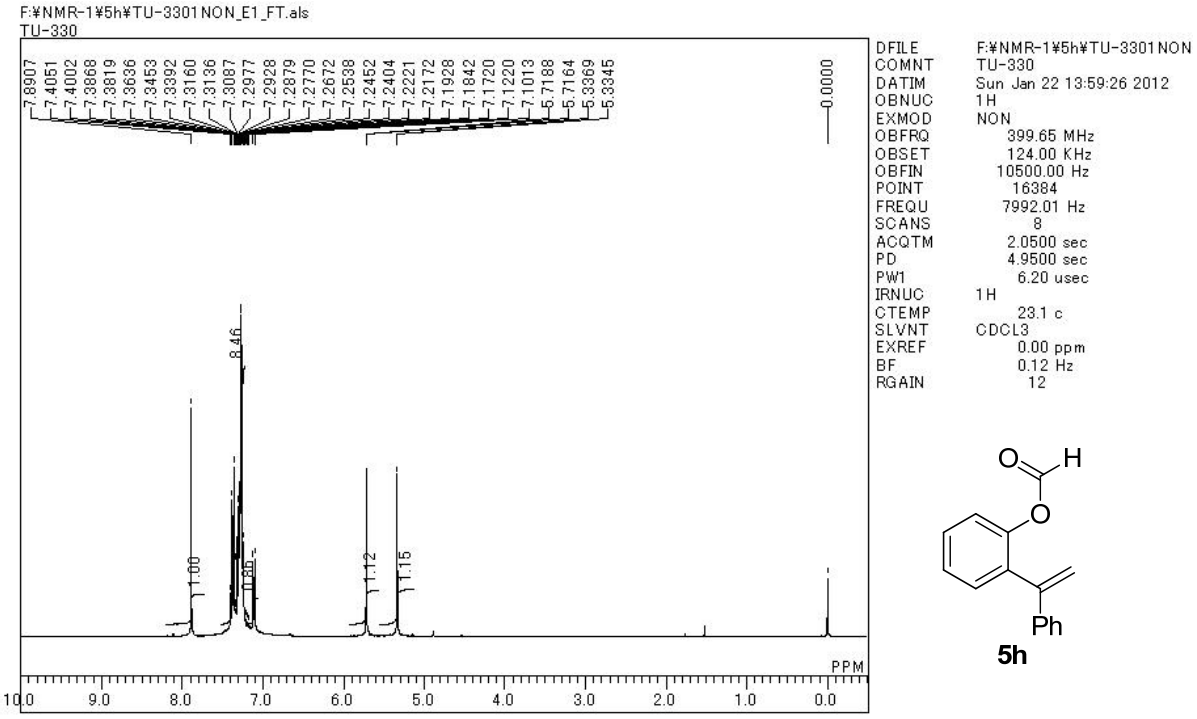

C:¥Documents and Settings¥Administrator¥デスクトップ¥ヒドロエステル化NMR¥ueda NMR¥元のNMR¥NMR-1¥S7¥S7-H.als
TU-011
8.0042
7.9895
7.9810
7.3075
7.2977
7.2928
7.2843
7.2562
7.2245
7.2159
7.1391
7.1305
7.1244
7.1208
7.1135
7.0671
7.0561
7.0488
7.0439
7.0354
6.6632
6.6327
3.8849
0.0000
0.93
9.25
1.00
3.16
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE C:¥Documents and Settings¥
COMNT TU-011
DATIM Thu Oct 06 21:20:37 2011
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 24.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16

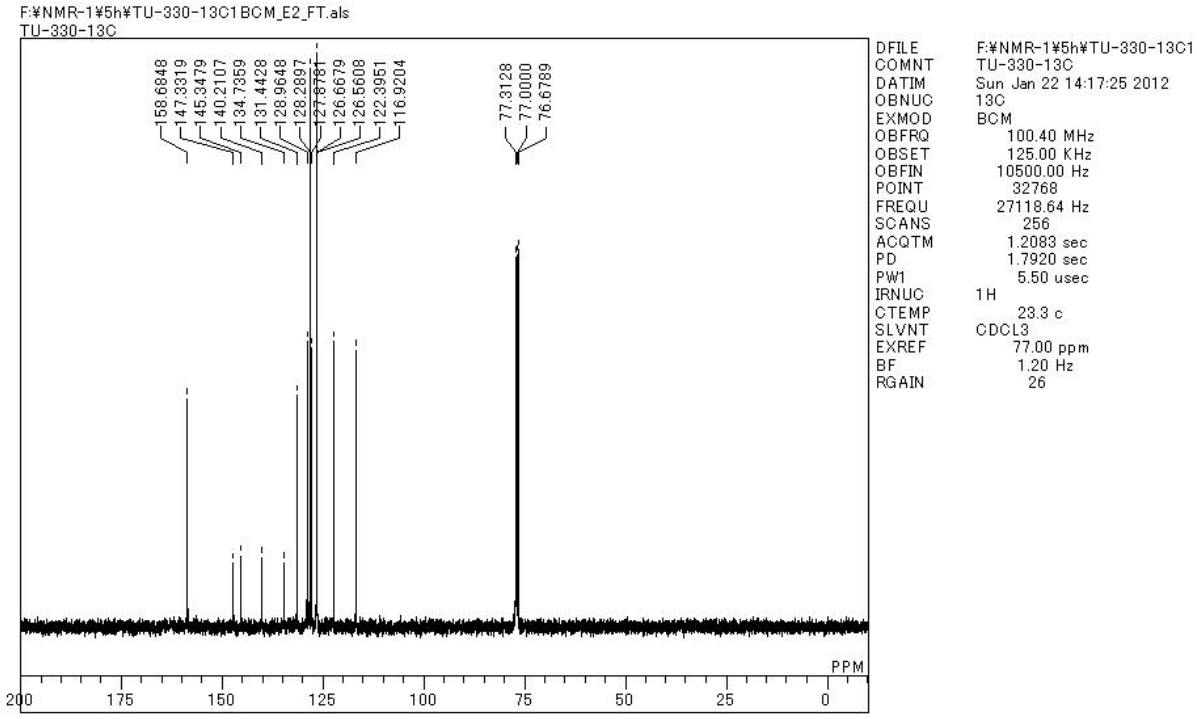
OH
Me
Ph
OH

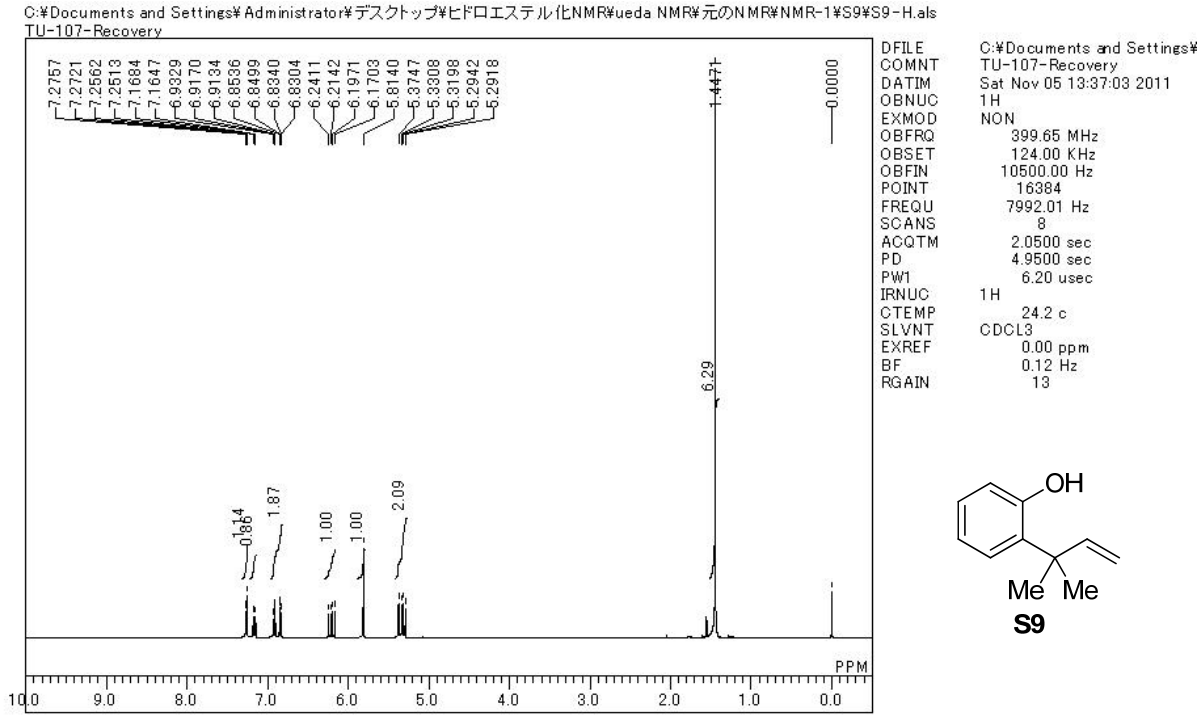
S7


C:¥Documents and Settings¥Administrator¥デスクトップ¥ヒドロエステル化NMR¥ueda NMR¥元のNMR¥NMR-1¥S8¥S8-H.als
TU-112
7.3880
7.3831
7.3770
7.3672
7.3624
7.3550
7.3514
7.3453
7.3392
7.3355
7.3331
7.3270
7.2818
7.2782
7.2562
7.2440
7.2391
7.1501
7.1464
7.1318
7.1269
6.9622
6.9512
6.9451
6.9426
6.9317
6.9134
6.9109
5.8774
5.8750
5.4248
5.1454
0.0000
6.09
0.83
1.86
1.00
0.97
0.87
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE C:¥Documents and Settings¥
COMNT TU-112
DATIM Mon Nov 28 08:59:40 2011
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17
OH
Ph

S8


F:¥NMR-1¥5h¥TU-3301NON_E1_FT.als
TU-330
7.8907
7.4051
7.4002
7.3868
7.3819
7.3636
7.3453
7.3392
7.3160
7.3136
7.3087
7.2977
7.2928
7.2879
7.2770
7.2672
7.2538
7.2452
7.2404
7.2221
7.2172
7.1928
7.1842
7.1720
7.1220
7.1013
5.7188
5.7164
5.3369
5.3345
0.0000
8.46
1.00
0.86
1.12
1.15
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥NMR-1¥5h¥TU-3301NON
COMNT TU-330
DATIM Sun Jan 22 13:59:26 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 23.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 12
O
H
O
Ph
5h

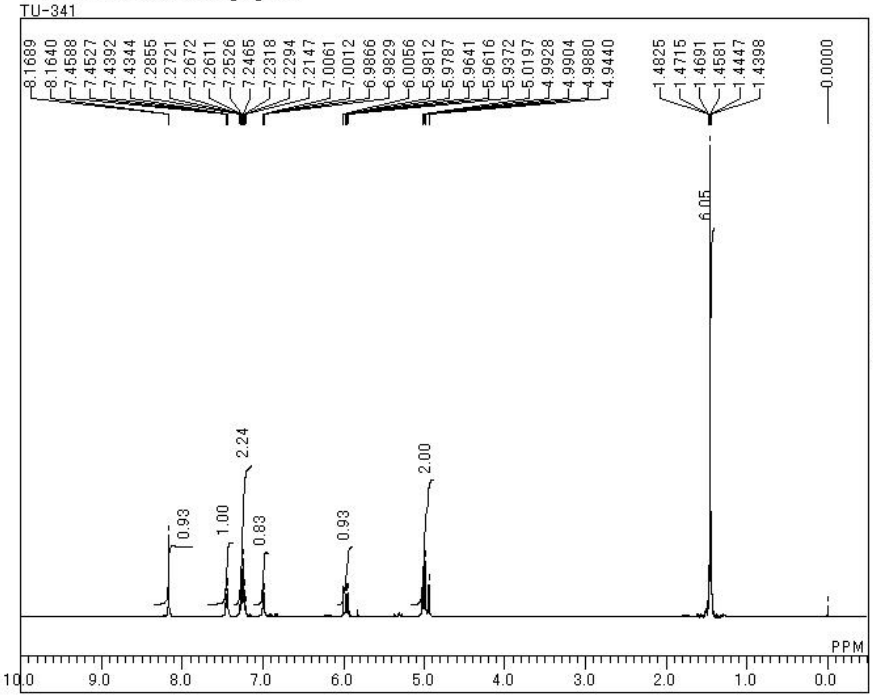

F:¥NMR-1¥5h¥TU-330-13C1BCM_E2_FT.als
TU-330-13C
158.6848
147.3319
145.3479
140.2107
134.7359
131.4428
128.9648
128.2897
127.8781
126.6679
126.5608
122.3951
116.9204
77.3128
77.0000
76.6789
PPM
200
175
150
125
100
75
50
25
0
DFILE F:¥NMR-1¥5h¥TU-330-13C1
COMNT TU-330-13C
DATIM Sun Jan 22 14:17:25 2012
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 256
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 23.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 26


C:¥Documents and Settings¥Administrator¥デスクトップ¥ヒドロエステル化NMR¥ueda NMR¥元のNMR¥NMR-1¥S9¥S9-H.als
TU-107-Recovery
7.2757
7.2721
7.2562
7.2513
7.1684
7.1647
6.9329
6.9170
6.9134
6.8536
6.8499
6.8340
6.8304
6.2411
6.2142
6.1971
6.1703
5.8140
5.3747
5.3308
5.3198
5.2942
5.2918
1.4471
0.0000
6.29
0.86
0.94
1.87
1.00
1.00
2.09
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE C:¥Documents and Settings¥
COMNT TU-107-Recovery
DATIM Sat Nov 05 13:37:03 2011
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 24.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 13

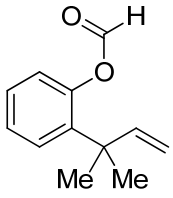
OH
Me
Me

S9

F:¥NMR-1¥5i¥TU-3411NON_E1_FT.als
TU-341

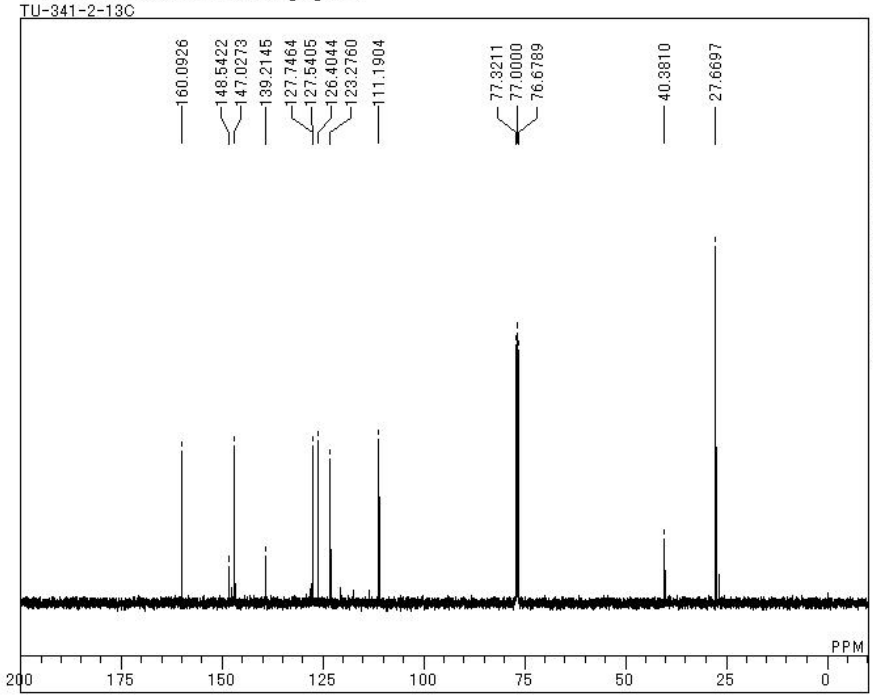


DFILE	F:¥NMR-1¥5i¥TU-3411NON_
COMNT	TU-341
DATIM	Sat Jan 28 09:38:16 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	23.1 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	10

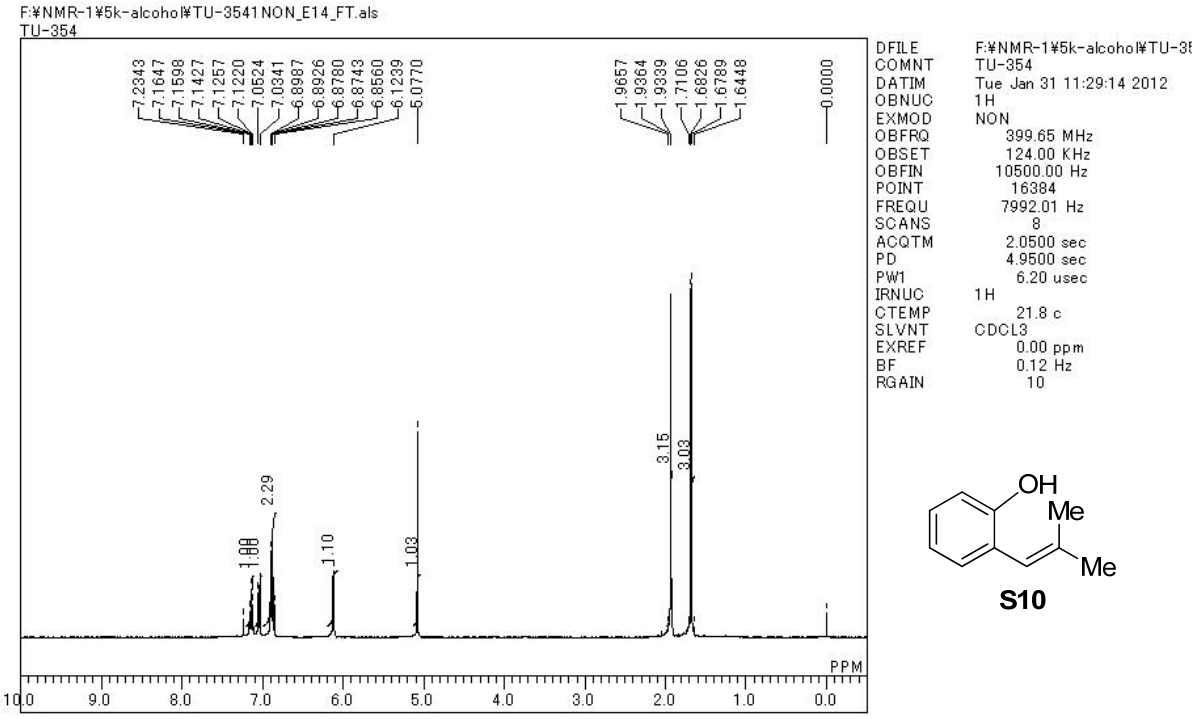


5i

F:¥NMR-1¥5i¥TU-341-2-13C1BCM_E4_FT.als
TU-341-2-13C

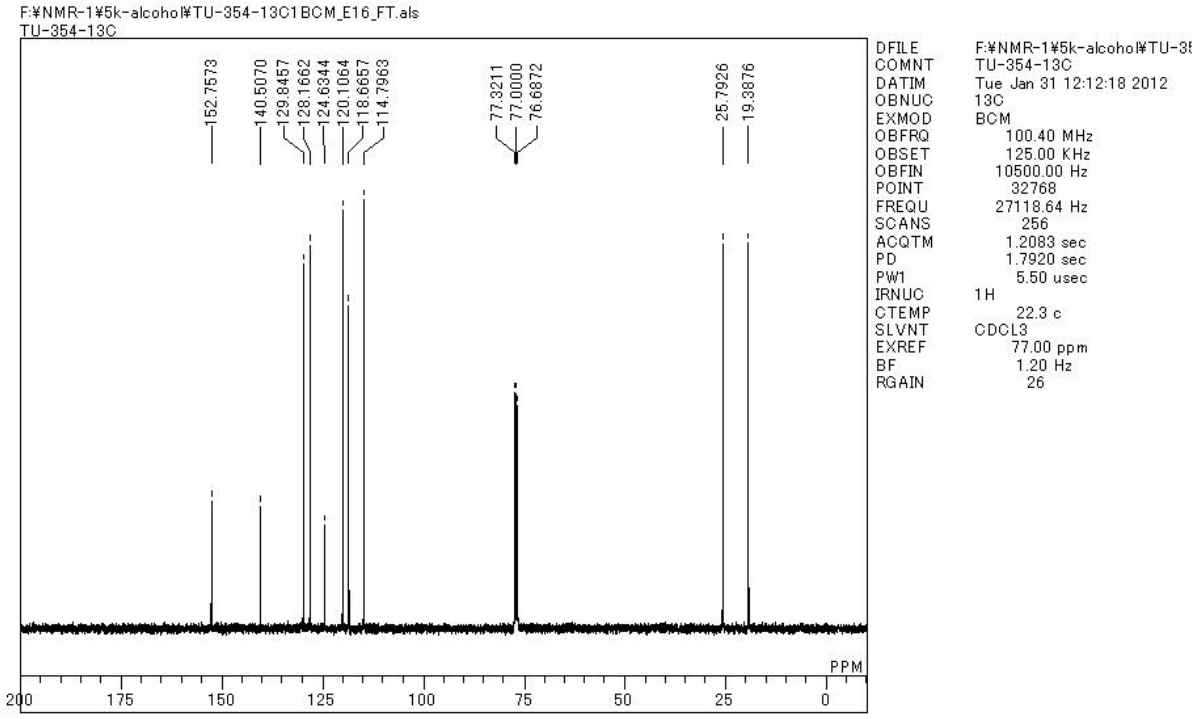


DFILE	F:¥NMR-1¥5i¥TU-341-2-13C
COMNT	TU-341-2-13C
DATIM	Sat Jan 28 11:23:19 2012
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	128
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	22.3 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	28

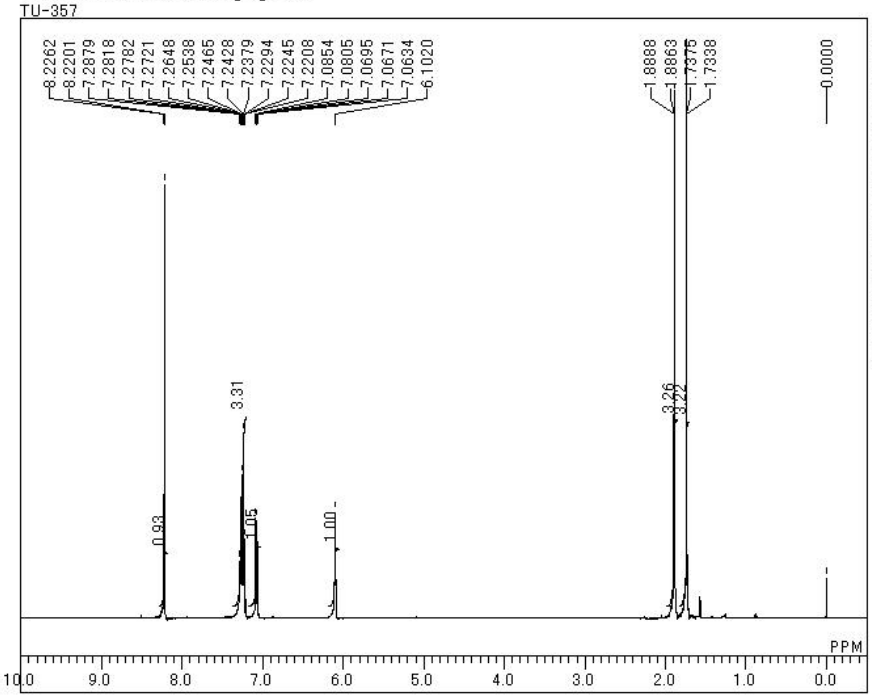

F:¥NMR-1¥5k-alcohol¥TU-3541NON_E14_FT.als
TU-354
7.2343
7.1647
7.1598
7.1427
7.1257
7.1220
7.0524
7.0341
6.8987
6.8926
6.8780
6.8743
6.8560
6.1239
5.0770
1.9657
1.9364
1.9339
1.7106
1.6826
1.6789
1.6448
0.0000
3.15
3.03
2.29
1.00
1.10
1.03
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥NMR-1¥5k-alcohol¥TU-3
COMNT TU-354
DATIM Tue Jan 31 11:29:14 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 21.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 10

OH
Me
Me

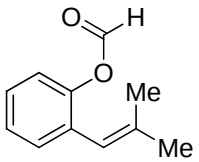
S10


F:¥NMR-1¥5k-alcohol¥TU-354-13C1BCM_E16_FT.als
TU-354-13C
152.7573
140.6070
129.8457
128.1662
124.6344
120.1064
118.6657
114.7963
77.3211
77.0000
76.6872
25.7926
19.3876
PPM
200
175
150
125
100
75
50
25
0
DFILE F:¥NMR-1¥5k-alcohol¥TU-3
COMNT TU-354-13C
DATIM Tue Jan 31 12:12:18 2012
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 256
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 26

F:¥NMR-1¥5k¥TU-3571NON_E3_FT.als
TU-357

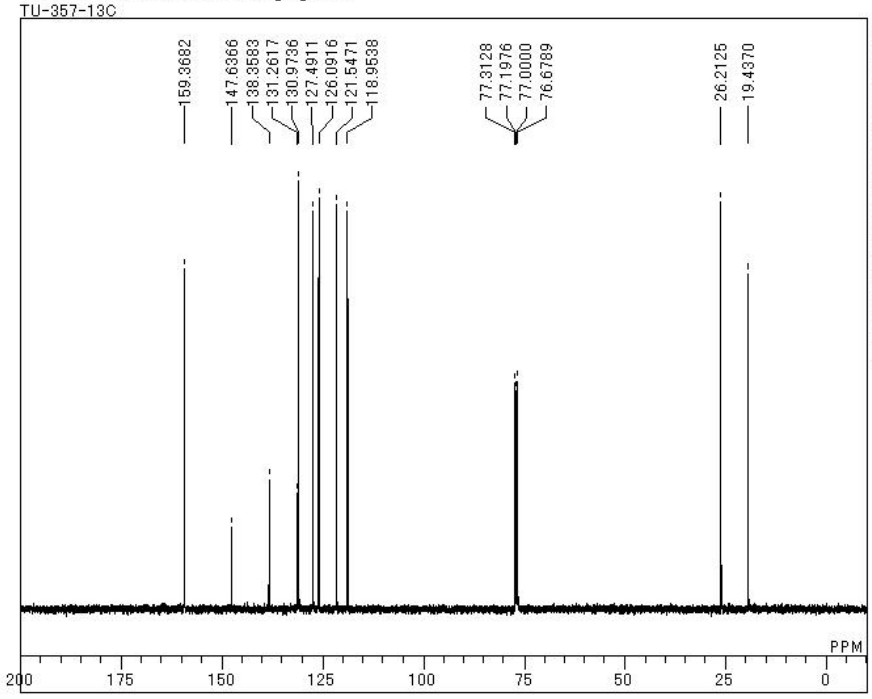


DFILE	F:¥NMR-1¥5k¥TU-3571NON_
COMNT	TU-357
DATIM	Wed Feb 01 18:17:33 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	23.1 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	9

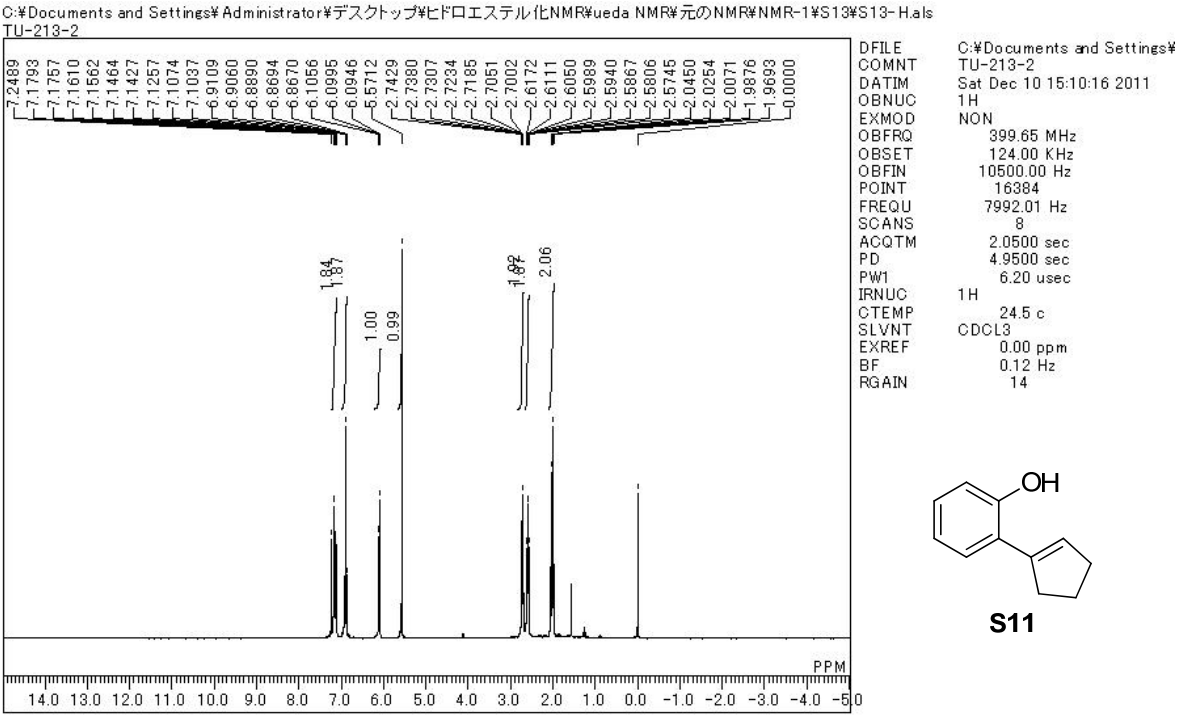


5j

F:¥NMR-1¥5k¥TU-357-13C1BCM_E4_FT.als
TU-357-13C



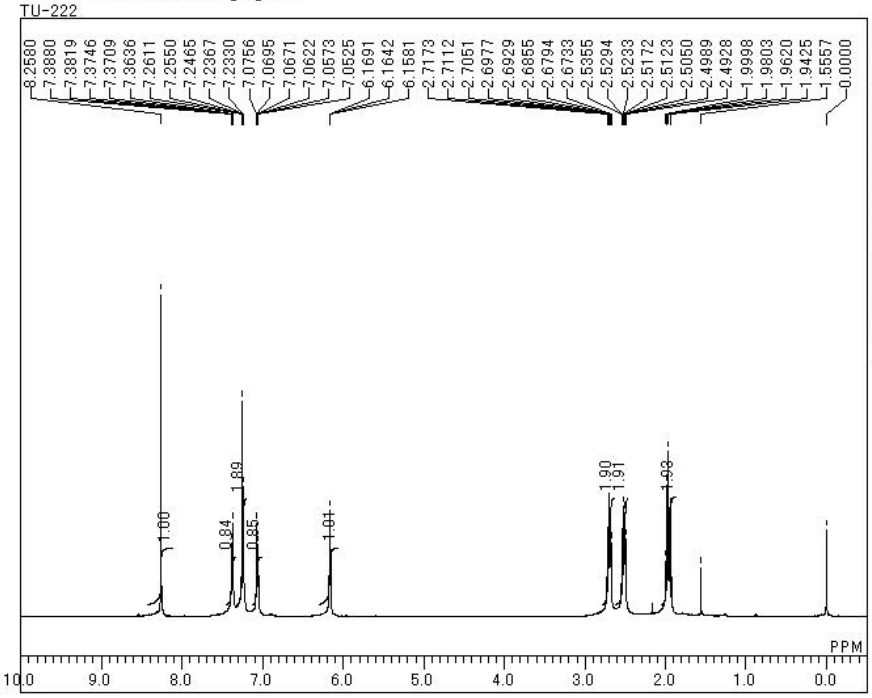
DFILE	F:¥NMR-1¥5k¥TU-357-13C1
COMNT	TU-357-13C
DATIM	Wed Feb 01 18:35:01 2012
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	256
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	23.0 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	26


C:¥Documents and Settings¥ Administrator¥デスクトップ¥ヒドロエステル化NMR¥ueda NMR¥元のNMR¥NMR-1¥S13¥S13-H.als
TU-213-2
7.2489
7.1793
7.1757
7.1610
7.1562
7.1464
7.1427
7.1257
7.1074
7.1037
6.9109
6.9060
6.8890
6.8694
6.8670
6.1056
6.0995
6.0946
5.5712
2.7429
2.7380
2.7307
2.7234
2.7185
2.7051
2.7002
2.6172
2.6111
2.6050
2.5989
2.5940
2.5867
2.5806
2.5745
2.0450
2.0254
2.0071
1.9876
1.9693
0.0000
1.84
1.87
1.00
0.99
1.97
2.06
PPM
14.0 13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0 -3.0 -4.0 -5.0
DFILE C:¥Documents and Settings¥
COMNT TU-213-2
DATIM Sat Dec 10 15:10:16 2011
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 24.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 14

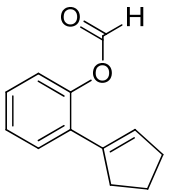
OH

S11

F:¥NMR-1¥5¥TU-2221NON_E4_FT.als
TU-222

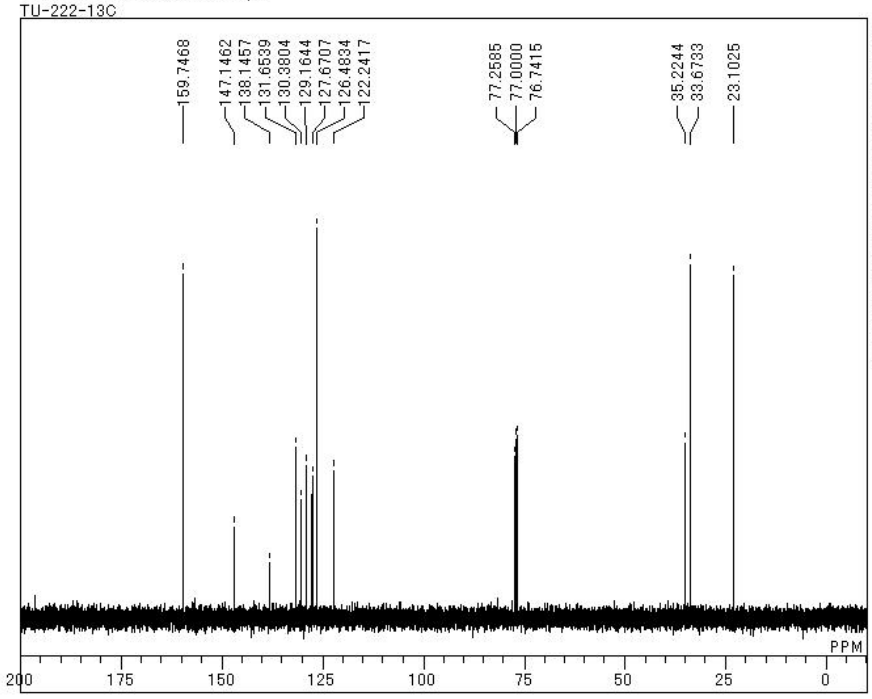


DFILE	F:¥NMR-1¥5¥TU-2221NON_
COMNT	TU-222
DATIM	Mon Dec 12 23:17:21 2011
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	22.8 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	13

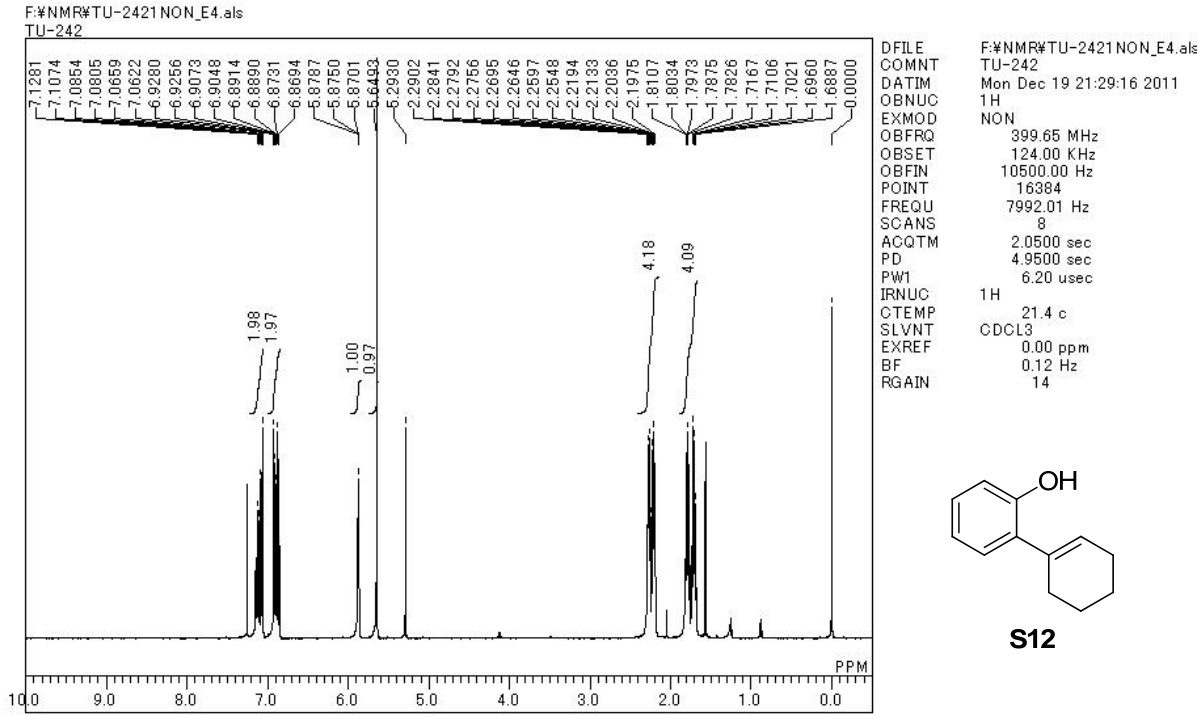


5k

F:¥NMR-1¥5¥TU-222-13C-1.jdf
TU-222-13C

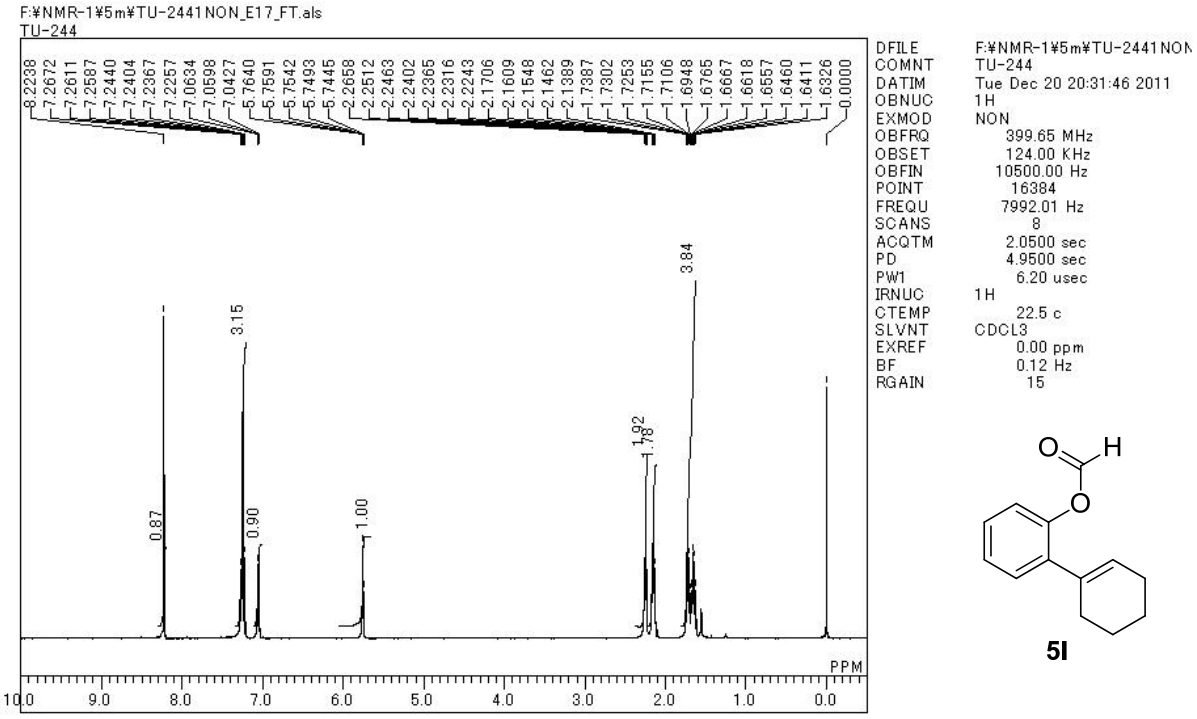


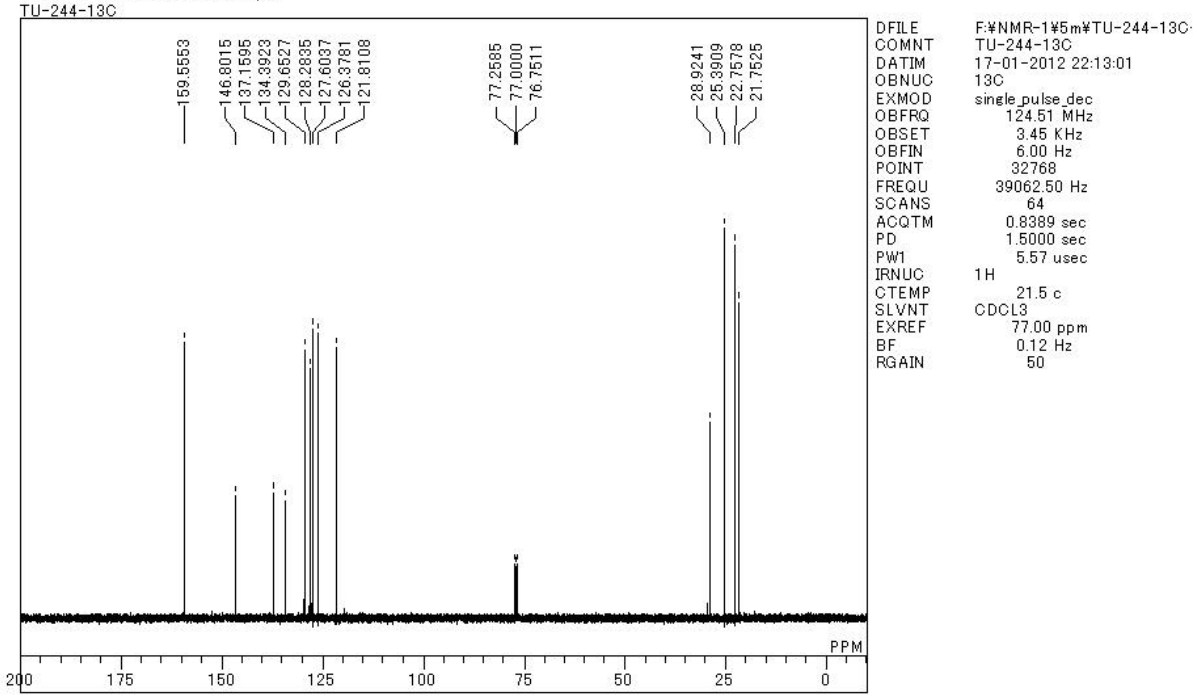
DFILE	F:¥NMR-1¥5¥TU-222-13C-1
COMNT	TU-222-13C
DATIM	17-01-2012 21:59:42
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	124.51 MHz
OBSET	3.45 KHz
OBFIN	6.00 Hz
POINT	32768
FREQU	39062.50 Hz
SCANS	64
ACQTM	0.8389 sec
PD	1.5000 sec
PW1	5.57 usec
IRNUC	1H
CTEMP	21.4 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50

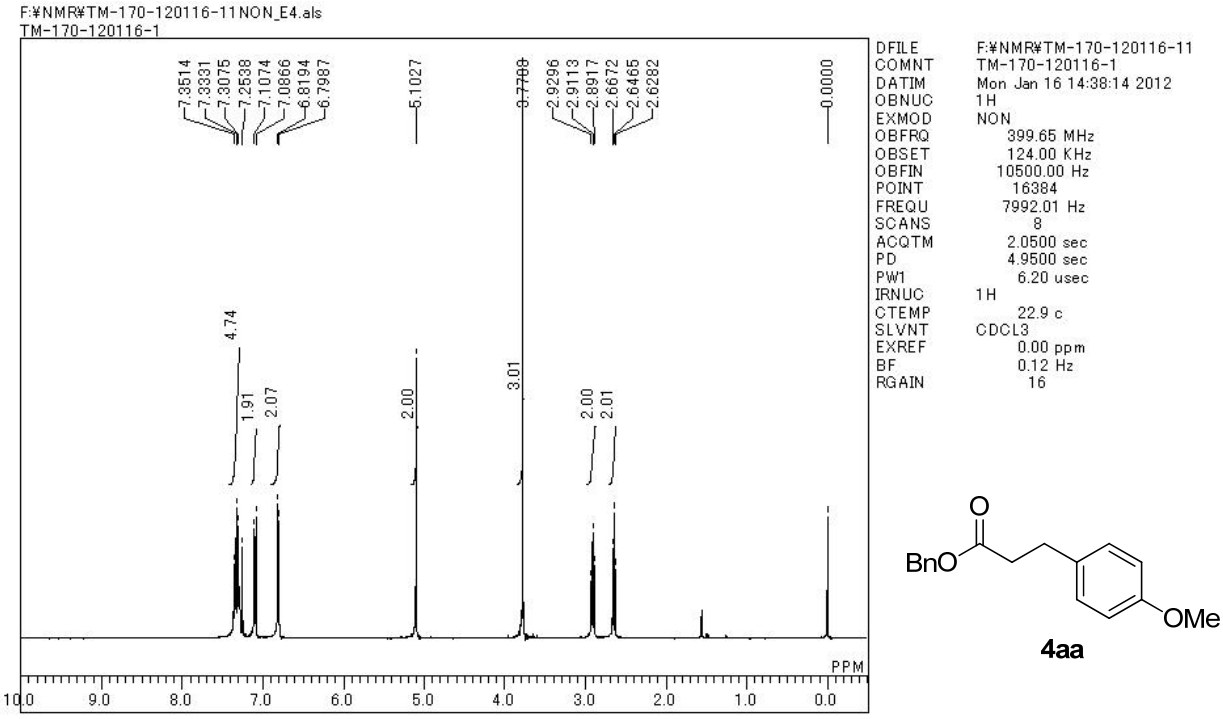


DFILE	F:¥NMR¥TU-2421NON_E4.als
COMNT	TU-242
DATIM	Mon Dec 19 21:29:16 2011
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	21.4 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	14

S12

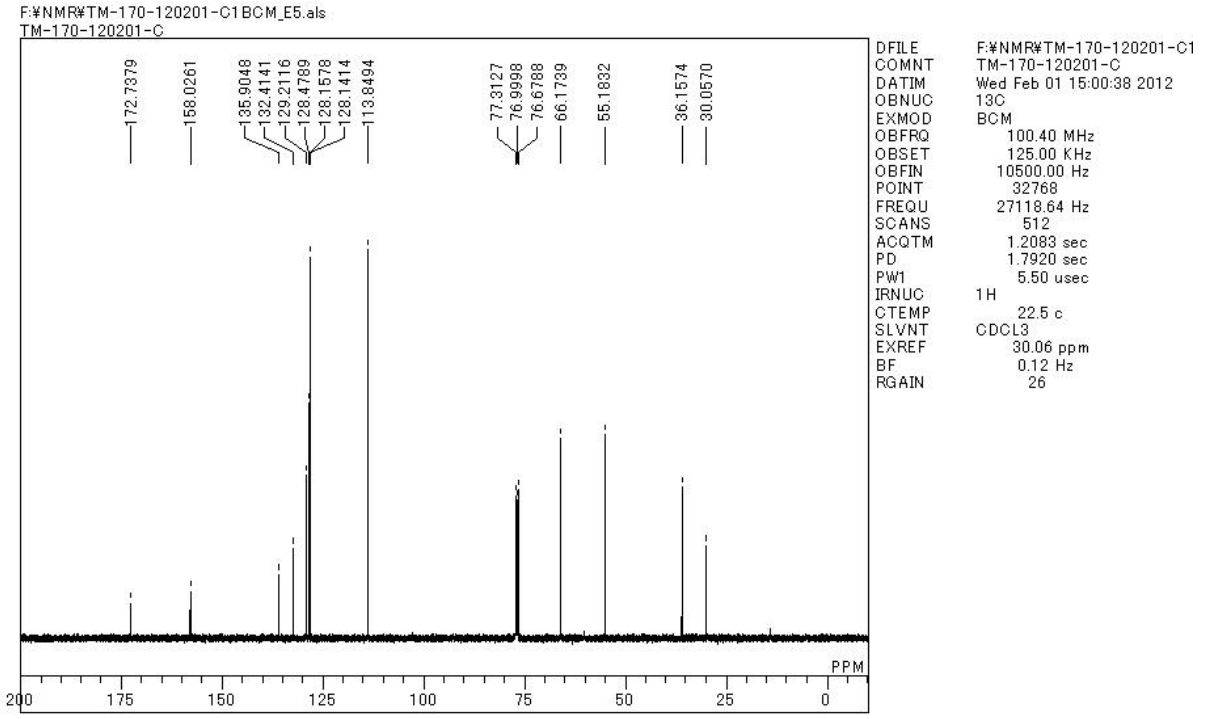

F:¥NMR-1¥5m¥TU-2441NON_E17_FT.als
TU-244
8.2238
7.2672
7.2611
7.2587
7.2440
7.2404
7.2367
7.2257
7.0634
7.0598
7.0427
5.7640
5.7591
5.7542
5.7493
5.7445
2.2658
2.2512
2.2463
2.2402
2.2365
2.2316
2.2243
2.1706
2.1609
2.1548
2.1462
2.1389
2.1387
2.1302
1.7253
1.7155
1.7106
1.6948
1.6765
1.6667
1.6618
1.6557
1.6460
1.6411
1.6326
0.0000
3.84
3.15
1.92
1.78
0.87
0.90
1.00
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥NMR-1¥5m¥TU-2441NON
COMNT TU-244
DATIM Tue Dec 20 20:31:46 2011
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15
O
H
O
5l


F:¥NMR-1¥5m¥TU-244-13C-1.jdf
TU-244-13C
159.5553
146.8015
137.1595
134.3923
129.6527
128.2835
127.6037
126.3781
121.8108
77.2585
77.0000
76.7511
28.9241
25.3909
22.7578
21.7525
PPM
200
175
150
125
100
75
50
25
0
DFILE F:¥NMR-1¥5m¥TU-244-13C
COMNT TU-244-13C
DATIM 17-01-2012 22:13:01
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 124.51 MHz
OBSET 3.45 KHz
OBFIN 6.00 Hz
POINT 32768
FREQU 39062.50 Hz
SCANS 64
ACQTM 0.8389 sec
PD 1.5000 sec
PW1 5.57 usec
IRNUC 1H
CTEMP 21.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50

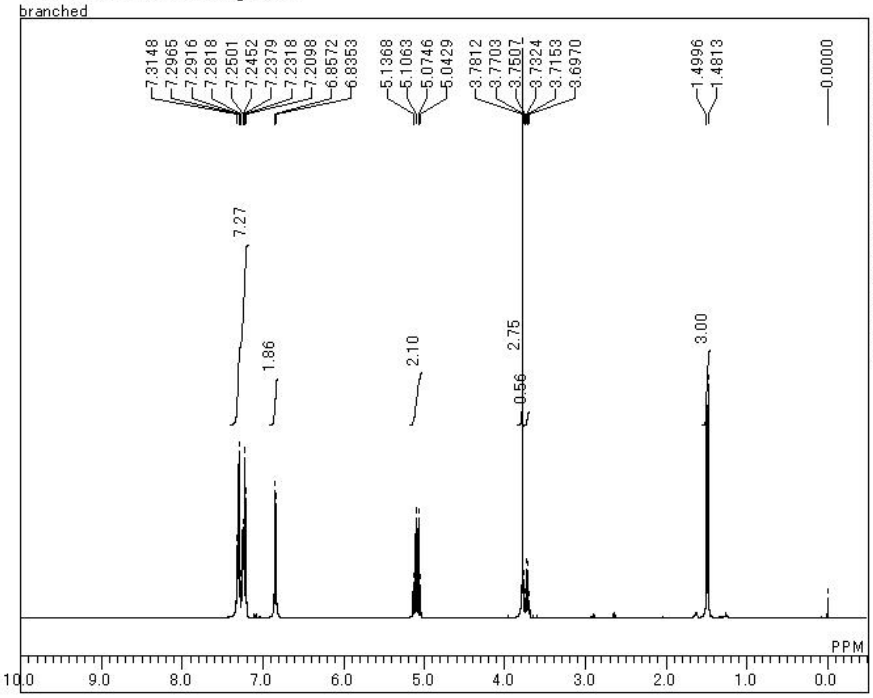

F:¥NMR¥TM-170-120116-11NON_E4.als
TM-170-120116-1
7.3514
7.3331
7.3075
7.2638
7.1074
7.0866
6.8194
6.7987
5.1027
3.7708
2.9296
2.9113
2.8917
2.6672
2.6465
2.6282
0.0000
4.74
1.91
2.07
2.00
3.01
2.00
2.01
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥NMR¥TM-170-120116-11
COMNT TM-170-120116-1
DATIM Mon Jan 16 14:38:14 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16

O
BnO
OMe

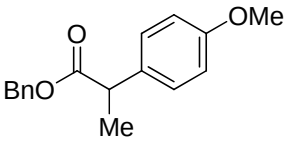
4aa


F:¥NMR¥TM-170-120201-C1BCM_E5.als
TM-170-120201-C
172.7379
158.0261
135.9048
132.4141
129.2116
128.4789
128.1578
128.1414
113.8494
77.3127
76.9998
76.6788
66.1739
55.1832
36.1574
30.0570
PPM
200
175
150
125
100
75
50
25
0
DFILE F:¥NMR¥TM-170-120201-C1
COMNT TM-170-120201-C
DATIM Wed Feb 01 15:00:38 2012
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 512
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 30.06 ppm
BF 0.12 Hz
RGAIN 26

F:¥NMR¥TM-120207-11NON_E13.als
branched

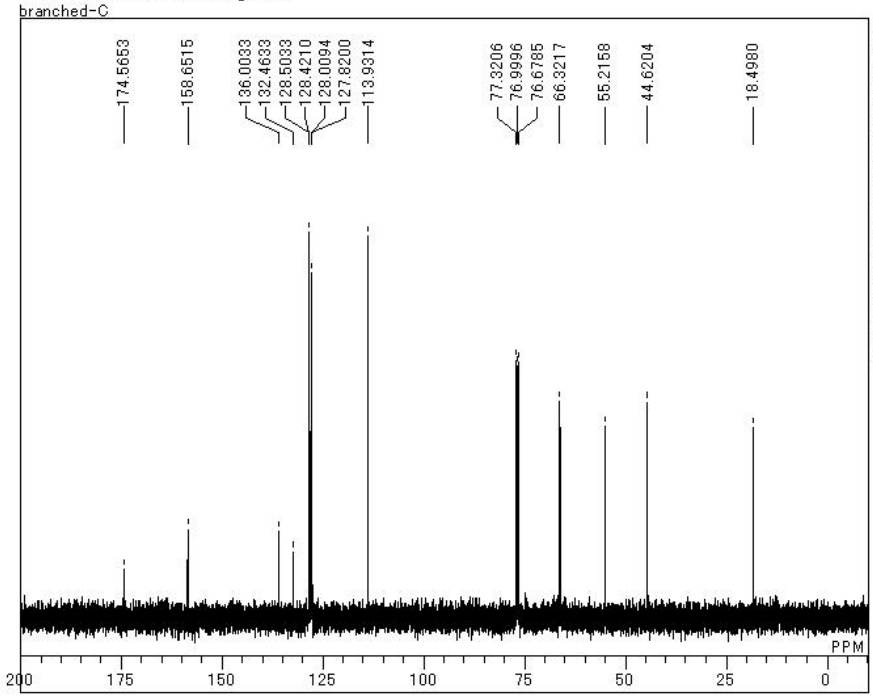


DFILE	F:¥NMR¥TM-120207-11NON
COMNT	branched
DATIM	Tue Feb 07 15:18:17 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	19.2 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	10

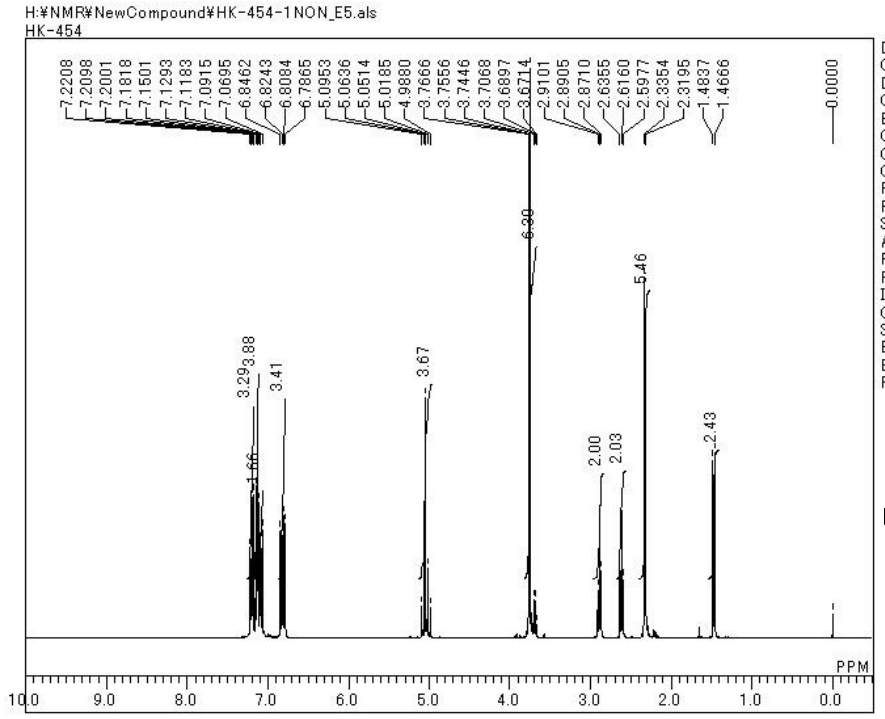


4ab

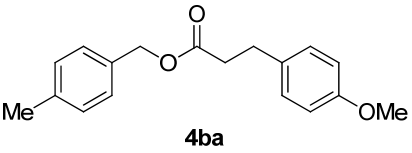
F:¥NMR¥TM-120207-21BCM_E6.als
branched-C



DFILE	F:¥NMR¥TM-120207-21BCM
COMNT	branched-C
DATIM	Tue Feb 07 18:33:21 2012
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	512
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	21.1 c
SLVNT	CDCL3
EXREF	18.50 ppm
BF	0.12 Hz
RGAIN	22



DFILE	H:¥NMR¥NewCompound¥HK-
COMNT	HK-454
DATIM	Tue Jan 24 23:55:33 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	21.3 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	8



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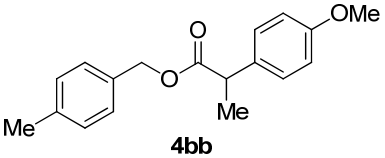
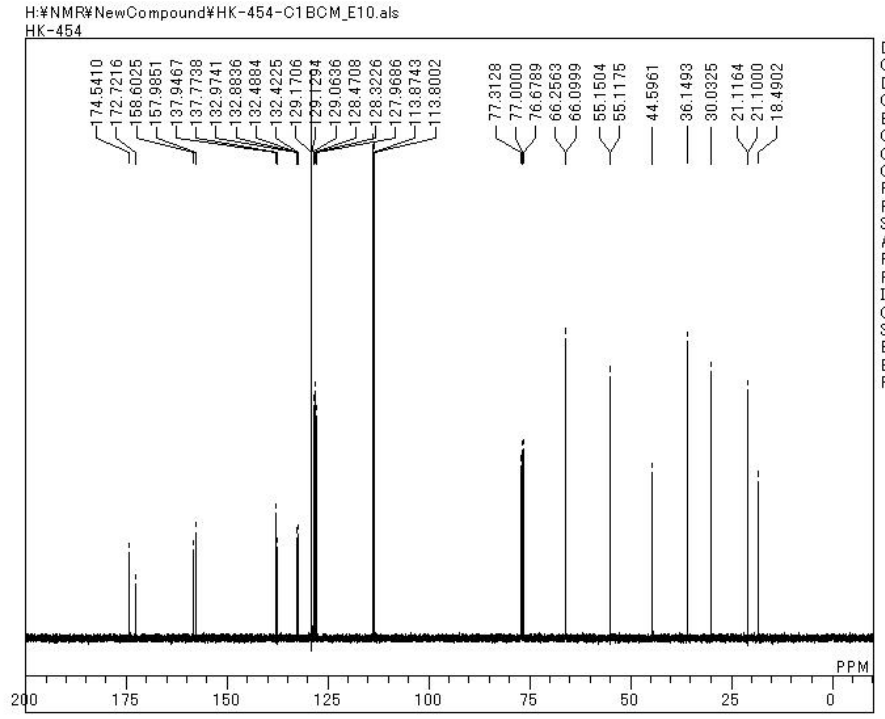
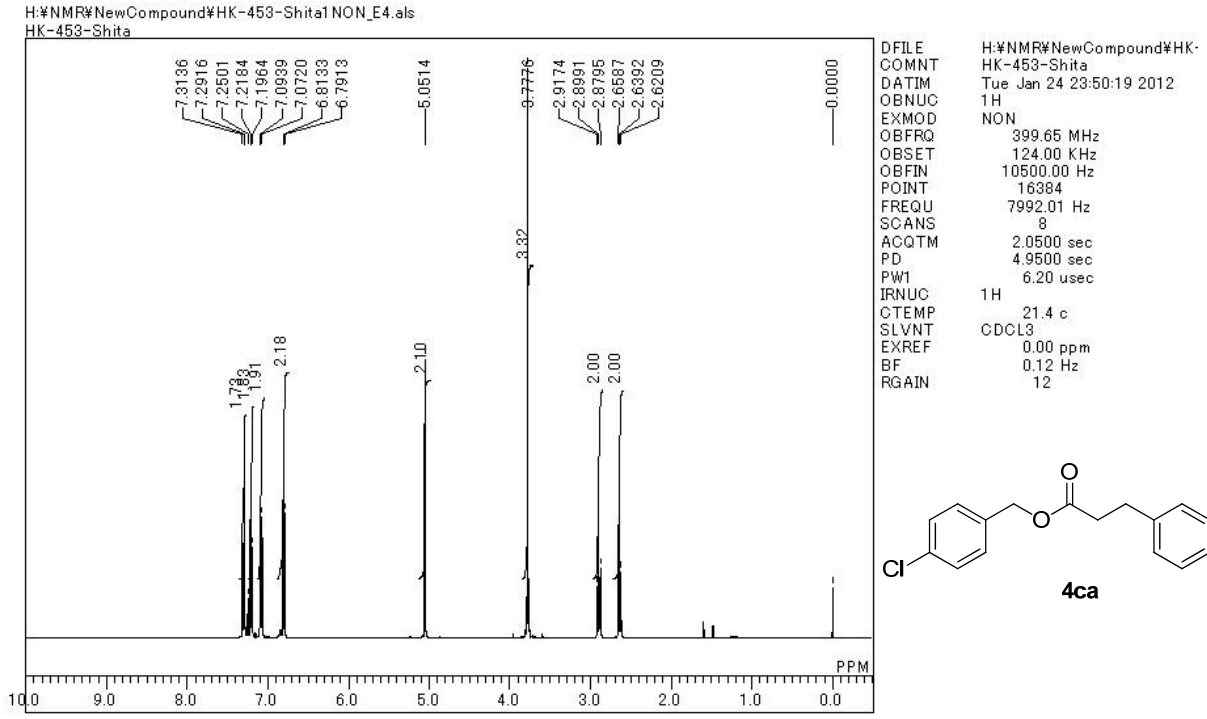
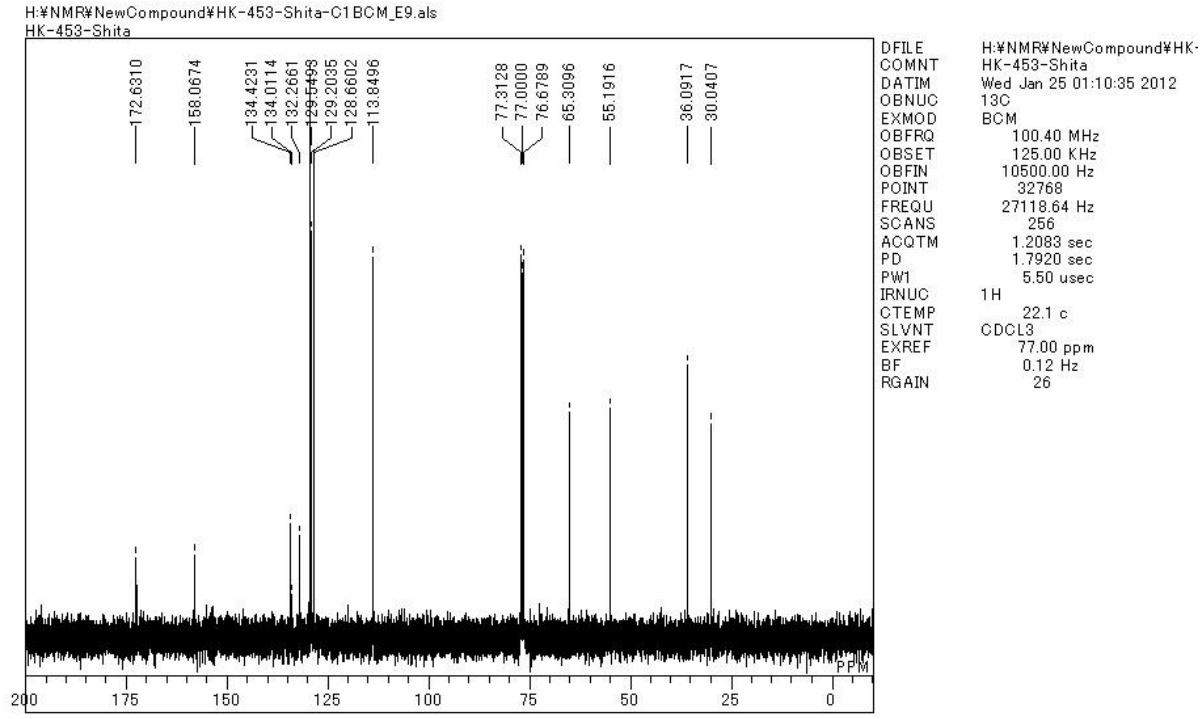


4bb

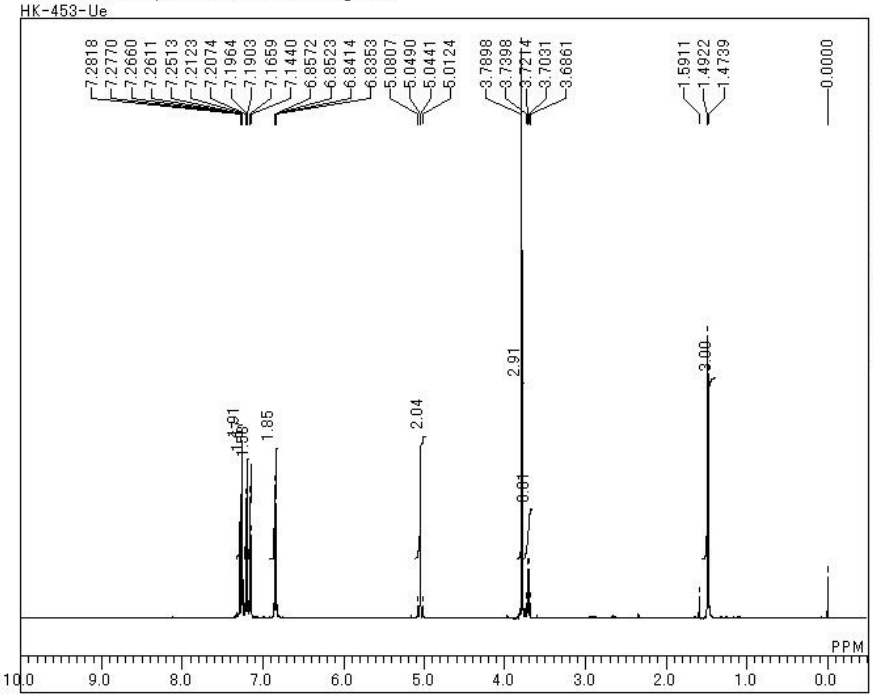


DFILE	H:¥NMR¥NewCompound¥HK-
COMNT	HK-454
DATIM	Wed Jan 25 01:29:58 2012
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	256
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	22.1 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	26

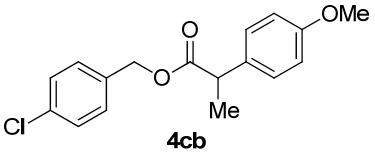

H:¥NMR¥NewCompound¥HK-453-Shita1NON_E4.als
HK-453-Shita
7.3136
7.2916
7.2501
7.2184
7.1964
7.0939
7.0720
6.8133
6.7913
5.0514
3.7776
2.9174
2.8991
2.8795
2.6587
2.6392
2.6209
0.0000
3.32
1.72
1.83
1.91
2.18
2.10
2.00
2.00
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE H:¥NMR¥NewCompound¥HK-
COMNT HK-453-Shita
DATIM Tue Jan 24 23:50:19 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 21.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 12
O
O
Cl
OMe
4ca


H:¥NMR¥NewCompound¥HK-453-Shita-C1BCM_E9.als
HK-453-Shita
172.6310
158.0674
134.4231
134.0114
132.2661
129.5498
129.2035
128.6602
113.8496
77.3128
77.0000
76.6789
65.3096
55.1916
36.0917
30.0407
PPM
200
175
150
125
100
75
50
25
0
DFILE H:¥NMR¥NewCompound¥HK-
COMNT HK-453-Shita
DATIM Wed Jan 25 01:10:35 2012
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 256
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 22.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 26

H:¥NMR¥NewCompound¥HK-453-Ue1NON_E3.als
HK-453-Ue

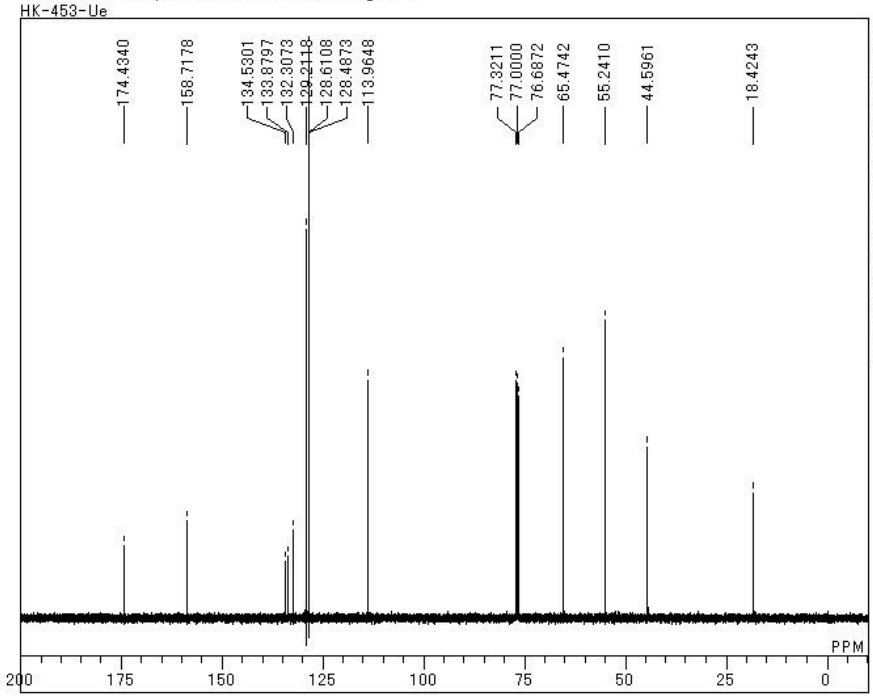


DFILE	H:¥NMR¥NewCompound¥HK-
COMNT	HK-453-Ue
DATIM	Tue Jan 24 23:43:42 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	21.4 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	12



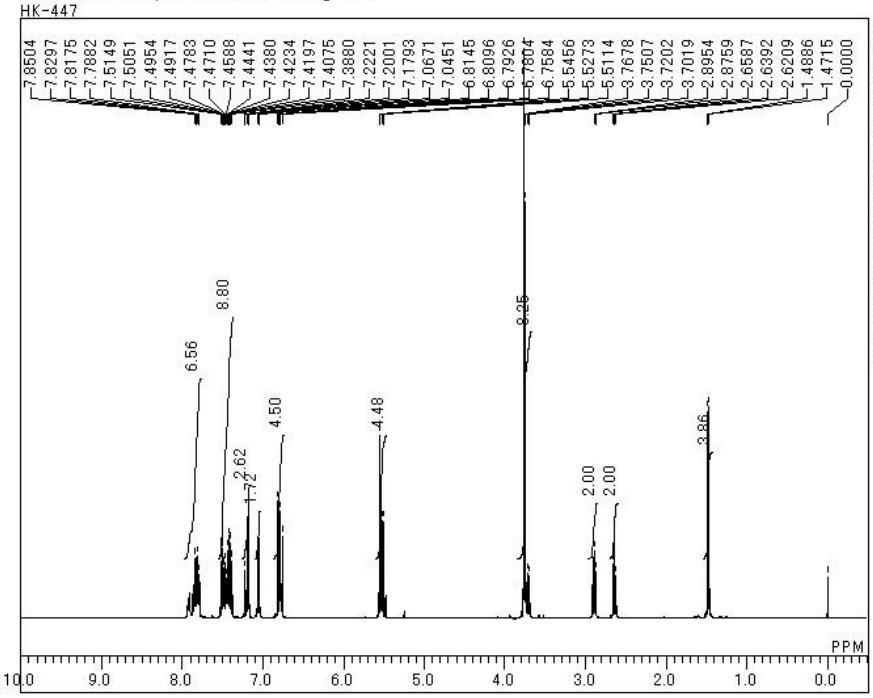
4cb

H:¥NMR¥NewCompound¥HK-453-Ue-C1BCM_E8.als
HK-453-Ue

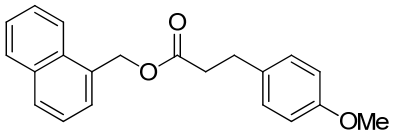


DFILE	H:¥NMR¥NewCompound¥HK-
COMNT	HK-453-Ue
DATIM	Wed Jan 25 00:50:50 2012
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	256
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	22.1 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	26

H:¥NMR¥NewCompound¥HK-447-1NON_E3.als
HK-447



DFILE	H:¥NMR¥NewCompound¥HK-
COMNT	HK-447
DATIM	Wed Jan 25 23:21:12 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	21.8 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	10



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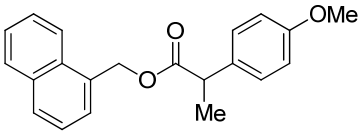
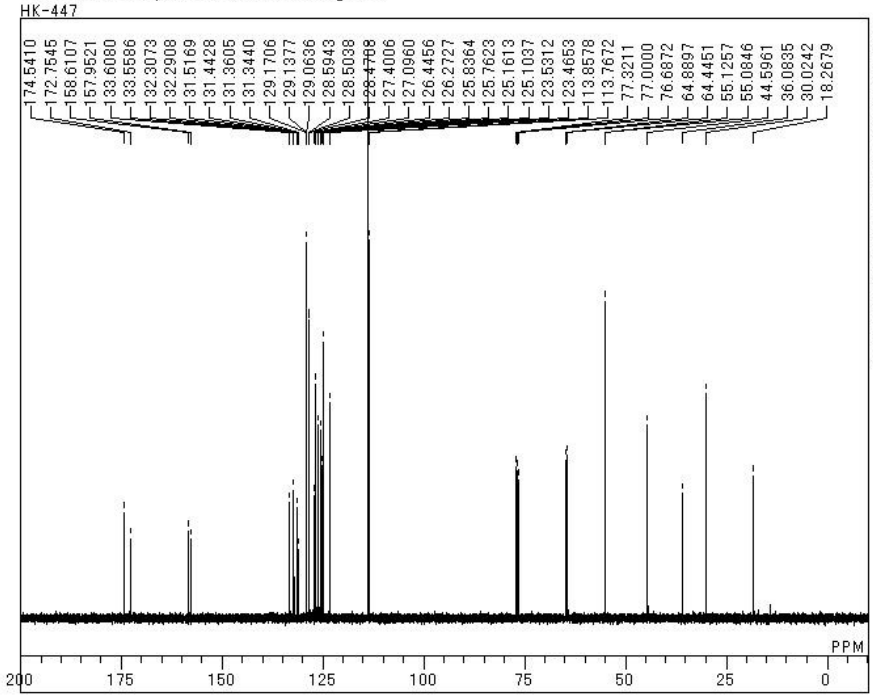


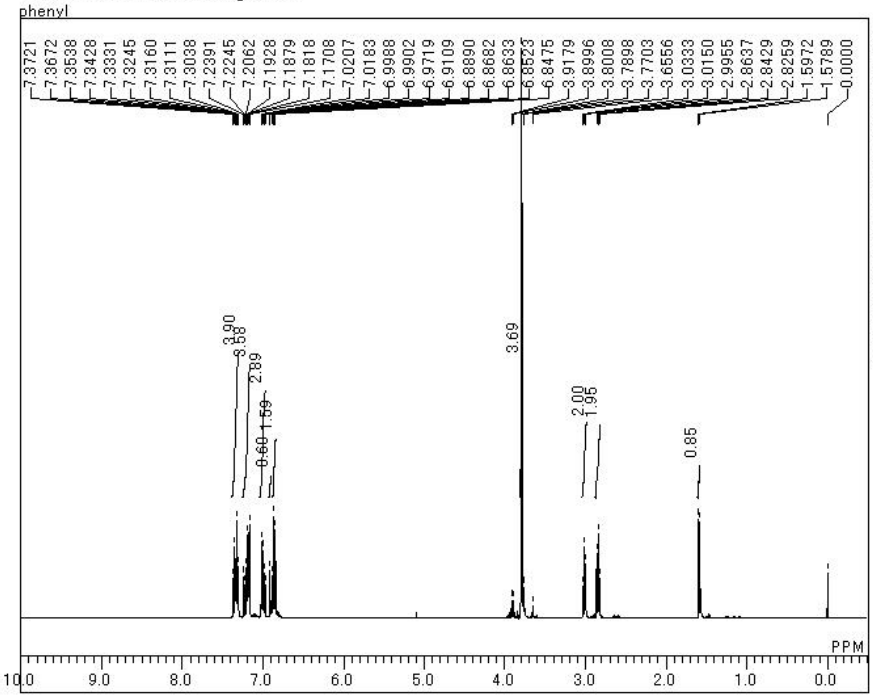
4db

H:¥NMR¥NewCompound¥HK-447-C1BCM_E6.als
HK-447

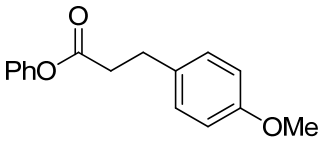


DFILE	H:¥NMR¥NewCompound¥HK-
COMNT	HK-447
DATIM	Wed Jan 25 00:14:51 2012
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	256
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	22.3 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	26

F:¥NMR¥TM-120119-11NON_E26.als
phenyl



DFILE	F:¥NMR¥TM-120119-11NON
COMNT	phenyl
DATIM	Thu Jan 19 15:10:27 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	22.0 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	12



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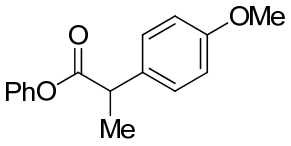
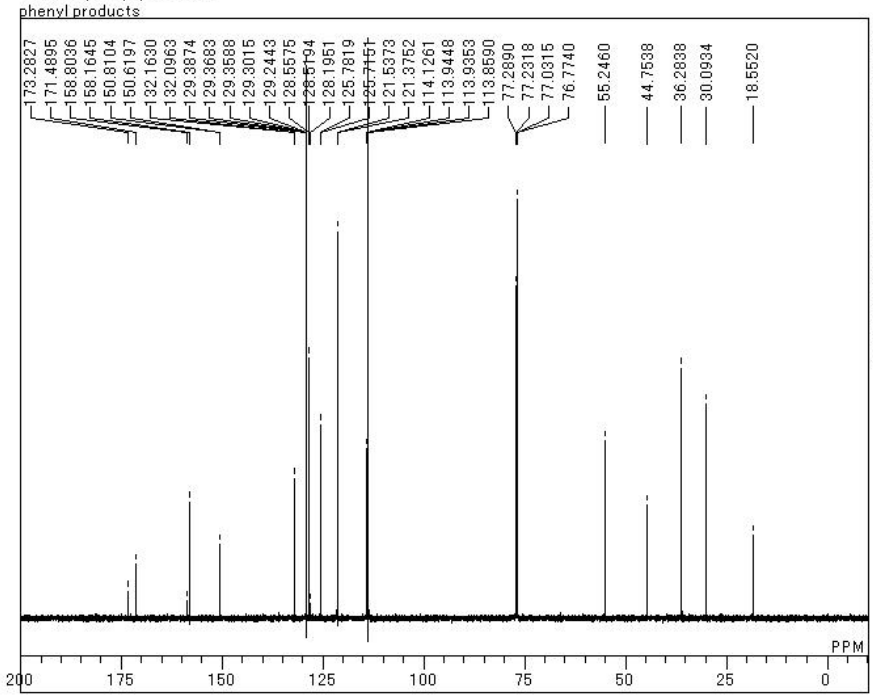
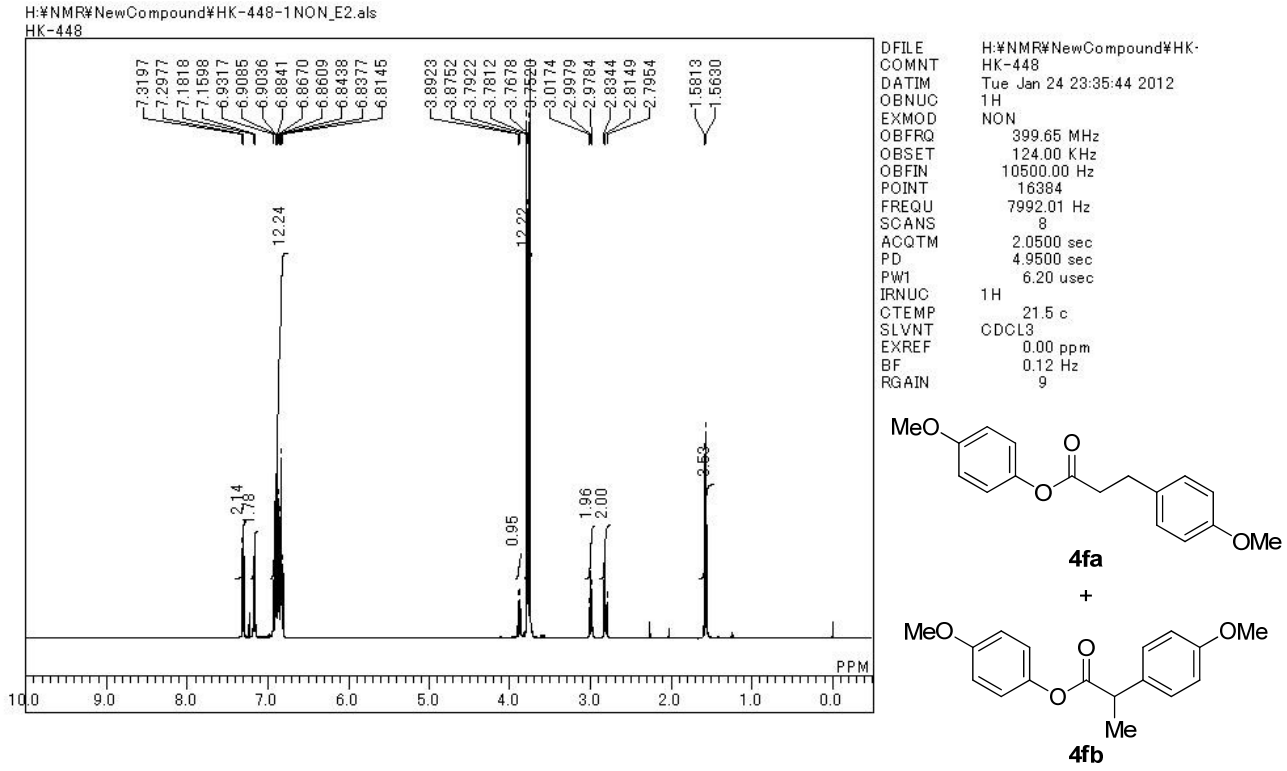


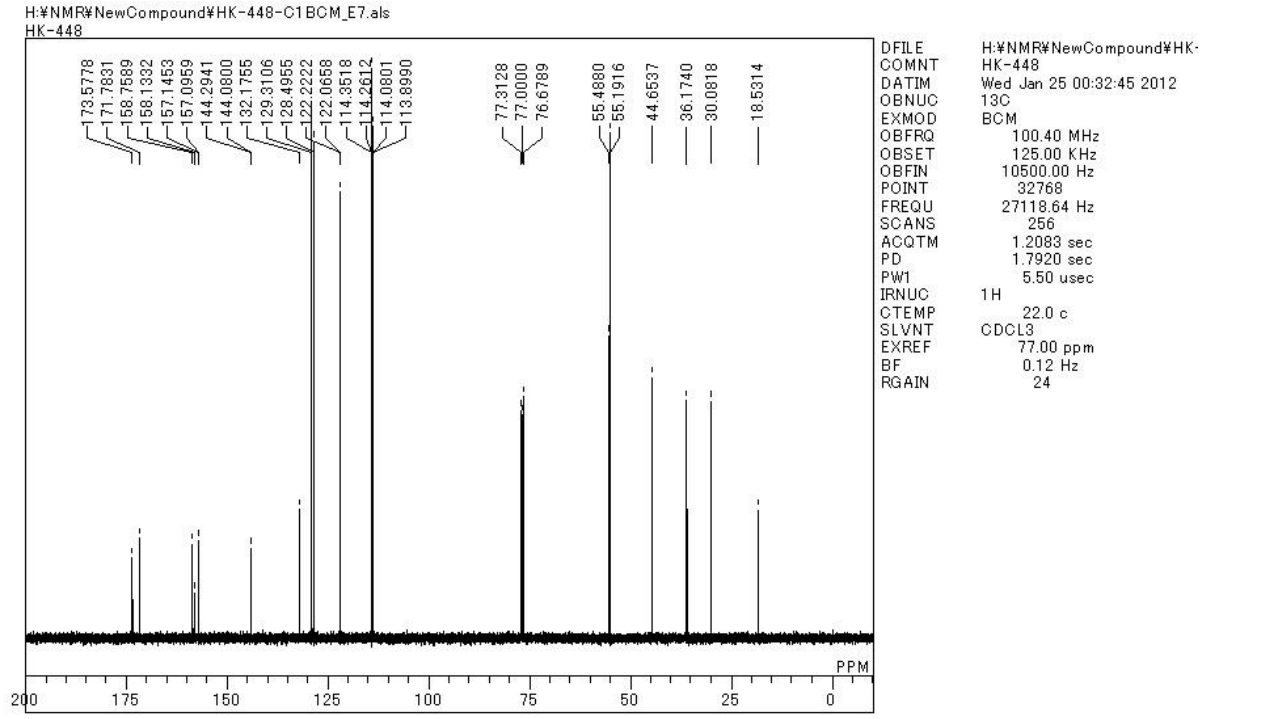
4eb

F:¥NMR¥phenyl products.1
phenyl products

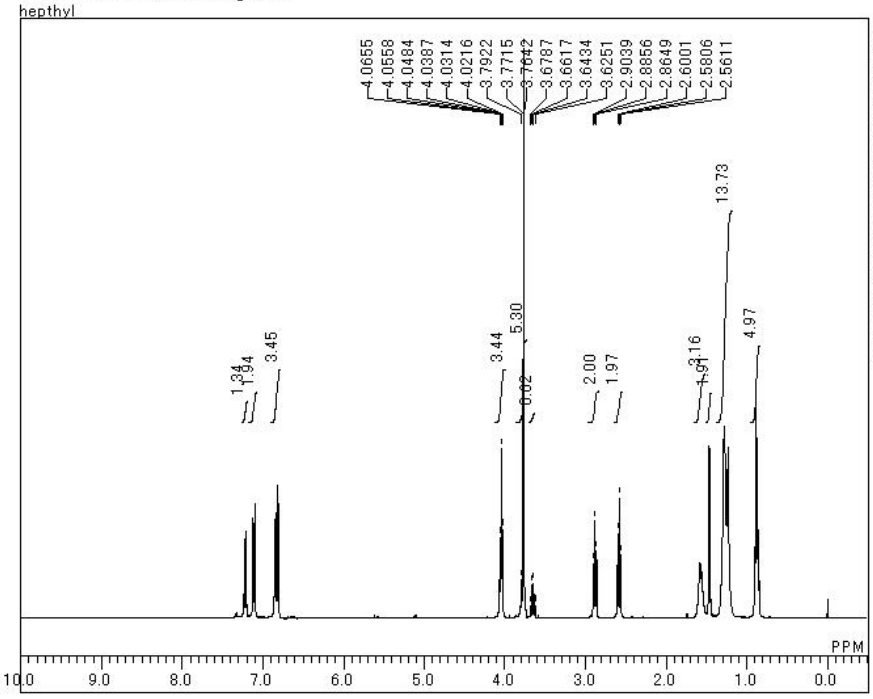


DFILE	F:¥NMR¥phenyl products.1
COMNT	phenyl products
DATIM	20-01-2012 16:41:24
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	32768
FREQU	39308.18 Hz
SCANS	1000
ACQTM	0.8336 sec
PD	1.5000 sec
PW1	3.33 usec
IRNUC	1H
CTEMP	19.6 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	58

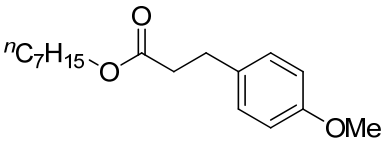

H:¥NMR¥NewCompound¥HK-448-1NON_E2.als
HK-448
7.3197
7.2977
7.1818
7.1598
6.9317
6.9085
6.9036
6.8841
6.8670
6.8609
6.8438
6.8377
6.8145
3.8923
3.8752
3.7922
3.7812
3.7678
3.7520
3.0174
2.9979
2.9784
2.8344
2.8149
2.7954
1.5813
1.5630
12.24
12.22
2.14
1.78
0.95
1.96
2.00
3.53
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE H:¥NMR¥NewCompound¥HK-
COMNT HK-448
DATIM Tue Jan 24 23:35:44 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 21.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 9
MeO
O
O
OMe
4fa
+
MeO
O
O
OMe
Me
4fb


H:¥NMR¥NewCompound¥HK-448-C1BCM_E7.als
HK-448
173.5778
171.7831
158.7589
158.1332
157.1453
157.0959
144.2941
144.0800
132.1755
129.3106
128.4955
122.2222
122.0658
114.3518
114.2612
114.0801
113.8990
77.3128
77.0000
76.6789
55.4880
55.1916
44.6537
36.1740
30.0818
18.5314
PPM
200
175
150
125
100
75
50
25
0
DFILE H:¥NMR¥NewCompound¥HK-
COMNT HK-448
DATIM Wed Jan 25 00:32:45 2012
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 256
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 22.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 24

F:¥NMR¥TM-120126-11NON_E2.als
heptyl

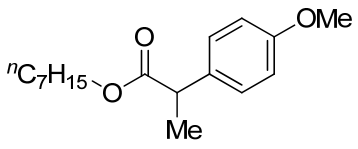


DFILE	F:¥NMR¥TM-120126-11NON
COMNT	heptyl
DATIM	Fri Jan 27 10:45:28 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	23.4 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	6



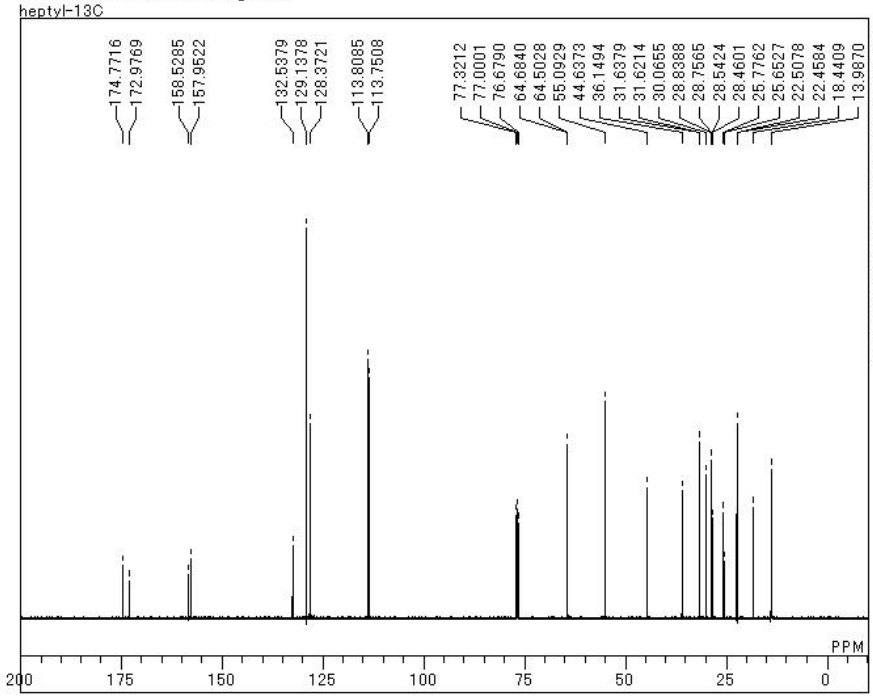
4ga

+



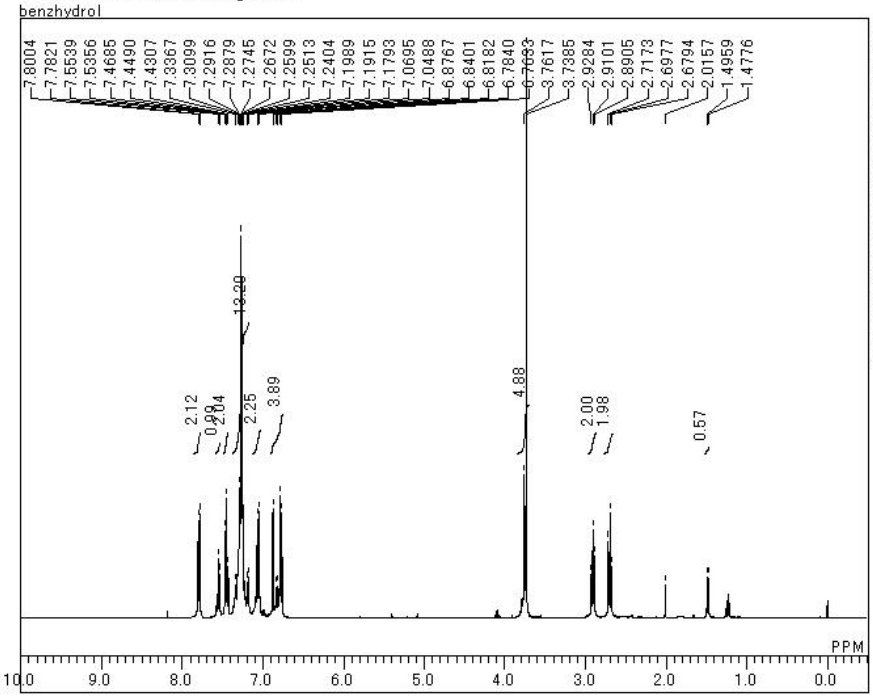
4gb

F:¥NMR¥TM-120206-31BCM_E8.als
heptyl-13C

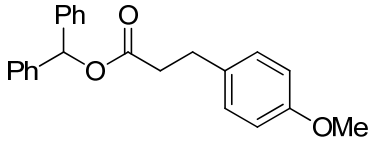


DFILE	F:¥NMR¥TM-120206-31BCM
COMNT	heptyl-13C
DATIM	Tue Feb 07 00:44:59 2012
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	1024
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	19.5 c
SLVNT	CDCL3
EXREF	13.99 ppm
BF	0.12 Hz
RGAIN	26

F:¥NMR¥TM-120126-31NON_E15.als
benzhydrol

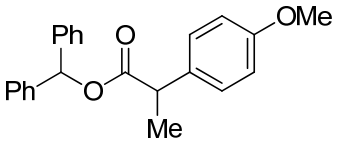


DFILE	F:¥NMR¥TM-120126-31NON
COMNT	benzhydrol
DATIM	Thu Jan 26 13:31:14 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	21.6 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	7



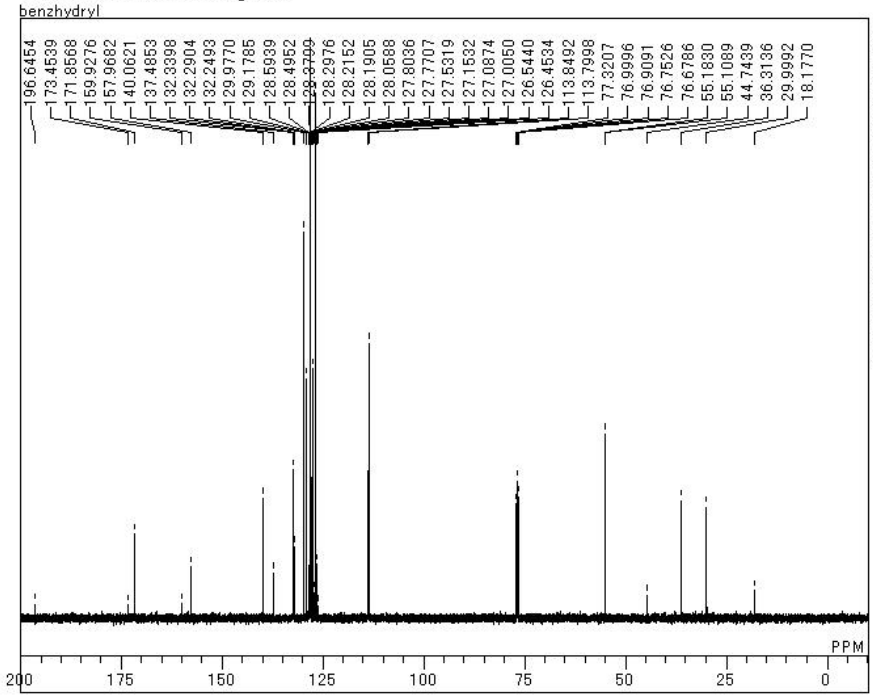
4ha

+

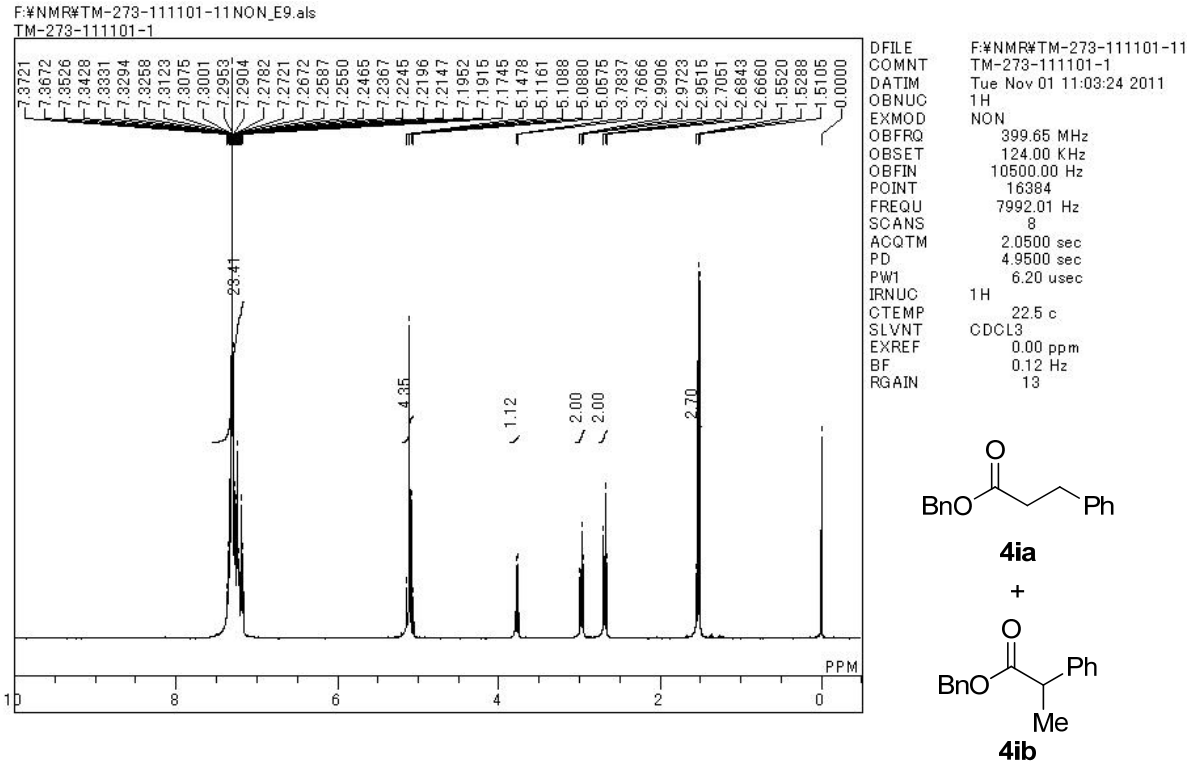


4hb

F:¥NMR¥TM-120206-11BCM_E7.als
benzhydryl



DFILE	F:¥NMR¥TM-120206-11BCM
COMNT	benzhydryl
DATIM	Mon Feb 06 10:31:35 2012
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	512
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	19.4 c
SLVNT	CDCL3
EXREF	18.18 ppm
BF	0.12 Hz
RGAIN	22


F:¥NMR¥TM-273-111101-11NON_E9.als
TM-273-111101-1
7.3721
7.3672
7.3526
7.3428
7.3331
7.3294
7.3258
7.3123
7.3075
7.3001
7.2953
7.2904
7.2782
7.2721
7.2672
7.2587
7.2550
7.2465
7.2367
7.2245
7.2196
7.2147
7.1952
7.1915
7.1745
5.1478
5.1161
5.1088
5.0880
5.0575
3.7837
3.7666
2.9906
2.9723
2.9515
2.7051
2.6843
2.6660
1.5520
1.5288
1.5105
0.0000
9.41
4.35
1.12
2.00
2.00
2.70
PPM
10
8
6
4
2
0
DFILE F:¥NMR¥TM-273-111101-11
COMNT TM-273-111101-1
DATIM Tue Nov 01 11:03:24 2011
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 13

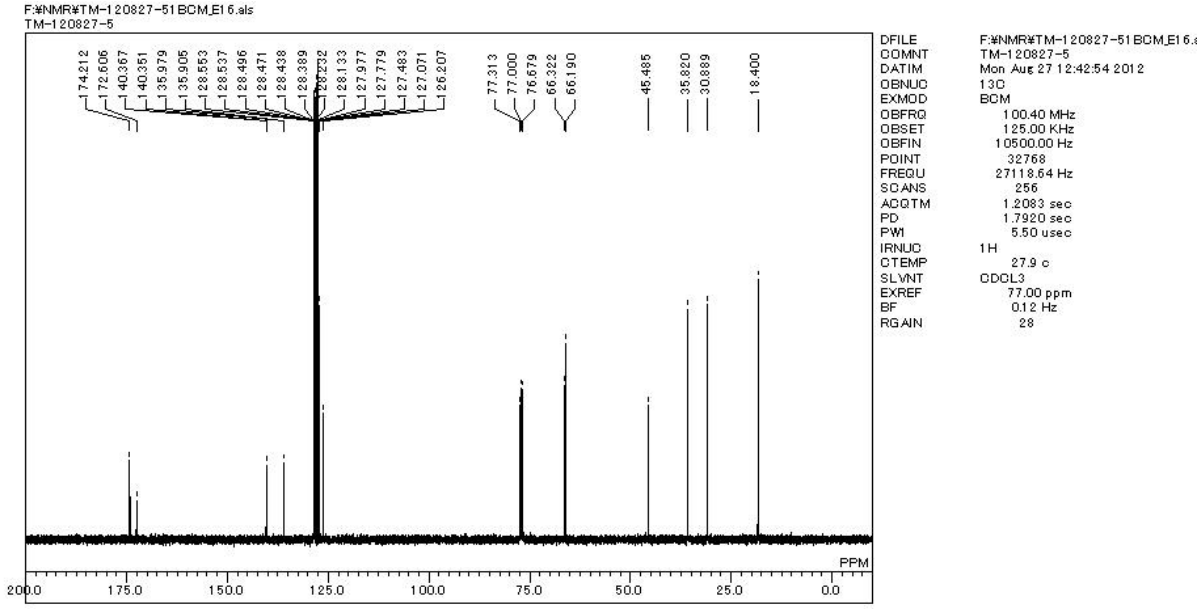
O
BnO
Ph

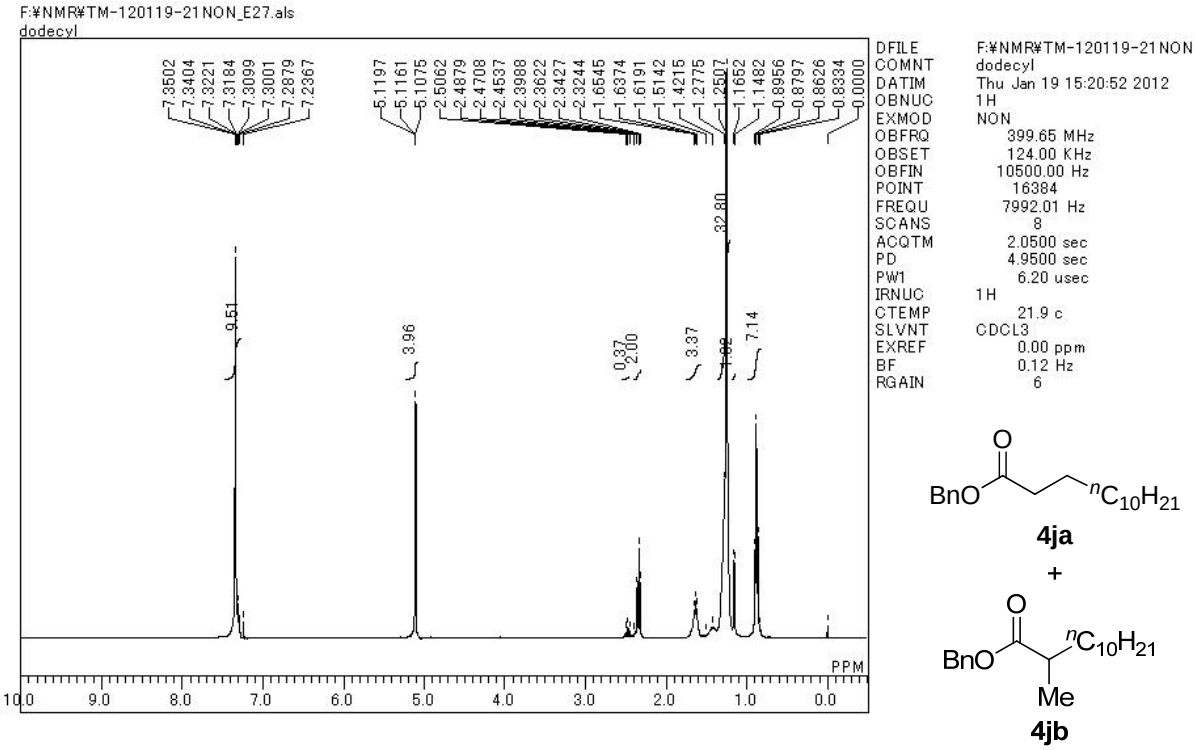
4ia

+

O
BnO
Ph
Me

4ib


F:¥NMR¥TM-120827-51BCM_E16.als
TM-120827-5
174.212
172.606
140.367
140.351
135.979
135.905
128.553
128.537
128.496
128.471
128.438
128.389
128.232
128.133
127.977
127.779
127.483
127.071
126.207
77.313
77.000
76.679
66.322
66.190
45.485
35.820
30.889
18.400
PPM
200.0
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0
DFILE F:¥NMR¥TM-120827-51BCM_E16.
COMNT TM-120827-5
DATIM Mon Aug 27 12:42:54 2012
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 256
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 27.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 28


F:¥NMR¥TM-120119-21NON_E27.als
dodecyl
7.3502
7.3404
7.3221
7.3184
7.3099
7.3001
7.2879
7.2367
5.1197
5.1161
5.1075
2.5062
2.4879
2.4708
2.4537
2.3988
2.3622
2.3427
2.3244
1.6545
1.6374
1.6191
1.5142
1.4215
1.2775
1.2507
1.1652
1.1482
0.8956
0.8797
0.8626
0.8334
0.0000
9.51
3.96
0.37
2.00
3.37
1.68
7.14
32.80
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
DFILE F:¥NMR¥TM-120119-21NON
COMNT dodecyl
DATIM Thu Jan 19 15:20:52 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 21.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 6

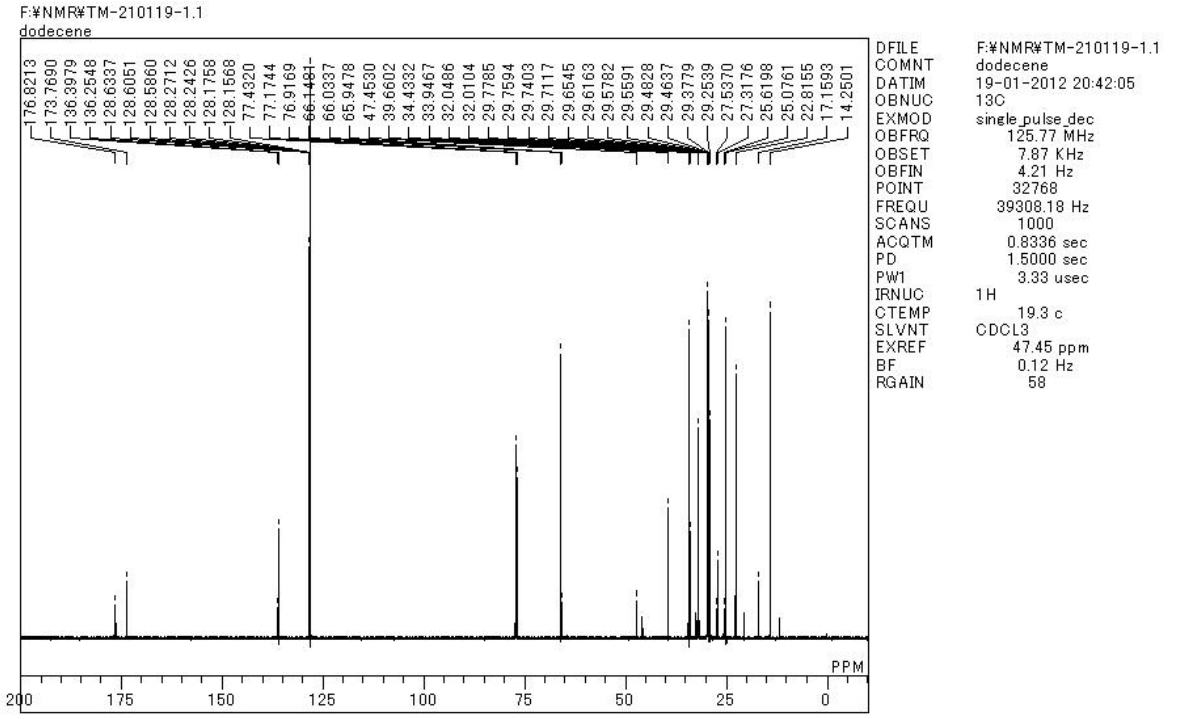
O
BnO
nC10H21

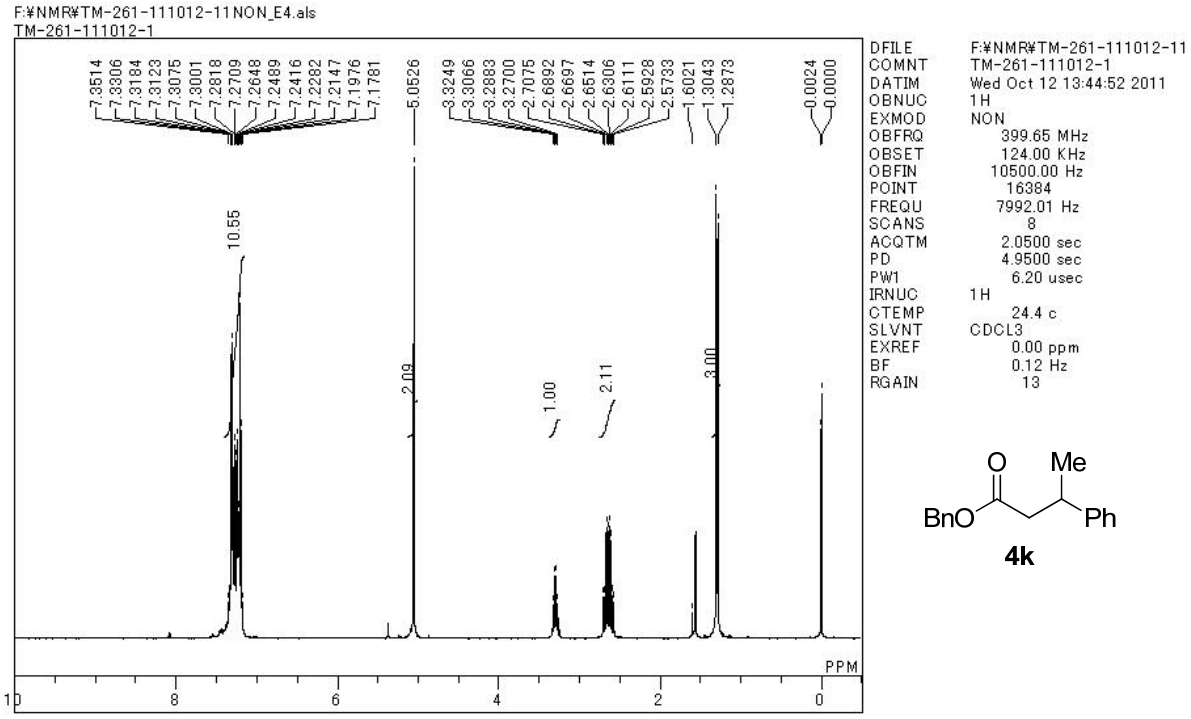
4ja

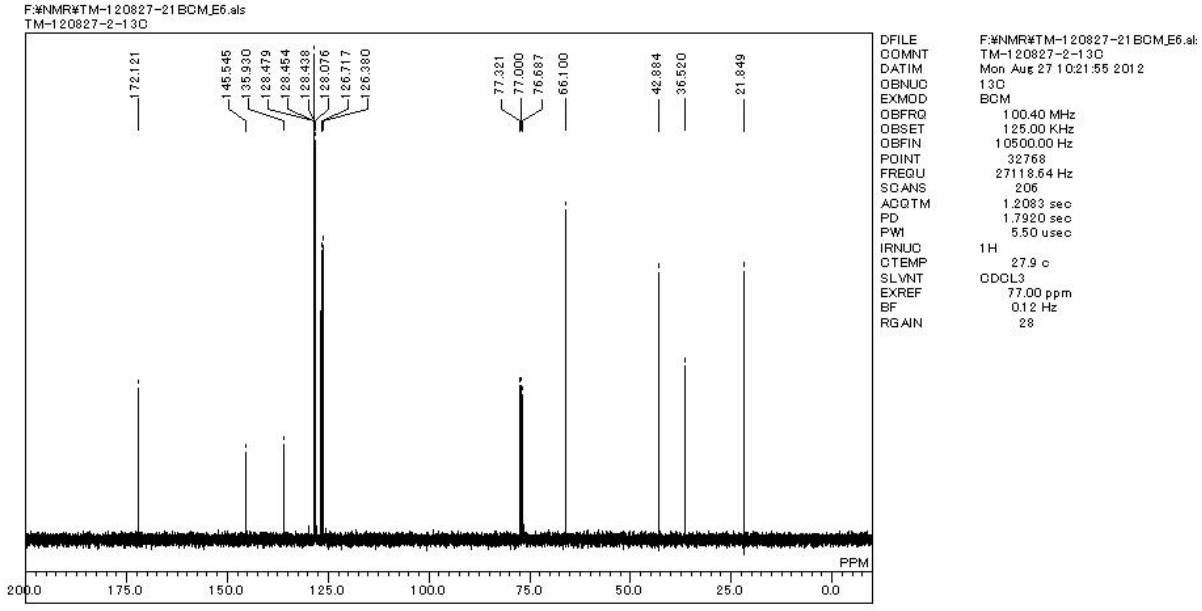
+

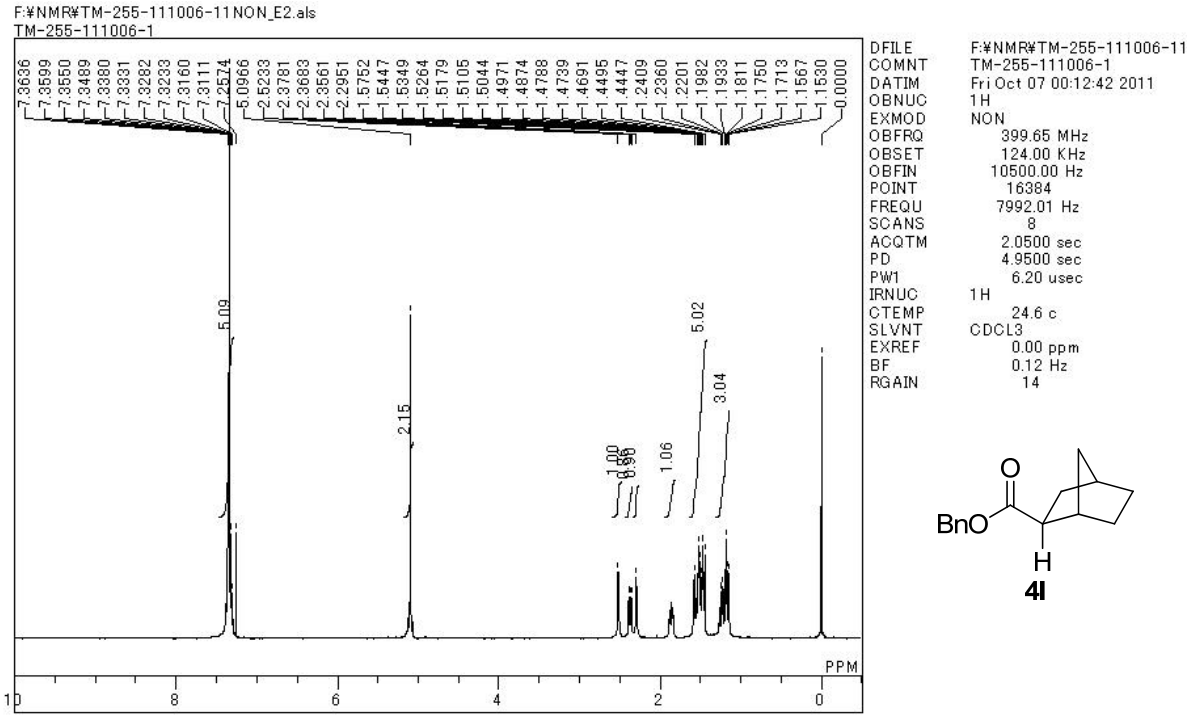
O
BnO
nC10H21
Me

4jb

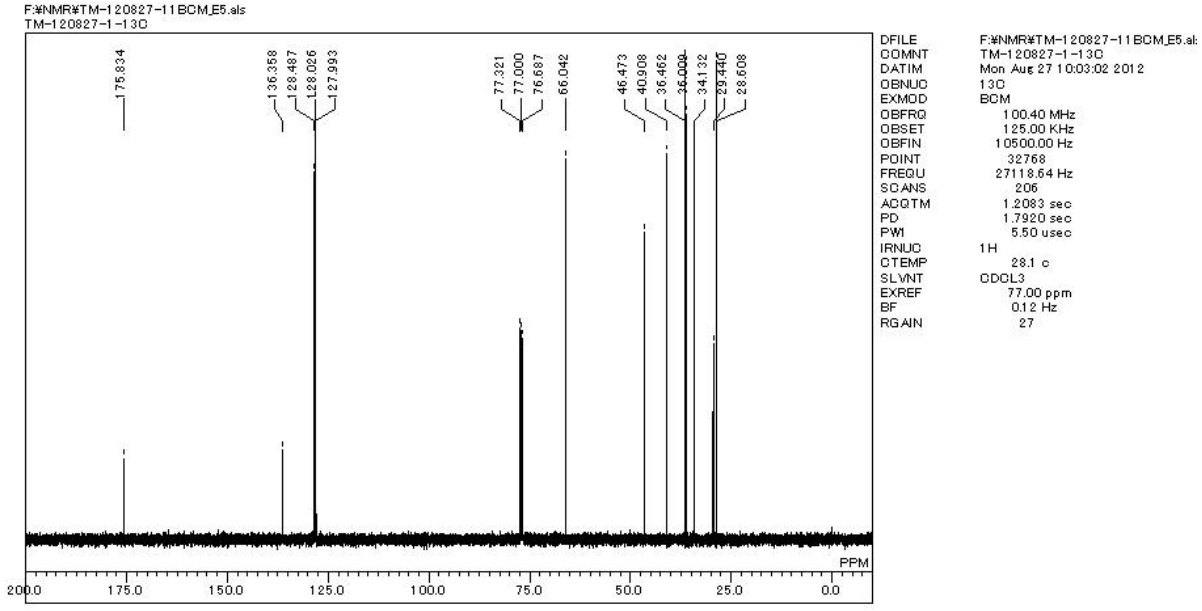

F:¥NMR¥TM-210119-1.1
dodecene
176.8213
173.7690
136.8979
136.2548
128.6337
128.6051
128.5860
128.2712
128.2426
128.1758
128.1568
77.4320
77.1744
76.9169
66.1481
66.0337
65.9478
47.4530
39.6602
34.4332
33.9467
32.0486
32.0104
29.7785
29.7594
29.7403
29.7117
29.6545
29.6163
29.5782
29.5591
29.4828
29.4637
29.3779
29.2539
27.5370
27.3176
25.6198
25.0761
22.8155
17.1593
14.2501
PPM
200
175
150
125
100
75
50
25
0
DFILE F:¥NMR¥TM-210119-1.1
COMNT dodecene
DATIM 19-01-2012 20:42:05
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 32768
FREQU 39308.18 Hz
SCANS 1000
ACQTM 0.8336 sec
PD 1.5000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 19.3 c
SLVNT CDCL3
EXREF 47.45 ppm
BF 0.12 Hz
RGAIN 58


F:¥NMR¥TM-261-111012-11NON_E4.als
TM-261-111012-1
7.3514
7.3306
7.3184
7.3123
7.3075
7.3001
7.2818
7.2709
7.2648
7.2489
7.2416
7.2282
7.2147
7.1976
7.1781
5.0526
3.3249
3.3066
3.2883
3.2700
3.2517
2.7075
2.6892
2.6697
2.6514
2.6306
2.6111
2.5928
2.5733
1.6021
1.3043
1.2873
0.0024
0.0000
10.55
2.09
1.00
2.11
3.00
PPM
10
8
6
4
2
0
DFILE F:¥NMR¥TM-261-111012-11
COMNT TM-261-111012-1
DATIM Wed Oct 12 13:44:52 2011
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 24.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 13
O
Me
BnO
Ph
4k


F:¥NMR¥TM-120827-21BCM_E6.als
TM-120827-2-13C
172.121
145.545
135.930
128.479
128.454
128.438
128.076
126.717
126.380
77.321
77.000
76.687
66.100
42.884
36.520
21.849
PPM
200.0
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0
DFILE F:¥NMR¥TM-120827-21BCM_E6.als
COMNT TM-120827-2-13C
DATIM Mon Aug 27 10:21:55 2012
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 206
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 27.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 28

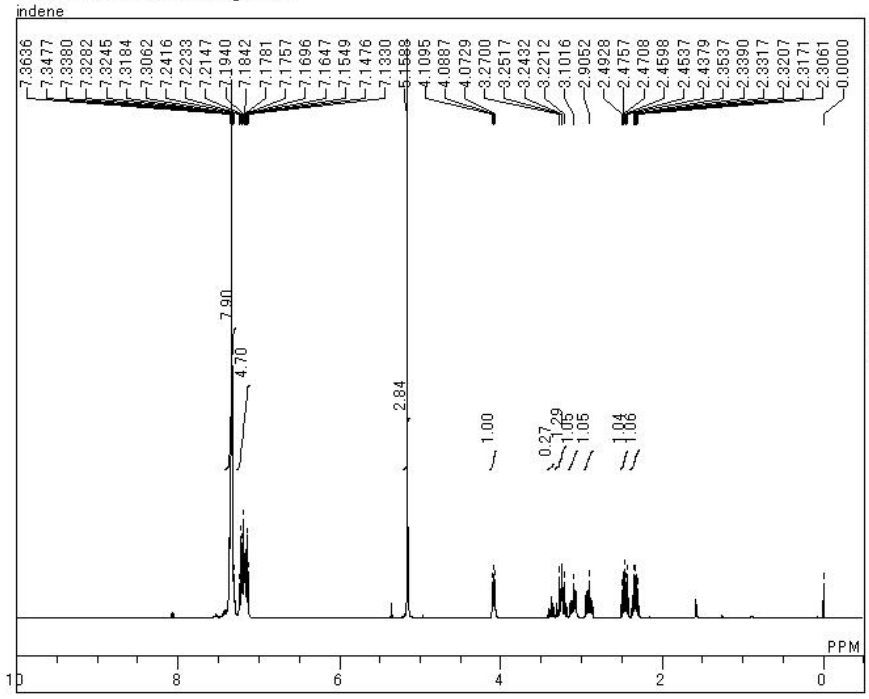

F:¥NMR¥TM-255-111006-11NON_E2.als
TM-255-111006-1
7.3636
7.3599
7.3550
7.3489
7.3380
7.3331
7.3282
7.3233
7.3160
7.3111
7.2574
5.0966
2.5233
2.3781
2.3683
2.3561
2.2951
1.5752
1.5447
1.5349
1.5264
1.5179
1.5105
1.5044
1.4971
1.4874
1.4788
1.4739
1.4691
1.4495
1.4447
1.2409
1.2360
1.2201
1.1982
1.1933
1.1811
1.1750
1.1713
1.1567
1.1530
0.0000
5.09
2.15
1.00
0.96
0.96
1.06
5.02
3.04
PPM
10
8
6
4
2
0
DFILE F:¥NMR¥TM-255-111006-11
COMNT TM-255-111006-1
DATIM Fri Oct 07 00:12:42 2011
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 24.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 14
O
BnO
H

4l

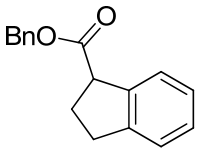

F:¥NMR¥TM-120827-11BCM_E5.als
TM-120827-1-13C
175.834
136.358
128.487
128.026
127.993
77.321
77.000
76.687
66.042
46.473
40.908
36.462
36.000
34.132
29.440
28.608
PPM
200.0
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0
DFILE F:¥NMR¥TM-120827-11BCM_E5.als
COMNT TM-120827-1-13C
DATIM Mon Aug 27 10:03:02 2012
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 206
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 28.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 27

F:¥NMR¥TM-120125-11NON_E10.als

indene



DFILE	F:¥NMR¥TM-120125-11NON
COMNT	indene
DATIM	Wed Jan 25 12:05:42 2012
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
POINT	16384
FREQU	7992.01 Hz
SCANS	8
ACQTM	2.0500 sec
PD	4.9500 sec
PW1	6.20 usec
IRNUC	1H
CTEMP	22.0 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	10



4ma

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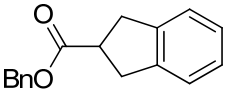
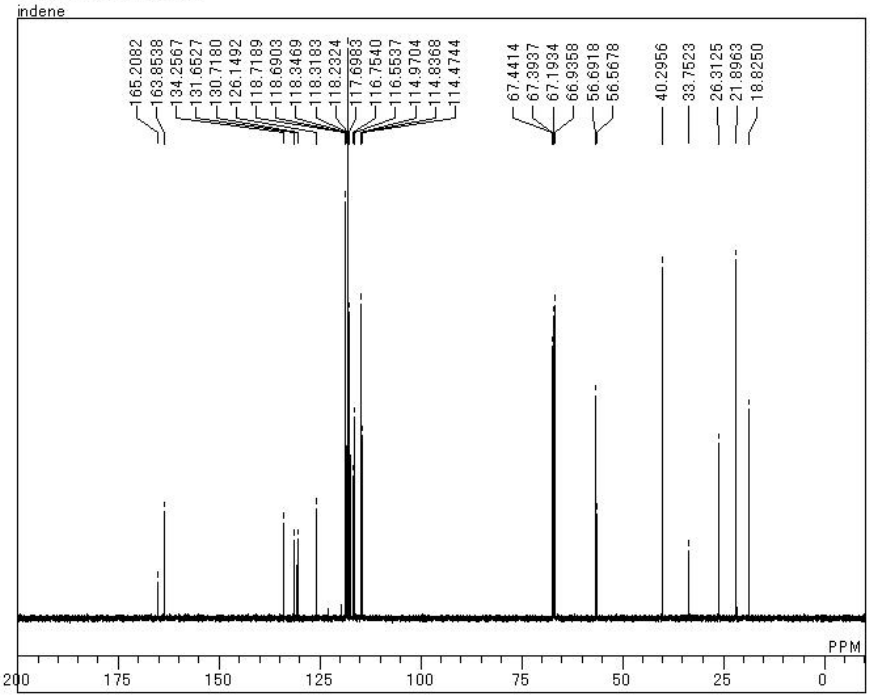


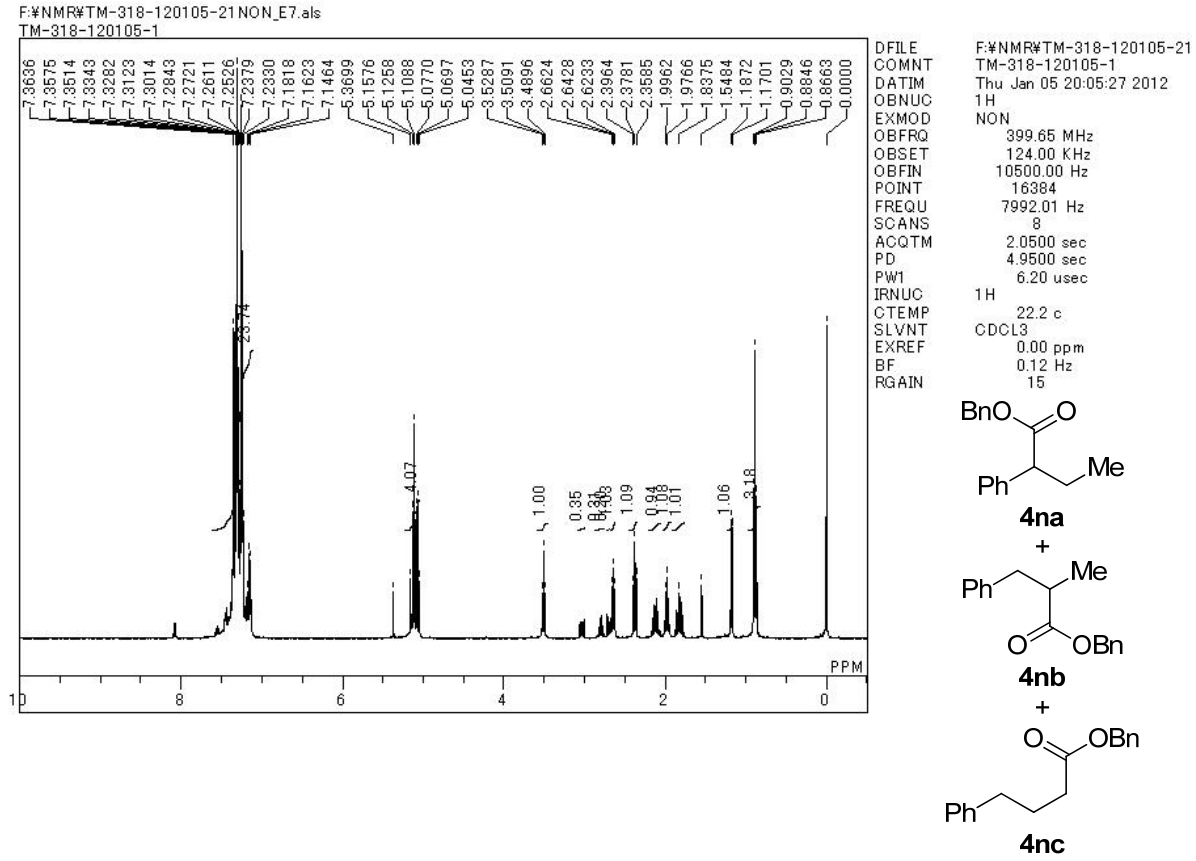
4mb

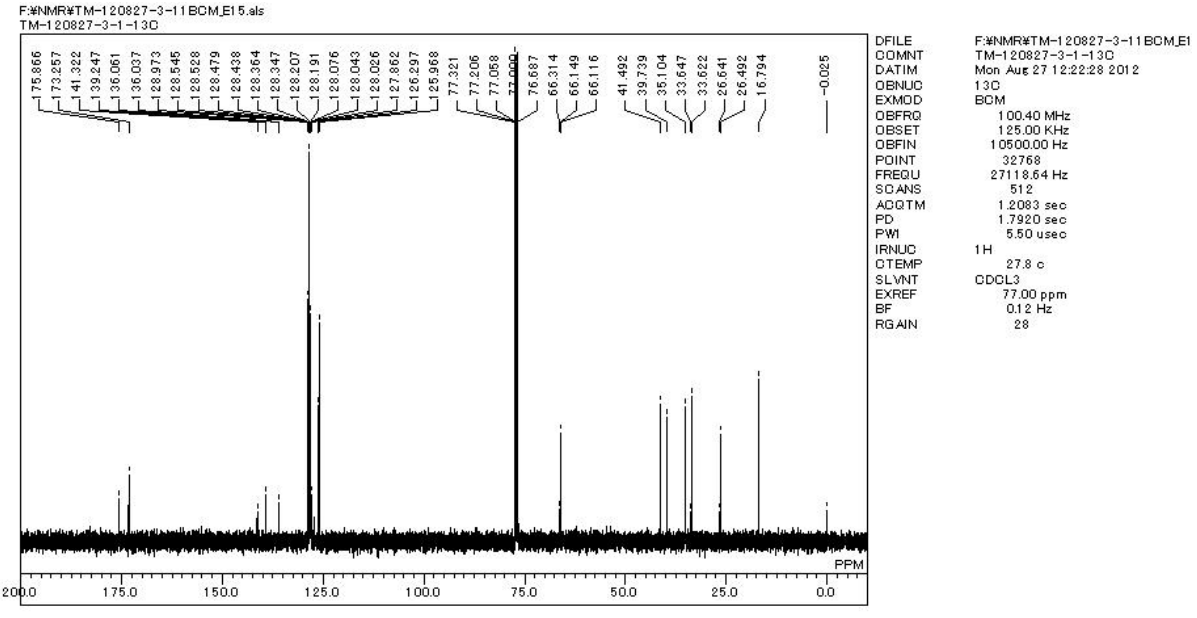
F:¥NMR¥TM-120125-1.1

indene



DFILE	F:¥NMR¥TM-120125-1.1
COMNT	indene
DATIM	25-01-2012 16:45:20
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	32768
FREQU	39308.18 Hz
SCANS	500
ACQTM	0.8336 sec
PD	1.5000 sec
PW1	3.33 usec
IRNUC	1H
CTEMP	19.7 c
SLVNT	CDCL3
EXREF	18.83 ppm
BF	0.12 Hz
RGAIN	60


F:¥NMR¥TM-318-120105-21 NON_E7.als
TM-318-120105-1
DFILE F:¥NMR¥TM-318-120105-21
COMNT TM-318-120105-1
DATIM Thu Jan 05 20:05:27 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC 1H
CTEMP 22.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15
PPM
BnO
O
Me
Ph
4na
+
Ph
Me
O
OBn
4nb
+
O
OBn
Ph
4nc


F:¥NMR¥TM-120827-3-11BCM_E15.als
TM-120827-3-1-13C
DFILE F:¥NMR¥TM-120827-3-11BCM_E1
COMNT TM-120827-3-1-13C
DATIM Mon Aug 27 12:22:28 2012
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 512
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 27.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 28
PPM

7. References

(1) Sofuku, S.; Muramatsu, I.; Hagitani, A. *Bull. Chem. Soc. Jpn*. **1967**, *40*, 2942–2945.
(2) Shi, M.; Shen, Y. M. *Molecules* **2002**, *7*, 386–393.
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