Supporting Information

Catalytic Enantioselective Petasis-type Reaction of Quinolines Catalyzed by a Newly Designed Thiourea Catalyst

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Table of contents

Experimental procedure for preparation of catalyst **1b** and its characterization data: S2.

Characterization data of catalysts **1c-i**: S4.

The results of Petasis-type reaction of **2a**, **2b** and **3** with **4A** using catalysts **1a-i**: S6.

General procedure for Petasis-type reaction of **2a-f**: S7.

Characterization data of obtained compounds **5a-6aF**: S7.

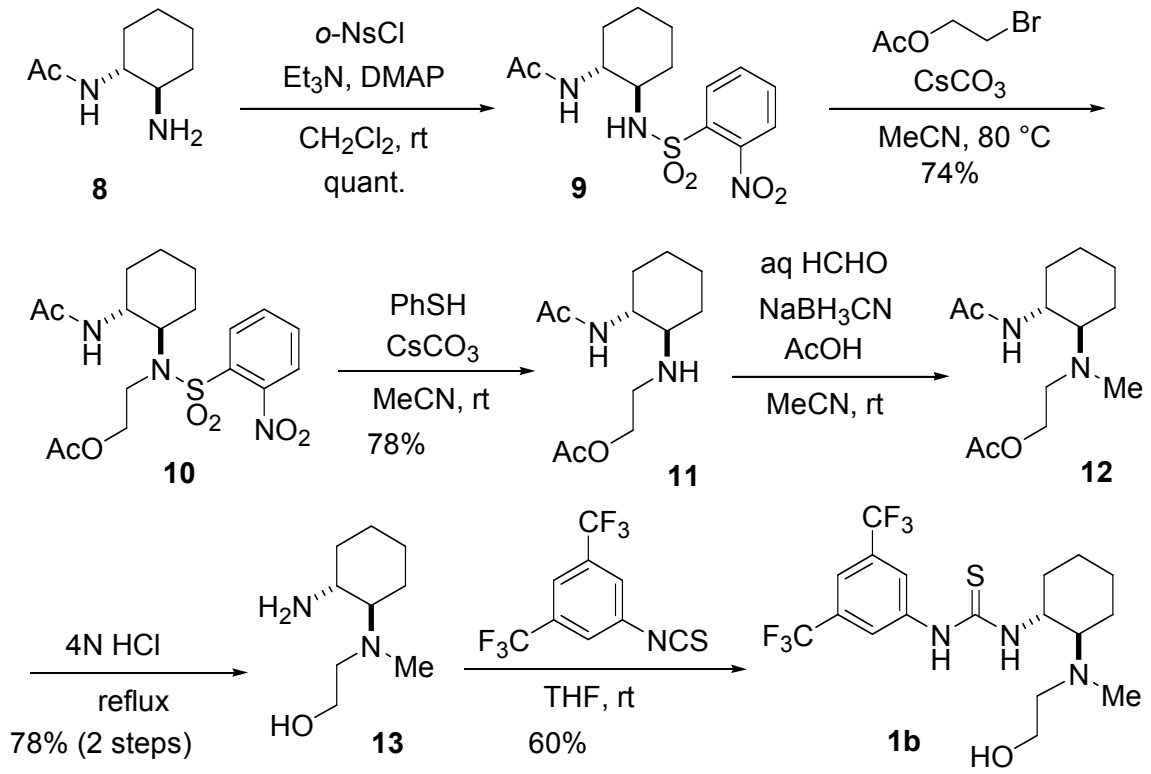
Conversion of the adduct **6aC** to (+)-galipinine **7** and characterization data: S10.

Copies of ^{1}H and ^{13}C NMR spectrum of all obtained compounds: S12.

Copies of HPLC of **5a-6aF**: S68.

General. Melting points were taken on a YANAGIMOTO micromelting point apparatus and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ at 500 or 400 MHz, and at 125 or 100 MHz, respectively; Tetramethylsilane (TMS) was used as an internal standard. IR spectra were recorded on a JASCO FT/IR-410 Fourier-transfer infrared spectrometer. Low and high resolution mass spectra were obtained by EI or FAB method. Optical rotations were recorded on a JASCO DIP-360 polarimeter with a path length of 1 cm; concentrations are quoted in mg (2 mL). $[\alpha]^{D}$ values are measured in 10^{-1} deg cm^2 g^{-1}. Enantiomeric excess was determined by high performance liquid chromatography (HPLC) analysis.

Experimental procedure for preparation of catalyst 1b and characterization data.



Scheme 1.

Amide 9: To a solution of amine **8** (4.7 g, 30 mmol), Et_3N (6.3 mL, 45 mmol) and DMAP (0.4 g, 3.0 mmol) in CH_2Cl_2 (30 mL) was added *o*-NsCl (6.3 g, 33 mmol) under argon atmosphere at 0 °C. After being stirred at the room temperature for 5 h, the reaction mixture was diluted with $CHCl_3$. The organic phase was washed with 1N HCl and saturated $NaHCO_3$, dried over $MgSO_4$ and concentrated at reduced pressure. Purification of the residue by column chromatography ($CHCl_3$:MeOH=20:1-10:1) afforded product **9** (10.2 g, quant.) as an amorphous. IR ($CHCl_3$) 1665 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ 8.12 (1H, dd, J = 7.0, 1.6 Hz), 7.81 (1H, dd, J = 7.6, 1.5 Hz), 7.78-7.68 (2H, m), 5.97 (1H, br s), 5.80 (1H, br s), 3.72 (1H, m), 3.23 (1H, m), 2.04 (1H, br m), 1.88

(1H, br m), 1.85 (3H, s), 1.69 (2H, br m), 1.43-1.15 (4H, br m). ^{13}C NMR ($CDCl_3$) δ 171.0, 147.8, 135.2, 133.4, 132.7, 130.2, 125.0, 58.7, 52.6, 33.4, 32.5, 24.7, 24.3, 23.1. MS (EI^+) m/z: 341 (M^+, 3), 96 (100). HRMS calcd for $C_{14}H_{19}N_3O_5S$: 341.1045, Found: 341.1043. $[\alpha]^{26}_D$ –66.2 (*c* 1.3, $CHCl_3$).

Acetate 10: A solution of amide **9** (10.2 g, 30 mmol), 2-bromoethyl acetate (6.6 mL, 60 mmol) and $CsCO_3$ (11.6 g, 60 mmol) in MeCN (60 mL) was stirred at 80 °C for 6 h. The reaction mixture was diluted with $CHCl_3$, washed with water, dried over K_2CO_3 and concentrated at reduced pressure. Purification of the residue by column chromatography ($CHCl_3$:MeOH=20:1-10:1) afforded product **10** (17.3 g, 74%) as an amorphous. IR ($CHCl_3$) 1739, 1667 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ 8.11 (1H, br m), 7.77-7.71 (2H, br m), 7.68 (1H, br m), 5.96 (1H, br d, *J* = 8.5 Hz), 4.03 (2H, br m), 3.92 (1H, br m), 3.72 (1H, br m), 3.61-3.45 (2H, m), 2.13 (1H, br d, *J* = 10.7 Hz), 1.98 (3H, s), 1.88 (3H, s), 1.82 (2H, br m), 1.73 (1H, br d, *J* = 10.7 Hz), 1.52 (1H, m), 1.44-1.20 (3H, br m). ^{13}C NMR ($CDCl_3$) δ 170.5, 169.8, 147.7, 134.1, 133.8, 132.1, 131.0, 124.3, 62.2, 61.4, 49.6, 42.0, 33.5, 31.0, 25.4, 24.5, 23.2, 20.6. MS (FAB^+) m/z: 428 ($M+H^+$, 100). HRMS calcd for $C_{18}H_{26}N_3O_7S$ ($M+H^+$): 428.1491, Found: 428.1497. $[\alpha]^{26}_D$ +148.3 (*c* 1.7, $CHCl_3$).

Amine 11: To a solution of acetate **10** (10 g, 23.4 mmol) in MeCN (50 mL) were added benzenethiol (2.9 mL, 28 mmol) and $CsCO_3$ (7.9 g, 28 mmol) under argon atmosphere at the room temperature. After being stirred at the same temperature for 2.5 h, the reaction mixture was diluted with $CHCl_3$, washed with water, dried over K_2CO_3 and concentrated at reduced pressure. Purification of the residue by column chromatography ($CHCl_3$:MeOH=5:1) afforded product **11** (4.4 g, 78%) as an amorphous. IR ($CHCl_3$) 1734, 1665 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ 5.75 (1H, br d, *J* = 6.7 Hz), 4.26 (1H, m), 4.04 (1H, m), 3.57 (1H, m), 2.95 (1H, m), 2.79 (1H, m), 2.34 (1H, m), 2.15 (1H, br m), 2.08 (3H, s), 2.05 (1H, br m), 1.99 (3H, s), 1.90 (1H, br m), 1.74 (1H, br m), 1.68 (1H, br m), 1.38-1.08 (4H, br m). ^{13}C NMR ($CDCl_3$) δ 171.4, 170.4, 63.9, 60.1, 53.0, 44.5, 32.6, 31.5, 24.6 (2C), 23.5, 21.0. MS (FAB^+) m/z: 243 ($M+H^+$, 100). HRMS calcd for $C_{12}H_{23}N_2O_3$ ($M+H^+$): 243.1709, Found: 243.1705. $[\alpha]^{26}_D$ -25.3 (*c* 1.0, $CHCl_3$).

Alcohol 13: A solution of amine **11** (4.4 g, 18 mmol) and formaldehyde solution (3.4 mL, 45 mmol) in MeCN (60 mL) was stirred at the room temperature for 15 min. To the reaction mixture was added $NaBH_3CN$ (1.3 g, 20 mmol) at the room temperature. After being stirred at the same temperature for 15 min, AcOH (3.3 mL) was added to the reaction mixture at the room temperature. After being stirred at the same temperature for 2 h, the reaction mixture was concentrated at reduced pressure. The residue was diluted with AcOEt, washed with 1N NaOH, water and brine, dried over K_2CO_3 and concentrated at reduced pressure to afford **12** as a colorless oil. IR ($CHCl_3$) 1733, 1660 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ 6.25 (1H, br m), 4.22 (1H, m), 4.04 (1H, m), 3.49 (1H, m), 2.70 (1H, m), 2.63 (1H, m), 2.48 (1H, br d, *J* = 12.2 Hz), 2.32 (1H, m), 2.22 (3H, s), 2.07 (3H, s), 1.97 (3H, s), 1.81 (2H, br m), 1.65 (1H, br d, *J* = 13.4 Hz), 1.36-1.12 (3H, m), 1.04 (1H, m). ^{13}C NMR ($CDCl_3$) δ 171.2,

170.2, 65.5, 62.4, 51.7, 50.8, 36.8, 32.6, 25.2, 24.4, 23.3, 22.4, 20.8. MS (EI^+) m/z: 256 (M^+, 2), 43 (100). HRMS calcd for $C_{13}H_{24}N_2O_3$: 256.1787, Found: 256.1790. $[\alpha]^{26}_D$ -40.8 (*c* 1.6, $CHCl_3$). A solution of the crude product **12** in 4N HCl (30 mL) was refluxed for 12 h. After being cooling to ambient temperature, the reaction mixture was basic with 4N NaOH, extracted with $CHCl_3$, dried over K_2CO_3 and concentrated at reduced pressure to afford **13** (2.46 g, 78% from amine **11**) as a pale yellow oil, which was used in next reaction without purification. IR ($CHCl_3$) 3370 cm^{-1}. ^1H NMR ($CDCl_3$) δ 3.70-3.50 (2H, br m), 2.85-2.53 (5H, br m), 2.44 (1H, br m), 2.29 (3H, s), 2.13 (1H, br m), 1.93 (1H, br m), 1.78 (2H, br m), 1.66 (1H, br m), 1.26-1.04 (4H, br m). ^{13}C NMR ($CDCl_3$) δ 69.2, 59.3, 54.4, 51.5, 37.0, 35.6, 25.5, 25.0, 22.4. MS (FAB^+) m/z: 173 ($M+H^+$, 100). HRMS calcd for $C_9H_{20}N_2O$ ($M+H^+$): 173.1654, Found: 173.1656. $[\alpha]^{27}_D$ -34.6 (*c* 1.5, $CHCl_3$).

Catalyst 1b: To a solution of alcohol **13** (2.5 g, 14 mmol) in THF (20 mL) was added 3,5-bis(triflouoromethyl)phenyl isothiocyanate (2.6 mL, 14 mmol) under argon atmosphere at the room temperature. After being stirred at the same temperature for 3 h, the reaction mixture was concentrated at reduced pressure. Purification of the residue by column chromatography ($CHCl_3$:MeOH=9:1) afforded product **1b** (3.8 g, 60%) as a colorless crystal. mp 167-170 ^oC (hexane/AcOEt). IR ($CHCl_3$) 3320, 1534, 1470 cm^{-1}. ^1H NMR ($CDCl_3$) δ 7.98 (2H, s), 7.61 (1H, s), 4.07 (1H, br s), 3.62 (2H, br m), 2.71 (1H, m), 2.60-2.41 (3H, m), 2.28 (3H, s), 1.86 (2H, br m), 1.73 (1H, br m), 1.30 (2H, m), 1.27-1.06 (2H, m). ^{13}C NMR ($CDCl_3$) δ 180.4, 140.3, 132.1 (q, *J* = 33 Hz), 123.3, 123.0 (q, *J* = 271 Hz), 118.1, 66.6, 58.7, 55.7, 54.9, 36.4, 32.7, 24.9, 24.5, 22.9. MS (FAB^+) m/z: 444 ($M+H^+$, 100). HRMS calcd for $C_{18}H_{24}F_6N_3OS$ ($M+H^+$): 444.1544, Found: 444.1547. Anal. Calcd for $C_{18}H_{23}F_6N_3OS$: C, 48.75; H, 5.23; F, 25.71, N, 9.48. Found: C, 48.77; H, 5.10; F, 25.50, N, 9.52. $[\alpha]^{27}_D$ -20.5 (*c* 1.0, $CHCl_3$).

Characterization data of catalysts 1c-i.

Catalyst 1c: Amorphous. IR ($CHCl_3$) 3319, 1531, 1471 cm^{-1}. ^1H NMR ($CDCl_3$) δ 7.95 (2H, s), 7.47 (1H, s), 4.46 (1H, br s), 3.85 (2H, br m), 2.87 (1H, br m), 2.73 (1H, br m), 2.61 (1H, br m), 2.41 (1H, br m), 2.35 (3H, s), 1.98-1.05 (9H, m). ^{13}C NMR ($CDCl_3$) δ 180.8, 141.5, 131.4 (q, *J* = 33 Hz), 123.2 (q, *J* = 273 Hz), 122.1, 116.7, 66.6, 56.6, 55.5, 50.2, 44.9, 35.7, 32.4, 25.0, 24.3, 22.4. MS (FAB^+) m/z: 458 ($M+H^+$, 100). HRMS calcd for $C_{19}H_{26}F_6N_3OS$ ($M+H^+$): 458.1701, Found: 458.1707. $[\alpha]^{28}_D$ -2.2 (*c* 1.2, $CHCl_3$).

Catalyst 1d: Amorphous. IR ($CHCl_3$) 3289, 1518, 1469 cm^{-1}. ^1H NMR ($CDCl_3$) δ 8.11 (2H, s), 7.56 (1H, s), 3.79 (1H, br s), 2.67 (1H, br m), 2.58-2.20 (5H, br m), 2.28 (3H, s), 2.24 (6H, s), 1.85 (2H, br t, *J* = 12.8 Hz), 1.72 (1H, br d, *J* = 12.8 Hz), 1.37-1.10 (4H, m). The presence of rotamers precluded a comprehensive assignment of all proton resonances. ^{13}C NMR ($CDCl_3$) δ 180.7, 141.5, 131.4 (q, *J* = 33 Hz), 123.2 (q, *J* = 272 Hz), 122.1, 116.7, 66.6, 56.6, 55.5, 50.1, 44.9, 35.7, 32.4, 25.0, 24.3, 22.4. MS (FAB^+) m/z: 471 ($M+H^+$, 100).

HRMS calcd for $C_{20}H_{29}F_6N_4S$ ($M+H^+$): 471.2017, Found: 471.2026. $[\alpha]^{27}_D$ -1.5 (*c* 0.9, $CHCl_3$).

Catalyst 1e: Amorphous. IR ($CHCl_3$) 3350, 1495, 1471, 1451 cm^{-1}. ^1H NMR ($CDCl_3$) δ 7.48-7.15 (18H, m), 3.87 (1H, br s), 3.27 (1H, br m), 3.12 (1H, br m), 2.90-2.65 (3H, br m), 2.64 (1H, br m), 2.25 (3H, s), 1.92-1.65 (3H, m), 1.43-1.05 (4H, m). The presence of rotamers precluded a comprehensive assignment of all proton resonances. ^{13}C NMR ($CDCl_3$) δ 181.0, 143.7, 140.1, 131.5 (q, *J* = 34 Hz), 128.6, 128.1, 127.3, 123.0 (q, *J* = 273 Hz), 122.7, 117.5, 86.7, 67.3, 61.3, 55.8, 54.4, 35.8, 32.2, 25.1, 24.3, 23.4. MS (FAB^+) m/z: 686 ($M+H^+$, 6), 243 (100). HRMS calcd for $C_{37}H_{38}F_6N_3OS$ ($M+H^+$): 686.2640, Found: 686.2632. $[\alpha]^{28}_D$ +10.8 (*c* 1.5, $CHCl_3$).

Catalyst 1f: Amorphous. IR ($CHCl_3$) 3404, 1496, 1471, 1381 cm^{-1}. ^1H NMR ($CDCl_3$) δ 7.96 (2H, br s), 7.63 (1H, br s), 3.80-3.30 (2H, br m), 2.40-2.00 (3H, br m), 1.85-1.65 (2H, br m), 1.50-1.10 (4H, br m). The presence of rotamers precluded a comprehensive assignment of all proton resonances. ^{13}C NMR ($CDCl_3$) δ 181.7, 140.7, 131.9 (q, *J* = 32 Hz), 123.5, 123.0 (q, *J* = 273 Hz), 118.3, 75.7, 60.5, 34.2, 31.2, 24.2, 23.6. MS (FAB^+) m/z: 387 ($M+H^+$, 100). HRMS calcd for $C_{15}H_{17}F_6N_2OS$ ($M+H^+$): 387.0966, Found: 387.0971. $[\alpha]^{28}_D$ +46.1 (*c* 2.5, $CHCl_3$).

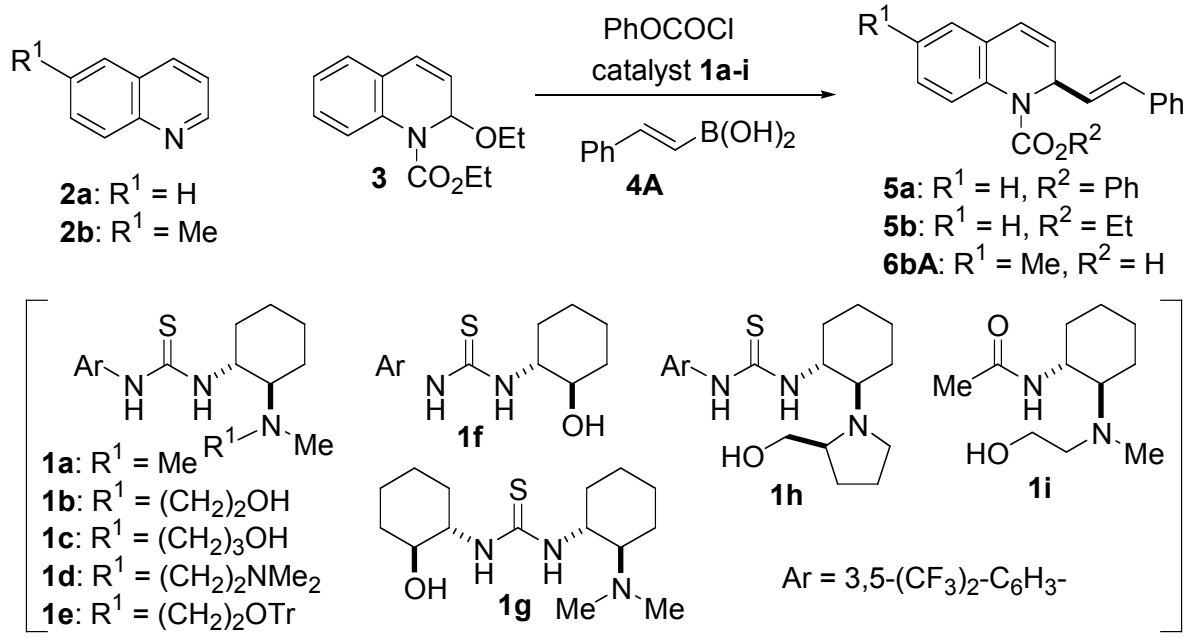
Catalyst 1g: Amorphous. IR ($CHCl_3$) 3412, 1562, 1499 cm^{-1}. ^1H NMR ($CDCl_3$) δ 4.10 (1H, br s), 3.38 (1H, br m), 2.43 (1H, br m), 2.29 (6H, s), 2.26 (2H, br m), 2.02 (2H, br m), 1.89 (1H, d, *J* = 12.2 Hz), 1.82 (1H, d, *J* = 12.2 Hz), 1.74-1.65 (4H, m), 1.40-1.10 (8H, m). ^{13}C NMR ($CDCl_3$) δ 182.1, 75.4, 67.2, 60.0, 56.4, 40.4, 34.0, 33.6, 31.9, 24.8, 24.7, 24.6, 24.1, 21.7. MS (FAB^+) m/z: 300 ($M+H^+$, 90), 125 (100). HRMS calcd for $C_{15}H_{30}N_3OS$ ($M+H^+$): 300.2110, Found: 300.2102. $[\alpha]^{28}_D$ +64.3 (*c* 1.7, $CHCl_3$).

Catalyst 1h: Amorphous. IR ($CHCl_3$) 3330, 1537, 1472, 1384 cm^{-1}. ^1H NMR ($CDCl_3$) δ 8.00 (2H, s), 7.59 (1H, s), 4.12 (1H, br m), 3.61 (1H, br d, *J* = 8.6 Hz), 3.39 (1H, br d, *J* = 8.6 Hz), 3.02 (1H, br m), 2.95 (1H, br m), 2.74 (1H, br m), 2.62 (1H, br m), 2.46 (1H, br m), 1.95-1.08 (12H, m). ^{13}C NMR ($CDCl_3$) δ 181.1, 140.6, 132.0 (q, *J* = 33 Hz), 123.4, 123.1 (q, *J* = 273 Hz), 118.1, 62.4, 56.9, 46.0, 33.0, 28.2, 25.0, 24.6, 24.3, 23.4. Two carbon peaks were missing due to overlapping. MS (FAB^+) m/z: 470 ($M+H^+$, 100). HRMS calcd for $C_{20}H_{26}F_6N_3OS$ ($M+H^+$): 470.1701, Found: 470.1708. $[\alpha]^{28}_D$ +5.3 (*c* 1.1, $CHCl_3$).

Catalyst 1i: A colorless oil. IR ($CHCl_3$) 3433, 1660 cm^{-1}. ^1H NMR ($CDCl_3$) δ 5.99 (1H, br m), 3.76 (1H, m), 3.57 (2H, t, *J* = 6.7 Hz), 2.70 (1H, m), 2.55 (1H, m), 2.31 (1H, m), 2.25 (3H, s), 2.22 (2H, br m), 1.97 (3H, s), 1.88-1.75 (2H, br m), 1.68 (1H, br m), 1.38-1.03 (4H, m). ^{13}C NMR ($CDCl_3$) δ 170.2, 66.7, 58.3, 54.7, 50.3, 35.9, 33.4, 25.2, 24.8, 23.6, 23.4. MS (EI^+) m/z: 214 (M^+, 1), 114 (100). HRMS calcd for $C_{11}H_{22}N_2O_2$: 214.1681, Found: 214.1677. $[\alpha]^{28}_D$ -6.7 (*c* 1.0, $CHCl_3$).

The results of Petasis-type reaction of 2a, 2b and 3 with 4A using catalysts 1a-I under various conditions.

Table 1. Reaction of **2a**, **2b** and **3** with **4A** in the presence of catalyst **1a-i**.[a]



entry	catalyst	substrate	additive	Yield (%)	ee (%)
1	**1a**	**2a**	none	34	-9
2	**1b**	**2a**	none	70	90
3	**1b**	**3a**	none	88	rac
4	**1c**	**2a**	none	47	27
5	**1d**	**2a**	none	31	4
6	**1e**	**2a**	none	44	rac
7	**1f**	**2a**	none	33	rac
8	**1g**	**2a**	none	57	rac
9	**1h**	**2a**	none	60	68
10	**1i**	**2a**	none	70	50
11	*rac*-**1a** and **1i**	**2a**	none	28	20
12	**1b**	**2a**	H_2O (56 eq)[b]	27	93
13	**1b**	**2a**	CF_3CH_2OH (1 eq)	77	46
14	**1b**	**2a**	H_2O (2 eq)[b] and $NaHCO_3$[c]	68	88
15	**1b**	**2a**	H_2O (10 eq)[b] and $NaHCO_3$[c]	70	89

16	**1b**	**2a**	H_2O (28 eq)[b] and $NaHCO_3$[c]	70	90
17	**1b**	**2a**	H_2O (56 eq)[b] and $NaHCO_3$[c]	65	94
18	**1b**	**2a**	H_2O (112 eq)[b] and $NaHCO_3$[c]	56	90
19	**1b**	**2b**	none	70	86
20	**1b**	**2b**	H_2O (56 eq)[b]	32	95
21	**1b**	**2b**	H_2O (56 eq)[b] and $NaHCO_3$[c]	75	95

[a] Reaction was carried out in the presence of catalyst **1** (10 mol%) in CH_2Cl_2 by using PhOCOCl (2 equiv) for 24 h. [b] H_2O (2-112 equivalent) was added. [c] $NaHCO_3$ (2 equiv) was added.

General procedure for Petasis-type reaction of 2a-f.

To a solution of substrate **2a-f** (0.2 mmol), boronic acid **4A-F** (0.4 mmol), catalyst **1a-i** (0.02 mmol) and $NaHCO_3$ (34 mg, 0.4 mmol) in CH_2Cl_2 (2 mL) were added H_2O (0.2 mL) and phenyl chloroformate (0.051 mL, 0.4 mmol) under argon atmosphere at the temperature shown in text. After being stirred at the same temperature for 24 h, the reaction mixture was diluted with $CHCl_3$, washed with 1N NaOH, 1N HCl and water, dried over $MgSO_4$ and concentrated at reduced pressure. Purification of the residue by column chromatography (hexane:AcOEt=10:1) afforded products **5a-6aF**.

Characterization data of obtained compounds 5a-6aF

Adduct 5a: A colorless oil. IR ($CHCl_3$) 1712 cm^{-1}. ^1H NMR ($CDCl_3$) δ 7.73 (1H, br m), 7.39 (2H, t, *J* = 7.6 Hz), 7.31 (2H, d, *J* = 7.0 Hz), 7.28-7.18 (7H, m), 7.14 (1H, d, *J* = 6.4 Hz), 7.10 (1H, t, *J* = 7.3 Hz), 6.63 (1H, d, *J* = 9.8 Hz), 6.60 (1H, d, *J* = 16.2 Hz), 6.17-6.07 (2H, m), 5.82 (1H, br t, *J* = 5.8 Hz). ^{13}C NMR ($CDCl_3$) δ 152.8, 151.1, 136.4, 134.2, 132.1, 129.4, 128.5, 127.9, 127.1, 126.6 (2C), 125.7 (2C), 125.1, 124.7, 124.4, 121.7, 115.3, 54.9. One carbon peak was missing due to overlapping. MS (EI^+) m/z: 353 (M^+, 44), 260 (100). HRMS calcd for $C_{24}H_{19}NO_2$: 353.1416, Found: 353.1410. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 0.5 mL/min, 254 nm) t_r (minor) = 28.7 min, t_r (major) = 34.9 min. A sample of 94% ee by HPLC analysis gave $[\alpha]^{28}_D$ -454 (*c* 1.8, $CHCl_3$).

Adduct 5b: A colorless oil. IR ($CHCl_3$) 1693 cm^{-1}. ^1H NMR ($CDCl_3$) δ 7.62 (1H, br m), 7.30-7.16 (6H, br m), 7.09 (1H, dd, *J* = 7.7, 1.9 Hz), 7.05 (1H, t, *J* = 7.6 Hz), 6.57 (1H, d, *J* = 9.8 Hz), 6.51 (1H, d, *J* = 15.9 Hz), 6.09-6.02 (2H, m), 5.70 (1H, br t, *J* = 6.1 Hz), 4.33 (1H, m), 4.26 (1H, m), 1.34 (3H, t, *J* = 7.0 Hz). ^{13}C NMR

($CDCl_3$) δ 154.3, 136.4, 134.7, 131.4, 128.4, 127.7, 127.6, 127.1, 126.9, 126.5, 126.4, 125.6, 124.3, 124.0, 62.1, 54.2, 14.4. One carbon peak was missing due to overlapping. MS (EI^+) m/z: 305 (M^+, 31), 130 (100). HRMS calcd for $C_{20}H_{19}NO_2$: 305.1416, Found: 305.1411. HPLC (Chiralcel AD-H, hexane/2-propanol=90/10, 0.5 mL/min, 254 nm) t_r (major) = 15.2 min, t_r (minor) = 16.5 min. A sample of 42% ee by HPLC analysis gave $[\alpha]^{25}_D$ -17.8 (*c* 0.64, $CHCl_3$).

Adduct 5c: A colorless oil. IR ($CHCl_3$) 1696 cm^{-1}. ^1H NMR ($CDCl_3$) δ 7.65 (1H, br m), 7.42-7.12 (11H, m), 7.10-7.01 (2H, m), 6.55 (1H, d, *J* = 6.5 Hz), 6.48 (1H, d, *J* = 15.9 Hz), 6.09-5.97 (2H, m), 5.71 (1H, br m), 5.32 (1H, br d, *J* = 12.5 Hz), 5.24 (1H, br d, *J* = 12.5 Hz). ^{13}C NMR ($CDCl_3$) δ 154.1, 136.4, 136.1, 134.5, 131.6, 128.6, 128.4, 128.2, 128.0, 127.8, 127.7, 126.9, 126.5, 126.4, 125.6, 125.4, 124.2, 67.8, 54.4. Two carbon peaks were missing due to overlapping. MS (EI^+) m/z: 367 (M^+, 4), 91 (100). HRMS calcd for $C_{25}H_{21}NO_2$: 367.1572, Found: 367.1575. HPLC (Chiralcel AD-H, hexane/2-propanol=95/5, 0.5 mL/min, 254 nm) t_r (minor) = 29.3 min, t_r (major) = 32.3 min. A sample of 67% ee by HPLC analysis gave $[\alpha]^{25}_D$ -56.4 (*c* 0.83, $CHCl_3$).

Adduct 6bA: A colorless crystal. mp 141-144 ^oC (hexane/AcOEt). IR ($CHCl_3$) 1696 cm^{-1}. ^1H NMR ($CDCl_3$) δ 7.61 (1H, br m), 7.37 (2H, t, *J* = 7.9 Hz), 7.29 (2H, d, *J* = 7.3 Hz), 7.26-7.17 (6H, m), 7.03 (1H, br d, *J* = 8.2 Hz), 6.94 (1H, s), 6.59 (1H, d, *J* = 15.8 Hz), 6.57 (1H, d, *J* = 9.1 Hz), 6.12 (1H, dd, *J* = 15.8, 6.7 Hz), 6.08 (1H, dd, *J* = 9.1, 6.1 Hz), 5.79 (1H, br t, *J* = 6.1 Hz), 2.30 (3H, s). ^{13}C NMR ($CDCl_3$) δ 152.8, 151.2, 136.4, 134.2, 132.0, 131.7, 129.4, 128.5, 127.8, 127.0, 126.9, 126.6, 125.8, 125.6, 125.2, 124.2, 121.7, 54.9, 20.7. Two carbon peaks were missing due to overlapping. MS (EI^+) m/z: 367 (M^+, 50), 44 (100). HRMS calcd for $C_{25}H_{21}NO_2$: 367.1572, Found: 367.1570. Anal. Calcd for $C_{25}H_{21}NO_2$: C, 81.72; H, 5.76; N, 3.81. Found: C, 81.73; H, 5.67; N, 3.79. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 0.5 mL/min, 254 nm) t_r (minor) = 25.4 min, t_r (major) = 35.1 min. A sample of 95% ee by HPLC analysis gave $[\alpha]^{25}_D$ -388 (*c* 1.1, $CHCl_3$).

Adduct 6cA: A colorless crystal. mp 161-164 ^oC (hexane/AcOEt). IR ($CHCl_3$) 1712 cm^{-1}. ^1H NMR ($CDCl_3$) δ 7.70 (1H, br m), 7.38 (2H, t, *J* = 7.9 Hz), 7.30 (2H, d, *J* = 7.0 Hz), 7.28-7.15 (10H, m), 7.09 (2H, m), 6.61 (1H, d, *J* = 15.6 Hz), 6.36 (1H, s), 6.07 (1H, dd, *J* = 15.6, 7.4 Hz), 5.55 (1H, d, *J* = 7.4 Hz). ^{13}C NMR ($CDCl_3$) δ 152.7, 151.2, 136.4, 132.9, 132.5, 129.6, 129.5, 129.4, 128.5, 127.9, 126.9, 126.7, 125.8, 125.6, 124.7, 123.9, 121.7, 121.5, 120.9, 59.5, 20.6. MS (EI^+) m/z: 367 (M^+, 28), 246 (100). HRMS calcd for $C_{25}H_{21}NO_2$: 367.1572, Found: 367.1579. Anal. Calcd for $C_{25}H_{21}NO_2$: C, 81.72; H, 5.76; N, 3.81. Found: C, 81.61; H, 5.60; N, 3.70. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 0.5 mL/min, 254 nm) t_r (minor) = 23.7 min, t_r (major) = 41.9 min. A sample of 96% ee by HPLC analysis gave $[\alpha]^{25}_D$ -482 (*c* 1.4, $CHCl_3$).

Adduct 6dA: A colorless crystal. mp 152-155 ^oC (hexane/AcOEt). IR ($CHCl_3$) 1715 cm^{-1}. ^1H NMR ($CDCl_3$) δ 7.69 (1H, br m), 7.40 (2H, t, *J* = 8.5 Hz), 7.34-7.12 (10H, m), 6.58 (1H, d, *J* = 16.2 Hz), 6.57 (1H, d, *J* = 9.4

Hz), 6.17 (1H, dd, J = 9.4, 6.1 Hz), 6.11 (1H, dd, J = 16.2, 7.2 Hz), 5.83 (1H, br t, J = 6.1 Hz). ^{13}C NMR ($CDCl_3$) δ 152.6, 151.0, 136.2, 132.8, 132.5, 129.9, 129.5, 128.6, 128.1, 127.7, 126.7, 126.2, 125.9, 125.7, 124.8, 124.6, 121.7, 54.9. Two carbon peaks were missing due to overlapping. MS (EI$^+$) m/z: 387 (M$^+$, 21), 44 (100). HRMS calcd for $C_{24}H_{18}ClNO_2$: 387.1026, Found: 387.1033. Anal. Calcd for $C_{24}H_{18}ClNO_2$: C, 74.32; H, 4.68; Cl, 9.14; N, 3.61. Found: C, 74.54; H, 4.63; Cl, 8.99; N, 3.59. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 0.5 mL/min, 254 nm) t_r (minor) = 27.3 min, t_r (major) = 37.3 min. A sample of 94% ee by HPLC analysis gave $[\alpha]^{25}_D$ -435 (c 0.75, $CHCl_3$).

Adduct 6eA: A colorless crystal. mp 143-145 ^{o}C (hexane/AcOEt). IR ($CHCl_3$) 1714 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ 7.63 (1H, br m), 7.39 (2H, t, J = 7.6 Hz), 7.35-7.15 (10H, m), 6.58 (1H, d, J = 15.6 Hz), 6.56 (1H, d, J = 9.4 Hz), 6.15 (1H, dd, J = 9.4, 6.1 Hz), 6.11 (1H, dd, J = 15.6, 7.0 Hz), 5.82 (1H, br t, J = 7.0 Hz). ^{13}C NMR ($CDCl_3$) δ 152.5, 150.9, 136.2, 133.3, 132.5, 130.6, 129.5, 129.2, 129.0, 128.6, 128.1, 126.7, 126.0, 125.9, 124.7, 124.6, 121.6, 117.6, 54.9. One carbon peak was missing due to overlapping. MS (EI$^+$) m/z: 431 (M$^+$, 22), 77 (100). HRMS calcd for $C_{24}H_{18}{}^{79}BrNO_2$: 431.0521, Found: 431.0515. Anal. Calcd for $C_{24}H_{18}BrNO_2$: C, 66.68; H, 4.20; Br, 18.48; N, 3.24. Found: C, 66.81; H, 4.19; Br, 18.46; N, 3.23. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 0.5 mL/min, 254 nm) t_r (minor) = 25.3 min, t_r (major) = 35.1 min. A sample of 95% ee by HPLC analysis gave $[\alpha]^{25}_D$ -413 (c 1.6, $CHCl_3$).

Adduct 6fA: A colorless crystal. mp 129-131 ^{o}C (hexane/AcOEt). IR ($CHCl_3$) 1746, 1713 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ 7.72 (1H, br m), 7.39 (2H, t, J = 7.6 Hz), 7.32 (2H, d, J = 7.3 Hz), 7.30-7.16 (6H, m), 6.95-6.90 (2H, m), 6.60 (1H, d, J = 15.9 Hz), 6.58 (1H, d, J = 9.7 Hz), 6.17-6.10 (2H, m), 5.83 (1H, br t, J = 6.4 Hz), 1.35 (9H, s). ^{13}C NMR ($CDCl_3$) δ 177.2, 155.7, 152.8, 151.0, 147.7, 136.3, 132.4, 131.5, 129.6, 129.4, 128.5, 128.0, 126.7, 125.8, 125.2, 124.8, 121.7, 120.6, 119.2, 115.3, 55.0, 39.0, 27.1. MS (EI$^+$) m/z: 453 (M$^+$, 18), 207 (100). HRMS calcd for $C_{29}H_{27}NO_4$: 453.1940, Found: 453.1943. Anal. Calcd for $C_{29}H_{27}NO_4$: C, 76.80; H, 6.00; N, 3.09. Found: C, 76.95; H, 5.98; N, 2.93. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 1.0 mL/min, 254 nm) t_r (minor) = 12.3 min, t_r (major) = 32.3 min. A sample of 96% ee by HPLC analysis gave $[\alpha]^{25}_D$ -533 (c 2.1, $CHCl_3$).

Adduct 6aB: Amorphous. IR ($CHCl_3$) 1712 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ 7.72 (1H, br m), 7.39 (2H, t, J = 7.8 Hz), 7.27-7.07 (8H, m), 6.79 (2H, d, J = 8.7 Hz), 6.61 (1H, d, J = 9.5 Hz), 6.54 (1H, d, J = 15.6 Hz), 6.09 (1H, dd, J = 9.5, 6.1 Hz), 5.99 (1H, dd, J = 15.6, 7.1 Hz), 5.79 (1H, br t, J = 6.8 Hz), 3.77 (3H, s). ^{13}C NMR ($CDCl_3$) δ 159.5, 152.8, 151.1, 134.3, 131.7, 129.4, 129.1, 127.9, 127.8, 127.2, 126.6, 125.7, 125.5, 124.7, 124.4, 122.8, 121.7, 113.9, 55.2, 55.0. One carbon peak was missing due to overlapping. MS (EI$^+$) m/z: 383 (M$^+$, 16), 262 (100). HRMS calcd for $C_{25}H_{21}NO_3$: 383.1521, Found: 383.1525. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 0.5 mL/min, 254 nm) t_r (minor) = 27.5 min, t_r (major) = 41.6 min. A sample of 97%

ee by HPLC analysis gave $[\alpha]^{25}_{D}$ -456 (*c* 1.3, $CHCl_3$).

Adduct 6aC: A colorless crystal. mp 165-167 ^{o}C (hexane/AcOEt). IR ($CHCl_3$) 1727 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ 7.72 (1H, br m), 7.39 (2H, t, *J* = 7.7 Hz), 7.26-7.07 (6H, m), 6.84 (1H, s), 6.74 (1H, d, *J* = 8.0 Hz), 6.69 (1H, d, *J* = 8.0 Hz), 6.61 (1H, d, *J* = 9.5 Hz), 6.50 (1H, d, *J* = 15.9 Hz), 6.09 (1H, dd, *J* = 9.5, 6.1 Hz), 5.96 (1H, dd, *J* = 15.9, 7.0 Hz), 5.91 (2H, s), 5.78 (1H, br t, *J* = 6.4 Hz). ^{13}C NMR ($CDCl_3$) δ 152.8, 151.1, 148.0, 147.5, 134.2, 131.8, 130.9, 129.4, 127.9, 127.2, 126.6, 125.7, 125.6, 124.7, 124.4, 123.3, 121.7, 121.5, 108.2, 105.9, 101.1, 54.9, 29.6. MS (EI^+) m/z: 397 (M^+, 2), 45 (100). HRMS calcd for $C_{25}H_{19}NO_4$: 397.1314, Found: 397.1317. Anal. Calcd for $C_{25}H_{19}NO_4$: C, 75.55; H, 4.82; N, 3.52. Found: C, 75.32; H, 4.69; N, 3.43. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 0.5 mL/min, 254 nm) t_r (minor) = 30.1 min, t_r (major) = 43.4 min. A sample of 83% ee by HPLC analysis gave $[\alpha]^{30}_{D}$ -470 (*c* 1.7, $CHCl_3$).

Adduct 6aD: A colorless crystal. mp 122-126 ^{o}C (hexane/AcOEt). IR ($CHCl_3$) 1712 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ 7.74 (1H, br m), 7.39 (2H, t, *J* = 7.3 Hz), 7.26-7.17 (4H, m), 7.16-7.07 (2H, m), 6.86 (2H, m), 6.76 (1H, d, *J* = 8.8 Hz), 6.63 (1H, d, *J* = 9.5 Hz), 6.54 (1H, d, *J* = 15.8 Hz), 6.10 (1H, dd, *J* = 9.5, 6.1 Hz), 6.01 (1H, dd, *J* = 15.8, 7.0 Hz), 5.81 (1H, br t, *J* = 6.1 Hz), 3.86 (3H, s), 3.85 (3H, s). ^{13}C NMR ($CDCl_3$) δ 152.8, 151.1, 149.1, 149.0, 134.2, 132.1, 129.4, 127.8, 127.4, 127.1, 126.5, 125.7, 125.5, 124.6, 124.4, 123.0, 121.7, 120.0, 111.0, 108.8, 55.8, 55.1. Two carbon peaks were missing due to overlapping. MS (EI^+) m/z: 413 (M^+, 20), 292 (100). HRMS calcd for $C_{26}H_{23}NO_4$: 413.1627, Found: 413.1631. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 1.0 mL/min, 254 nm) t_r (minor) = 51.8 min, t_r (major) = 71.5 min. A sample of 89% ee by HPLC analysis gave $[\alpha]^{25}_{D}$ -476 (*c* 1.4, $CHCl_3$).

Adduct 6aE: A colorless crystal. mp 113-115 ^{o}C (hexane/AcOEt). IR ($CHCl_3$) 1713 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ 7.73 (1H, br m), 7.37 (2H, t, *J* = 7.7 Hz), 7.24-7.04 (10H, m), 6.60 (1H, d, *J* = 9.5 Hz), 6.56 (1H, d, *J* = 15.6 Hz), 6.12-6.04 (2H, m), 5.80 (1H, br t, *J* = 6.4 Hz), 2.28 (3H, s). ^{13}C NMR ($CDCl_3$) δ 152.8, 151.1, 137.8, 134.2, 133.6, 132.0, 129.4, 129.2, 127.8, 127.1, 126.5, 125.6, 125.5, 124.6, 124.3, 124.0, 121.7, 55.0, 21.1. Two carbon peaks were missing due to overlapping. MS (EI^+) m/z: 367 (M^+, 32), 246 (100). HRMS calcd for $C_{25}H_{21}NO_2$: 367.1572, Found: 367.1574. Anal. Calcd for $C_{25}H_{21}NO_2$: C, 81.72; H, 5.76; N, 3.81. Found: C, 81.90; H, 5.94; N, 3.74. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 0.5 mL/min, 254 nm) t_r (minor) = 25.6 min, t_r (major) = 30.8 min. A sample of 91% ee by HPLC analysis gave $[\alpha]^{28}_{D}$ -364 (*c* 1.1, $CHCl_3$).

Adduct 6aF: Amorphous. IR ($CHCl_3$) 1712 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ 7.74 (1H, br m), 7.50 (2H, d, *J* = 8.3 Hz), 7.42-7.35 (4H, m), 7.27-7.08 (6H, m), 6.65 (1H, d, *J* = 9.5 Hz), 6.60 (1H, d, *J* = 15.9 Hz), 6.23 (1H, dd, *J* = 15.9, 6.7 Hz), 6.10 (1H, dd, *J* = 9.5, 6.1 Hz), 5.84 (1H, br t, *J* = 6.5 Hz). ^{13}C NMR ($CDCl_3$) δ 152.8, 151.0, 139.9, 134.1, 130.6, 129.7 (q, *J* = 32 Hz), 129.5, 128.0, 127.8, 127.0, 126.8, 126.7, 126.1, 125.4 (q, *J* = 4 Hz),

125.2, 124.8, 124.4 (q, J = 271 Hz), 124.3, 121.7, 54.7. One carbon peak was missing due to overlapping. MS (EI^+) m/z: 421 (M^+, 58), 328 (100). HRMS calcd for $C_{25}H_{18}F_3NO_2$: 421.1290, Found: 421.1284. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 0.5 mL/min, 254 nm) t_r (minor) = 33.9 min, t_r (major) = 36.3 min. A sample of 95% ee by HPLC analysis gave $[\alpha]^{25}_D$ -396 (c 0.71, $CHCl_3$).

Conversion of the adduct 6aC to (+)-galipinine 7 and characterization data.[1)]

A suspension of adduct **6aC** (80 mg, 0.20 mmol) and 10% Pd-C (120 mg) in MeOH (4 mL) was stirred under a hydrogen atmosphere at 20 °C for 12 h. After the reaction mixture was filtered, the filtrate was concentrated at reduced pressure. Purification of the residue by column chromatography (hexane:AcOEt=10:1) afforded product (79 mg, 98%) as a colorless crystal. mp 119-121 °C (hexane/AcOEt). IR ($CHCl_3$) 1708 cm^{-1}. ^1H NMR ($CDCl_3$) δ 7.57 (1H, br m), 7.37 (2H, t, J = 7.3 Hz), 7.23-7.10 (5H, m), 7.09 (1H, t, J = 7.3 Hz), 6.68 (1H, d, J = 7.9 Hz), 6.63-6.57 (2H, m), 5.88 (2H, AB q, J = 14.0 Hz), 4.73 (1H, m), 2.78 (2H, m), 2.63 (2H, m), 2.34 (1H, m), 1.91 (1H, m), 1.80-1.60 (2H, m). ^{13}C NMR ($CDCl_3$) δ 153.4, 151.3, 147.6, 145.7, 136.2, 135.5, 129.3, 128.1, 126.2, 125.7, 125.4, 124.8, 121.7, 121.0, 108.8, 108.1, 100.7, 53.2, 34.8, 32.1, 28.6, 24.5. One carbon peak was missing due to overlapping. MS (EI^+) m/z: 401 (M^+, 19), 135 (100). HRMS calcd for $C_{25}H_{23}NO_4$: 401.1627, Found: 401.1632. Anal. Calcd for $C_{25}H_{23}NO_4$: C, 74.79; H, 5.77; N, 3.49. Found: C, 74.57; H, 5.56; N, 3.26. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 0.5 mL/min, 254 nm) t_r (minor) = 24.7 min, t_r (major) = 26.2 min. A sample of 83% ee by HPLC analysis gave $[\alpha]^{28}_D$ -97.2 (c 2.1, $CHCl_3$). To a stirred solution of product (39 mg, 0.097 mmol) in dry THF (5 mL) was $LiAlH_4$ (11 mg, 0.29 mmol) under argon atmosphere at 0 °C for 12 h. After being stirred at the room temperature for 12 h, the reaction mixture was slowly hydrolyzed with water. The solid residue was filtered and washed with diethyl ether. The filtration was dried over Na_2SO_4 and concentrated at reduced pressure. Purification of the residue by column chromatography (hexane:AcOEt=6:1) afforded product **7** (19 mg, 65%) as a colorless oil. IR ($CHCl_3$) 2940, 1501, 1442 cm^{-1}. ^1H NMR ($CDCl_3$) δ 7.07 (1H, t, J = 7.3 Hz), 6.97 (1H, d, J = 7.3 Hz), 6.72 (1H, d, J = 7.9 Hz), 6.68 (1H, s), 6.63 (1H, d, J = 7.3 Hz), 6.58 (1H, t, J = 7.3 Hz), 6.52 (1H, d, J = 7.9 Hz), 5.91 (2H, s), 3.26 (1H, m), 2.90 (3H, s), 2.83 (1H, m), 2.72-2.58 (2H, m), 2.50 (1H, m), 1.97-1.83 (3H, m), 1.71 (1H, m). ^{13}C NMR ($CDCl_3$) δ 147.7, 145.7, 145.3, 135.9, 128.7, 127.1, 121.8, 121.0, 115.5, 110.7, 108.7, 108.2, 100.8, 58.2, 38.0, 33.1, 32.0, 24.3, 23.5. MS (EI^+) m/z: 295 (M^+, 21), 146 (100). HRMS calcd for $C_{19}H_{21}NO_2$: 295.1572, Found: 295.1566. HPLC (Chiralcel OD-H, hexane/2-propanol=95/5, 0.5 mL/min, 254 nm) t_r (major) = 15.3 min, t_r (minor) = 18.1 min. A sample of 83% ee by HPLC analysis gave $[\alpha]^{31}_D$ +24.8 (c 0.8, $CHCl_3$).

References

1) Rueping, M.; Antonchick, A. P.; Theissmann, T. *Angew. Chem. Int. Ed.* **2006**, *45*, 3683.

Copies of ^{1}H and ^{13}C NMR spectrum of all obtained compounds.

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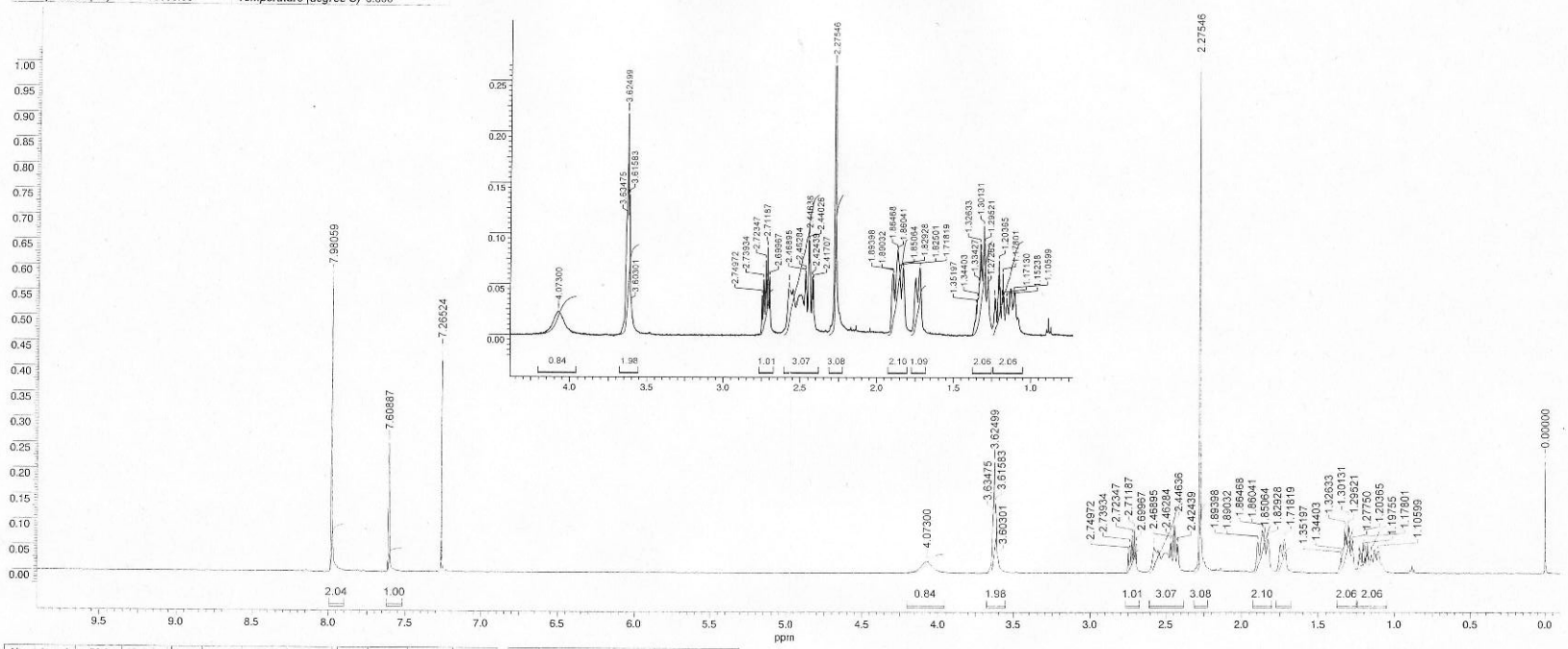
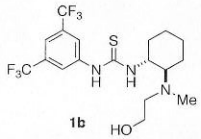


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	-0.00	-0.0	0.2208	18	1.33	663.2	0.0901	35	2.45	1223.2	0.0948
2	1.11	553.0	0.0428	19	1.33	667.1	0.0519	36	2.46	1231.4	0.0633
3	1.15	576.2	0.0367	20	1.34	672.0	0.0371	37	2.47	1234.5	0.0606
4	1.17	585.7	0.0381	21	1.35	676.0	0.0304	38	2.58	1287.6	0.0519
5	1.18	589.0	0.0610	22	1.72	859.1	0.0668	39	2.70	1349.8	0.0578
6	1.18	592.4	0.0375	23	1.83	912.5	0.0659	40	2.71	1355.9	0.0867
7	1.20	598.8	0.0485	24	1.83	914.6	0.0671	41	2.72	1361.7	0.0742
8	1.20	601.8	0.0737	25	1.85	925.3	0.0649	42	2.74	1369.7	0.0549
9	1.21	604.9	0.0426	26	1.86	930.2	0.0826	43	2.75	1374.9	0.0394
10	1.22	611.9	0.0288	27	1.86	932.3	0.0845	44	3.60	1801.5	0.0313
11	1.23	614.3	0.0372	28	1.88	941.5	0.0382	45	3.62	1807.9	0.1383
12	1.27	636.3	0.0483	29	1.89	945.2	0.0599	46	3.62	1812.5	0.2179
13	1.28	638.8	0.0584	30	1.89	947.0	0.0613	47	3.63	1817.4	0.1177
14	1.30	647.6	0.0909	31	2.28	1137.7	1.0000	48	4.07	2036.5	0.0233
15	1.30	650.7	0.1079	32	2.42	1208.5	0.0546	49	7.27	3632.6	0.4329
16	1.31	653.7	0.0715	33	2.42	1212.2	0.0576	50	7.61	3804.4	0.2522
17	1.32	659.8	0.0825	34	2.44	1220.1	0.0931	51	7.98	3990.3	0.5790

No.	(ppm)	Value	Absolute Value
1	[1.05 .. 1.24]	2.063	1.58085e+3
2	[1.25 .. 1.38]	2.064	1.58185e+3
3	[1.68 .. 1.77]	1.090	8.35507e+2
4	[1.80 .. 1.92]	2.104	1.61288e+3
5	[2.23 .. 2.31]	3.077	2.35849e+3
6	[2.38 .. 2.61]	3.070	2.35298e+3
7	[2.68 .. 2.77]	1.008	7.72302e+2
8	[3.56 .. 3.68]	1.977	1.51547e+3
9	[3.96 .. 4.20]	0.839	6.42848e+2
10	[7.52 .. 7.62]	1.000	7.66409e+2
11	[7.90 .. 8.00]	2.044	1.56635e+3

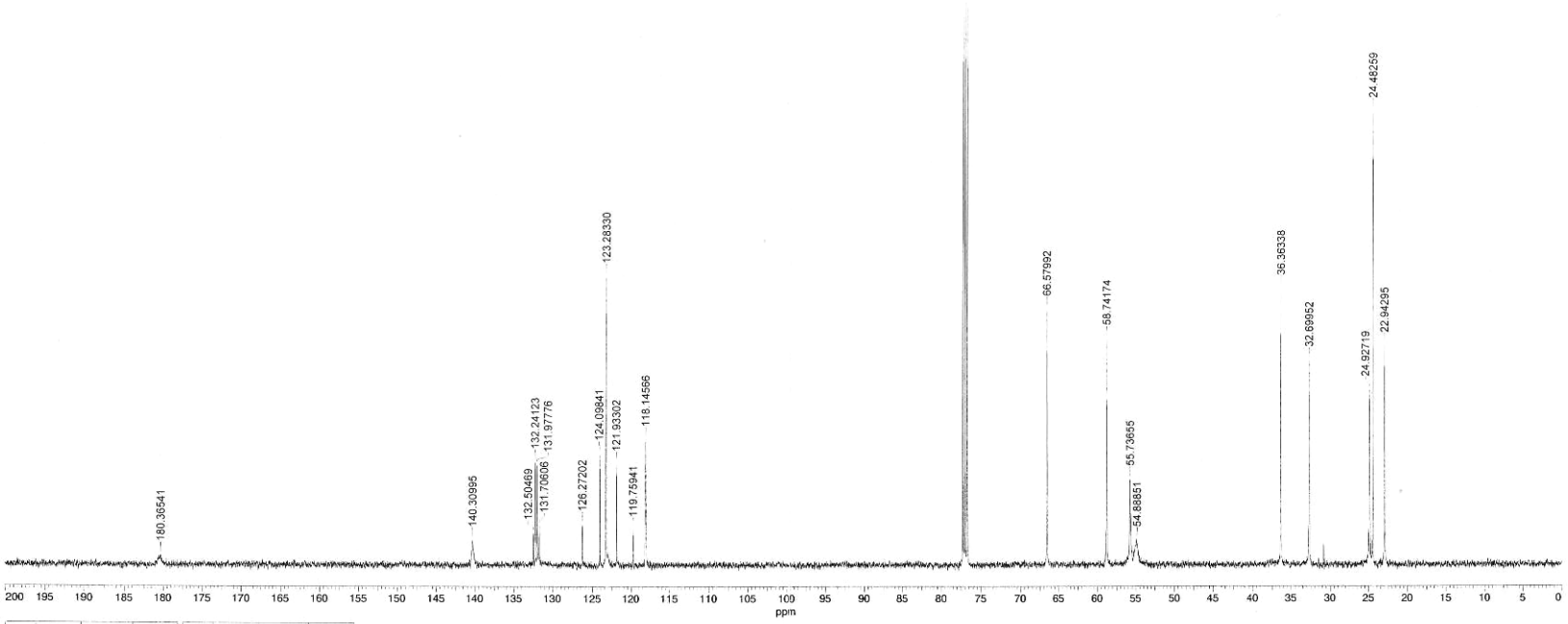


1b

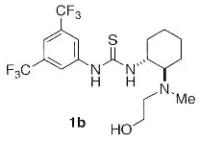
C:\Documents and Settings\Owner\My Documents\%–I–I\urea1-1h\urea1-1h.nmdata

20 May 2006
noe

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Sat May 20 03:05:47 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\ureaOH\ureaOH.nmdata
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	1024	*Original Points Coun:*	32768	*Points Count*	32768
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	22.94	2882.8	0.3873	12	121.93	15320.9	0.1788
2	24.48	3076.2	0.8037	13	123.28	15490.5	0.5111
3	24.93	3132.1	0.3094	14	124.10	15593.0	0.1968
4	32.70	4108.7	0.3613	15	126.27	15866.1	0.0724
5	36.36	4569.1	0.4891	16	131.71	16548.9	0.0691
6	54.89	6896.7	0.0437	17	131.98	16583.0	0.1767
7	55.74	7003.3	0.1520	18	132.24	16616.1	0.1819
8	58.74	7380.9	0.4009	19	132.50	16649.2	0.0568
9	66.58	8365.8	0.4530	20	140.31	17629.9	0.0437
10	118.15	14845.0	0.2219	21	180.37	22662.9	0.0167
11	119.76	15047.8	0.0626				

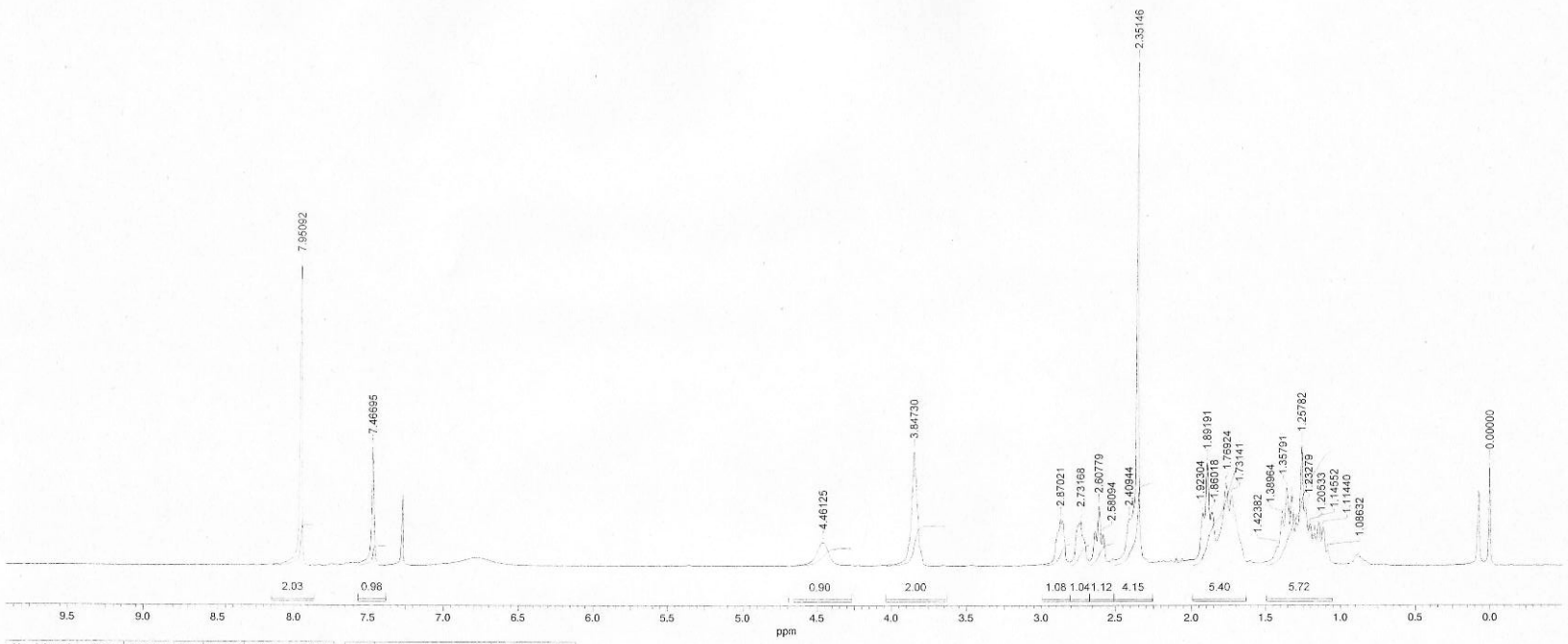


1b

C:\Documents and Settings\Owner\My Documents\ R‰ª\ureaOH\ureaOH.nmdata

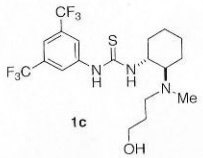
5 Jul 2006

Acquisition Time (sec)	4.1001	*Date*	05 Jul 2006 12:35:12		*File Name*	C:\Documents and Settings\Owner\My Documents\ R%-%\YD91NON_E104_FT.als		*Frequency (MHz)*	399.65
Nucleus	1H	*Number of Transients*	8	*Original Points Count*	32768	*Points Count*	32768	*Pulse Sequence*	NON	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	7992.01	*Temperature (degree C)*	19.700						



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	-0.00	-0.0	0.1844	15	1.77	707.1	0.1484
2	1.09	434.1	0.0273	16	1.86	743.4	0.0965
3	1.11	445.4	0.0688	17	1.89	756.1	0.1852
4	1.15	457.8	0.0792	18	1.92	768.5	0.0949
5	1.17	469.0	0.0567	19	2.35	939.8	0.9073
6	1.21	481.7	0.0730	20	2.41	962.9	0.0839
7	1.23	492.7	0.1056	21	2.58	1031.5	0.0572
8	1.26	502.7	0.2168	22	2.61	1042.2	0.1071
9	1.30	517.6	0.0772	23	2.73	1091.7	0.0823
10	1.32	529.5	0.1273	24	2.87	1147.1	0.0835
11	1.36	542.7	0.1395	25	3.85	1537.6	0.2054
12	1.39	555.4	0.0885	26	4.46	1782.9	0.0425
13	1.42	569.0	0.0342	27	7.47	2984.2	0.2122
14	1.73	692.0	0.1267	28	7.95	3177.6	0.5403

No.	(ppm)	Value	Absolute Value
1	[1.06 .. 1.49]	5.719	2.30272e+3
2	[1.63 .. 1.99]	5.400	2.17439e+3
3	[2.26 .. 2.51]	4.146	1.66931e+3
4	[2.51 .. 2.67]	1.122	4.51954e+2
5	[2.67 .. 2.80]	1.045	4.20598e+2
6	[2.80 .. 2.99]	1.076	4.33127e+2
7	[3.63 .. 4.04]	2.000	8.05308e+2
8	[4.27 .. 4.69]	0.901	3.62645e+2
9	[7.38 .. 7.57]	0.975	3.92662e+2
10	[7.86 .. 8.15]	2.029	8.17084e+2



1c

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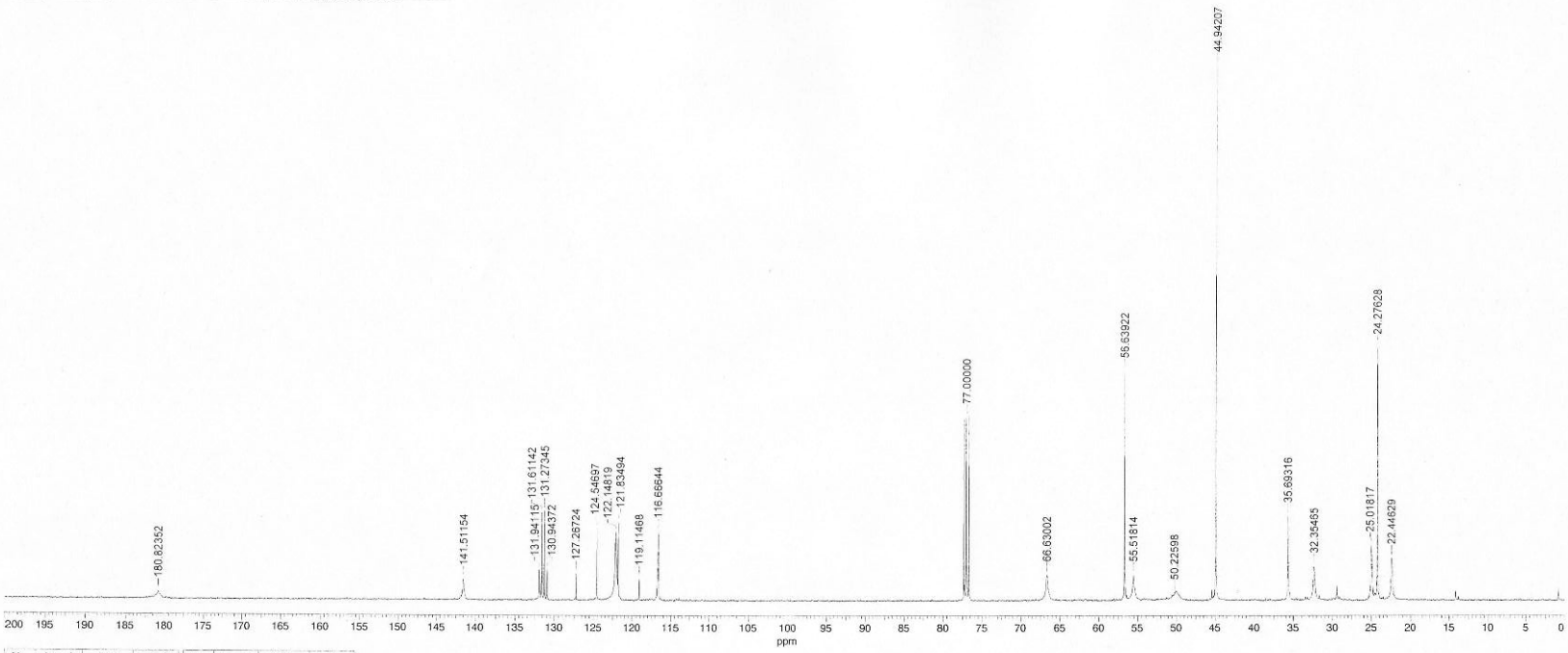
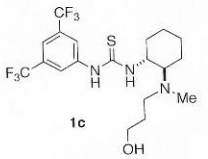
5 Jul 2006

Acquisition Time (sec)	1.2083	*Date*	05 Jul 2006 12:33:14			*File Name*	C:\Documents and Settings\Owner\My Documents\ R%‰%YD8C1BCM_E111_FT.als			*Frequency (MHz)*	100.40
Nucleus	13C	*Number of Transients*	2048	*Original Points Count*	32768	*Points Count*	32768	*Pulse Sequence*	BCM	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	27118.64	*Temperature (degree C)*	20.200								



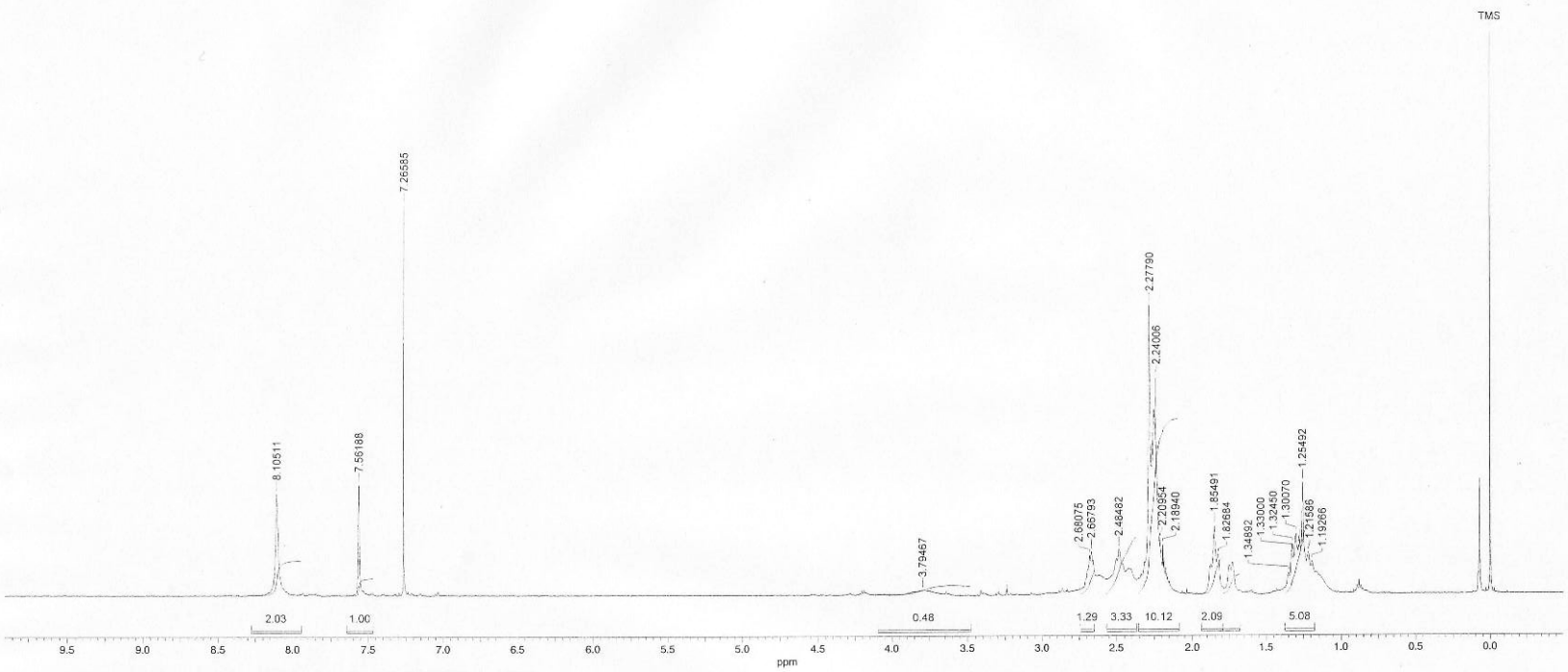
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	22.45	2253.6	0.0793	13	119.11	11959.1	0.0402
2	24.28	2437.3	0.4718	14	121.83	12232.2	0.1477
3	25.02	2511.8	0.1026	15	122.15	12263.7	0.1277
4	32.35	3248.4	0.0632	16	124.55	12504.5	0.1347
5	35.69	3583.6	0.1581	17	127.27	12777.6	0.0502
6	44.94	4512.2	1.0000	18	130.94	13146.8	0.0573
7	50.23	5042.7	0.0137	19	131.27	13179.9	0.1668
8	55.52	5574.0	0.0475	20	131.61	13213.8	0.1640
9	56.64	5686.6	0.4281	21	131.94	13246.9	0.0573
10	66.63	6689.7	0.0481	22	141.51	14207.8	0.0395
11	77.00	7730.8	0.3421	23	180.82	18154.7	0.0139
12	116.67	11713.3	0.1286				



1c

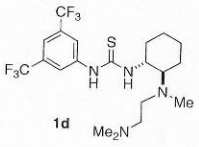
C:\Documents and Settings\Owner\My Documents\ R%‰%YD8C1BCM_E111_FT.als

Acquisition Time (sec)	3.2768	*Comment*	pos	*Date*	Thu Feb 22 17:03:28 2007			*File Name*	C:\Documents and Settings\–ôïÿ¾ ¢%…Šw\ftfX/N/¤fb/¤\NMR\NMR DATA\yamaoka\5H\5H.nmdata		
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.19	596.3	0.0589	13	2.18	1091.0	0.0664
2	1.22	607.9	0.0732	14	2.19	1094.7	0.0881
3	1.25	627.5	0.1986	15	2.21	1104.8	0.0978
4	1.28	637.5	0.0974	16	2.24	1120.0	0.3842
5	1.28	640.6	0.0876	17	2.28	1139.0	0.5151
6	1.30	650.3	0.1077	18	2.48	1242.4	0.0798
7	1.30	652.5	0.1022	19	2.67	1334.0	0.0761
8	1.32	662.3	0.0885	20	2.68	1340.4	0.0692
9	1.33	665.0	0.0775	21	3.79	1897.3	0.0082
10	1.35	674.5	0.0378	22	7.27	3632.9	0.6952
11	1.83	913.4	0.0699	23	7.56	3780.9	0.1964
12	1.85	927.5	0.1222	24	8.11	4052.6	0.1819

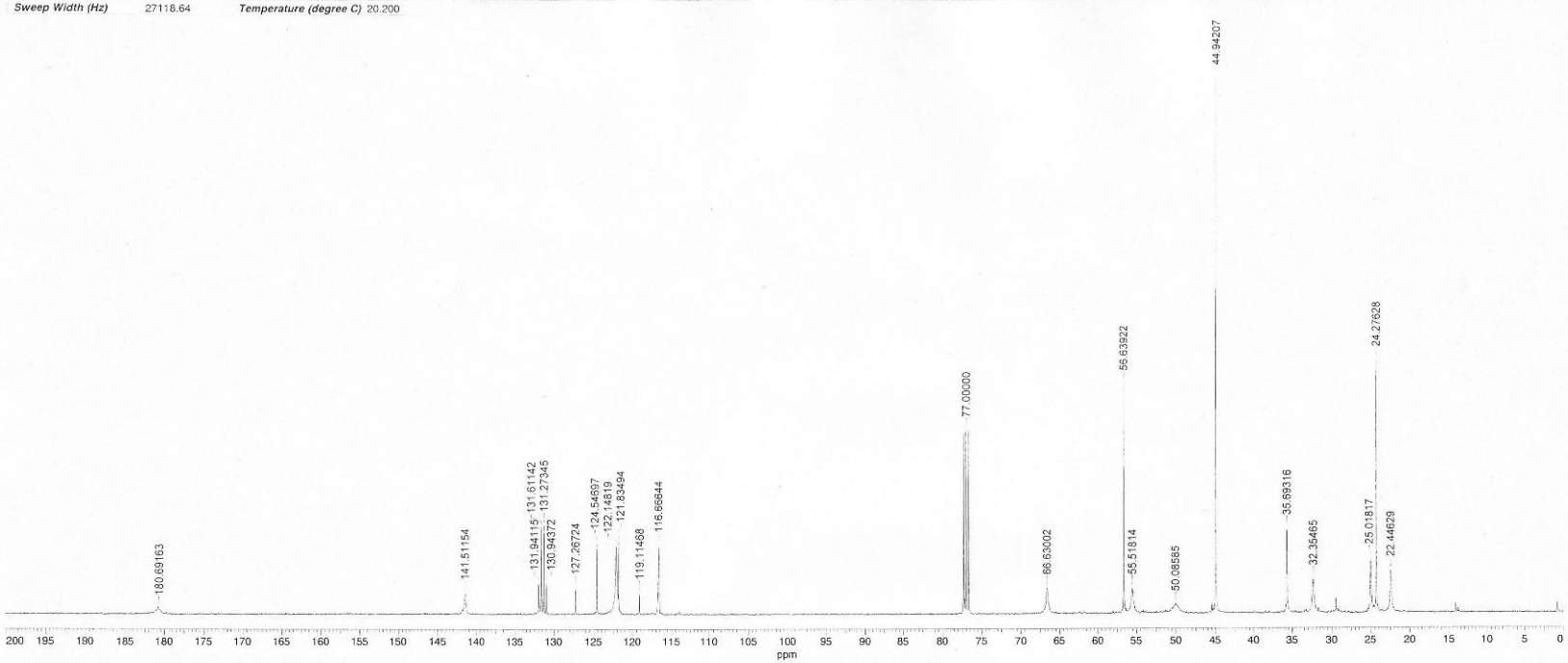
No.	(ppm)	Value	Absolute Value
1	[1.17 .. 1.37]	5.075	2.68594e+3
2	[1.68 .. 1.79]	1.111	5.87982e+2
3	[1.79 .. 1.94]	2.088	1.10520e+3
4	[2.09 .. 2.35]	10.121	5.35596e+3
5	[2.37 .. 2.57]	3.328	1.76122e+3
6	[2.65 .. 2.74]	1.291	6.83060e+2
7	[3.48 .. 4.10]	0.480	2.54287e+2
8	[7.47 .. 7.64]	1.000	5.29203e+2
9	[7.94 .. 8.28]	2.028	1.07342e+3



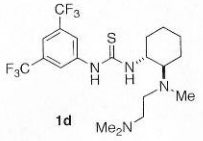
1d

5 Jul 2006

Acquisition Time (sec)	1.2083	*Date*	05 Jul 2006 12:33:14		*File Name*	C:\Documents and Settings\Owner\My Documents\ R%‰\YD8C1BCM_E111_FT.als		*Frequency (MHz)*	100.40
Nucleus	13C	*Number of Transients*	2048	*Original Points Count*	32768	*Points Count*	32768	*Pulse Sequence*	BCM
Sweep Width (Hz)	27118.64	*Temperature (degree C)*	20.200					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	22.45	2253.6	0.0793	13	119.11	11959.1	0.0402
2	24.28	2437.3	0.4718	14	121.83	12232.2	0.1477
3	25.02	2511.8	0.1026	15	122.15	12263.7	0.1277
4	32.35	3248.4	0.0632	16	124.55	12504.5	0.1347
5	35.69	3583.6	0.1581	17	127.27	12777.6	0.0502
6	44.94	4512.2	1.0000	18	130.94	13146.8	0.0573
7	50.09	5028.6	0.0160	19	131.27	13179.9	0.1668
8	55.52	5574.0	0.0475	20	131.61	13213.8	0.1640
9	56.64	5686.6	0.4281	21	131.94	13246.9	0.0573
10	66.63	6689.7	0.0481	22	141.51	14207.8	0.0395
11	77.00	7730.8	0.3421	23	180.69	18141.4	0.0100
12	116.67	11713.3	0.1286				

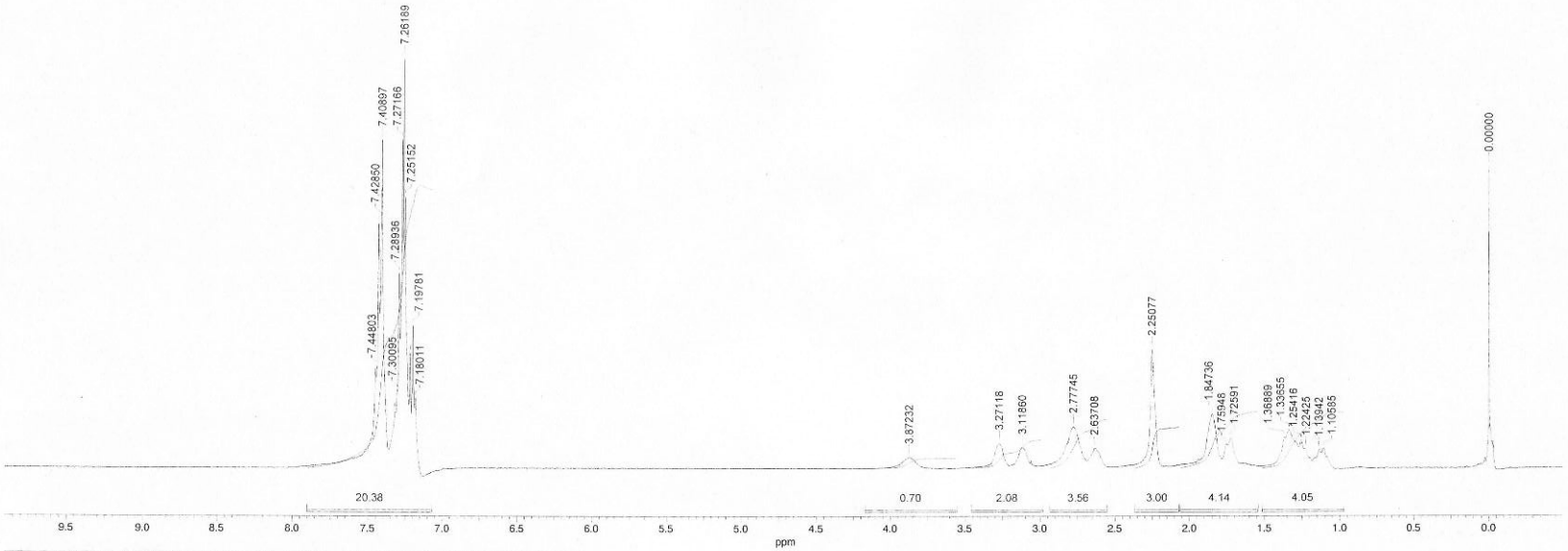


1d

C:\Documents and Settings\Owner\My Documents\ R%‰\YD8C1BCM_E111_FT.als

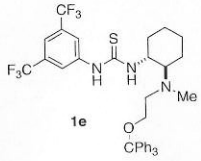
5 Jul 2006

Acquisition Time (sec)	4.1001	*Date*	05 Jul 2006 12:34:36			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD71NON_E103_FT.als			*Frequency (MHz)*	399.65
Nucleus	1H	*Number of Transients*	8	*Original Points Count*	32768	*Points Count*	32768	*Pulse Sequence*	NON	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	7992.01	*Temperature (degree C)*	20.900								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.5532	15	3.27	1307.3	0.0456
2	1.11	442.0	0.0364	16	3.87	1547.6	0.0203
3	1.14	455.4	0.0332	17	7.18	2869.5	0.1286
4	1.22	489.3	0.0344	18	7.20	2876.6	0.2608
5	1.25	501.2	0.0498	19	7.22	2884.2	0.2099
6	1.34	534.2	0.0699	20	7.25	2898.1	0.4958
7	1.37	547.1	0.0561	21	7.26	2902.2	0.7498
8	1.73	689.8	0.0562	22	7.27	2906.1	0.6006
9	1.76	703.2	0.0418	23	7.29	2913.2	0.3551
10	1.85	738.3	0.0989	24	7.30	2917.8	0.1429
11	2.25	899.5	0.2170	25	7.32	2923.9	0.1030
12	2.64	1053.9	0.0360	26	7.41	2961.0	0.5994
13	2.78	1110.0	0.0762	27	7.43	2968.8	0.4593
14	3.12	1246.4	0.0381	28	7.45	2976.6	0.1843

No.	(ppm)	Value	Absolute Value
1	[0.97 .. 1.51]	4.048	1.04814e+3
2	[1.54 .. 2.06]	4.135	1.07079e+3
3	[2.07 .. 2.37]	3.000	7.76855e+2
4	[2.55 .. 2.93]	3.564	9.22882e+2
5	[2.98 .. 3.46]	2.084	5.39620e+2
6	[3.55 .. 4.17]	0.701	1.81459e+2
7	[7.07 .. 7.90]	20.384	5.27859e+3

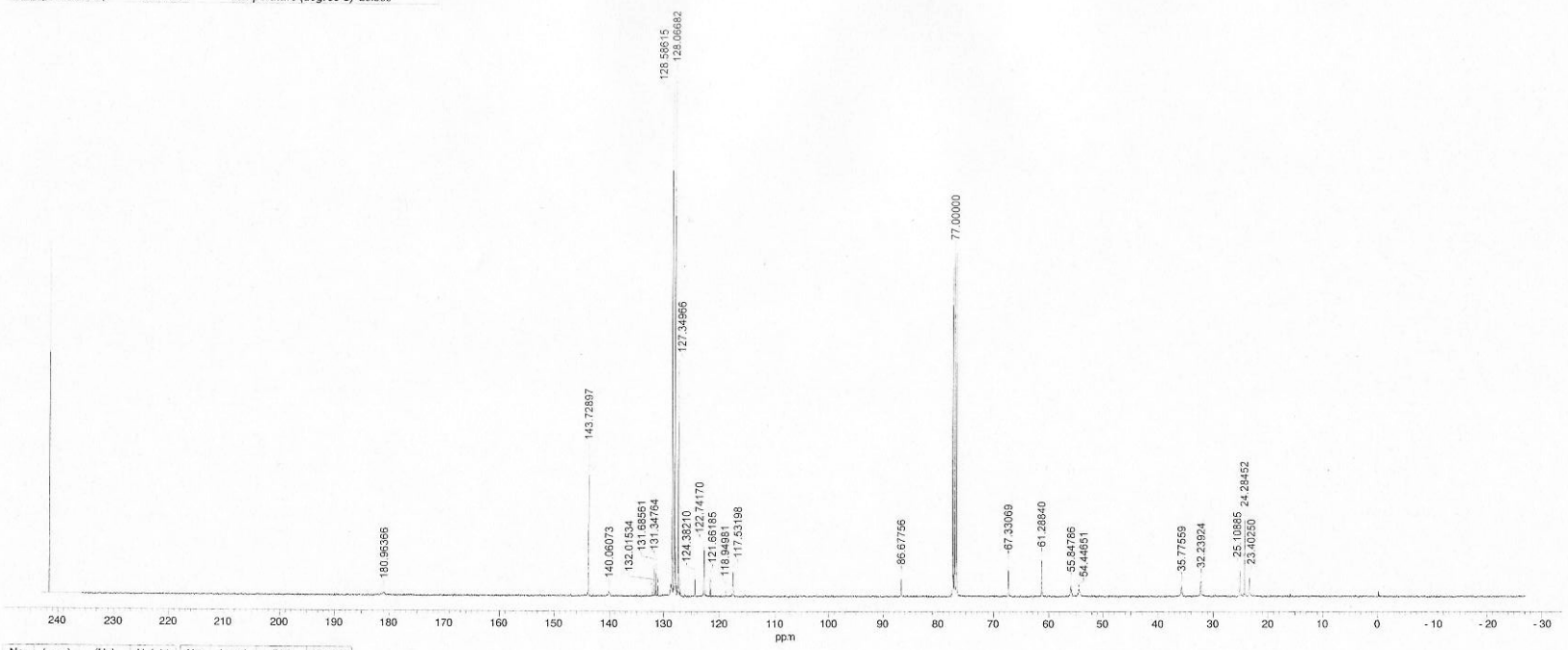


1e

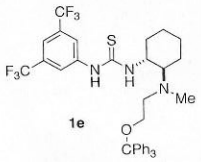
C:\Documents and Settings\Owner\My Documents\ R‰ª\YD71NON_E103_FT.als

17 Jul 2006
Tr

Acquisition Time (sec)	1.2083	*Comment*	Tr	*Date*	17 Jul 2006 03:32:40			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\Tr\Tr1BCM_E6_FT.als		
Frequency (MHz)	100.40	*Nucleus*	13C	*Number of Transients*	4096	*Original Points Count*	32768	*Points Count*	32768	*Pulse Sequence*	BCM	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	27118.64	*Temperature (degree C)*	20.300								



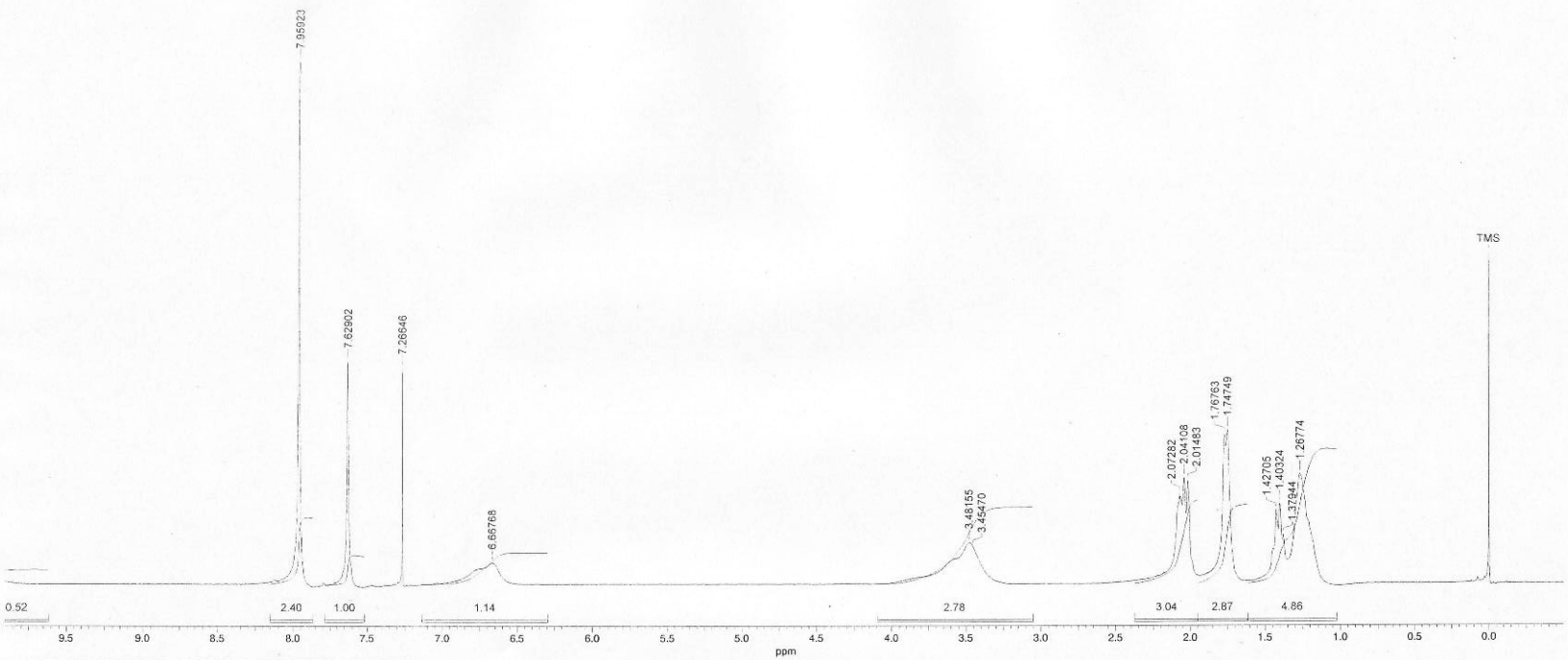
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	23.40	2349.6	0.0364	17	118.95	11942.6	0.0120
2	24.28	2438.2	0.1470	18	121.66	12214.8	0.0383
3	25.11	2520.9	0.0500	19	122.74	12323.3	0.0954
4	32.24	3236.8	0.0293	20	124.38	12488.0	0.0399
5	35.78	3591.9	0.0230	21	127.10	12761.1	0.0147
6	54.45	5466.4	0.0123	22	127.35	12785.9	0.4411
7	55.85	5607.1	0.0218	23	128.07	12857.9	1.0000
8	61.29	6153.4	0.0705	24	128.59	12910.0	0.9644
9	67.33	6760.0	0.0643	25	131.02	13154.2	0.0206
10	77.00	7730.8	0.6593	26	131.35	13187.3	0.0625
11	86.68	8702.4	0.0353	27	131.69	13221.2	0.0602
12	117.46	11792.8	0.0169	28	132.02	13254.3	0.0210
13	117.49	11796.1	0.0358	29	140.06	14062.1	0.0088
14	117.53	11800.2	0.0482	30	143.73	14430.4	0.2728
15	117.56	11803.5	0.0356	31	180.96	18168.8	0.0054
16	117.61	11807.7	0.0173				



1e

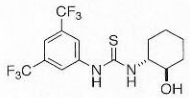
C:\Documents and Settings\Owner\My Documents\ R‰ª\Tr\Tr1BCM_E6_FT.als

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Thu Feb 22 05:25:15 2007			*File Name*	C:\Documents and Settings\–ò·ì® ¢%»Šw\ƒfƒXƒNƒgƒbƒv\NMR\NMR DATA\yamaoka\2H\2H.nmdata		
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000								



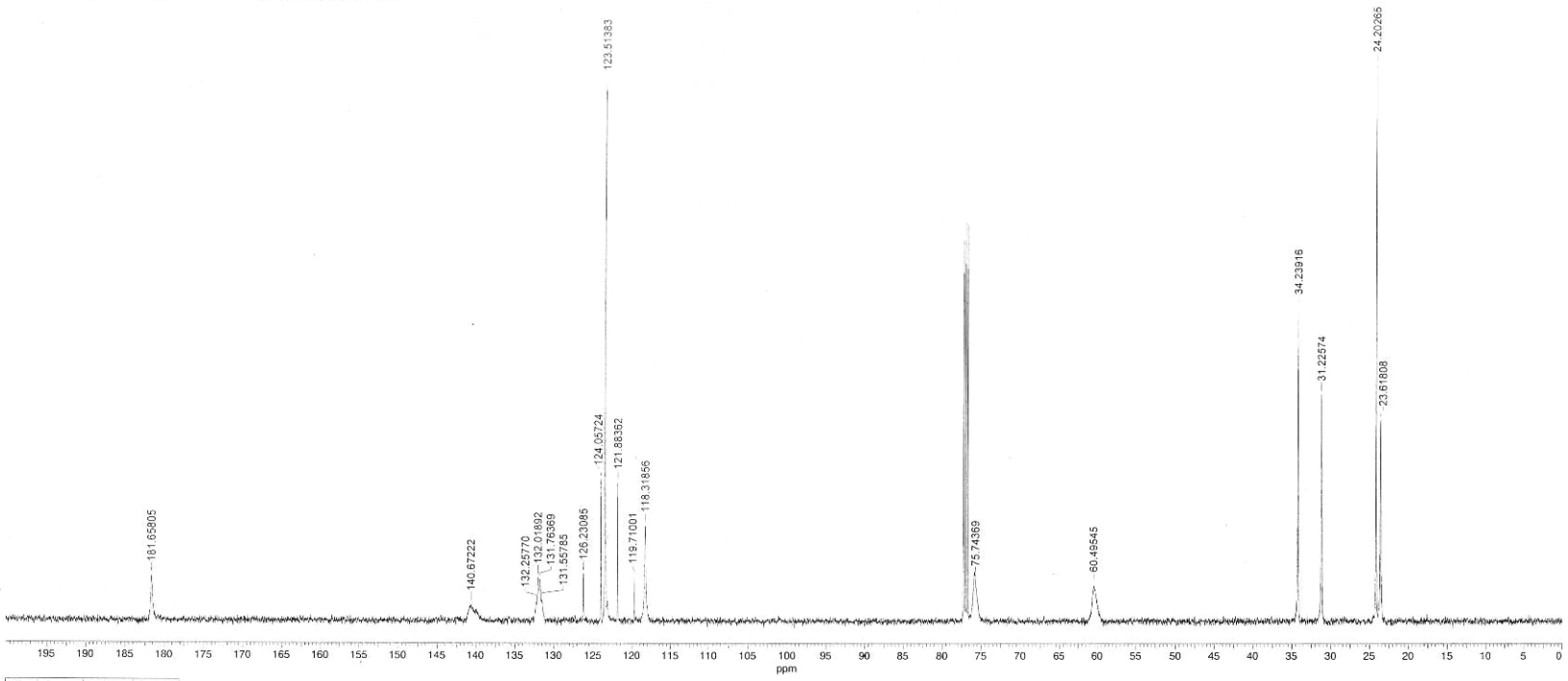
No.	(ppm)	(Hz)	Height
1	1.27	633.9	0.2099
2	1.38	689.7	0.0935
3	1.40	701.6	0.1533
4	1.43	713.5	0.1411
5	1.75	873.7	0.2939
6	1.77	883.8	0.2857
7	2.01	1007.4	0.1975
8	2.04	1020.5	0.2022
9	2.07	1036.4	0.1734
10	3.45	1727.3	0.0726
11	3.48	1740.8	0.0796
12	6.67	3333.8	0.0416
13	7.27	3633.2	0.4133
14	7.63	3814.5	0.4255
15	7.96	3979.6	1.0000
16	10.03	5014.2	0.0192

No.	(ppm)	Value	Absolute Value
1	[1.02 .. 1.61]	4.856	4.25131e+3
2	[1.61 .. 1.95]	2.875	2.51656e+3
3	[1.95 .. 2.38]	3.043	2.66369e+3
4	[3.05 .. 4.10]	2.781	2.43422e+3
5	[6.29 .. 7.14]	1.142	9.99472e+2
6	[7.52 .. 7.79]	1.000	8.75424e+2
7	[7.87 .. 8.15]	2.401	2.10174e+3
8	[9.62 .. 10.48]	0.520	4.55657e+2

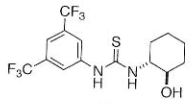


1f

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Thu Feb 22 09:10:12 2007			*File Name*	C:\Documents and Settings\–ôˆ¡ª ¤¾¤ÊŠw\ƒfƒXƒN\ƒofbƒ‹\NMR\NMR DATA\yamaoka\2C\2C.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	512	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000								

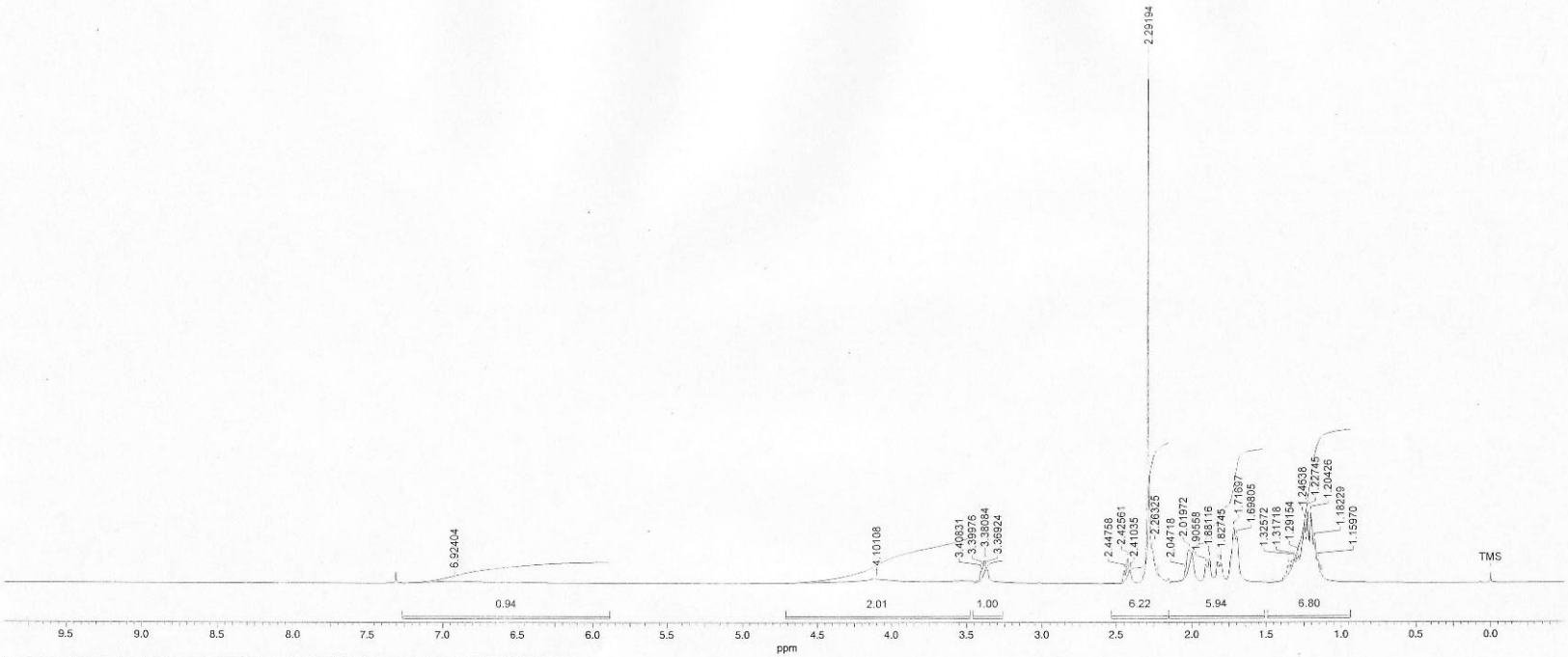


No.	(ppm)	(Hz)	Height
1	23.62	2967.6	0.3619
2	24.20	3041.1	1.0000
3	31.23	3923.5	0.4068
4	34.24	4302.2	0.5629
5	60.50	7601.3	0.0647
6	75.74	9517.2	0.0755
7	118.32	14866.7	0.1713
8	119.71	15041.6	0.0784
9	121.88	15314.7	0.2471
10	123.51	15519.5	0.9647
11	124.06	15587.8	0.2542
12	126.23	15860.9	0.0857
13	131.56	16530.2	0.0395
14	131.76	16556.1	0.0757
15	132.02	16588.2	0.0785
16	132.26	16618.2	0.0361
17	140.67	17675.5	0.0297
18	181.66	22825.3	0.0795



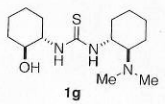
1f

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Thu Feb 22 06:09:48 2007			*File Name*	C:\Documents and Settings\		
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000								



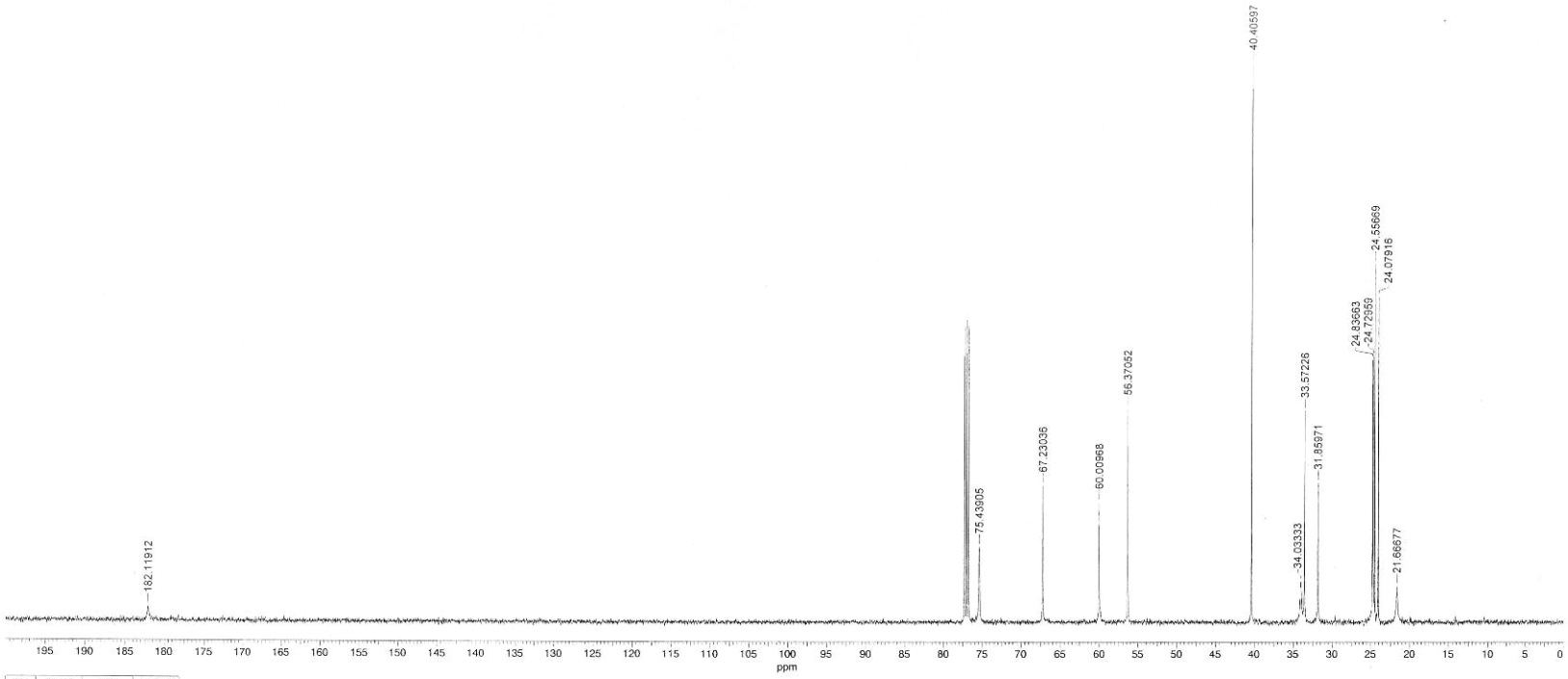
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.14	567.6	0.0173	18	2.02	1009.9	0.0632
2	1.16	579.9	0.0451	19	2.05	1023.6	0.0240
3	1.18	591.1	0.0824	20	2.22	1111.8	0.0181
4	1.20	602.1	0.1340	21	2.26	1131.6	0.0671
5	1.23	613.7	0.1391	22	2.29	1146.0	1.0000
6	1.25	623.2	0.1204	23	2.40	1202.1	0.0236
7	1.29	645.8	0.0551	24	2.41	1205.2	0.0251
8	1.32	658.6	0.0453	25	2.43	1212.8	0.0474
9	1.33	662.9	0.0431	26	2.45	1223.8	0.0243
10	1.35	677.2	0.0327	27	3.36	1680.0	0.0259
11	1.70	849.0	0.0883	28	3.37	1684.6	0.0305
12	1.72	858.5	0.1055	29	3.38	1690.4	0.0436
13	1.81	902.7	0.0378	30	3.39	1693.8	0.0426
14	1.83	913.7	0.0408	31	3.40	1699.9	0.0298
15	1.88	940.6	0.0463	32	3.41	1704.2	0.0238
16	1.89	947.3	0.0298	33	4.10	2050.5	0.0086
17	1.91	952.8	0.0358	34	6.92	3462.0	0.0039

No.	(ppm)	Value	Absolute Value
1	[0.94 .. 1.49]	6.799	4.12123e+3
2	[1.51 .. 2.15]	5.945	3.60327e+3
3	[2.15 .. 2.53]	6.219	3.76946e+3
4	[3.26 .. 3.46]	1.000	6.06132e+2
5	[3.48 .. 4.72]	2.012	1.21980e+3
6	[5.89 .. 7.26]	0.940	5.69785e+2

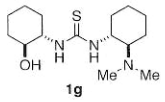


1g

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Thu Feb 22 06:36:00 2007			*File Name*	C:\Documents and Settings\~drix1~q%~$w\/f\X\fN\fg\fb\NMR\NMR DATA\yamaoka\3C\3C.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	512	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000								

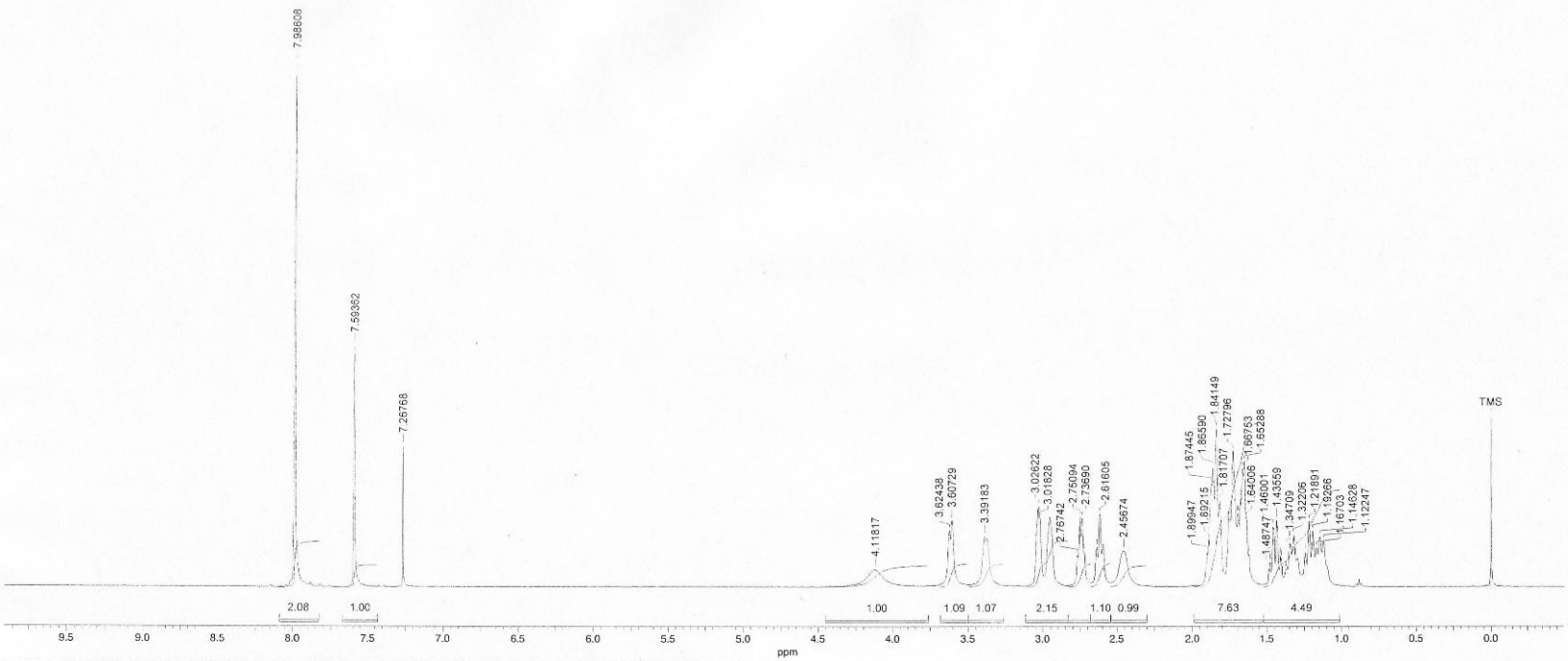


No.	(ppm)	(Hz)	Height
1	21.67	2722.4	0.0645
2	24.08	3025.5	0.5820
3	24.56	3085.5	0.6409
4	24.73	3107.3	0.4755
5	24.84	3120.7	0.4692
6	31.86	4003.2	0.2487
7	33.57	4218.4	0.3769
8	34.03	4276.3	0.0722
9	40.41	5077.0	1.0000
10	56.37	7083.0	0.3817
11	60.01	7540.2	0.2139
12	67.23	8447.5	0.2439
13	75.44	9478.9	0.1347
14	182.12	22883.3	0.0248



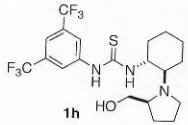
1g

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Thu Feb 22 07:06:18 2007			*File Name*	C:\Documents and Settings\~ÁÌ‚ g%~ŠwÌ‡fÌX‡N‡o‡b‡v\NMR\NMR DATA\yamaoka\4H\4H.nmdata		
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000								



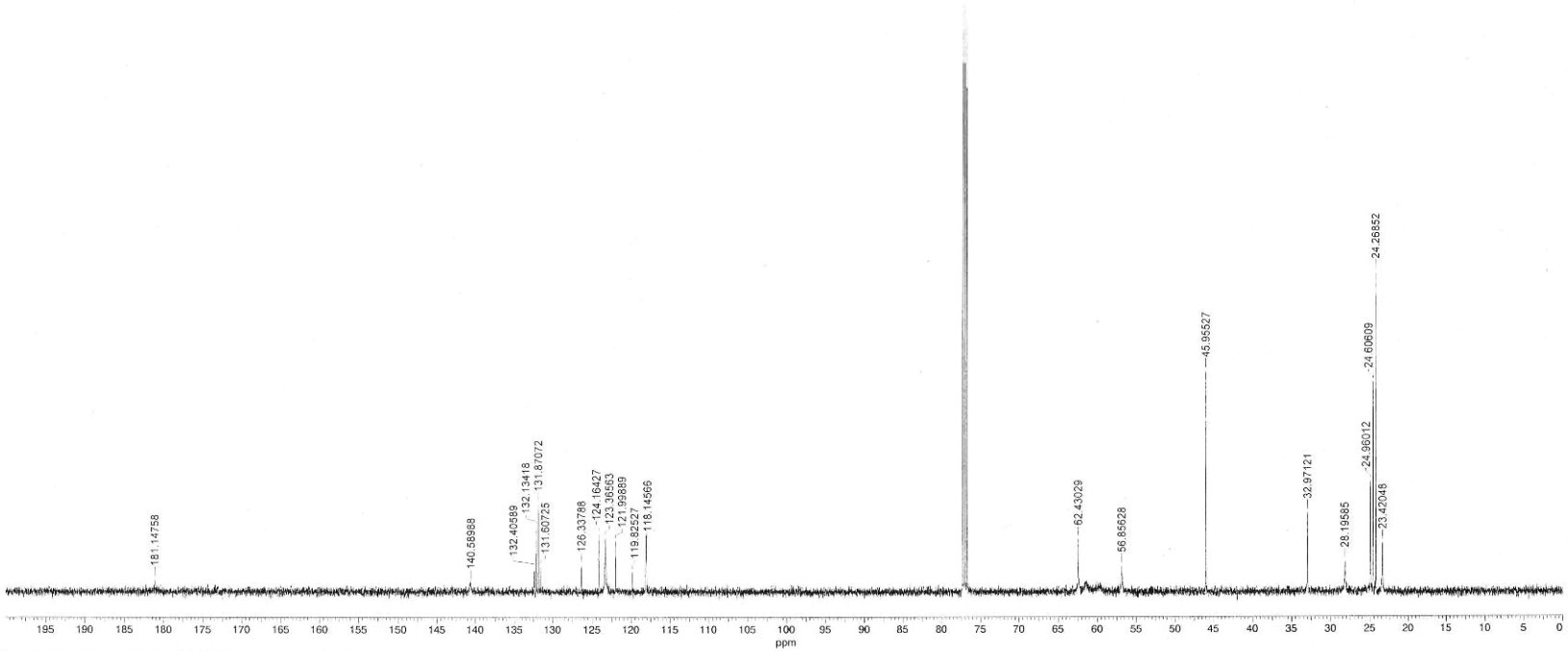
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.12	561.2	0.0877	17	1.49	743.7	0.0349	33	2.62	1308.0	0.1391
2	1.15	573.1	0.0955	18	1.62	810.9	0.0621	34	2.64	1318.4	0.0757
3	1.17	583.5	0.0746	19	1.64	820.0	0.1311	35	2.72	1360.5	0.0651
4	1.19	596.3	0.1067	20	1.65	826.4	0.2387	36	2.74	1368.5	0.1310
5	1.22	609.5	0.1248	21	1.67	833.8	0.2252	37	2.75	1375.5	0.1344
6	1.24	622.3	0.0657	22	1.68	840.5	0.1687	38	2.77	1383.7	0.0600
7	1.32	661.0	0.0999	23	1.70	848.4	0.1387	39	3.02	1509.1	0.1315
8	1.35	673.5	0.0831	24	1.73	864.0	0.2591	40	3.03	1513.1	0.1536
9	1.37	687.0	0.0336	25	1.82	908.5	0.1641	41	3.03	1517.1	0.1485
10	1.41	702.5	0.0538	26	1.84	920.7	0.3008	42	3.39	1695.9	0.0963
11	1.41	705.6	0.0586	27	1.86	930.2	0.2024	43	3.61	1803.6	0.1266
12	1.43	715.0	0.1163	28	1.87	933.0	0.2270	44	3.62	1812.2	0.1079
13	1.44	717.8	0.1268	29	1.87	937.2	0.1963	45	4.12	2059.1	0.0334
14	1.46	727.6	0.1121	30	1.89	946.1	0.0896	46	7.27	3633.8	0.2674
15	1.46	730.0	0.1158	31	1.90	949.7	0.0654	47	7.59	3796.8	0.4589
16	1.48	739.5	0.0468	32	2.46	1228.4	0.0690	48	7.99	3993.0	1.0000

No.	(ppm)	Value	Absolute Value
1	[1.01 .. 1.52]	4.486	4.09162e+3
2	[1.52 .. 1.99]	7.633	6.96155e+3
3	[2.30 .. 2.54]	0.989	9.02448e+2
4	[2.54 .. 2.68]	1.097	1.00039e+3
5	[2.68 .. 2.83]	1.064	9.70187e+2
6	[2.83 .. 3.12]	2.149	1.95957e+3
7	[3.26 .. 3.50]	1.073	9.78586e+2
8	[3.50 .. 3.68]	1.086	9.90568e+2
9	[3.76 .. 4.45]	1.005	9.16391e+2
10	[7.43 .. 7.67]	1.000	9.12076e+2
11	[7.83 .. 8.09]	2.081	1.89760e+3

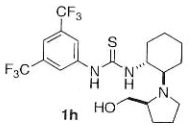


1h

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	22 Feb 2007 12:16:24			*File Name*	C:\Documents and Settings\–ô•ï•³ q‰=Šw\ƒfƒXƒNƒgƒbƒv\NMR\NMR DATA\yamaoka\4C\4C.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	1763	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000								



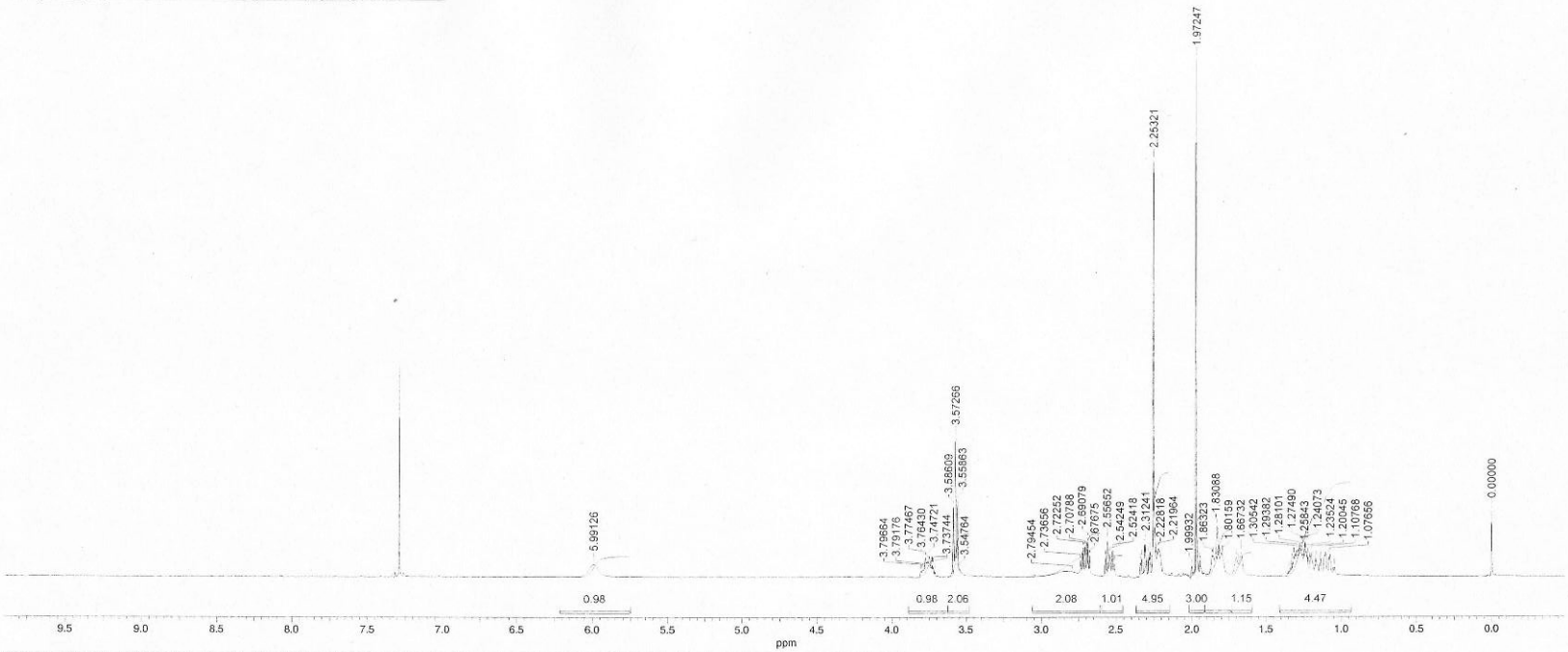
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	23.42	2942.8	0.0805	12	122.00	15329.2	0.0849
2	24.27	3049.3	0.5332	13	123.37	15500.9	0.0906
3	24.61	3091.8	0.3495	14	124.16	15601.2	0.0970
4	24.96	3136.2	0.1842	15	126.34	15874.4	0.0446
5	28.20	3542.8	0.0497	16	131.61	16536.5	0.0415
6	32.97	4142.8	0.1316	17	131.87	16569.6	0.1458
7	45.96	5774.3	0.3688	18	132.13	16602.7	0.1079
8	56.86	7144.0	0.0426	19	132.41	16636.8	0.0369
9	62.43	7844.4	0.0884	20	140.59	17665.1	0.0156
10	118.15	14845.0	0.0785	21	181.15	22761.2	0.0205
11	119.83	15056.0	0.0332				



1h

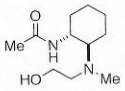
5 Jul 2006

Acquisition Time (sec)	4.1001	*Date*	05 Jul 2006 12:35:28			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD101NON_E105_FT.als			*Frequency (MHz)*	399.65
Nucleus	1H	*Number of Transients*	8	*Original Points Count*	32768	*Points Count*	32768	*Pulse Sequence*	NON	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	7992.01	*Temperature (degree C)*	19.600								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	-0.00	-0.0	0.1246	25	1.32	528.8	0.0271	49	2.25	900.5	0.8032	73	3.59	1434.4	0.1106
2	1.04	417.6	0.0179	26	1.33	529.8	0.0277	50	2.26	901.7	0.6601	74	3.71	1481.7	0.0097
3	1.05	421.2	0.0176	27	1.33	533.4	0.0165	51	2.28	910.0	0.0488	75	3.71	1483.4	0.0100
4	1.08	430.2	0.0433	28	1.34	534.6	0.0164	52	2.28	912.9	0.0416	76	3.72	1486.1	0.0146
5	1.09	433.9	0.0383	29	1.35	538.3	0.0109	53	2.30	921.0	0.0628	77	3.72	1488.5	0.0204
6	1.11	442.7	0.0465	30	1.67	666.3	0.0461	54	2.31	924.2	0.0629	78	3.73	1490.5	0.0233
7	1.11	445.4	0.0419	31	1.69	675.4	0.0271	55	2.33	932.4	0.0352	79	3.73	1492.2	0.0174
8	1.14	454.4	0.0349	32	1.70	679.8	0.0366	56	2.34	935.4	0.0278	80	3.74	1493.7	0.0187
9	1.15	457.8	0.0266	33	1.79	717.1	0.0426	57	2.51	1003.7	0.0255	81	3.75	1497.6	0.0414
10	1.17	467.1	0.0348	34	1.80	718.8	0.0455	58	2.52	1008.8	0.0508	82	3.75	1499.0	0.0374
11	1.18	470.2	0.0223	35	1.80	720.0	0.0455	59	2.54	1016.1	0.0435	83	3.76	1501.2	0.0296
12	1.20	479.8	0.0468	36	1.81	723.7	0.0381	60	2.56	1021.7	0.0688	84	3.76	1503.2	0.0289
13	1.21	482.9	0.0311	37	1.83	731.7	0.0973	61	2.57	1026.8	0.0365	85	3.76	1504.4	0.0309
14	1.22	489.0	0.0384	38	1.86	741.5	0.0396	62	2.68	1069.8	0.0402	86	3.77	1506.6	0.0283
15	1.23	490.5	0.0414	39	1.86	742.9	0.0393	63	2.69	1075.4	0.0734	87	3.77	1508.5	0.0373
16	1.24	493.7	0.0487	40	1.86	744.6	0.0410	64	2.71	1082.2	0.0577	88	3.79	1514.2	0.0137
17	1.24	495.9	0.0657	41	1.94	776.8	0.0228	65	2.72	1088.1	0.0557	89	3.79	1515.4	0.0145
18	1.25	497.6	0.0612	42	1.95	778.5	0.0301	66	2.74	1093.7	0.0313	90	3.80	1517.3	0.0122
19	1.26	502.9	0.0434	43	1.97	788.3	1.0000	67	2.79	1116.8	0.0101	91	3.80	1519.8	0.0121
20	1.27	509.5	0.0666	44	1.98	789.8	0.8385	68	3.55	1417.8	0.0165	92	3.81	1521.5	0.0097
21	1.28	512.0	0.0551	45	2.00	799.0	0.0210	69	3.56	1422.2	0.1466	93	5.99	2394.4	0.0243
22	1.29	517.1	0.0509	46	2.22	885.4	0.0513	70	3.56	1423.4	0.1327				

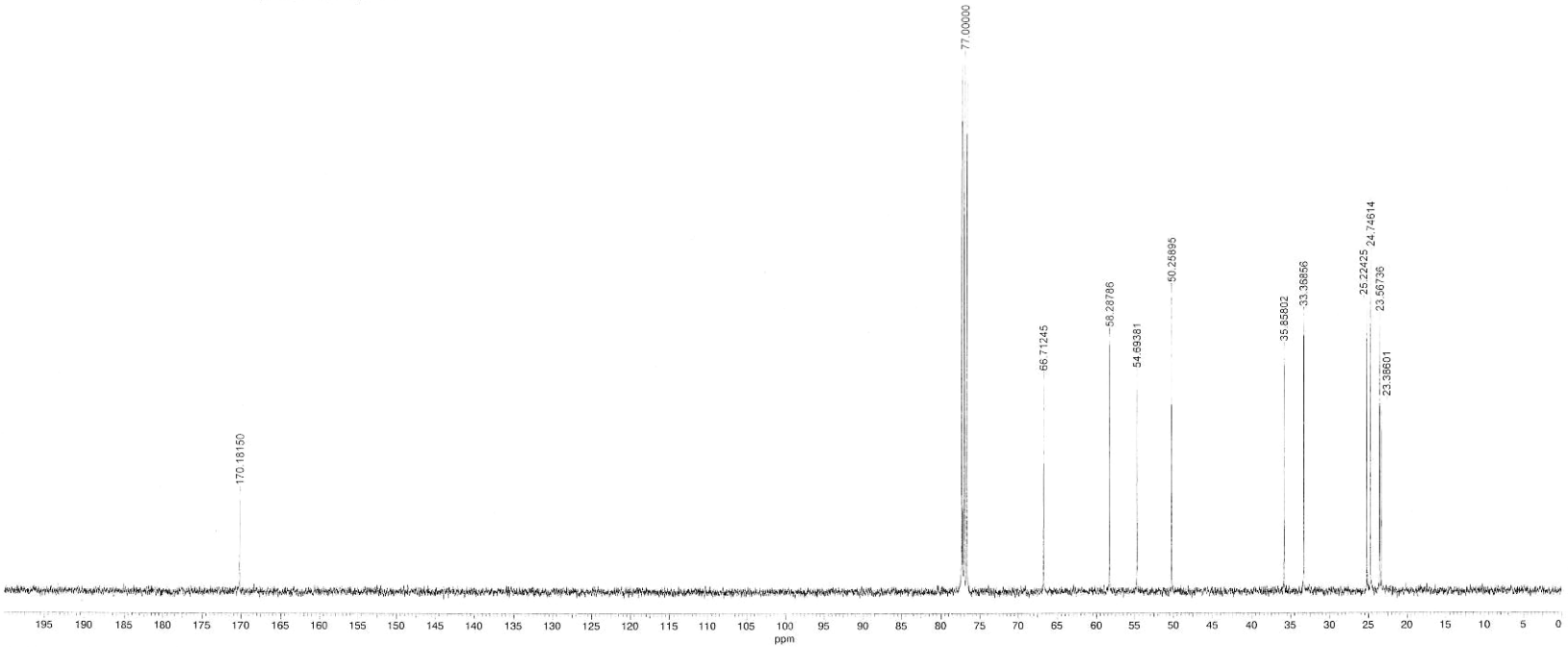
No.	(ppm)	Value	Absolute Value
1	[0.93 .. 1.41]	4.471	1.46383e+3
2	[1.60 .. 1.73]	1.148	3.75854e+2
3	[1.74 .. 1.91]	2.235	7.31631e+2
4	[1.92 .. 2.02]	3.000	9.82199e+2
5	[2.15 .. 2.37]	4.954	1.62181e+3
6	[2.46 .. 2.60]	1.013	3.31686e+2
7	[2.61 .. 3.06]	2.076	6.79583e+2
8	[3.48 .. 3.63]	2.058	6.73856e+2
9	[3.63 .. 3.89]	0.981	3.21147e+2
10	[5.75 .. 6.22]	0.975	3.19235e+2



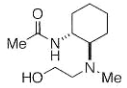
1i

5 Jul 2006

Acquisition Time (sec)	1.2083	*Date*	05 Jul 2006 12:34:00		*File Name*	C:\Documents and Settings\Owner\My Documents\ R%-®\YD10C1BCM_E110_FT.als			*Frequency (MHz)*	100.40
Nucleus	13C	*Number of Transients*	512	*Original Points Count*	32768	*Points Count*	32768	*Pulse Sequence*	BCM	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	27118.64	*Temperature (degree C)*	20.900								



No.	(ppm)	(Hz)	Height
1	23.39	2348.0	0.3404
2	23.57	2366.2	0.5011
3	24.75	2484.5	0.6242
4	25.22	2532.5	0.5326
5	33.37	3350.2	0.5116
6	35.86	3600.1	0.4452
7	50.26	5046.0	0.5568
8	54.69	5491.3	0.3949
9	58.29	5852.1	0.4722
10	66.71	6697.9	0.3901
11	77.00	7730.8	0.9979
12	170.18	17086.2	0.1729



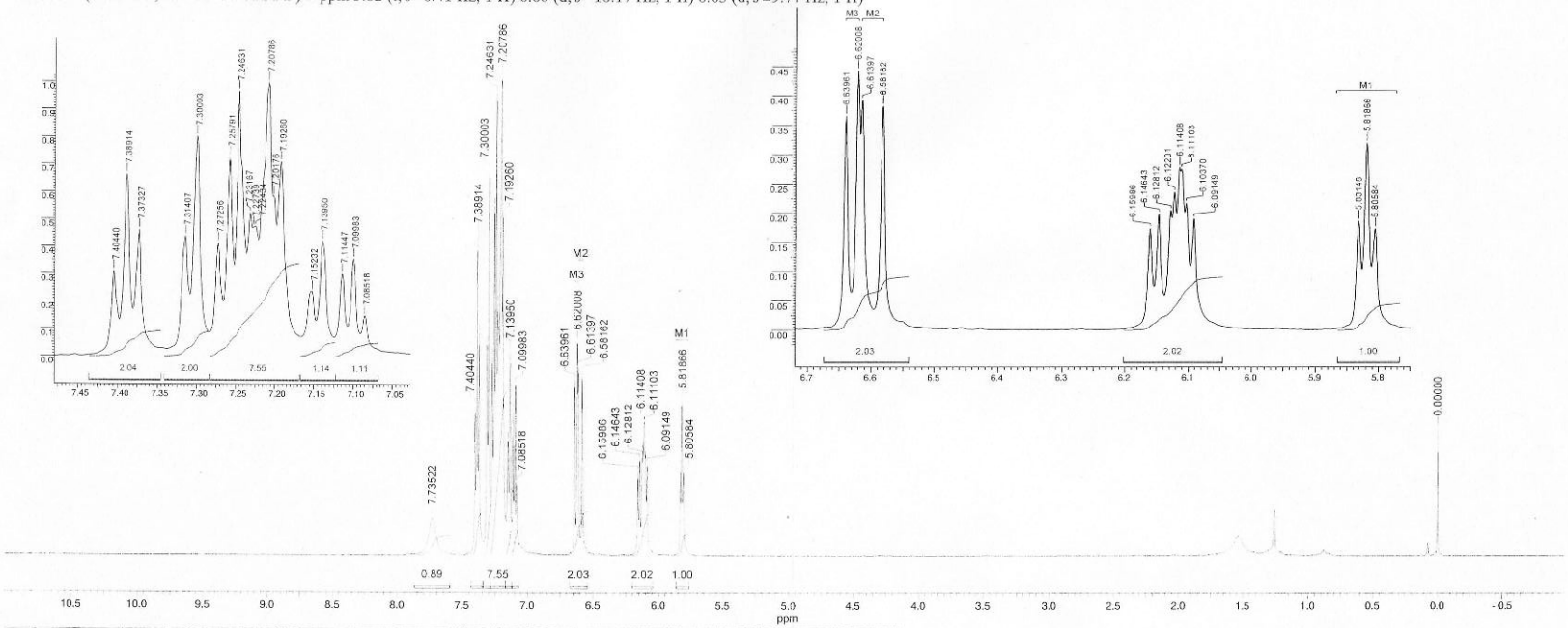
1i

C:\Documents and Settings\Owner\My Documents\ R%-®\YD10C1BCM_E110_FT.als

8 Oct 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Sun Oct 8 05:35:54 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\Š˜–ØŒ˜\ik0105pro2\ik0105pro2.nmdata
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	16	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D

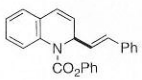
1H NMR (500 MHz, CHLOROFORM-D) d ppm 5.82 (t, *J*=6.41 Hz, 1 H) 6.60 (d, *J*=16.17 Hz, 1 H) 6.63 (d, *J*=9.77 Hz, 1 H)



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	-0.00	-0.0	0.2636	19	7.11	3557.2	0.3015
2	5.81	2902.9	0.1742	20	7.14	3569.8	0.4235
3	5.82	2909.3	0.3208	21	7.15	3576.2	0.2385
4	5.83	2915.7	0.1870	22	7.19	3596.3	0.7111
5	6.09	3045.7	0.1908	23	7.20	3600.9	0.5850
6	6.10	3051.9	0.2176	24	7.21	3603.9	1.0000
7	6.11	3055.5	0.2755	25	7.22	3612.2	0.4762
8	6.11	3057.0	0.2787	26	7.23	3613.7	0.4732
9	6.12	3061.0	0.2363	27	7.23	3615.8	0.5244
10	6.13	3064.1	0.2056	28	7.25	3623.2	0.9672
11	6.15	3073.2	0.1994	29	7.26	3629.0	0.7280
12	6.16	3079.9	0.1741	30	7.27	3636.3	0.4137
13	6.58	3290.8	0.3825	31	7.30	3650.0	0.8030
14	6.61	3307.0	0.3929	32	7.31	3657.0	0.4393
15	6.62	3310.0	0.4432	33	7.37	3686.6	0.4623
16	6.64	3319.8	0.3660	34	7.39	3694.6	0.6658
17	7.09	3542.6	0.1496	35	7.40	3702.2	0.3118
18	7.10	3549.9	0.3574	36	7.74	3867.6	0.0766

No.	(ppm)	Value	Absolute Value
1	[5.77 .. 5.86]	1.000	7.10081e+2
2	[6.05 .. 6.20]	2.018	1.43320e+3
3	[6.54 .. 6.67]	2.032	1.44299e+3
4	[7.07 .. 7.12]	1.107	7.86160e+2
5	[7.12 .. 7.17]	1.144	8.12449e+2
6	[7.17 .. 7.28]	7.546	5.35811e+3
7	[7.28 .. 7.34]	2.004	1.42302e+3
8	[7.35 .. 7.44]	2.036	1.44550e+3
9	[7.60 .. 7.87]	0.892	6.33291e+2

No.	Multiplet1	Shift1	(ppm)	J (Hz)	Type	H's
1	M1	5.82	[5.77 .. 5.87]	6.41	t	1
2	M1	5.82	[5.77 .. 5.87]	6.41	t	1
3	M2	6.60	[6.58 .. 6.61]	16.17	d	1
4	M3	6.63	[6.62 .. 6.64]	9.77	d	1

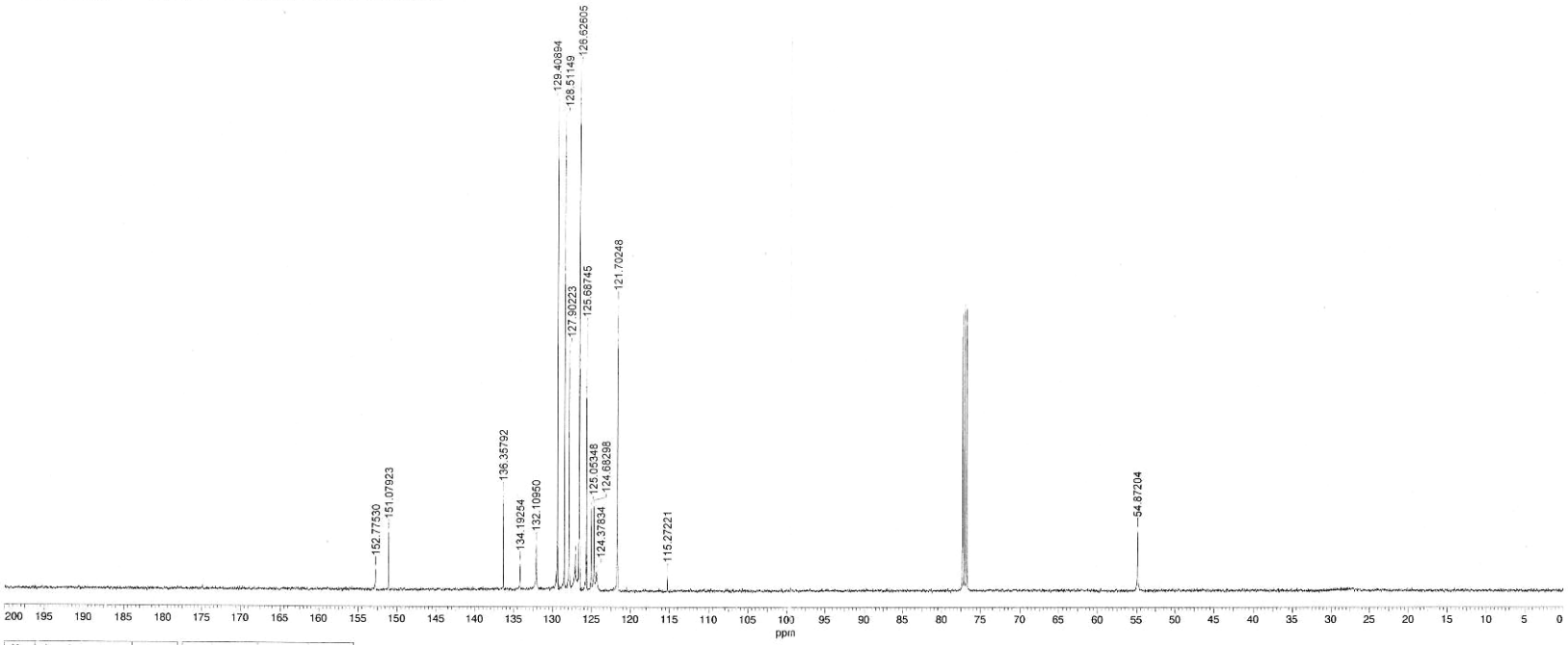


5a

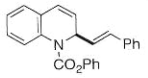
C:\Documents and Settings\Owner\My Documents\Š˜–ØŒ˜\ik0105pro2\ik0105pro2.nmdata

18 May 2006
noe

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Tue May 16 08:30:00 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\1\1.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	1024	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	54.87	6894.7	0.1177	11	127.11	15971.6	0.0710
2	115.27	14484.0	0.0301	12	127.90	16070.9	0.4598
3	121.70	15291.9	0.5502	13	128.51	16147.5	0.9034
4	124.38	15628.1	0.0379	14	129.41	16260.2	0.9324
5	124.68	15666.4	0.1632	15	132.11	16599.6	0.0883
6	125.05	15713.0	0.1580	16	134.19	16861.3	0.0512
7	125.69	15792.6	0.4995	17	136.36	17133.4	0.1847
8	125.70	15794.7	0.4753	18	151.08	18983.1	0.1117
9	126.57	15903.3	0.4717	19	152.78	19196.2	0.0408
10	126.63	15910.6	1.0000				



5a

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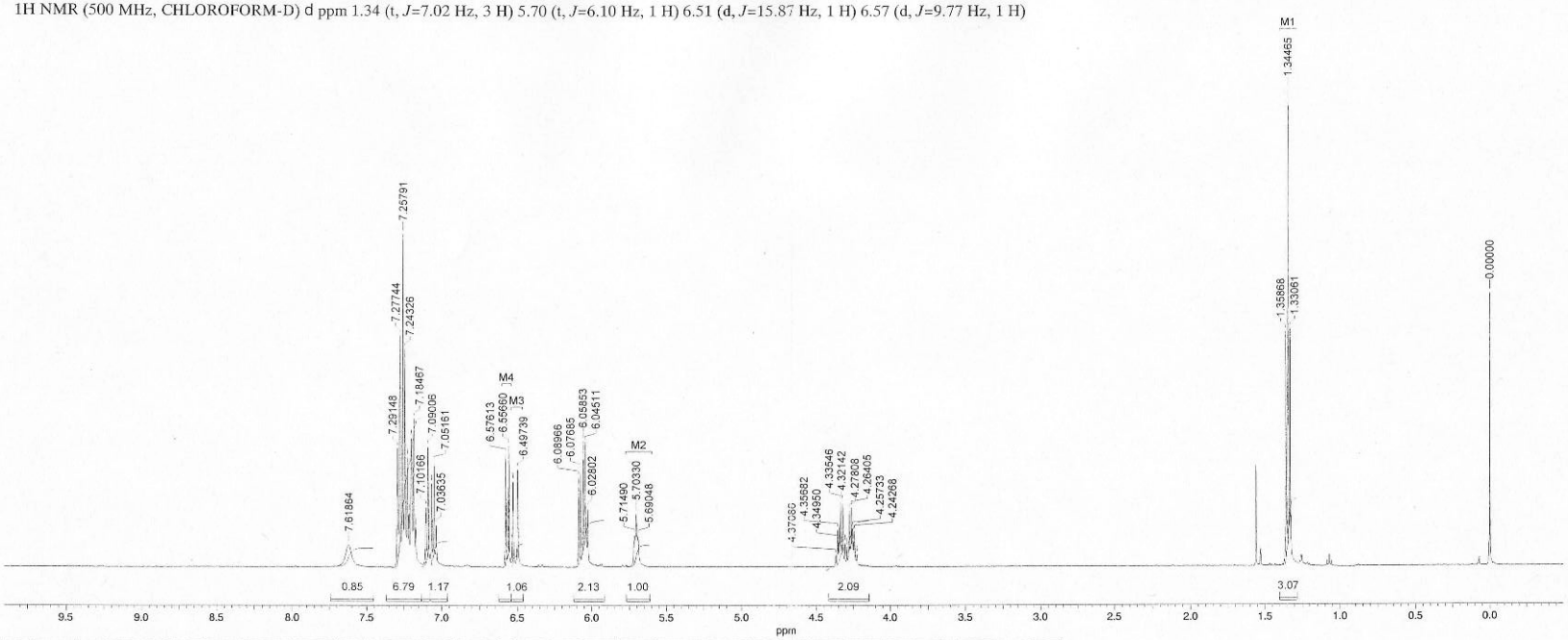
1 May 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Mon May 1 16:39:19 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰"\296-1\296-1.nmdata		
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	2	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000								

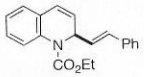
1H NMR (500 MHz, CHLOROFORM-D) d ppm 1.34 (t, *J*=7.02 Hz, 3 H) 5.70 (t, *J*=6.10 Hz, 1 H) 6.51 (d, *J*=15.87 Hz, 1 H) 6.57 (d, *J*=9.77 Hz, 1 H)



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.5722	19	4.36	2178.4	0.0780	37	7.09	3543.5	0.2237
2	1.33	665.3	0.4984	20	4.37	2185.4	0.0235	38	7.09	3545.0	0.2519
3	1.34	672.3	1.0000	21	5.69	2845.2	0.0654	39	7.10	3550.8	0.1255
4	1.36	679.3	0.4932	22	5.70	2851.6	0.1131	40	7.11	3552.7	0.1138
5	4.23	2114.3	0.0268	23	5.71	2857.4	0.0664	41	7.17	3585.0	0.0828
6	4.24	2121.3	0.0745	24	6.03	3014.0	0.1234	42	7.18	3592.3	0.3119
7	4.25	2125.0	0.0544	25	6.04	3020.4	0.1353	43	7.19	3594.5	0.1907
8	4.26	2128.7	0.0818	26	6.05	3022.6	0.2622	44	7.20	3599.7	0.2685
9	4.26	2132.0	0.1254	27	6.06	3029.3	0.2649	45	7.20	3600.9	0.2695
10	4.27	2135.4	0.0432	28	6.08	3038.4	0.2038	46	7.22	3608.2	0.1129
11	4.28	2139.0	0.1174	29	6.09	3044.8	0.1897	47	7.22	3609.7	0.1097
12	4.29	2146.4	0.0427	30	6.50	3248.7	0.2060	48	7.23	3614.0	0.2302
13	4.31	2153.4	0.0491	31	6.53	3264.6	0.1795	49	7.24	3621.6	0.4571
14	4.32	2160.7	0.1331	32	6.56	3278.3	0.2548	50	7.26	3629.0	0.6996
15	4.33	2164.1	0.0454	33	6.58	3288.1	0.2358	51	7.28	3638.7	0.4865
16	4.34	2167.7	0.1367	34	7.04	3518.2	0.0870	52	7.29	3645.7	0.2497
17	4.34	2171.1	0.0877	35	7.05	3525.8	0.2187	53	7.29	3647.3	0.1741
18	4.35	2174.7	0.0531	36	7.07	3533.1	0.1752	54	7.62	3809.3	0.0459

No.	(ppm)	Value	Absolute Value
1	[1.28 .. 1.40]	3.066	2.51255e+3
2	[4.14 .. 4.42]	2.087	1.71029e+3
3	[5.61 .. 5.77]	1.000	8.19426e+2
4	[5.92 .. 6.12]	2.132	1.74673e+3
5	[6.46 .. 6.54]	1.057	8.66129e+2
6	[6.54 .. 6.63]	0.981	8.03952e+2
7	[6.96 .. 7.08]	1.169	9.58339e+2
8	[7.08 .. 7.13]	1.019	8.35168e+2
9	[7.13 .. 7.37]	6.786	5.56098e+3
10	[7.45 .. 7.74]	0.846	6.92885e+2

No.	Multiplet1	Shift1	(ppm)	J (Hz)	Type	H's
1	M1	1.34	[1.29 .. 1.40]	7.02	t	3
2	M1	1.34	[1.29 .. 1.40]	7.02	t	3
3	M2	5.69	[5.60 .. 5.78]	6.10	t	1
4	M2	5.69	[5.60 .. 5.78]	6.10	t	1
5	M3	6.50	[6.47 .. 6.54]	15.87	d	1
6	M4	6.57	[6.54 .. 6.61]	9.77	d	1



5b

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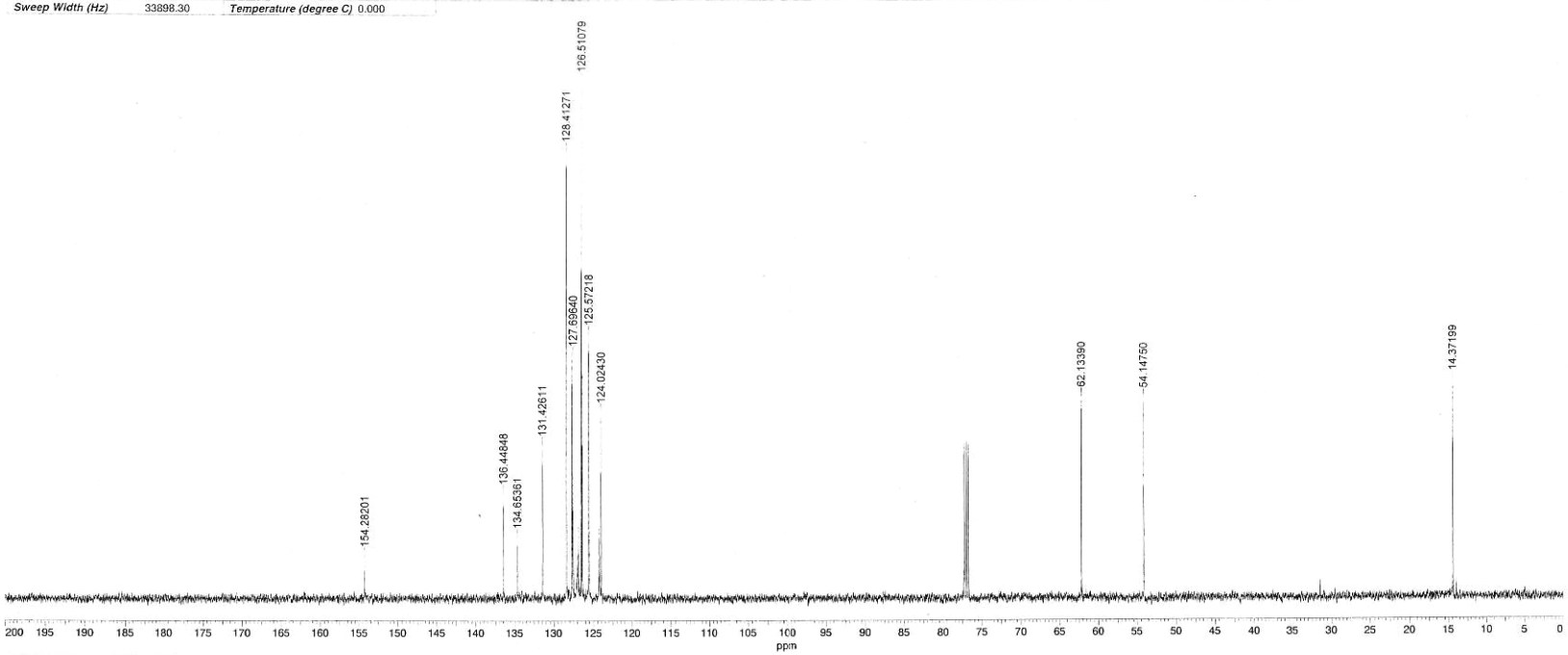
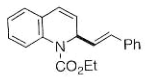
Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	20 May 2006 03:42:12			*File Name*	C:\Documents and Settings\Owner\My Documents\ R%-ᴿ\Et\Et.nmdata
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	29	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height
1	14.37	1805.8	0.4123
2	54.15	6803.6	0.3811
3	62.13	7807.1	0.3833
4	124.02	15583.7	0.3546
5	124.25	15611.6	0.1199
6	125.57	15778.1	0.5066
7	126.39	15880.6	0.4379
8	126.51	15896.1	1.0000
9	126.86	15939.5	0.1242
10	127.06	15965.4	0.0684
11	127.58	16030.6	0.2446
12	127.70	16045.1	0.4655
13	128.41	16135.1	0.8639
14	131.43	16513.7	0.2906
15	134.65	16919.2	0.1113
16	136.45	17144.8	0.1965
17	154.28	19385.5	0.0746



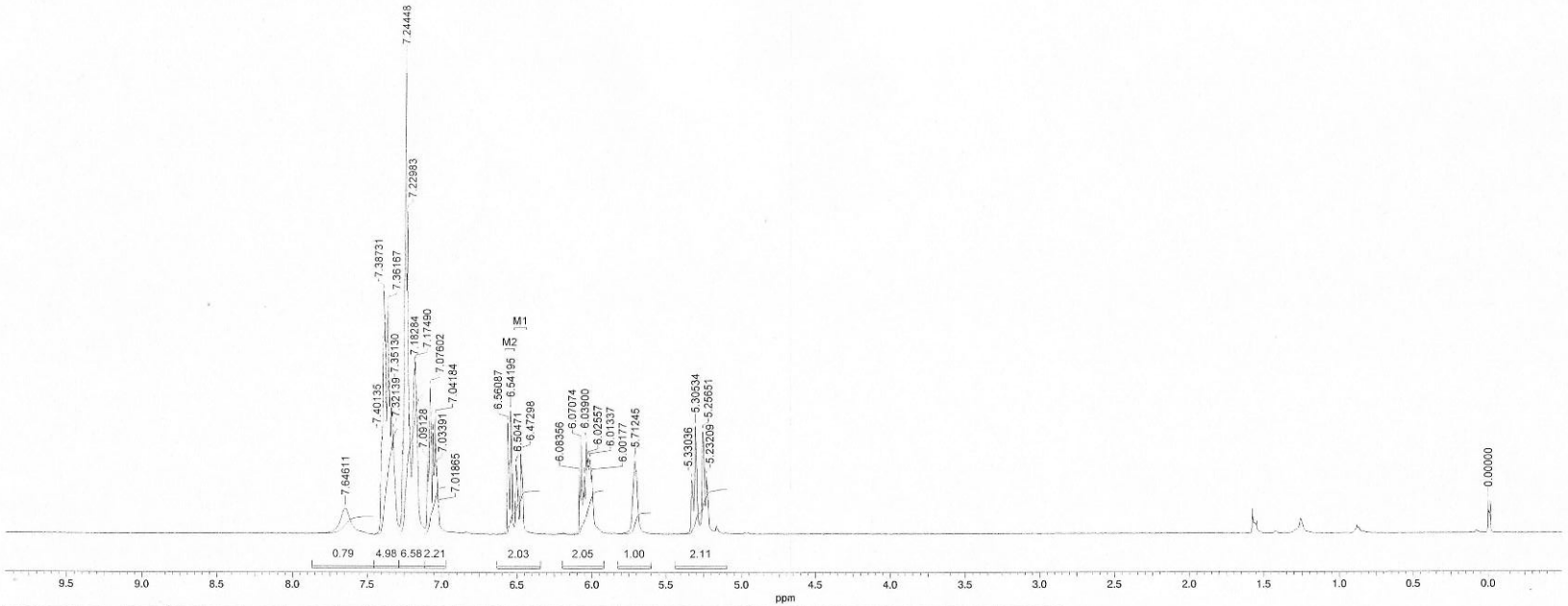
5b

C:\Documents and Settings\Owner\My Documents\ R%-ᴿ\Et\Et.nmdata

1 May 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Mon May 1 16:44:40 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\296-3\296-3.nmdata		
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	2	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000								

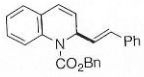
1H NMR (500 MHz, CHLOROFORM-D) d ppm 6.49 (d, *J*=15.87 Hz, 1 H) 6.55 (d, *J*=9.46 Hz, 1 H)



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.0676	15	6.07	3035.4	0.1935	29	7.22	3607.9	0.2512
2	5.23	2616.0	0.1199	16	6.08	3041.8	0.1247	30	7.23	3614.9	0.6777
3	5.26	2628.3	0.2157	17	6.47	3236.5	0.1694	31	7.23	3617.1	0.5464
4	5.31	2652.7	0.2265	18	6.50	3252.4	0.1456	32	7.24	3622.2	1.0000
5	5.33	2665.2	0.1138	19	6.54	3271.0	0.2597	33	7.26	3630.8	0.1762
6	5.71	2856.2	0.1538	20	6.56	3280.4	0.2341	34	7.32	3660.7	0.2170
7	6.00	3000.9	0.1233	21	7.02	3509.3	0.0588	35	7.34	3667.7	0.2661
8	6.01	3006.7	0.1569	22	7.03	3517.0	0.1431	36	7.35	3673.8	0.3013
9	6.02	3009.7	0.1429	23	7.04	3520.9	0.2467	37	7.35	3675.6	0.3095
10	6.03	3012.8	0.1602	24	7.06	3528.2	0.2116	38	7.36	3680.8	0.4848
11	6.03	3015.5	0.1561	25	7.08	3538.0	0.3090	39	7.38	3689.1	0.4435
12	6.04	3019.5	0.1942	26	7.09	3545.6	0.1521	40	7.39	3693.7	0.5098
13	6.05	3025.9	0.1214	27	7.17	3587.5	0.3616	41	7.40	3700.7	0.2028
14	6.06	3028.7	0.0867	28	7.18	3591.4	0.3464	42	7.65	3823.1	0.0525

No.	(ppm)	Value	Absolute Value
1	[5.10 .. 5.44]	2.107	1.17049e+3
2	[5.60 .. 5.83]	1.000	5.55527e+2
3	[5.92 .. 6.20]	2.053	1.14059e+3
4	[6.34 .. 6.63]	2.034	1.12989e+3
5	[6.97 .. 7.11]	2.214	1.22971e+3
6	[7.11 .. 7.28]	6.576	3.65330e+3
7	[7.28 .. 7.45]	4.977	2.76478e+3
8	[7.45 .. 7.87]	0.792	4.40049e+2

No.	Multiplet1	Shift1	(ppm)	J (Hz)	Type	H's
1	M1	6.48	[6.44 .. 6.52]	15.87	d	1
2	M2	6.55	[6.52 .. 6.58]	9.46	d	1



5c

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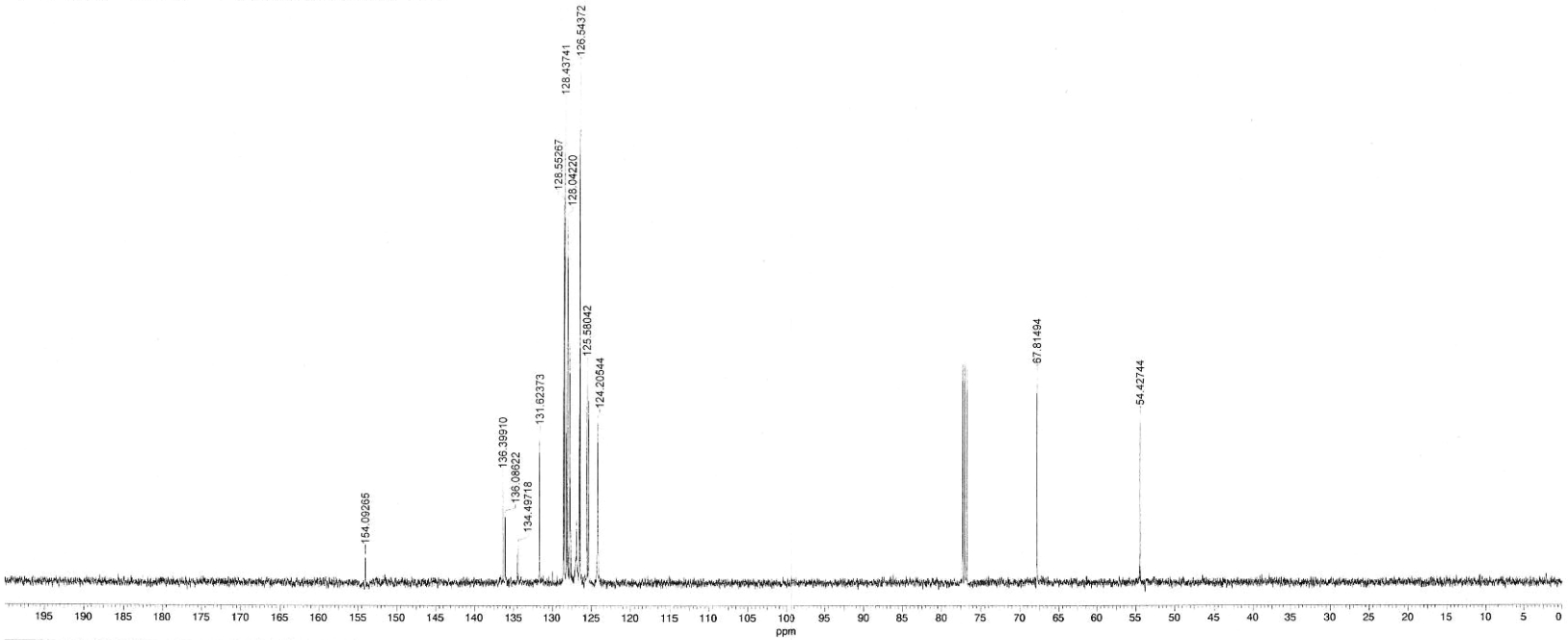
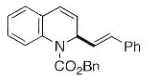
24 May 2006
noe

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Wed May 24 04:25:30 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD14-C\YD14-C.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	67	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	54.43	6838.8	0.3197	11	128.04	16088.5	0.7077
2	67.81	8520.9	0.4019	12	128.17	16104.0	0.4474
3	124.21	15606.4	0.3137	13	128.44	16138.2	0.9243
4	125.41	15757.5	0.3550	14	128.55	16152.6	0.7391
5	125.58	15779.2	0.4152	15	131.62	16538.5	0.2806
6	126.44	15886.8	0.4580	16	134.50	16899.6	0.0717
7	126.54	15900.2	1.0000	17	136.09	17099.2	0.1288
8	126.87	15941.6	0.1054	18	136.40	17138.5	0.1967
9	127.69	16044.0	0.1872	19	154.09	19361.7	0.0487
10	127.76	16053.3	0.4480				

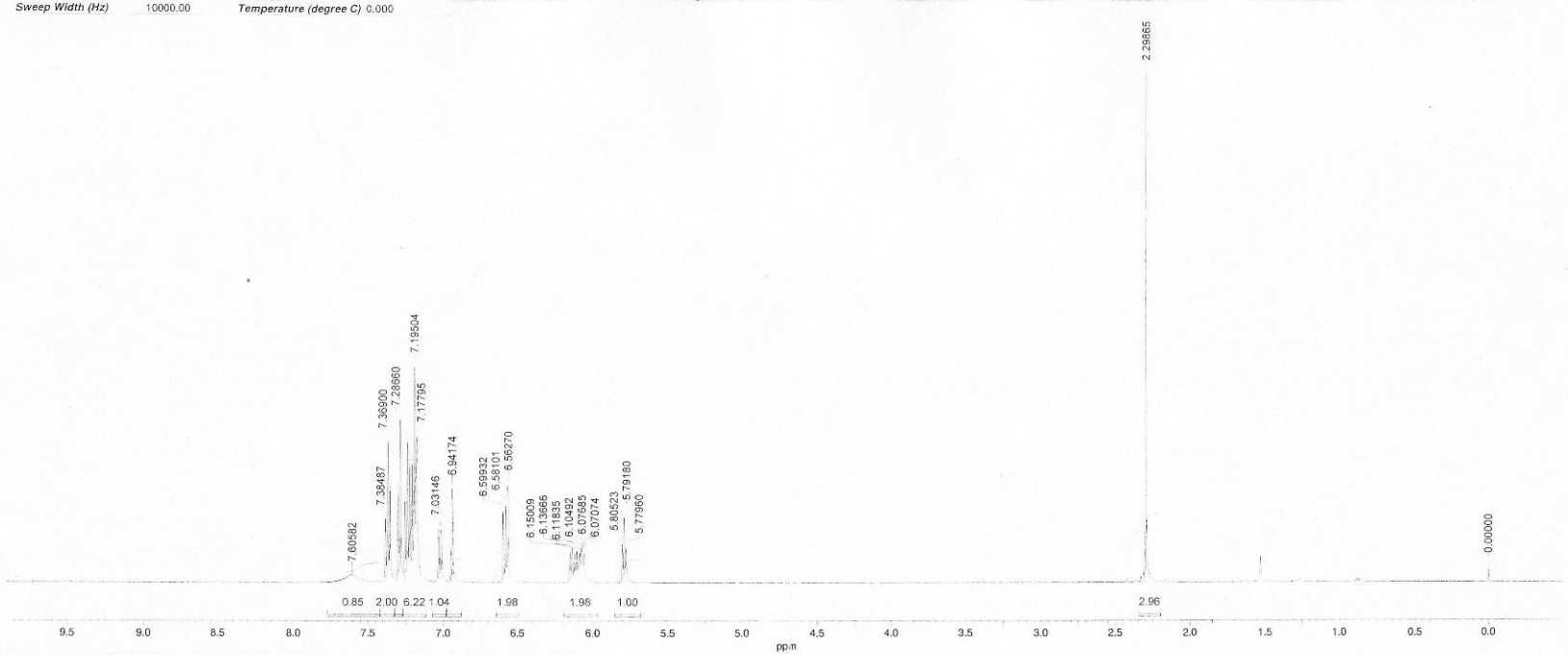


5c

C:\Documents and Settings\Owner\My Documents\ R‰ª\YD14-C\YD14-C.nmdata

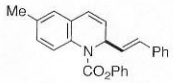
26 Sep 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Tue Sep 26 14:02:40 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R%‰\YD-26HH\YD-26HH.nmdata
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Coun*	32768	*Points Count*	32768
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.0293	17	6.60	3299.7	0.1432
2	2.30	1149.3	1.0000	18	6.94	3470.9	0.1843
3	5.78	2889.8	0.0703	19	7.01	3507.5	0.1035
4	5.79	2895.9	0.1361	20	7.03	3515.7	0.1066
5	5.81	2902.6	0.0761	21	7.18	3589.0	0.2887
6	6.06	3029.0	0.0576	22	7.20	3597.5	0.4248
7	6.07	3035.4	0.0641	23	7.21	3605.2	0.2322
8	6.08	3038.4	0.0690	24	7.23	3612.8	0.2428
9	6.09	3044.5	0.0583	25	7.24	3620.7	0.2856
10	6.10	3052.5	0.0641	26	7.26	3628.0	0.1603
11	6.12	3059.2	0.0581	27	7.29	3643.3	0.3203
12	6.14	3068.3	0.0692	28	7.30	3650.6	0.1780
13	6.15	3075.0	0.0621	29	7.35	3676.9	0.1954
14	6.56	3281.4	0.1938	30	7.37	3684.5	0.2756
15	6.57	3283.5	0.1902	31	7.38	3692.4	0.1254
16	6.58	3290.5	0.1556	32	7.61	3802.9	0.0151

No.	(ppm)	Value	Absolute Value
1	[2.20 .. 2.35]	2.965	2.01606e+3
2	[5.68 .. 5.86]	1.000	6.80044e+2
3	[5.97 .. 6.19]	1.978	1.34549e+3
4	[6.49 .. 6.64]	1.983	1.34846e+3
5	[6.88 .. 6.98]	1.012	6.88107e+2
6	[6.98 .. 7.07]	1.042	7.08709e+2
7	[7.11 .. 7.27]	6.218	4.22864e+3
8	[7.27 .. 7.32]	1.930	1.31263e+3
9	[7.32 .. 7.42]	1.997	1.35830e+3
10	[7.42 .. 7.77]	0.853	5.80328e+2

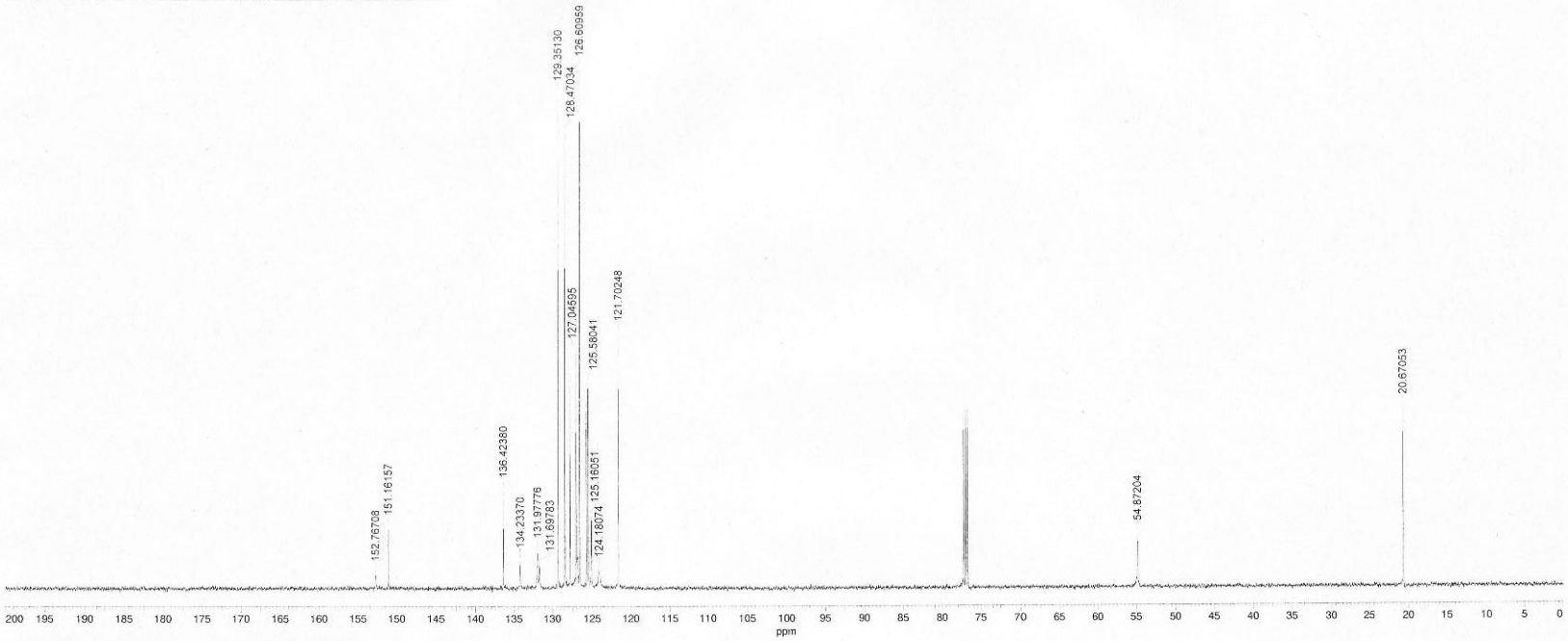


6bA

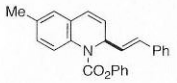
C:\Documents and Settings\Owner\My Documents\ R%‰\YD-26HH\YD-26HH.nmdata

26 Sep 2006
noe

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	26 Sep 2006 14:54:36			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD-26CC\YD-26CC.nmdata
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	262	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	20.67	2597.3	0.3418	11	127.84	16062.6	0.3908
2	54.87	6894.7	0.1015	12	128.47	16142.3	0.8816
3	121.70	15291.9	0.4888	13	129.35	16253.0	0.9524
4	124.18	15603.3	0.0353	14	131.70	16547.8	0.0462
5	125.16	15726.4	0.1404	15	131.98	16583.0	0.0718
6	125.58	15779.2	0.3946	16	134.23	16866.5	0.0520
7	125.75	15800.9	0.3417	17	136.42	17141.7	0.1884
8	126.61	15908.5	1.0000	18	151.16	18993.5	0.1164
9	126.93	15948.8	0.0646	19	152.77	19195.2	0.0270
10	127.05	15963.3	0.4550				

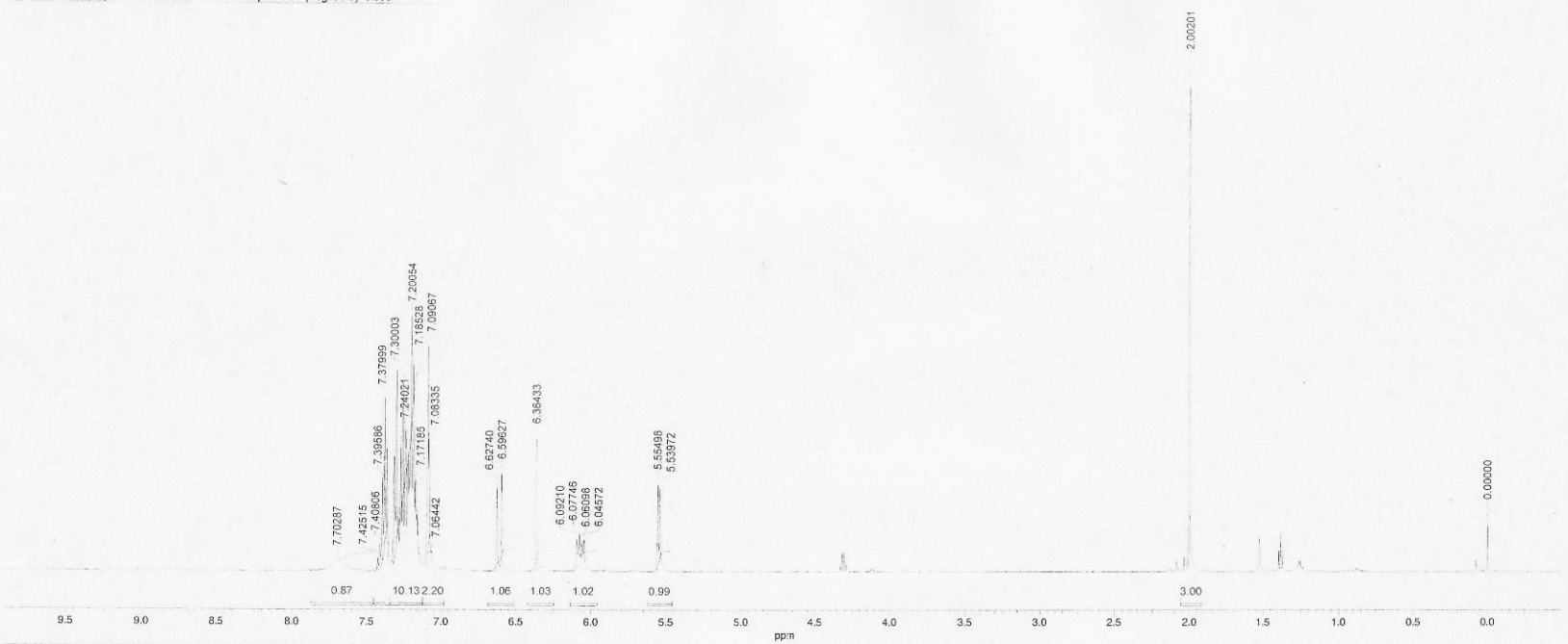


6bA

C:\Documents and Settings\Owner\My Documents\ R‰ª\YD-26CC\YD-26CC.nmdata

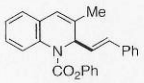
15 Sep 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Fri Sep 15 04:26:17 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R%-ª\YD-25H\YD-25H.nmdata		
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	-0.00	-0.0	0.1154	20	7.17	3585.9	0.1799
2	2.00	1001.0	1.0000	21	7.19	3592.6	0.4165
3	5.54	2769.9	0.1695	22	7.20	3600.3	0.5015
4	5.55	2777.5	0.1741	23	7.21	3607.3	0.1924
5	6.05	3022.9	0.0628	24	7.22	3611.3	0.2163
6	6.06	3030.5	0.0621	25	7.24	3618.3	0.2617
7	6.08	3038.7	0.0738	26	7.24	3620.1	0.2735
8	6.09	3046.1	0.0656	27	7.26	3628.0	0.3710
9	6.36	3182.2	0.2634	28	7.27	3635.1	0.2495
10	6.60	3298.1	0.1939	29	7.28	3642.4	0.1041
11	6.63	3313.7	0.1728	30	7.30	3650.0	0.3939
12	7.06	3532.2	0.0409	31	7.31	3657.0	0.2253
13	7.08	3541.7	0.2589	32	7.36	3682.1	0.2404
14	7.09	3545.3	0.4420	33	7.38	3690.0	0.3387
15	7.13	3563.6	0.0167	34	7.40	3697.9	0.1816
16	7.15	3573.4	0.0353	35	7.41	3704.0	0.0527
17	7.16	3577.7	0.1072	36	7.41	3705.3	0.0508
18	7.16	3581.3	0.1117	37	7.43	3712.6	0.0260
19	7.17	3583.5	0.1247	38	7.70	3851.4	0.0230

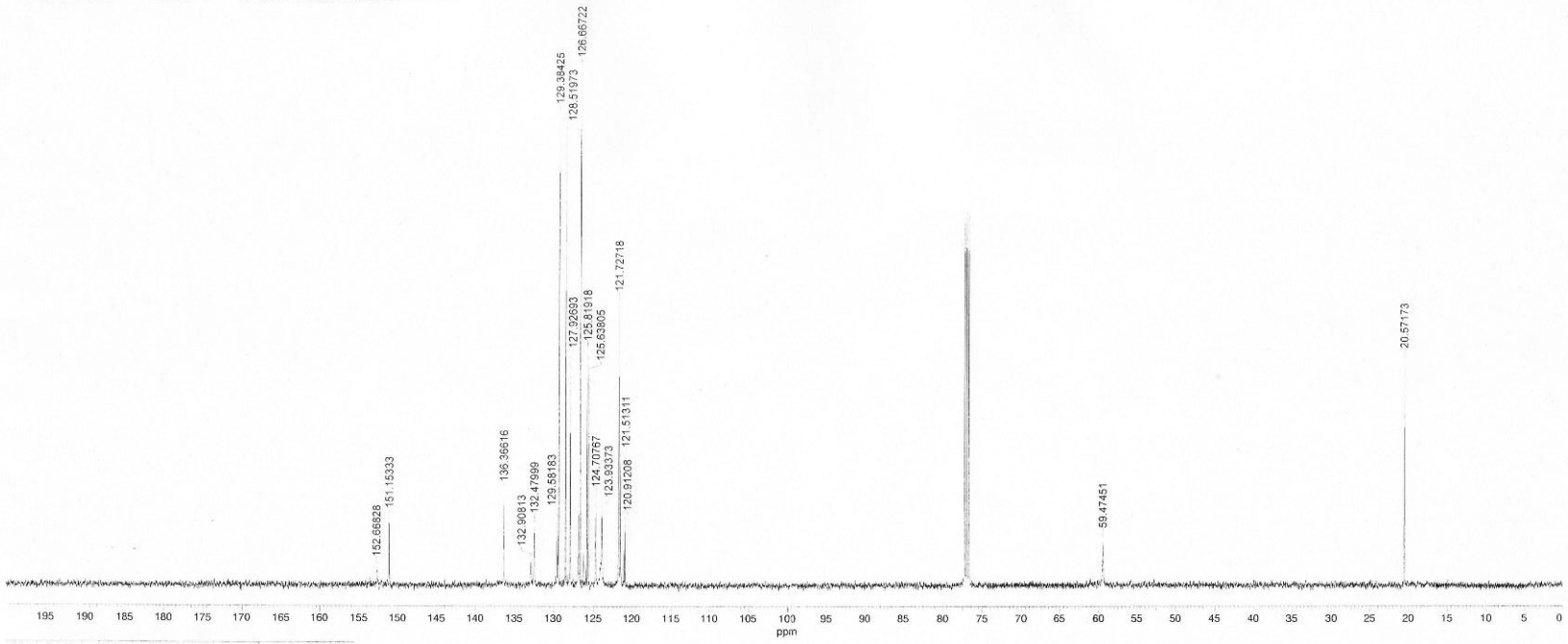
No.	(ppm)	Value	Absolute Value
1	[1.92 .. 2.06]	3.000	2.50369e+3
2	[5.46 .. 5.62]	0.991	8.27194e+2
3	[5.96 .. 6.14]	1.023	8.53642e+2
4	[6.25 .. 6.42]	1.032	8.61226e+2
5	[6.52 .. 6.69]	1.062	8.86573e+2
6	[6.98 .. 7.12]	2.200	1.83569e+3
7	[7.12 .. 7.34]	10.135	8.45801e+3
8	[7.34 .. 7.44]	2.400	2.00266e+3
9	[7.46 .. 7.88]	0.866	7.22607e+2



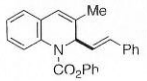
6cA

C:\Documents and Settings\Owner\My Documents\ R%-ª\YD-25H\YD-25H.nmdata

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Fri Sep 15 04:53:30 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰®\YD-25C\YD-25C.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	512	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	20.57	2584.8	0.4344	12	127.93	16074.0	0.4353
2	59.47	7473.0	0.0879	13	128.52	16148.5	0.8766
3	120.91	15192.6	0.1208	14	129.38	16257.1	0.9095
4	121.51	15268.1	0.2435	15	129.47	16267.5	0.0984
5	121.73	15295.0	0.5454	16	129.58	16282.0	0.1302
6	123.93	15572.3	0.1479	17	132.48	16646.1	0.1157
7	124.71	15669.5	0.1668	18	132.91	16699.9	0.0523
8	125.64	15786.4	0.4107	19	136.37	17134.4	0.1768
9	125.82	15809.2	0.4493	20	151.15	18992.4	0.1248
10	126.67	15915.7	1.0000	21	152.67	19182.8	0.0317
11	126.91	15946.8	0.1454				

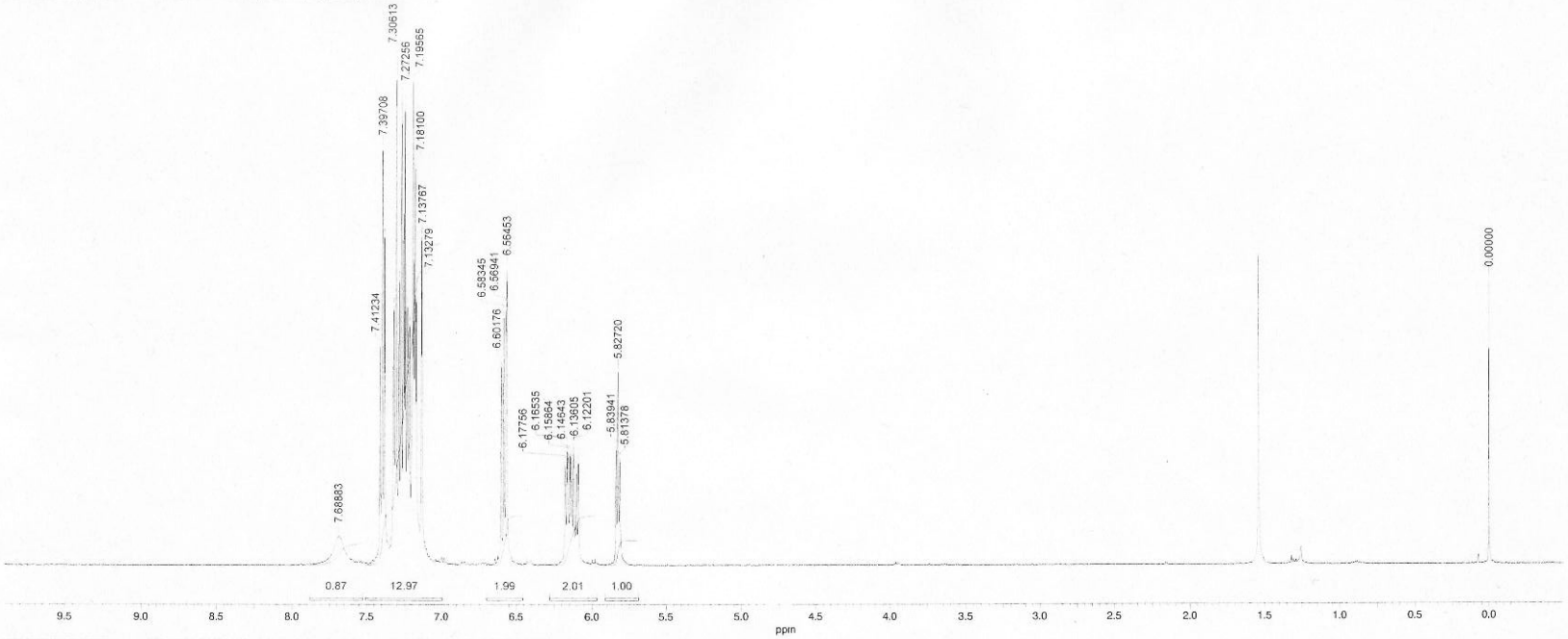


6cA

C:\Documents and Settings\Owner\My Documents\ R‰®\YD-25C\YD-25C.nmdata

18 Sep 2006
noe

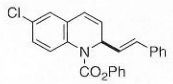
Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Mon Sep 18 02:23:14 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R%-%\YD-29H\YD-29H.nmdata
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	-0.00	-0.0	0.5555	20	7.18	3587.8	0.5224
2	5.81	2906.9	0.2097	21	7.18	3590.5	0.7892
3	5.83	2913.6	0.3790	22	7.19	3594.2	0.6005
4	5.84	2919.7	0.2336	23	7.20	3597.8	0.9523
5	6.09	3045.1	0.2032	24	7.22	3609.4	0.4730
6	6.10	3052.2	0.1925	25	7.23	3614.9	0.4595
7	6.12	3061.0	0.2388	26	7.23	3616.4	0.5083
8	6.14	3068.0	0.2270	27	7.24	3622.2	0.5807
9	6.15	3073.2	0.2208	28	7.25	3625.9	0.9063
10	6.16	3079.3	0.2193	29	7.26	3628.7	0.6913
11	6.17	3082.7	0.2379	30	7.27	3636.3	0.9260
12	6.18	3088.8	0.2032	31	7.29	3643.3	0.5602
13	6.56	3282.3	0.5824	32	7.31	3653.1	1.0000
14	6.57	3284.7	0.5120	33	7.32	3660.4	0.5081
15	6.58	3291.7	0.4993	34	7.34	3672.0	0.0383
16	6.60	3300.9	0.3992	35	7.38	3690.0	0.6436
17	7.13	3566.4	0.5578	36	7.40	3698.5	0.8188
18	7.14	3568.8	0.6444	37	7.41	3706.2	0.4312
19	7.17	3585.3	0.5240	38	7.69	3844.4	0.0567

No.	(ppm)	Value	Absolute Value
1	[5.69 .. 5.91]	1.000	6.01884e+2
2	[5.97 .. 6.28]	2.010	1.20949e+3
3	[6.46 .. 6.70]	1.986	1.19529e+3
4	[6.99 .. 7.51]	12.973	7.80813e+3
5	[7.52 .. 7.88]	0.875	5.26371e+2

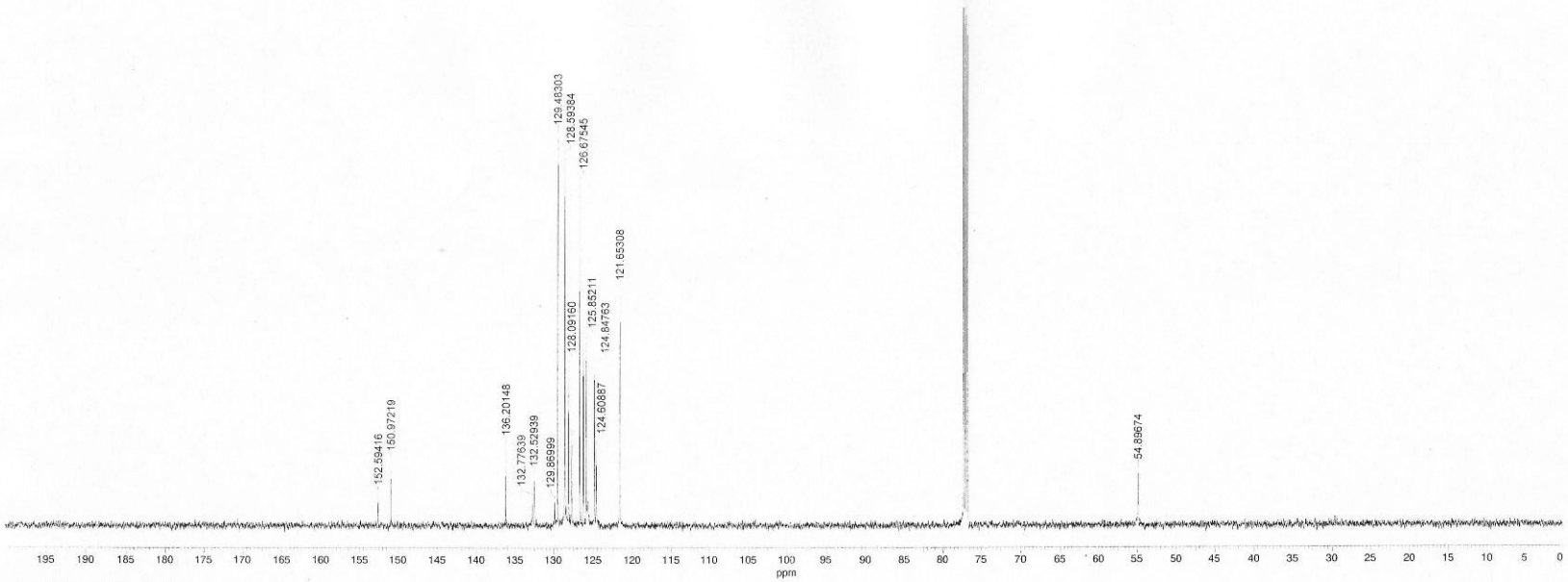
C:\Documents and Settings\Owner\My Documents\ R%-%\YD-29H\YD-29H.nmdata



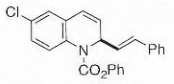
6dA

18 Sep 2006
noe

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Mon Sep 18 03:15:04 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD-29C\YD29C.nmdata
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	1024	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height
1	54.90	6897.8	0.0920
2	121.65	15285.7	0.4111
3	124.61	15657.1	0.1390
4	124.85	15687.1	0.2814
5	125.67	15790.6	0.0450
6	125.85	15813.3	0.3263
7	126.23	15860.9	0.2971
8	126.68	15916.8	0.6092
9	127.70	16046.1	0.1555
10	128.09	16094.7	0.2830
11	128.59	16157.8	0.6541
12	129.48	16269.5	0.6882
13	129.87	16318.2	0.0426
14	132.53	16652.3	0.0818
15	132.78	16683.4	0.0470
16	136.20	17113.7	0.1363
17	150.97	18969.7	0.1085
18	152.59	19173.5	0.0487

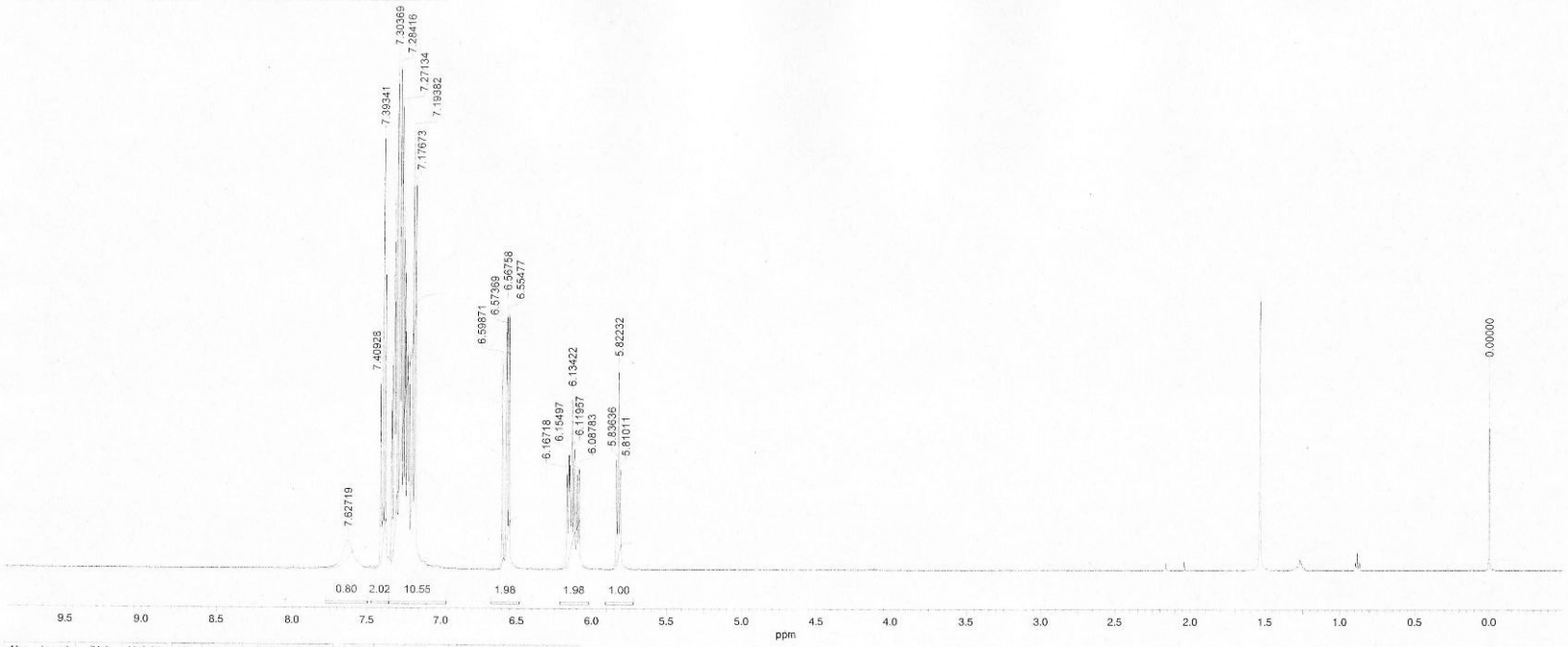


6dA

C:\Documents and Settings\Owner\My Documents\ R‰ª\YD-29C\YD29C.nmdata

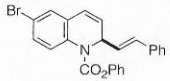
27 Oct 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Fri Oct 27 07:21:39 2006	*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD-30\YD-30.nmdata
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000			*Points Count*	32768
						Solvent	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	-0.00	-0.0	0.3921	18	7.22	3608.5	0.4074
2	5.81	2905.1	0.1961	19	7.23	3614.6	0.4233
3	5.82	2911.2	0.3910	20	7.24	3621.6	0.4927
4	5.84	2918.2	0.2152	21	7.25	3623.2	0.5871
5	6.09	3043.9	0.2005	22	7.26	3628.0	0.6926
6	6.10	3050.9	0.1859	23	7.27	3635.7	0.9091
7	6.12	3059.8	0.2359	24	7.28	3639.9	0.6748
8	6.13	3067.1	0.3323	25	7.28	3642.1	0.9845
9	6.15	3074.1	0.2062	26	7.30	3651.8	1.0000
10	6.15	3077.5	0.2244	27	7.31	3657.3	0.5236
11	6.17	3083.6	0.1896	28	7.32	3659.5	0.7054
12	6.55	3277.4	0.5030	29	7.33	3665.9	0.3987
13	6.57	3283.8	0.5205	30	7.33	3667.4	0.3077
14	6.57	3286.8	0.4716	31	7.38	3689.1	0.5762
15	6.60	3299.4	0.4144	32	7.39	3696.7	0.8434
16	7.18	3588.4	0.7560	33	7.41	3704.6	0.3613
17	7.19	3596.9	0.8601	34	7.63	3813.6	0.0553

No.	(ppm)	Value	Absolute Value
1	[5.72 .. 5.91]	1.000	7.15581e+2
2	[6.02 .. 6.21]	1.984	1.41956e+3
3	[6.48 .. 6.67]	1.984	1.41990e+3
4	[6.97 .. 7.35]	10.550	7.54955e+3
5	[7.35 .. 7.47]	2.017	1.44305e+3
6	[7.49 .. 7.78]	0.798	5.70939e+2

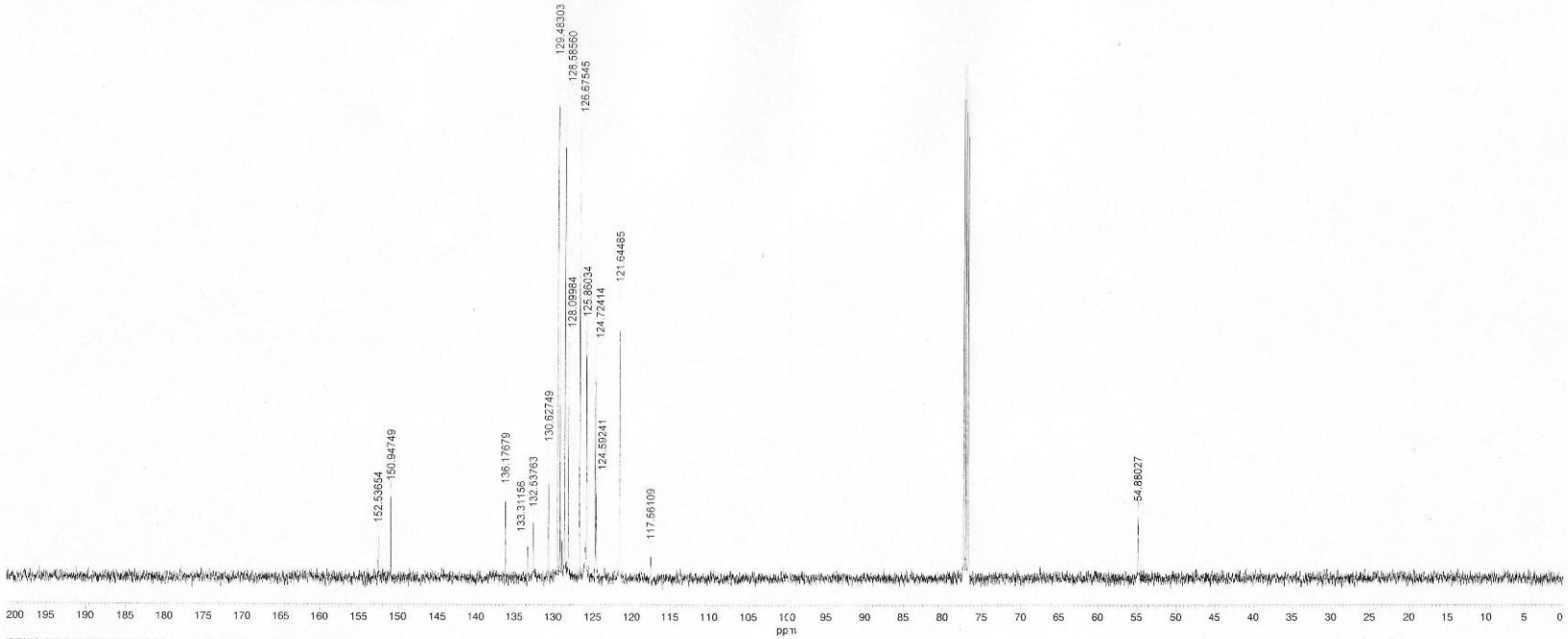


6eA

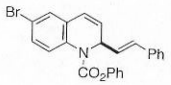
C:\Documents and Settings\Owner\My Documents\ R‰ª\YD-30\YD-30.nmdata

27 Oct 2006
noe

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Fri Oct 27 18:05:29 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R%.®\YD-30C\YD-30C.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	259	*Original Points Coun*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33896.30	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	54.88	6895.7	0.1241	11	128.98	16206.4	0.0771
2	117.56	14771.6	0.0488	12	129.17	16230.2	0.4975
3	121.64	15284.7	0.5481	13	129.48	16269.5	0.9888
4	124.59	15655.0	0.1832	14	130.63	16413.3	0.2382
5	124.72	15671.6	0.4383	15	132.54	16653.4	0.1104
6	125.86	15814.4	0.4805	16	133.31	16750.6	0.0631
7	125.98	15828.8	0.0674	17	136.18	17110.6	0.1564
8	126.68	15916.8	0.8781	18	150.95	18966.6	0.1614
9	128.10	16095.7	0.4594	19	152.54	19166.2	0.0803
10	128.59	16156.8	0.9362				

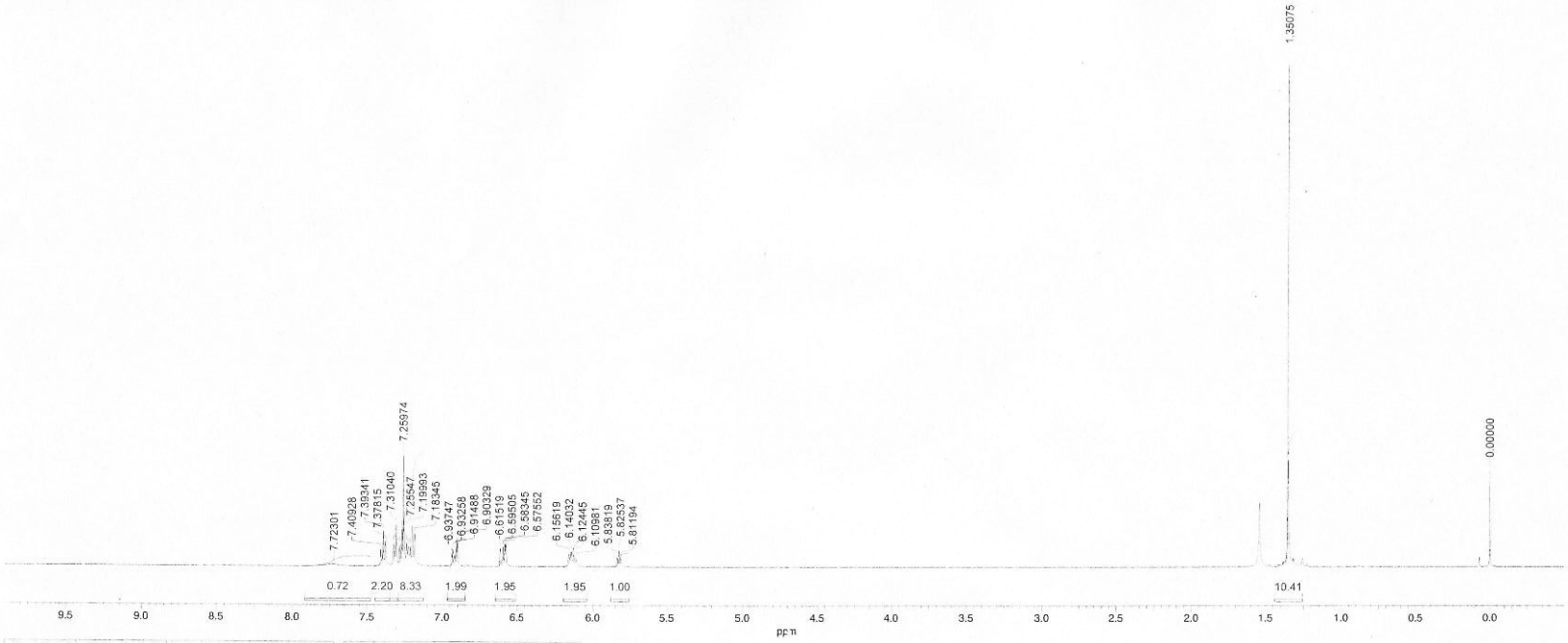


6eA

C:\Documents and Settings\Owner\My Documents\ R%.®\YD-30C\YD-30C.nmdata

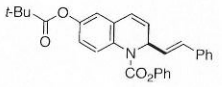
26 Sep 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Tue Sep 26 14:00:07 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R%₀ᴿ\YD-27H\YD-27H.nmdata
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	-0.00	-0.0	0.1884	18	6.93	3466.3	0.0334
2	1.35	675.4	1.0000	19	6.94	3468.7	0.0247
3	5.81	2906.0	0.0171	20	7.18	3591.7	0.0632
4	5.83	2912.7	0.0328	21	7.20	3600.0	0.0793
5	5.84	2919.1	0.0188	22	7.22	3607.6	0.0374
6	6.11	3054.9	0.0149	23	7.23	3614.3	0.0382
7	6.12	3062.2	0.0240	24	7.24	3619.5	0.0452
8	6.14	3070.2	0.0303	25	7.26	3627.7	0.0720
9	6.16	3078.1	0.0249	26	7.26	3629.9	0.2180
10	6.58	3287.8	0.0436	27	7.27	3635.7	0.0723
11	6.58	3291.7	0.0441	28	7.29	3642.7	0.0416
12	6.60	3297.5	0.0383	29	7.31	3655.2	0.0820
13	6.62	3307.6	0.0358	30	7.33	3662.5	0.0442
14	6.90	3449.2	0.0398	31	7.38	3689.1	0.0480
15	6.90	3451.6	0.0558	32	7.39	3696.7	0.0694
16	6.91	3457.4	0.0373	33	7.41	3704.6	0.0316
17	6.92	3460.2	0.0214	34	7.72	3861.5	0.0036

No.	(ppm)	Value	Absolute Value
1	[1.26 .. 1.44]	10.414	3.78623e+3
2	[5.75 .. 5.88]	1.000	3.63588e+2
3	[6.04 .. 6.19]	1.951	7.09411e+2
4	[6.51 .. 6.65]	1.950	7.09087e+2
5	[6.85 .. 6.97]	1.989	7.23136e+2
6	[7.12 .. 7.30]	8.325	3.02691e+3
7	[7.30 .. 7.35]	2.128	7.73764e+2
8	[7.35 .. 7.45]	2.202	8.00619e+2
9	[7.47 .. 7.91]	0.716	2.60173e+2

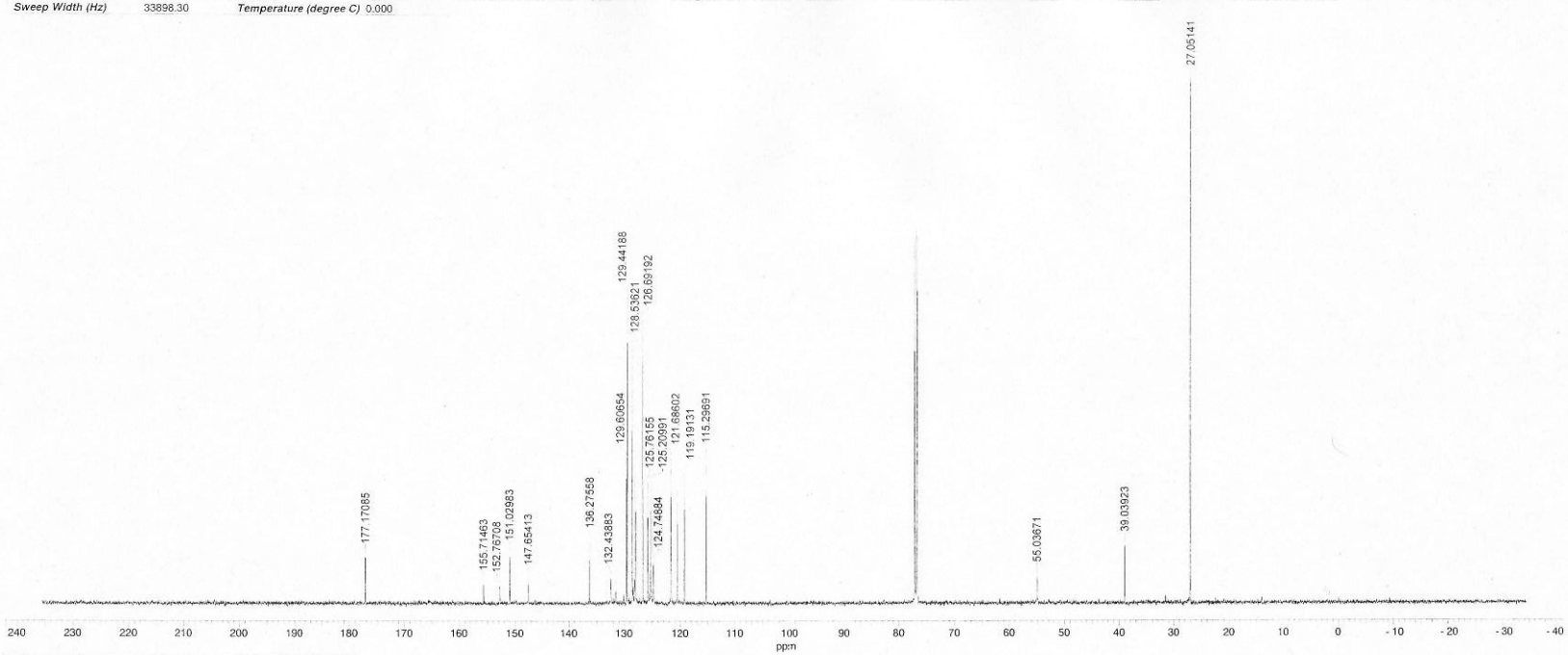


6fA

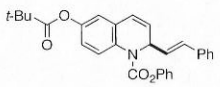
C:\Documents and Settings\Owner\My Documents\ R%₀ᴿ\YD-27H\YD-27H.nmdata

15 Sep 2006

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Fri Sep 15 05:55:45 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD-27C\YD-27C.nmdata
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	1024	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	27.05	3399.0	1.0000	13	128.54	16150.6	0.4910
2	39.04	4905.3	0.1103	14	129.44	16264.4	0.5869
3	55.04	6915.4	0.0529	15	129.61	16285.1	0.2794
4	115.30	14487.1	0.2802	16	131.52	16526.1	0.0283
5	119.19	14976.4	0.2489	17	132.44	16640.9	0.0494
6	120.60	15153.3	0.1982	18	136.28	17123.0	0.1183
7	121.69	15289.8	0.2780	19	147.65	18552.7	0.0475
8	124.75	15674.7	0.0810	20	151.03	18976.9	0.0944
9	125.21	15732.6	0.2328	21	152.77	19195.2	0.0333
10	125.76	15801.9	0.2330	22	155.71	19565.5	0.0379
11	126.69	15918.8	0.5421	23	177.17	22261.5	0.0879
12	128.00	16083.3	0.2304				



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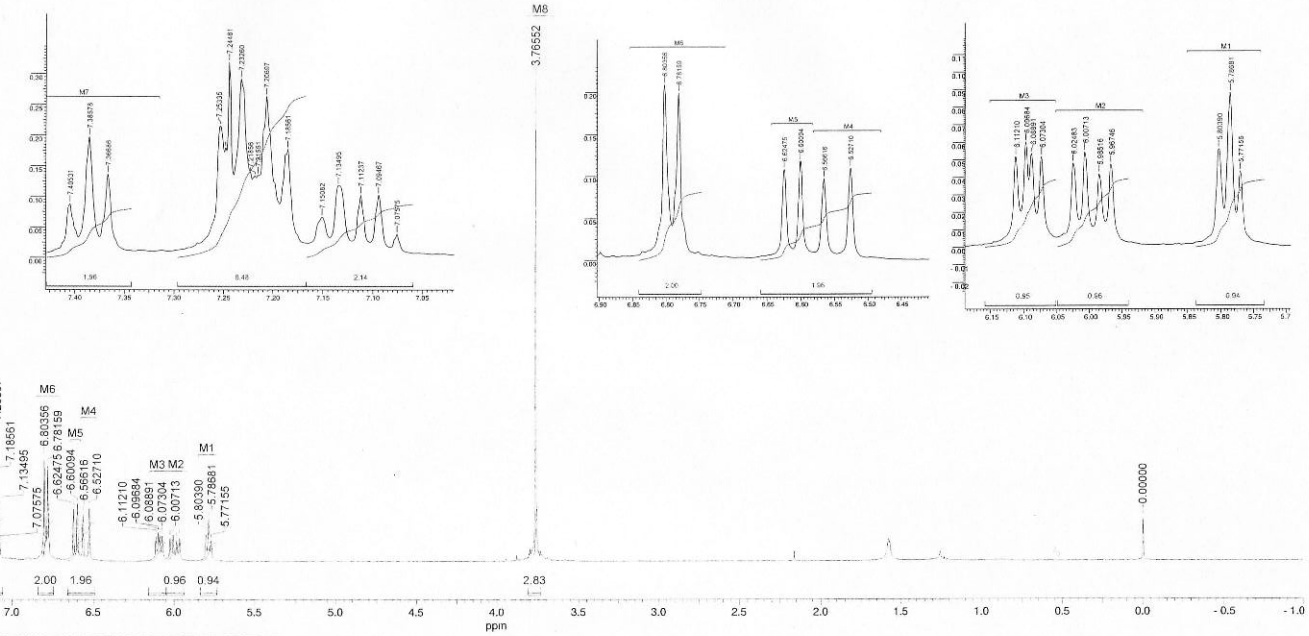
10 Jul 2006
PetasisOMe

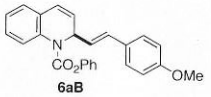
Acquisition Time (sec)	4.1001	*Comment*	PetasisOMe	*Date*	09 Jul 2006 23:30:52			*File Name*	C:\Documents and Settings\Owner\My Documents\Š`–ØŒ`\petasisOMe\petasisOMe1NON_E80_FT.als		
Frequency (MHz)	399.65	*Nucleus*	1H	*Number of Transients*	8	*Original Points Count*	32768	*Points Count*	32768	*Pulse Sequence*	NON
Solvent	CHLOROFORM-D			*Sweep Width (Hz)*	7992.01	*Temperature (degree C)*	20.400				

1H NMR (400 MHz, CHLOROFORM-D) d ppm 3.77 (s, 3 H) 5.79 (t, *J*=6.46 Hz, 1 H) 6.00 (dd, *J*=15.85, 7.07 Hz, 1 H) 6.09 (dd, *J*=9.39, 6.22 Hz, 4 H) 6.55 (d, *J*=15.61 Hz, 1 H) 6.61 (d, *J*=9.51 Hz, 1 H) 6.79 (d, *J*=8.78 Hz, 2 H) 7.39 (t, *J*=7.68 Hz, 2 H)



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.0875	19	6.80	2719.0	0.2096
2	3.77	1504.9	1.0000	20	7.08	2827.8	0.0391
3	5.77	2306.6	0.0433	21	7.09	2835.4	0.1027
4	5.79	2312.7	0.0883	22	7.11	2842.5	0.1030
5	5.80	2319.5	0.0562	23	7.13	2851.5	0.1179
6	5.97	2384.9	0.0474	24	7.15	2857.8	0.0668
7	5.99	2392.0	0.0418	25	7.19	2871.7	0.1777
8	6.01	2400.7	0.0544	26	7.21	2880.3	0.2637
9	6.02	2407.8	0.0480	27	7.22	2883.7	0.1350
10	6.07	2427.1	0.0519	28	7.22	2884.9	0.1341
11	6.09	2433.4	0.0535	29	7.23	2890.5	0.2923
12	6.10	2436.6	0.0600	30	7.24	2895.4	0.3192
13	6.11	2442.7	0.0519	31	7.25	2896.8	0.1800
14	6.53	2608.6	0.1099	32	7.25	2898.8	0.2156
15	6.57	2624.2	0.0974	33	7.37	2944.2	0.1365
16	6.60	2638.1	0.1186	34	7.39	2951.7	0.1973
17	6.62	2647.6	0.1086	35	7.41	2959.5	0.0879
18	6.78	2710.3	0.1994	36	7.72	3087.1	0.0211

No.	(ppm)	Value	Absolute Value
1	[3.73 .. 3.81]	2.830	1.37525e+3
2	[5.73 .. 5.84]	0.940	4.57046e+2
3	[5.94 .. 6.05]	0.957	4.64918e+2
4	[6.05 .. 6.16]	0.946	4.59932e+2
5	[6.49 .. 6.66]	1.962	9.53260e+2
6	[6.75 .. 6.84]	2.000	9.71925e+2
7	[7.06 .. 7.17]	2.142	1.04106e+3
8	[7.17 .. 7.30]	6.476	3.14694e+3
9	[7.34 .. 7.43]	1.961	9.53071e+2
10	[7.61 .. 7.84]	0.800	3.88678e+2



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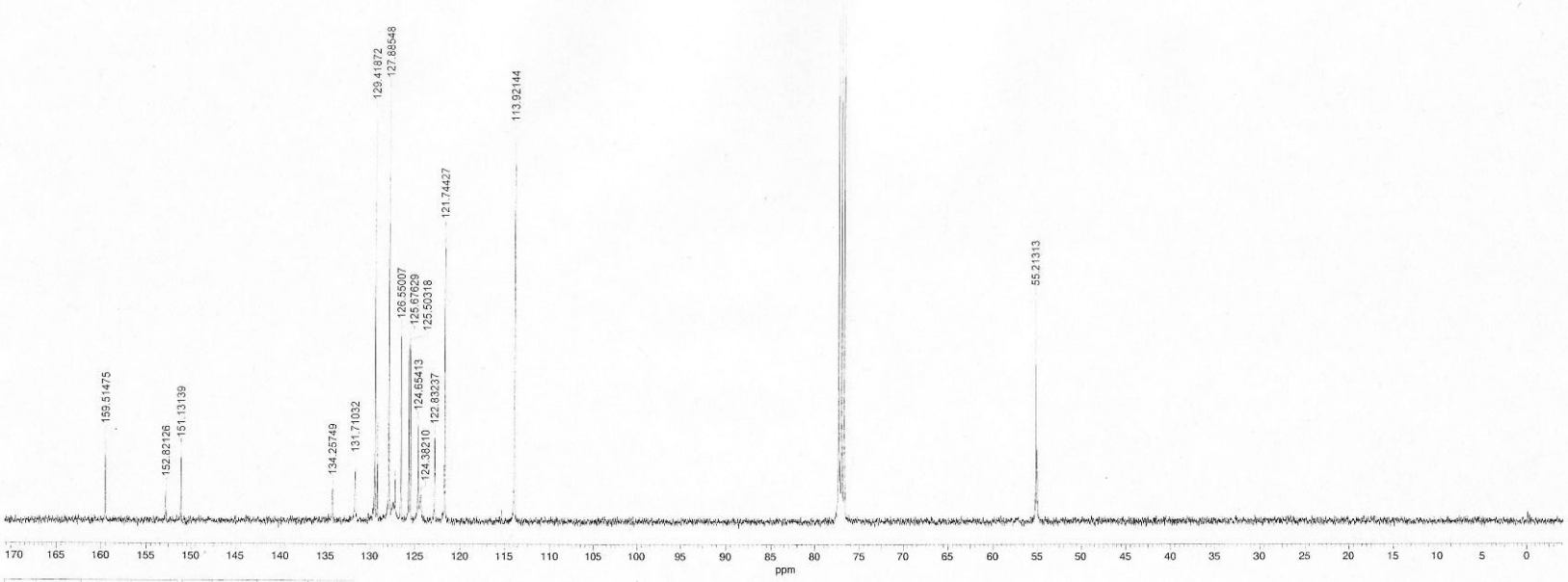
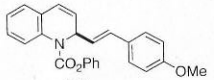
10 Jul 2006
petasisOMe

Acquisition Time (sec)	1.2063	*Comment*	petasisOMe	*Date*	09 Jul 2006 23:31:08						
File Name	C:\Documents and Settings\Owner\My Documents\Š`–ØŒ`\petasisOMe-carbon\petasisOMe1BCM_E70_FT.als					*Frequency (MHz)*	100.40	*Nucleus*	13C	*Number of Transients*	1024
Original Points Count	32768	*Points Count*	32768	*Pulse Sequence*	BCM	*Solvent*	CHLOROFORM-D	*Sweep Width (Hz)*	27118.64	*Temperature (degree C)*	20.100



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	55.21	5543.4	0.3945	11	127.83	12833.9	0.1743
2	113.92	11437.7	0.6863	12	127.89	12839.7	0.7639
3	121.74	12223.1	0.5123	13	129.14	12965.5	0.1761
4	122.83	12332.4	0.1469	14	129.42	12993.6	0.7245
5	124.38	12488.0	0.0462	15	131.71	13223.7	0.0966
6	124.65	12515.3	0.1711	16	134.26	13479.5	0.0565
7	125.50	12600.5	0.3126	17	151.13	15173.6	0.1218
8	125.68	12617.9	0.3226	18	152.82	15343.3	0.0525
9	126.55	12705.6	0.3345	19	159.51	16015.3	0.1455
10	127.19	12770.2	0.0726				



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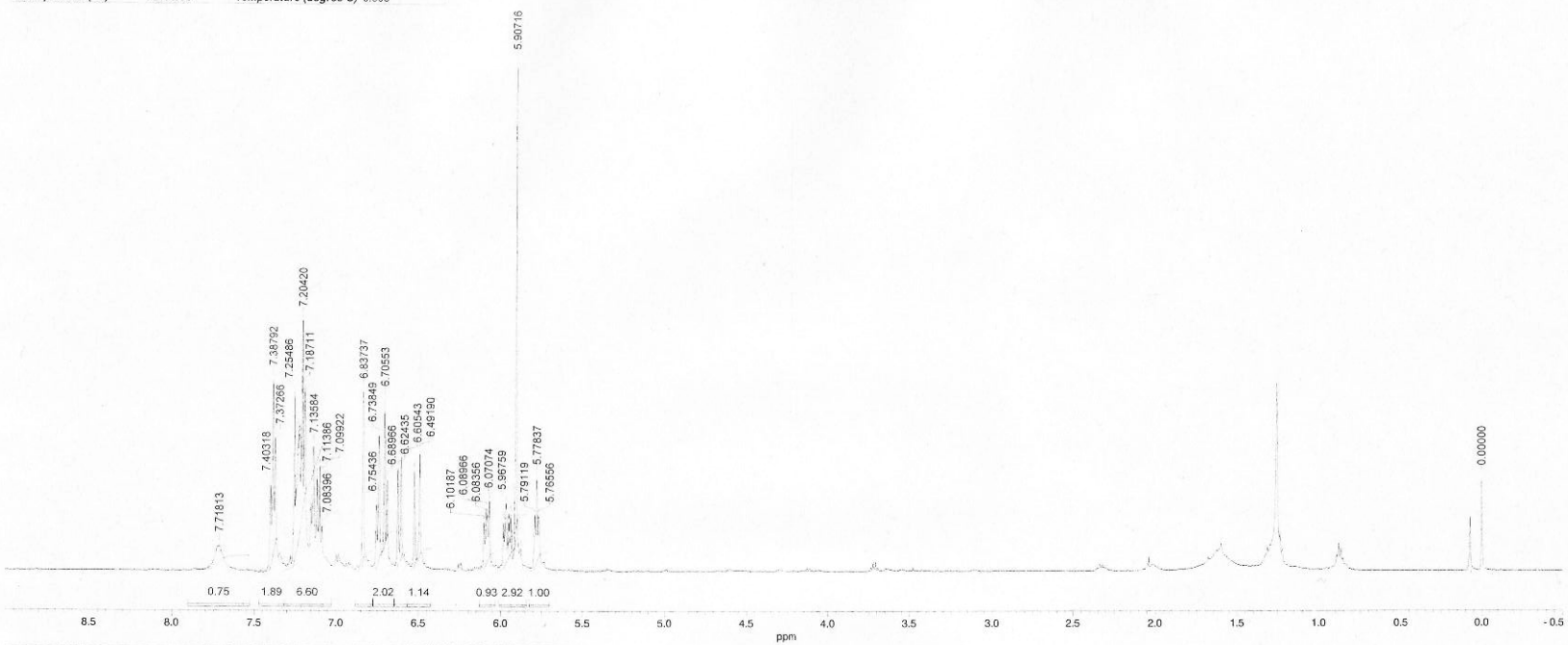
3 Oct 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Tue Oct 3 04:06:12 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R%-#\367H\367H.nmdata
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.1796	20	6.71	3352.8	0.3357
2	5.77	2882.8	0.1096	21	6.74	3369.2	0.2658
3	5.78	2889.2	0.1829	22	6.75	3377.2	0.1303
4	5.79	2895.6	0.1101	23	6.84	3418.7	0.3506
5	5.88	2939.2	0.0452	24	7.08	3542.0	0.0880
6	5.91	2953.6	1.0000	25	7.10	3549.6	0.2047
7	5.94	2968.2	0.1111	26	7.11	3556.9	0.1869
8	5.95	2975.2	0.0959	27	7.14	3567.9	0.2434
9	5.97	2983.8	0.1338	28	7.15	3574.9	0.1322
10	5.98	2990.8	0.0973	29	7.19	3593.6	0.3656
11	6.07	3035.4	0.1376	30	7.20	3602.1	0.4921
12	6.08	3041.8	0.1103	31	7.22	3611.3	0.2673
13	6.09	3044.8	0.1239	32	7.23	3615.2	0.2799
14	6.10	3050.9	0.0966	33	7.25	3622.5	0.1610
15	6.49	3245.9	0.2371	34	7.25	3627.4	0.3512
16	6.52	3261.8	0.1964	35	7.37	3686.3	0.2608
17	6.61	3302.7	0.2256	36	7.39	3694.0	0.3761
18	6.62	3312.2	0.2027	37	7.40	3701.6	0.1682
19	6.69	3344.8	0.1823	38	7.72	3859.1	0.0489

No.	(ppm)	Value	Absolute Value
1	[5.70 .. 5.83]	1.000	7.35517e+2
2	[5.84 .. 6.01]	2.915	2.14406e+3
3	[6.04 .. 6.13]	0.931	6.84421e+2
4	[6.42 .. 6.57]	1.141	8.39003e+2
5	[6.57 .. 6.64]	0.976	7.17655e+2
6	[6.65 .. 6.78]	2.023	1.48823e+3
7	[6.78 .. 6.88]	0.995	7.32058e+2
8	[7.03 .. 7.32]	6.601	4.85490e+3
9	[7.32 .. 7.47]	1.892	1.39164e+3
10	[7.53 .. 7.90]	0.752	5.52830e+2

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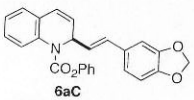
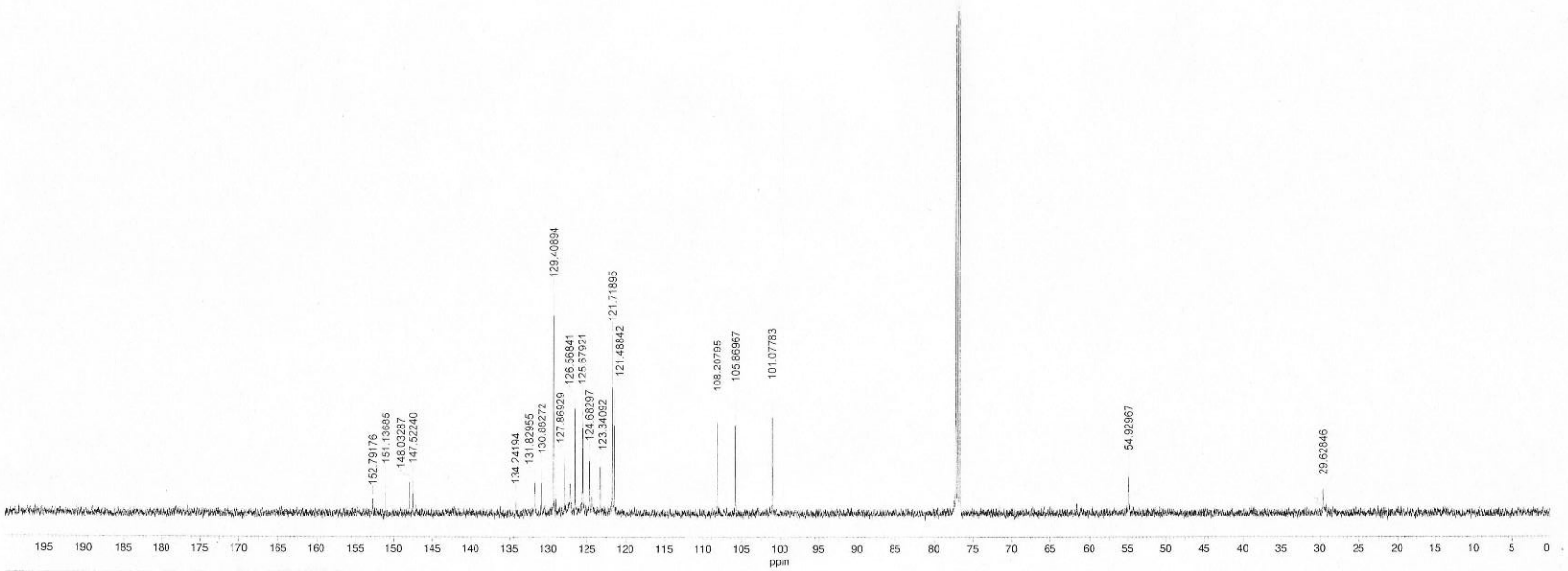


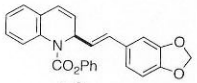
6aC

3 Oct 2006
noe

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Tue Oct 3 04:32:29 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R%-%367C\367C.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	512	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33896.30	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	29.63	3722.8	0.0449	13	126.57	15903.3	0.2055
2	54.93	6901.9	0.0890	14	127.16	15977.8	0.0548
3	101.08	12700.4	0.2157	15	127.87	16066.8	0.1012
4	105.87	13302.5	0.2113	16	129.41	16260.2	0.3967
5	108.21	13596.3	0.1940	17	130.88	16445.4	0.0821
6	121.49	15265.0	0.2203	18	131.83	16564.4	0.0635
7	121.72	15294.0	0.3188	19	134.24	16867.5	0.0286
8	123.34	15497.8	0.0895	20	147.52	18536.2	0.0645
9	124.37	15627.1	0.0276	21	148.03	18600.3	0.0560
10	124.68	15666.4	0.1058	22	151.14	18990.3	0.0643
11	125.61	15783.3	0.1663	23	152.79	19198.3	0.0254
12	125.68	15791.6	0.2067				



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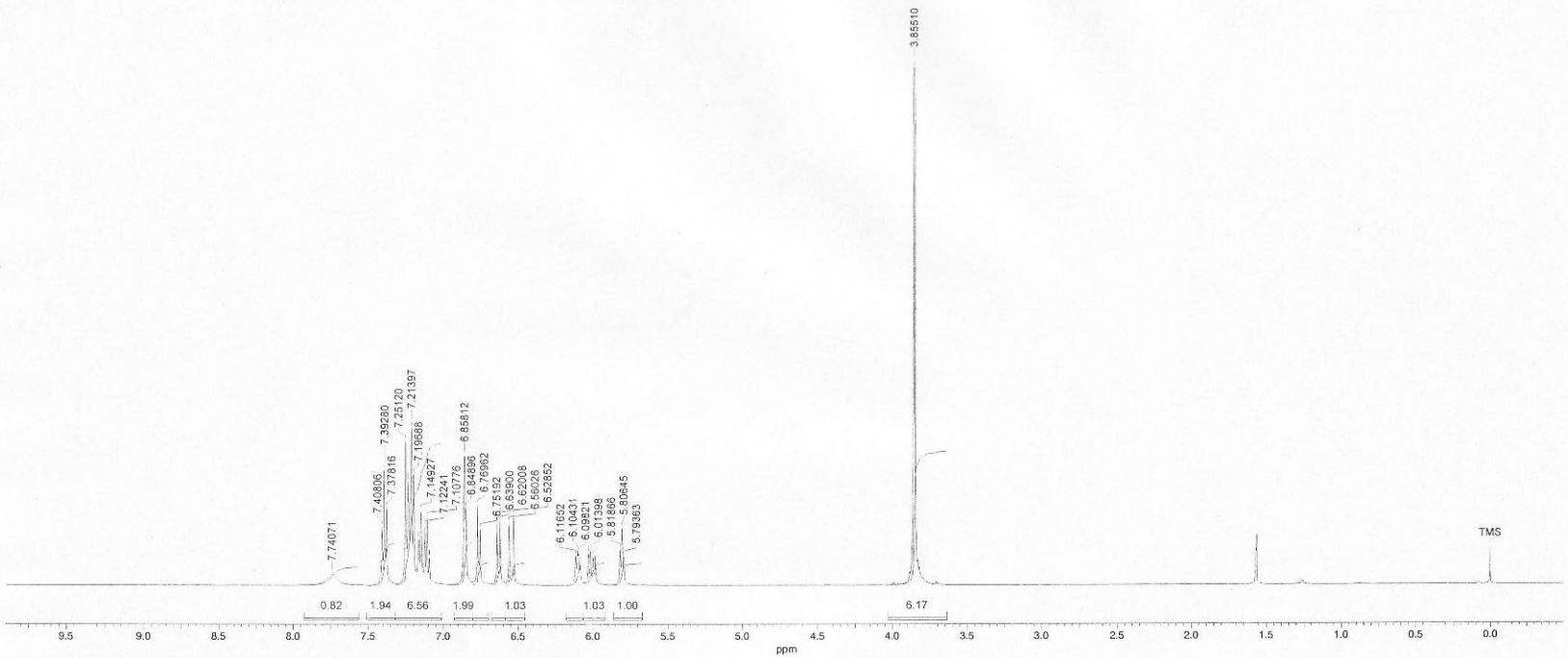
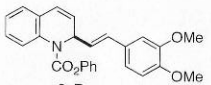
C:\Documents and Settings\Owner\My Documents\ R%-%367C\367C.nmdata

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Thu Feb 22 07:00:21 2007			*File Name*	C:\Documents and Settings\–ô•ï•ª ¢%••Šw\ƒ‡ƒXƒNƒgƒbƒv\NMR\NMR DATA\yamaoka\1H\1H.nmdata		
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000								



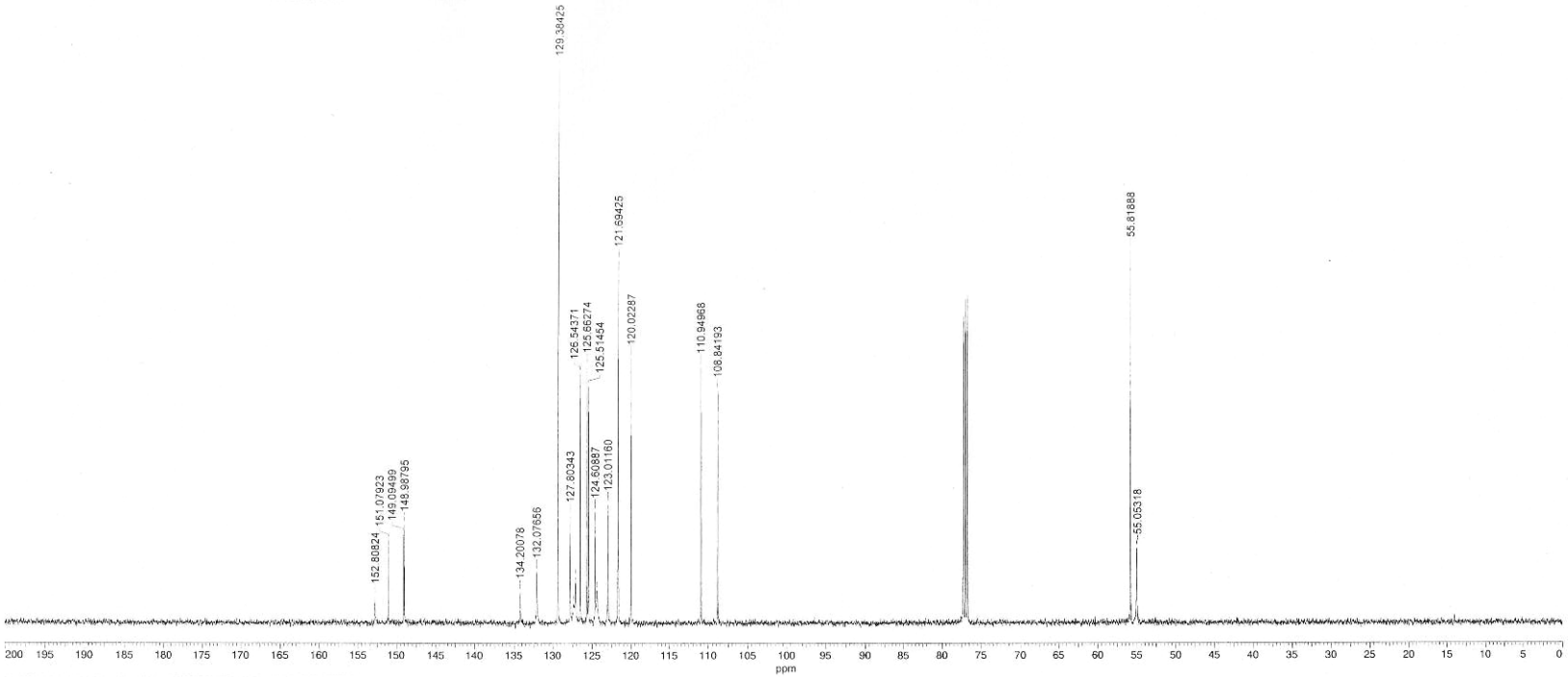
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	3.86	1927.5	1.0000	19	6.77	3384.8	0.1522
2	5.79	2896.8	0.0543	20	6.85	3424.5	0.1466
3	5.81	2903.2	0.1086	21	6.86	3429.1	0.2473
4	5.82	2909.3	0.0681	22	6.86	3430.9	0.2187
5	5.98	2991.1	0.0577	23	7.09	3546.3	0.0512
6	6.00	2998.1	0.0537	24	7.11	3553.9	0.1279
7	6.01	3007.0	0.0660	25	7.12	3561.2	0.1113
8	6.03	3014.0	0.0596	26	7.14	3567.9	0.0256
9	6.09	3043.0	0.0552	27	7.15	3574.6	0.1416
10	6.10	3049.1	0.0614	28	7.16	3582.0	0.0865
11	6.10	3052.2	0.0668	29	7.20	3598.4	0.2105
12	6.12	3058.3	0.0558	30	7.21	3607.0	0.3100
13	6.53	3264.3	0.1324	31	7.23	3617.4	0.1959
14	6.56	3280.1	0.1197	32	7.25	3625.6	0.2732
15	6.62	3310.0	0.1282	33	7.38	3689.1	0.1457
16	6.64	3319.5	0.1180	34	7.39	3696.4	0.2417
17	6.75	3376.0	0.1062	35	7.41	3704.0	0.1111
18	6.76	3380.8	0.0463	36	7.74	3870.4	0.0214

No.	(ppm)	Value	Absolute Value
1	[3.64 .. 4.03]	6.170	4.88974e+3
2	[5.67 .. 5.86]	1.000	7.92552e+2
3	[5.92 .. 6.07]	1.033	8.19002e+2
4	[6.07 .. 6.18]	0.916	7.25732e+2
5	[6.46 .. 6.58]	1.031	8.17382e+2
6	[6.59 .. 6.68]	0.985	7.80540e+2
7	[6.70 .. 6.80]	1.047	8.29551e+2
8	[6.80 .. 6.93]	1.986	1.57387e+3
9	[7.01 .. 7.32]	6.556	5.19549e+3
10	[7.32 .. 7.51]	1.939	1.53637e+3
11	[7.56 .. 7.92]	0.823	6.52222e+2

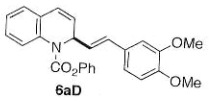


6aD

Acquisition Time (sec)	0.9667	*Comment*	008	*Date*	Thu Feb 22 05:19:38 2007			*File Name*	C:\Documents and Settings\–ôrí³ ¤%ª Šw\ff X fN f¤ f bf¤\NMR\NMR DATA\yamaoka\1C\1C.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	512	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000								



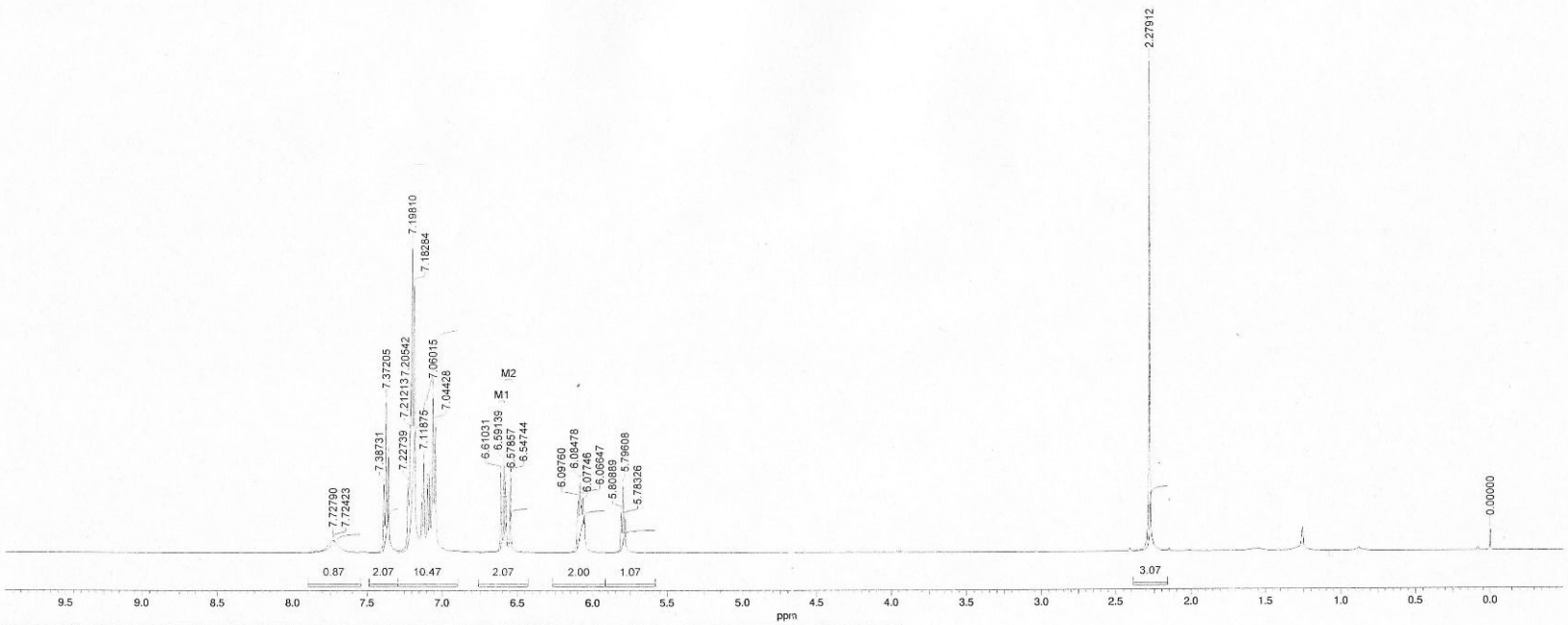
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	55.05	6917.4	0.1351	12	126.54	15900.2	0.4512
2	55.82	7013.6	0.6724	13	127.10	15970.6	0.0827
3	108.84	13676.0	0.4186	14	127.37	16003.7	0.0354
4	110.95	13940.8	0.4623	15	127.80	16058.5	0.1937
5	120.02	15080.9	0.4777	16	129.38	16257.1	1.0000
6	121.69	15290.9	0.6550	17	132.08	16595.4	0.0923
7	123.01	15456.4	0.2143	18	134.20	16862.3	0.0559
8	124.39	15630.2	0.0590	19	148.99	18720.3	0.1770
9	124.61	15657.1	0.2015	20	149.09	18733.8	0.1597
10	125.51	15770.9	0.4262	21	151.08	18983.1	0.1489
11	125.66	15789.5	0.4633	22	152.81	19200.4	0.0461



6aD

6 Jun 2006

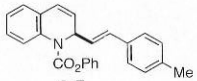
Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Tue Jun 6 22:12:59 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\Š`–ØŒ`\jk0038pro3\jk0038pro3.nmdata
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	8	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.0423	16	7.06	3530.1	0.3261
2	2.28	1139.6	1.0000	17	7.08	3540.1	0.1678
3	5.78	2891.6	0.0710	18	7.09	3547.5	0.1426
4	5.80	2898.0	0.1380	19	7.12	3559.4	0.1826
5	5.81	2904.4	0.0828	20	7.13	3566.4	0.1041
6	6.06	3027.7	0.0763	21	7.18	3591.4	0.5448
7	6.07	3033.2	0.1119	22	7.20	3599.0	0.6214
8	6.08	3038.7	0.0976	23	7.21	3602.7	0.3309
9	6.08	3042.4	0.1454	24	7.21	3606.1	0.2473
10	6.10	3048.8	0.1066	25	7.23	3613.7	0.1408
11	6.55	3273.7	0.1592	26	7.36	3678.4	0.1982
12	6.58	3289.3	0.1461	27	7.37	3686.0	0.3061
13	6.59	3295.7	0.1822	28	7.39	3693.7	0.1389
14	6.61	3305.2	0.1647	29	7.72	3862.1	0.0249
15	7.04	3522.1	0.2631	30	7.73	3863.9	0.0250

No.	(ppm)	Value	Absolute Value
1	[2.16 .. 2.39]	3.066	2.38906e+3
2	[5.58 .. 5.92]	1.067	8.31510e+2
3	[5.92 .. 6.27]	2.000	1.55827e+3
4	[6.43 .. 6.76]	2.075	1.61669e+3
5	[6.90 .. 7.29]	10.470	8.15743e+3
6	[7.29 .. 7.49]	2.066	1.60943e+3
7	[7.54 .. 7.90]	0.867	6.75643e+2

No.	Multiplet1	Shift1	(ppm)	J (Hz)	Type	H's
1	M1	6.60	[6.59 .. 6.62]	9.46	d	1
2	M2	6.56	[6.53 .. 6.58]	15.56	d	1

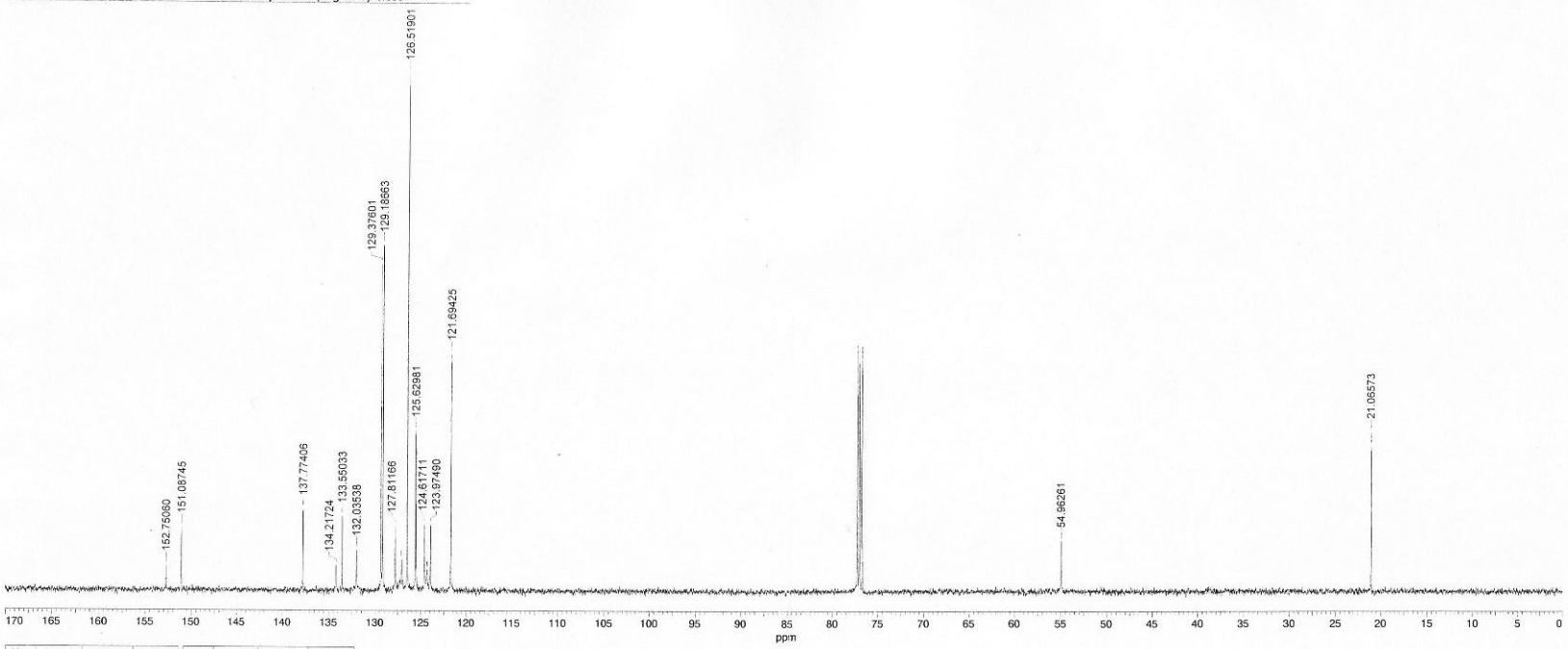


6aE

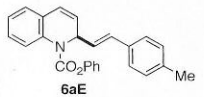
C:\Documents and Settings\Owner\My Documents\Š`–ØŒ`\jk0038pro3\jk0038pro3.nmdata

6 Jun 2006
noe

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Tue Jun 6 21:47:15 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\Š`–ØŒ`\ik0038carboin2\ik0038carboin2.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	256	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	21.07	2646.9	0.3076	11	127.81	16059.5	0.1250
2	54.96	6906.1	0.0982	12	129.19	16232.3	0.6668
3	121.69	15290.9	0.4571	13	129.38	16256.1	0.6303
4	123.97	15577.4	0.1288	14	132.04	16590.2	0.0790
5	124.33	15621.9	0.0404	15	133.55	16780.6	0.1426
6	124.62	15658.1	0.1285	16	134.22	16864.4	0.0491
7	125.55	15775.0	0.2762	17	137.77	17311.3	0.1572
8	125.63	15785.4	0.3084	18	151.09	18984.1	0.1212
9	126.52	15897.1	1.0000	19	152.75	19193.1	0.0480
10	127.13	15973.7	0.0610				

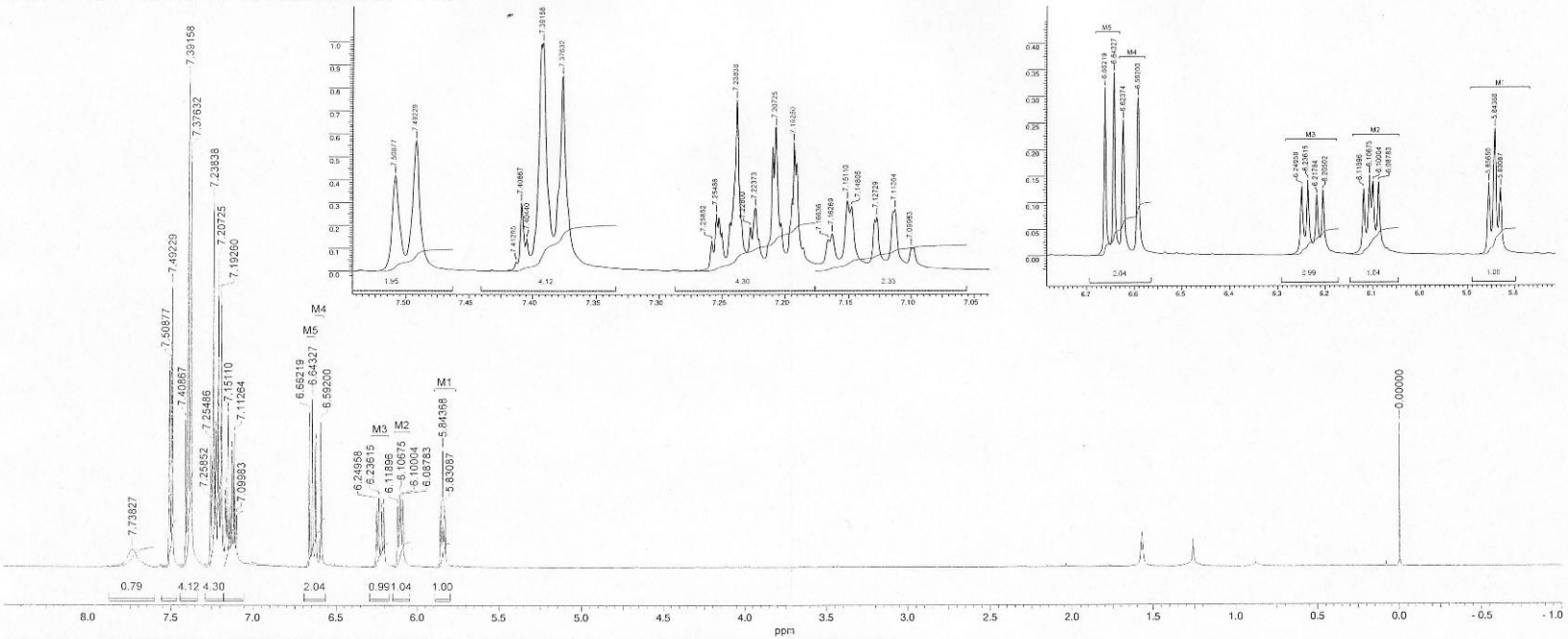


6aE

C:\Documents and Settings\Owner\My Documents\Š`–ØŒ`\ik0038carboin2\ik0038carboin2.nmdata

10 Jun 2006

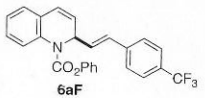
Acquisition Time (sec)	3.2768	*Comment*	nce	*Date*	Sat Jun 10 19:07:28 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\Š`–ØŒ`\ikCFpure\ikCFpure.nmdata
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	8	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.2930	20	7.15	3574.0	0.2851
2	5.83	2915.4	0.1267	21	7.15	3575.5	0.3100
3	5.84	2921.8	0.2384	22	7.16	3581.3	0.1651
4	5.86	2928.3	0.1358	23	7.17	3583.2	0.1403
5	6.09	3043.9	0.1382	24	7.19	3596.3	0.5632
6	6.10	3050.0	0.1390	25	7.21	3603.6	0.6313
7	6.11	3053.4	0.1504	26	7.22	3611.9	0.2801
8	6.12	3059.5	0.1251	27	7.23	3614.0	0.1944
9	6.21	3102.5	0.1222	28	7.24	3619.2	0.7499
10	6.22	3108.9	0.1143	29	7.25	3627.4	0.2528
11	6.24	3118.1	0.1419	30	7.26	3629.3	0.1352
12	6.25	3124.8	0.1300	31	7.38	3688.2	0.8546
13	6.59	3296.0	0.2975	32	7.39	3695.8	1.0000
14	6.62	3311.9	0.2551	33	7.40	3702.2	0.1448
15	6.64	3321.6	0.3445	34	7.41	3704.3	0.3012
16	6.66	3331.1	0.3166	35	7.41	3706.5	0.0432
17	7.10	3549.9	0.1062	36	7.49	3746.1	0.5737
18	7.11	3556.3	0.2726	37	7.51	3754.4	0.4209
19	7.13	3563.6	0.2388	38	7.74	3869.1	0.0361

No.	(ppm)	Value	Absolute Value
1	[5.80 .. 5.89]	1.000	7.93241e+2
2	[6.05 .. 6.15]	1.037	8.22440e+2
3	[6.17 .. 6.29]	0.994	7.88554e+2
4	[6.56 .. 6.69]	2.040	1.61819e+3
5	[7.06 .. 7.18]	2.330	1.84802e+3
6	[7.18 .. 7.29]	4.298	3.40912e+3
7	[7.33 .. 7.44]	4.119	3.26734e+3
8	[7.46 .. 7.56]	1.951	1.54801e+3
9	[7.60 .. 7.88]	0.788	6.25052e+2

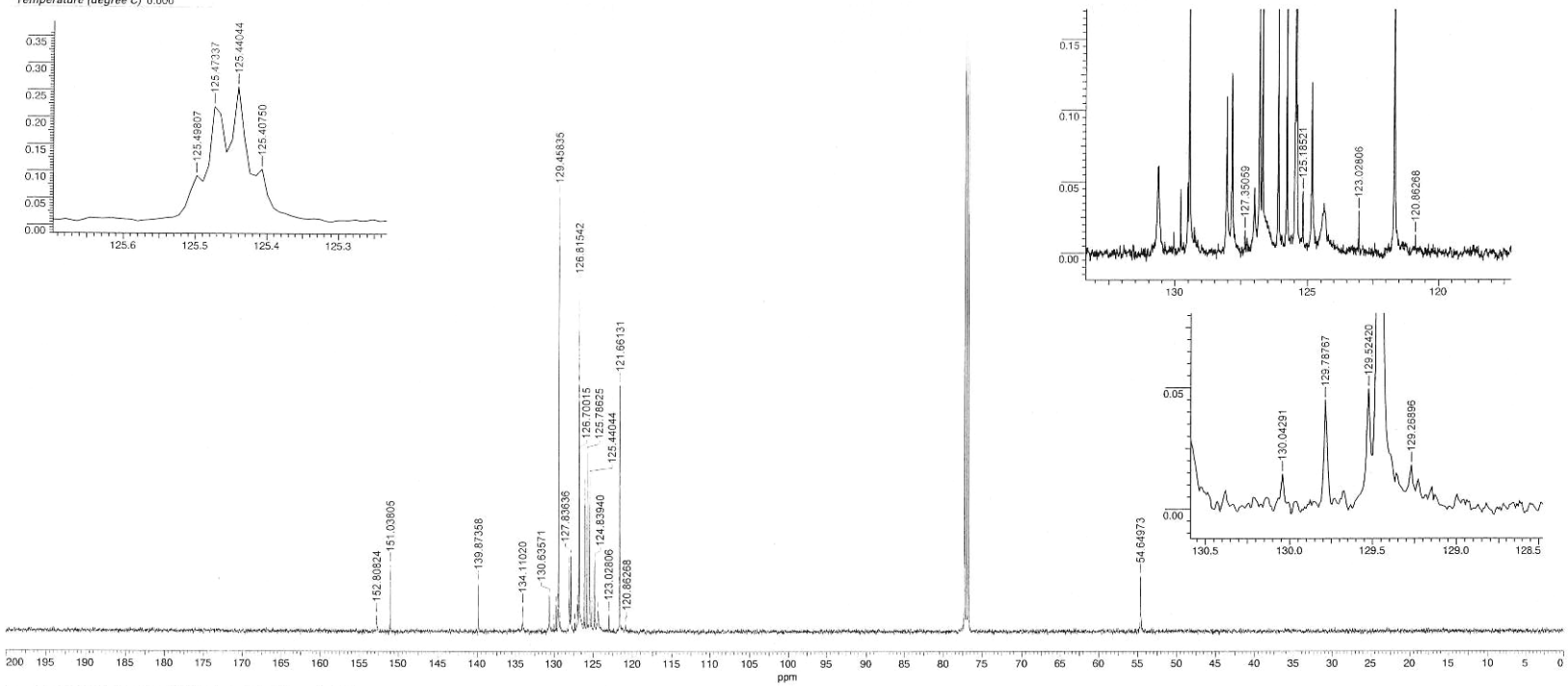
No.	Multiplet1	Shift1	(ppm)	J (Hz)	Type	H's
1	M1	5.83	[5.77 .. 5.89]	6.41	t	1
2	M1	5.83	[5.77 .. 5.89]	6.41	t	1
3	M2	6.09	[6.05 .. 6.14]	9.46	dd	1
4	M2	6.09	[6.05 .. 6.14]	6.10	dd	1
5	M3	6.23	[6.18 .. 6.28]	15.72	dd	1
6	M3	6.23	[6.18 .. 6.28]	6.56	dd	1
7	M4	6.60	[6.58 .. 6.63]	15.87	d	5
8	M5	6.66	[6.63 .. 6.68]	9.46	d	5



6aF

C:\Documents and Settings\Owner\My Documents\Š`–ØŒ`\ikCFpure\ikCFpure.nmdata

Acquisition Time (sec)	0.9667	Comment	noe	Date	Tue Jun 13 05:25:00 2006			File Name	F:\ikCF3carbon2\ikcf3carbon2.nmdata	Frequency (MHz)	125.65
Nucleus	13C	Number of Transients	2048	Original Points Count	32768	Points Count	32768	Solvent	CHLOROFORM-D	Sweep Width (Hz)	33898.30
Temperature (degree C)	0.000										

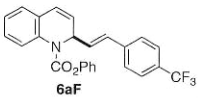


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	54.65	6866.7	0.0918	16	127.00	15957.1	0.0458
2	120.86	15186.4	0.0125	17	127.35	16001.6	0.0158
3	121.66	15286.7	0.4084	18	127.84	16062.6	0.1263
4	123.03	15458.5	0.0295	19	128.04	16088.5	0.1096
5	124.38	15628.1	0.0349	20	129.27	16242.6	0.0181
6	124.84	15686.1	0.1196	21	129.46	16266.4	0.7219
7	125.19	15729.5	0.0433	22	129.52	16274.7	0.0495
8	125.41	15757.5	0.1039	23	129.79	16307.8	0.0449
9	125.44	15761.6	0.2566	24	130.04	16339.9	0.0144
10	125.47	15765.7	0.2197	25	130.64	16414.4	0.0611
11	125.50	15768.8	0.0914	26	134.11	16850.9	0.0423
12	125.79	15805.0	0.2964	27	139.87	17575.1	0.0803
13	126.11	15845.4	0.2378	28	151.04	18977.9	0.1093
14	126.70	15919.9	0.2975	29	152.81	19200.4	0.0264
15	126.82	15934.4	0.5716				

⑥ 1本 124.4 (q, J=271)

1本 129.7 (q, J=32)

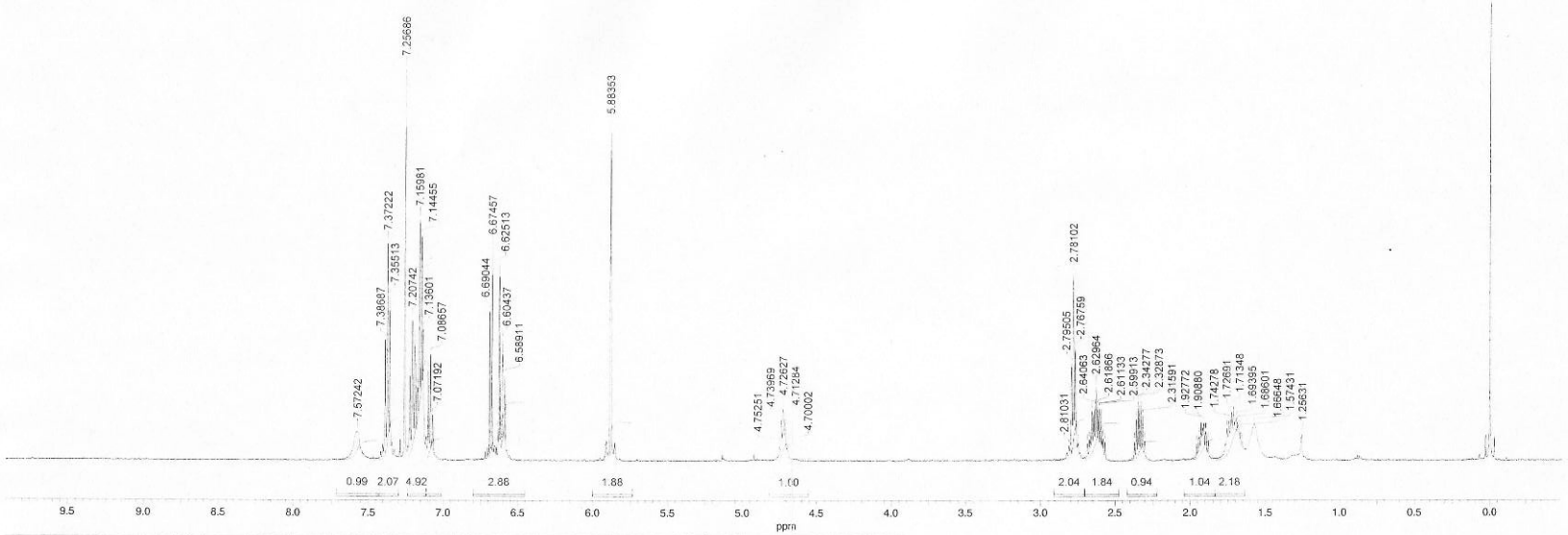
125.4 (q, J=4)



6aF

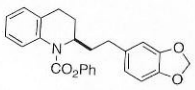
1 Sep 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Fri Sep 1 22:55:33 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰\358\358.nmdata		
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000								



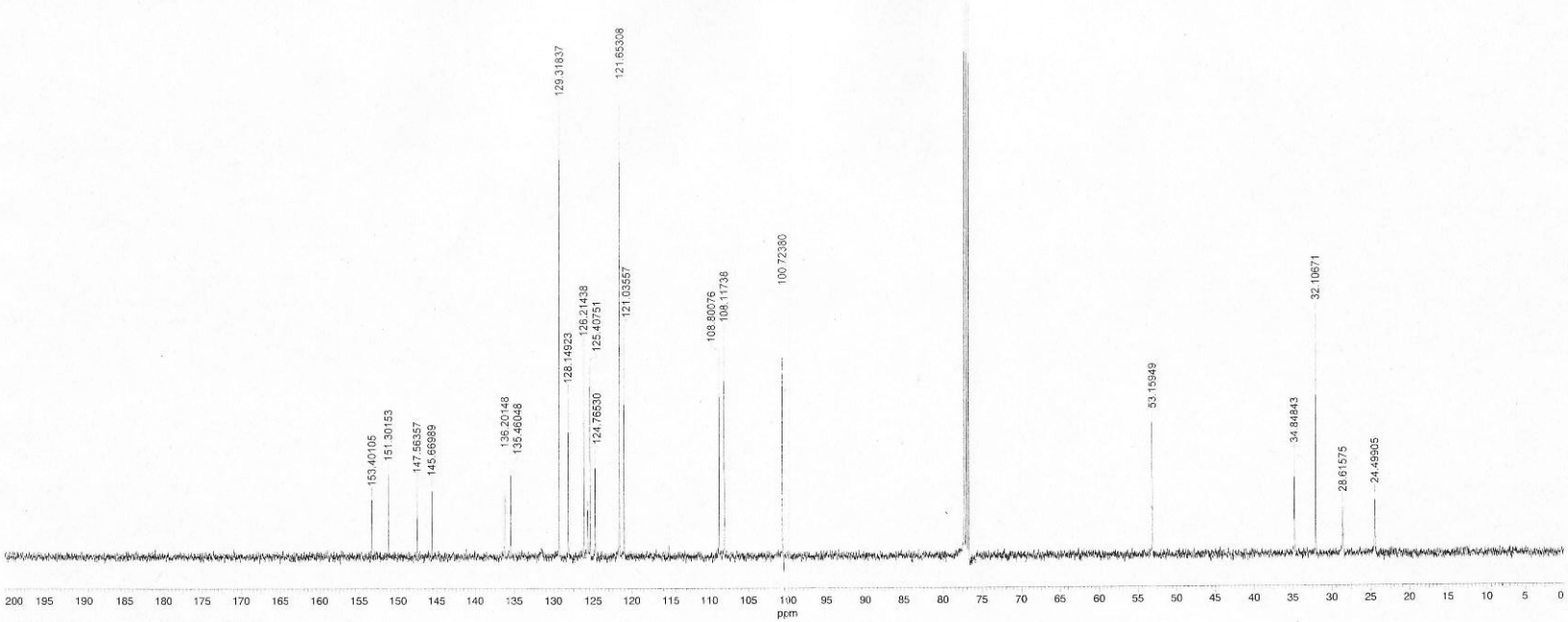
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.26	628.2	0.0474	21	1.94	969.7	0.0441	41	2.68	1338.0	0.0382	61	6.69	3345.2	0.2742
2	1.57	787.2	0.0661	22	1.94	971.5	0.0423	42	2.69	1344.1	0.0319	62	7.07	3536.0	0.0830
3	1.65	827.4	0.0341	23	1.96	977.6	0.0303	43	2.75	1376.5	0.0316	63	7.09	3543.3	0.1936
4	1.67	833.2	0.0540	24	2.30	1150.6	0.0355	44	2.77	1383.8	0.2049	64	7.10	3550.6	0.1652
5	1.69	843.0	0.0697	25	2.32	1158.0	0.0816	45	2.78	1390.5	0.3384	65	7.14	3568.0	0.2406
6	1.69	847.0	0.0766	26	2.33	1164.4	0.1091	46	2.80	1397.5	0.1779	66	7.14	3572.3	0.4110
7	1.70	850.3	0.0740	27	2.34	1171.4	0.1095	47	2.81	1405.2	0.0276	67	7.16	3579.9	0.4410
8	1.71	853.1	0.0697	28	2.36	1177.8	0.0750	48	4.70	2350.0	0.0312	68	7.17	3585.4	0.1330
9	1.71	856.7	0.0994	29	2.37	1184.8	0.0345	49	4.71	2356.4	0.0773	69	7.17	3586.9	0.1338
10	1.73	863.5	0.0885	30	2.57	1285.5	0.0335	50	4.73	2363.1	0.0959	70	7.19	3594.9	0.2203
11	1.74	871.4	0.0717	31	2.58	1291.9	0.0401	51	4.74	2369.8	0.0744	71	7.21	3603.7	0.2565
12	1.75	877.5	0.0585	32	2.59	1295.3	0.0378	52	4.75	2376.3	0.0286	72	7.22	3611.0	0.1556
13	1.88	940.1	0.0365	33	2.60	1299.6	0.0944	53	5.88	2939.9	0.6010	73	7.26	3628.4	0.7161
14	1.90	948.0	0.0520	34	2.61	1305.7	0.0946	54	5.88	2941.8	0.6102	74	7.36	3677.6	0.3009
15	1.90	949.8	0.0537	35	2.62	1309.3	0.1001	55	6.59	3294.6	0.1552	75	7.37	3686.1	0.3966
16	1.91	954.4	0.0679	36	2.63	1314.8	0.1341	56	6.60	3300.7	0.1820	76	7.39	3693.4	0.2203
17	1.92	957.8	0.0592	37	2.64	1320.3	0.0981	57	6.60	3302.2	0.2212	77	7.57	3786.2	0.0530
18	1.92	959.9	0.0470	38	2.65	1324.0	0.0921	58	6.63	3312.6	0.3581				
19	1.92	961.7	0.0497	39	2.66	1329.8	0.0910	59	6.63	3314.1	0.3150				
20	1.93	963.9	0.0695	40	2.67	1334.0	0.0378	60	6.67	3337.3	0.3894				

No.	(ppm)	Value	Absolute Value
1	[1.64 .. 1.83]	2.178	4.93272e+2
2	[1.83 .. 2.04]	1.038	2.35000e+2
3	[2.22 .. 2.42]	0.941	2.13083e+2
4	[2.48 .. 2.71]	1.842	4.17071e+2
5	[2.71 .. 2.91]	2.038	4.61542e+2
6	[4.56 .. 4.82]	1.000	2.26471e+2
7	[5.74 .. 6.00]	1.878	4.25368e+2
8	[6.45 .. 6.80]	2.881	6.52488e+2
9	[7.01 .. 7.11]	1.047	2.37127e+2
10	[7.12 .. 7.24]	4.917	1.11359e+3
11	[7.30 .. 7.43]	2.074	4.69716e+2
12	[7.43 .. 7.72]	0.993	2.24886e+2

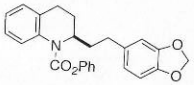


17 Dec 2006

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Sun Dec 17 04:31:32 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD-41C\YD-41C.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	512	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	24.50	3078.3	0.1010	12	125.41	15757.5	0.3440
2	28.62	3595.6	0.0864	13	125.71	15795.7	0.0857
3	32.11	4034.2	0.4317	14	126.21	15858.8	0.3714
4	34.85	4378.7	0.1755	15	128.15	16102.0	0.2869
5	53.16	6679.5	0.2383	16	129.32	16248.9	0.8036
6	100.72	12655.9	0.4629	17	135.46	17020.6	0.1600
7	108.12	13584.9	0.3966	18	136.20	17113.7	0.1717
8	108.80	13670.8	0.3603	19	145.67	18303.4	0.1215
9	121.04	15208.1	0.4052	20	147.56	18541.4	0.1269
10	121.65	15285.7	0.8344	21	151.30	19011.0	0.1478
11	124.77	15676.8	0.1780	22	153.40	19274.8	0.1026



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30 Oct 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Mon Oct 30 15:01:14 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD-42ent\YD-42ent.nmdata		
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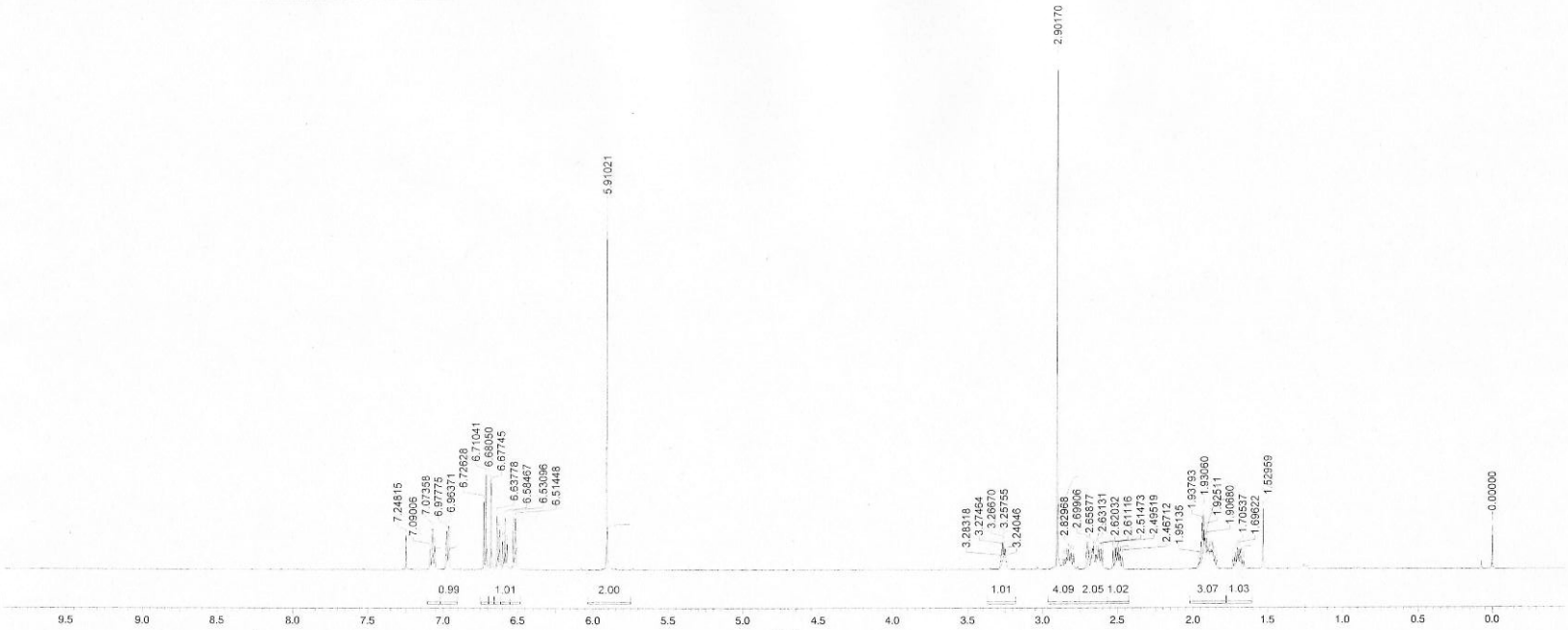
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000								



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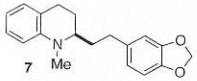
1	-0.00	-0.0	0.0862	22	1.91	953.4	0.0606	43	2.63	1315.7	0.0470	64	3.27	1637.3	0.0399
2	1.53	764.8	0.1185	23	1.92	958.9	0.0603	44	2.64	1319.3	0.0299	65	3.28	1641.6	0.0166
3	1.66	828.9	0.0160	24	1.92	960.7	0.0587	45	2.65	1324.2	0.0284	66	5.91	2955.1	0.7075
4	1.67	834.4	0.0184	25	1.93	962.6	0.0770	46	2.66	1329.4	0.0443	67	6.51	3257.2	0.1000
5	1.68	839.0	0.0251	26	1.93	965.3	0.1172	47	2.67	1333.0	0.0405	68	6.53	3265.5	0.1042
6	1.69	842.9	0.0385	27	1.94	969.0	0.0905	48	2.67	1337.3	0.0247	69	6.57	3285.9	0.0506
7	1.70	848.1	0.0404	28	1.94	972.3	0.0535	49	2.69	1345.3	0.0373	70	6.58	3292.3	0.1039
8	1.71	852.7	0.0434	29	1.95	975.7	0.0220	50	2.70	1349.5	0.0544	71	6.60	3299.7	0.0579
9	1.71	857.3	0.0335	30	1.96	978.7	0.0149	51	2.71	1353.5	0.0351	72	6.62	3311.3	0.0794
10	1.72	861.5	0.0251	31	1.96	982.1	0.0111	52	2.79	1397.1	0.0309	73	6.64	3318.9	0.1086
11	1.73	867.0	0.0228	32	2.47	1233.6	0.0263	53	2.81	1403.9	0.0323	74	6.68	3338.7	0.1675
12	1.84	921.7	0.0187	33	2.48	1240.3	0.0283	54	2.82	1408.7	0.0306	75	6.68	3340.3	0.1750
13	1.85	926.5	0.0232	34	2.49	1243.6	0.0294	55	2.83	1414.8	0.0392	76	6.71	3355.2	0.1858
14	1.86	928.1	0.0274	35	2.50	1247.6	0.0428	56	2.84	1419.7	0.0240	77	6.73	3363.1	0.1337
15	1.87	932.6	0.0336	36	2.50	1250.0	0.0340	57	2.85	1425.5	0.0212	78	6.96	3481.9	0.0858
16	1.87	936.3	0.0376	37	2.51	1254.0	0.0425	58	2.86	1431.6	0.0204	79	6.98	3488.9	0.0780
17	1.88	938.4	0.0357	38	2.51	1257.4	0.0427	59	2.90	1450.8	1.0000	80	7.06	3529.5	0.0460
18	1.88	940.3	0.0395	39	2.53	1264.1	0.0366	60	3.24	1620.2	0.0168	81	7.07	3536.8	0.0806
19	1.89	942.7	0.0362	40	2.60	1300.1	0.0380	61	3.25	1624.5	0.0409	82	7.09	3545.0	0.0394
20	1.89	945.5	0.0356	41	2.61	1305.6	0.0399	62	3.26	1628.8	0.0547	83	7.25	3624.1	0.0666
21	1.90	948.8	0.0393	42	2.62	1310.2	0.0396	63	3.27	1633.4	0.0535				

No.	(ppm)	Value	Absolute Value
1	[1.60 .. 1.78]	1.026	7.62034e+2
2	[1.78 .. 2.02]	3.066	2.27708e+3
3	[2.43 .. 2.57]	1.016	7.54590e+2
4	[2.57 .. 2.75]	2.053	1.52497e+3
5	[2.76 .. 2.96]	4.086	3.03541e+3
6	[3.18 .. 3.37]	1.014	7.53444e+2
7	[5.75 .. 6.03]	2.000	1.48556e+3
8	[6.48 .. 6.55]	0.997	7.40364e+2
9	[6.55 .. 6.61]	1.011	7.51083e+2
10	[6.61 .. 6.66]	0.997	7.40612e+2
11	[6.66 .. 6.69]	0.956	7.10408e+2
12	[6.70 .. 6.75]	0.953	7.08250e+2
13	[6.90 .. 7.02]	0.991	7.36032e+2
14	[7.02 .. 7.11]	0.974	7.23152e+2



7

18 Jan 2007

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Thu Jan 18 17:08:03 2007						
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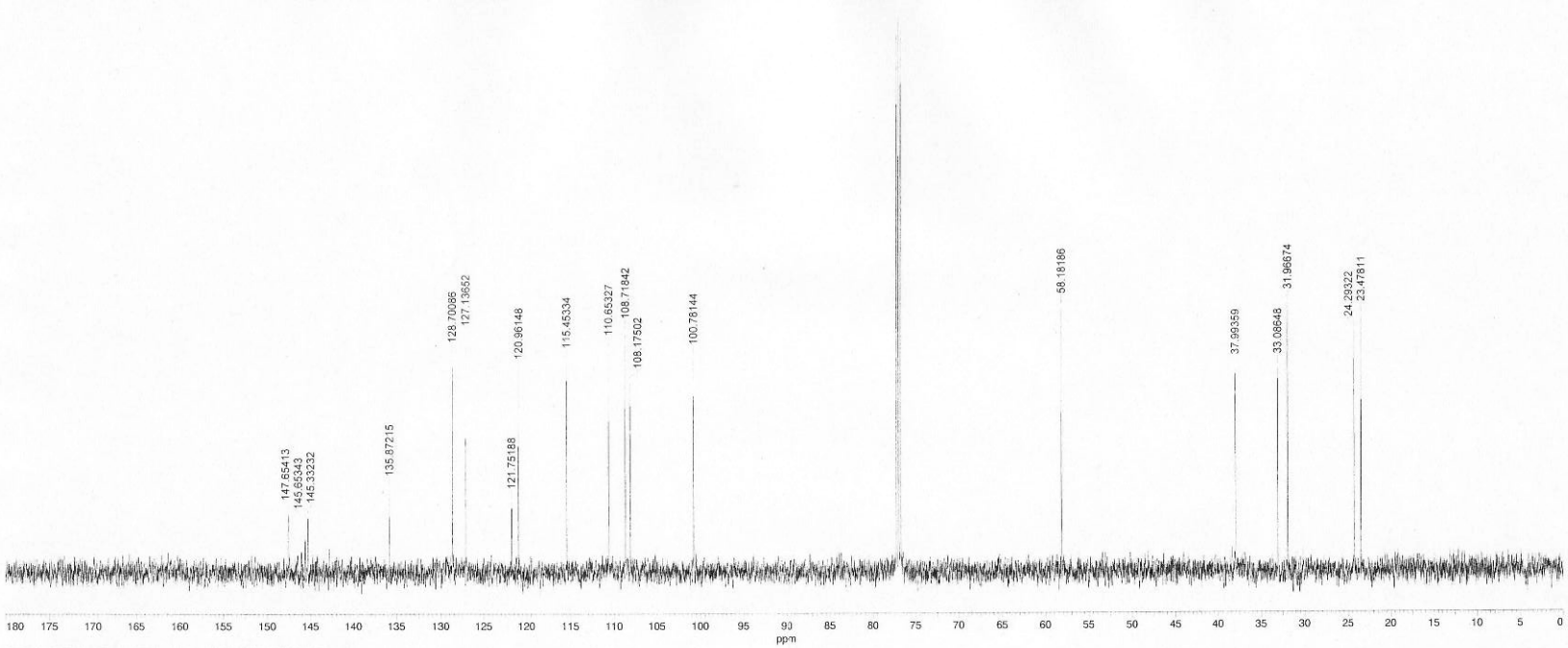
Original Points Count	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D	*Sweep Width (Hz)*	33898.30	*Temperature (degree C)*	0.000		



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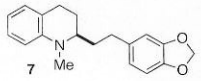
1	23.48	2950.0	0.4595	11	115.45	14506.7	0.3796
2	24.29	3052.4	0.4324	12	120.96	15198.8	0.3603
3	31.97	4016.6	0.4825	13	121.75	15298.1	0.1264
4	33.09	4157.3	0.3661	14	127.14	15974.7	0.4199
5	37.99	4773.9	0.3650	15	128.70	16171.3	0.3897
6	58.18	7310.6	0.4761	16	135.87	17072.3	0.1496
7	100.78	12663.2	0.3864	17	145.33	18261.0	0.1011
8	108.18	13592.2	0.3429	18	145.65	18301.4	0.0902
9	108.72	13660.5	0.4328	19	147.65	18552.7	0.1063
10	110.65	13903.6	0.4027				



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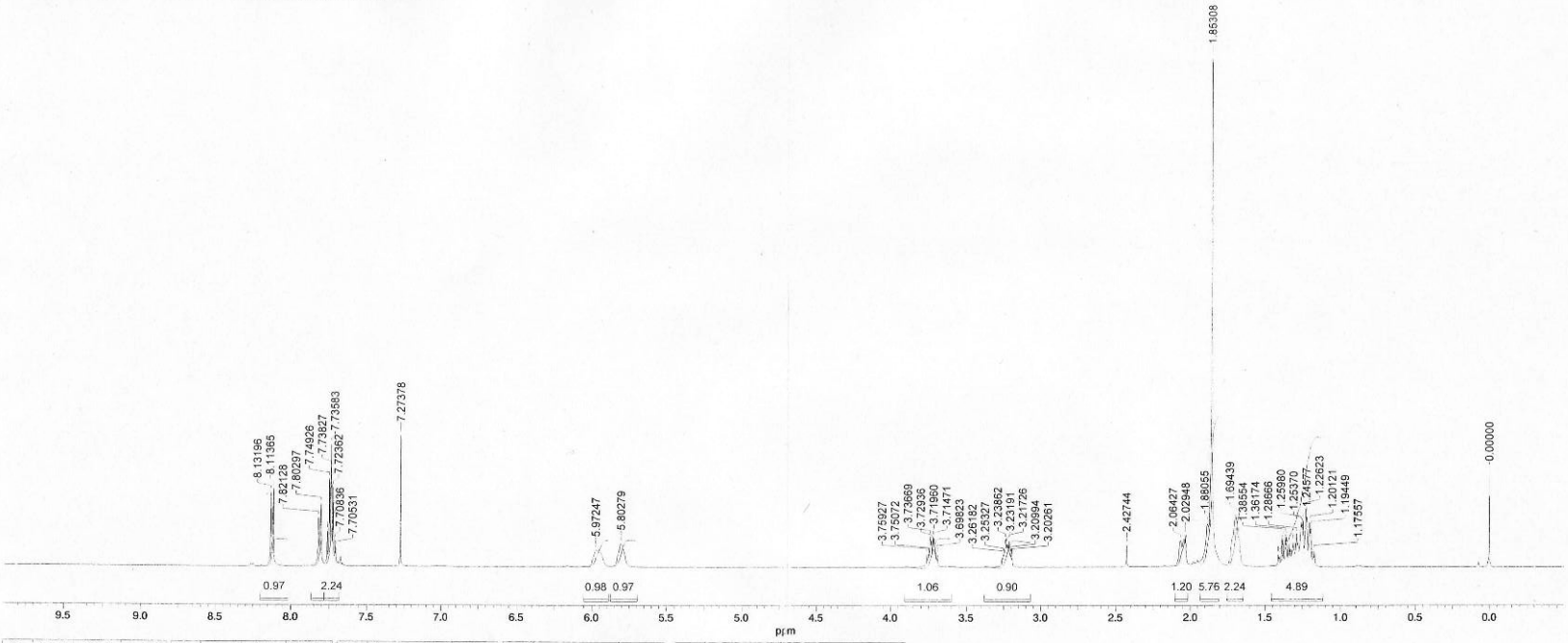
24 May 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Wed May 24 04:06:31 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R%-®\YD1-H\YD1-H.nmdata
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



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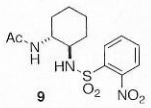
1	0.00	0.0	0.1789	20	1.36	677.5	0.0569	39	3.23	1616.0	0.0435	58	7.71	3854.2	0.0492
2	1.17	584.4	0.0230	21	1.36	680.9	0.0623	40	3.24	1619.3	0.0520	59	7.72	3860.0	0.1244
3	1.18	587.8	0.0289	22	1.38	689.4	0.0508	41	3.25	1623.0	0.0288	60	7.72	3861.8	0.1528
4	1.18	591.1	0.0146	23	1.39	692.8	0.0613	42	3.25	1626.6	0.0237	61	7.73	3865.5	0.1588
5	1.19	597.2	0.0756	24	1.40	701.9	0.0204	43	3.26	1630.9	0.0184	62	7.73	3866.7	0.2036
6	1.20	600.6	0.0865	25	1.41	705.6	0.0223	44	3.69	1845.5	0.0217	63	7.74	3867.9	0.2376
7	1.22	610.1	0.0962	26	1.68	837.7	0.0579	45	3.70	1849.1	0.0292	64	7.74	3869.1	0.1913
8	1.23	613.1	0.1129	27	1.69	847.2	0.1013	46	3.71	1853.7	0.0331	65	7.75	3872.8	0.1623
9	1.23	615.9	0.0695	28	1.85	926.5	1.0000	47	3.71	1857.4	0.0550	66	7.75	3874.6	0.1706
10	1.25	622.9	0.0898	29	1.88	940.3	0.0840	48	3.72	1859.8	0.0575	67	7.76	3880.4	0.0679
11	1.25	626.9	0.0827	30	1.88	942.4	0.0827	49	3.73	1864.7	0.0504	68	7.76	3882.3	0.0455
12	1.26	629.9	0.0856	31	2.03	1014.7	0.0610	50	3.74	1868.3	0.0584	69	7.80	3901.5	0.1210
13	1.28	640.3	0.0431	32	2.06	1032.1	0.0506	51	3.74	1871.1	0.0341	70	7.81	3903.6	0.1189
14	1.29	643.3	0.0636	33	2.43	1213.7	0.0413	52	3.75	1875.4	0.0252	71	7.82	3909.1	0.0787
15	1.29	646.1	0.0457	34	3.19	1597.0	0.0170	53	3.76	1879.6	0.0239	72	7.82	3910.6	0.0936
16	1.31	652.8	0.0305	35	3.20	1601.3	0.0228	54	5.80	2901.4	0.0444	73	8.11	4056.8	0.1512
17	1.31	655.8	0.0463	36	3.21	1605.0	0.0265	55	5.97	2986.2	0.0319	74	8.12	4058.4	0.1234
18	1.33	665.0	0.0350	37	3.22	1608.6	0.0501	56	7.27	3636.9	0.2553	75	8.13	4063.8	0.1411
19	1.34	668.1	0.0431	38	3.22	1612.3	0.0443	57	7.71	3852.7	0.0349	76	8.13	4066.0	0.1437

No.	(ppm)	Value	Absolute Value
1	[1.12 .. 1.46]	4.894	3.36552e+3
2	[1.65 .. 1.75]	2.235	1.53734e+3
3	[1.80 .. 1.93]	5.763	3.96342e+3
4	[2.02 .. 2.10]	1.202	8.26793e+2
5	[3.07 .. 3.38]	0.900	6.18714e+2
6	[3.60 .. 3.91]	1.057	7.26803e+2
7	[5.70 .. 5.88]	0.968	6.65903e+2
8	[5.89 .. 6.06]	0.980	6.73662e+2
9	[7.68 .. 7.78]	2.243	1.54275e+3
10	[7.78 .. 7.87]	1.000	6.87719e+2
11	[8.01 .. 8.20]	0.970	6.67184e+2



9

C:\Documents and Settings\Owner\My Documents\ R%-®\YD1-H\YD1-H.nmdata

24 May 2006
noe

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Wed May 24 04:10:39 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD1-C\YD1-C.nmdata		
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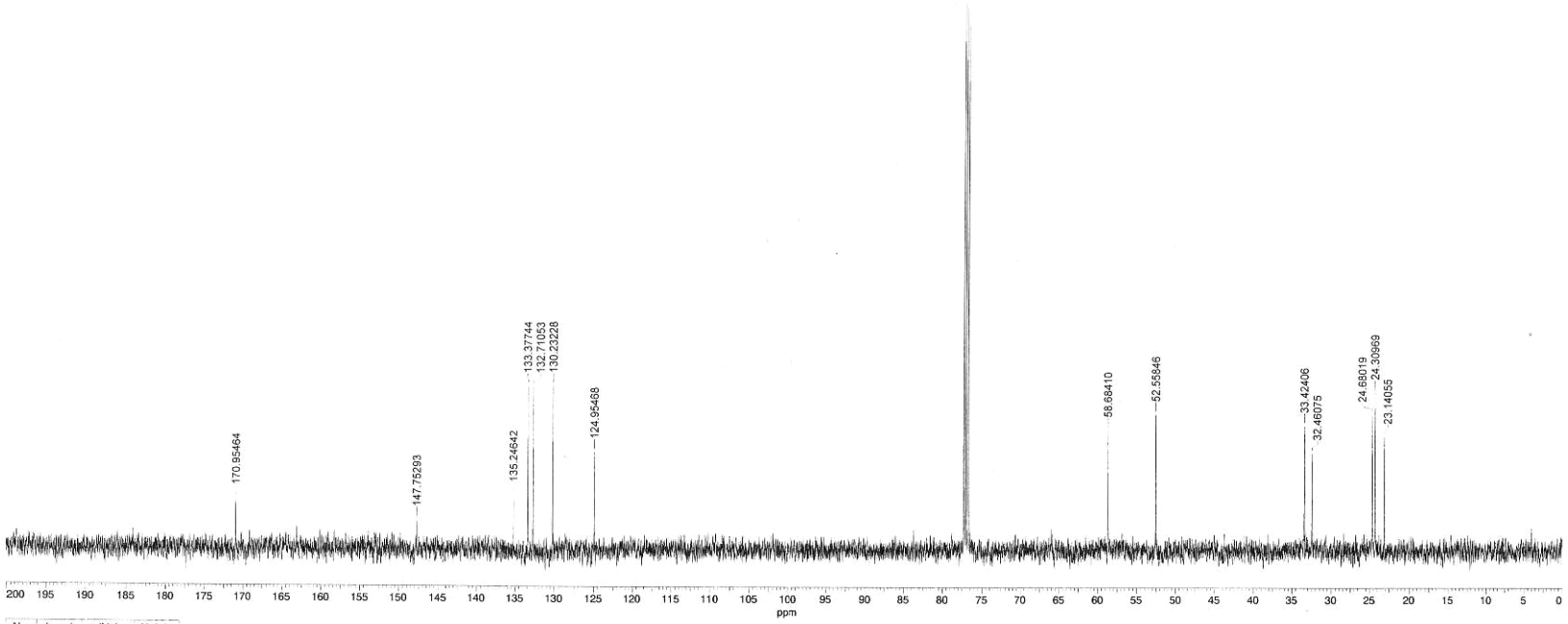
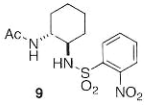
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height
1	23.14	2907.6	0.2073
2	24.31	3054.5	0.2881
3	24.68	3101.1	0.2478
4	32.46	4078.7	0.1780
5	33.42	4199.7	0.2277
6	52.56	6604.0	0.2476
7	58.68	7373.7	0.2191
8	124.95	15700.6	0.1779
9	130.23	16363.7	0.2972
10	132.71	16675.1	0.2964
11	133.38	16758.9	0.2964
12	135.25	16993.7	0.0984
13	147.75	18565.2	0.0527
14	170.95	21480.5	0.0903



9

C:\Documents and Settings\Owner\My Documents\ R‰ª\YD1-C\YD1-C.nmdata

24 May 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Wed May 24 04:15:38 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰®\YD2-H\YD2-H.nmdata
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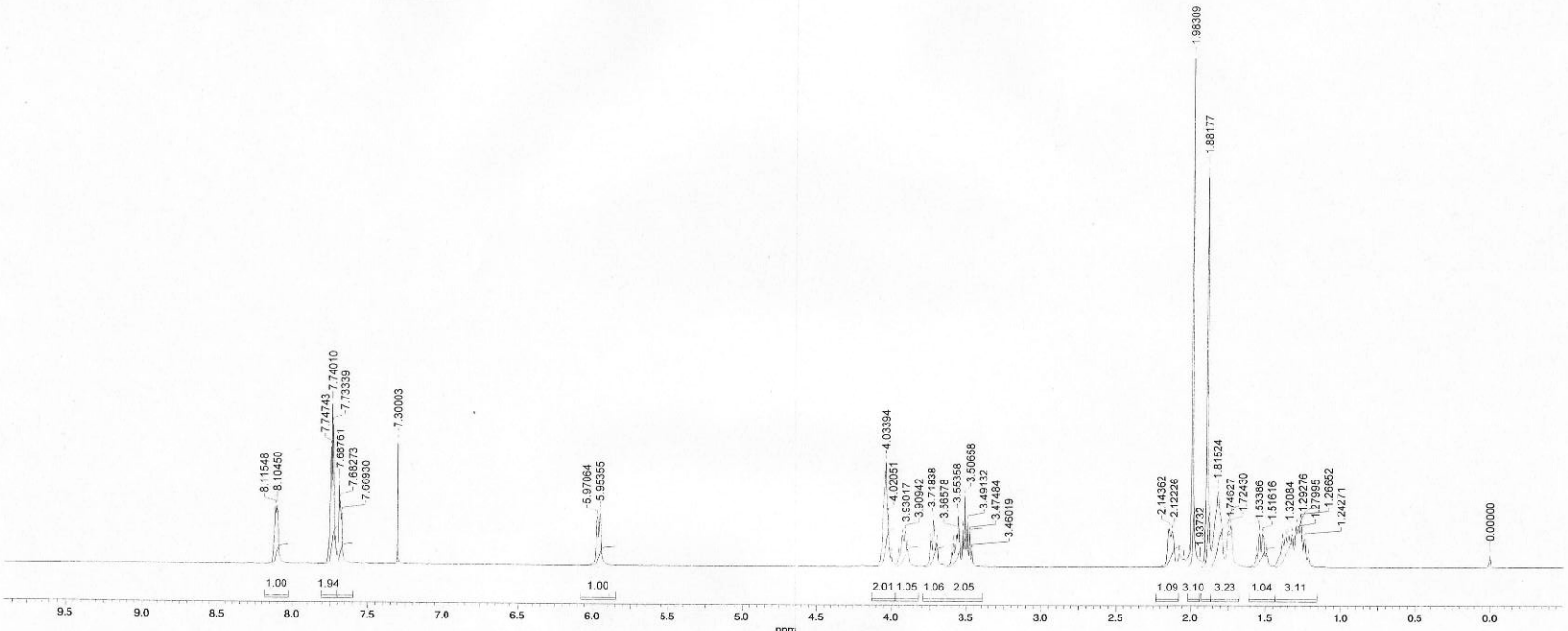
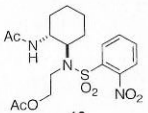
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.0258	17	1.56	779.1	0.0261	33	3.52	1760.3	0.0744	49	4.03	2017.0	0.2051
2	1.22	609.5	0.0212	18	1.72	862.1	0.0829	34	3.54	1771.3	0.0547	50	5.95	2976.8	0.1015
3	1.24	621.4	0.0558	19	1.75	873.1	0.0723	35	3.55	1776.8	0.1007	51	5.97	2985.3	0.0958
4	1.27	633.3	0.0933	20	1.82	907.6	0.1483	36	3.57	1782.9	0.0693	52	7.30	3650.0	0.2412
5	1.28	640.0	0.0703	21	1.88	940.9	0.7857	37	3.58	1792.4	0.0460	53	7.67	3834.7	0.0997
6	1.29	646.4	0.0830	22	1.94	968.7	0.0151	38	3.60	1798.8	0.0291	54	7.68	3841.4	0.1252
7	1.32	660.4	0.0658	23	1.98	991.5	1.0000	39	3.70	1847.9	0.0471	55	7.69	3843.8	0.1615
8	1.34	671.4	0.0625	24	2.01	1002.5	0.0276	40	3.72	1859.2	0.0923	56	7.73	3866.7	0.2751
9	1.36	680.9	0.0596	25	2.04	1019.6	0.0172	41	3.74	1868.3	0.0496	57	7.74	3870.1	0.3140
10	1.39	693.4	0.0506	26	2.07	1035.5	0.0266	42	3.74	1870.5	0.0524	58	7.75	3873.7	0.2303
11	1.48	742.2	0.0237	27	2.12	1061.1	0.0715	43	3.89	1945.2	0.0353	59	8.10	4052.2	0.1154
12	1.49	746.2	0.0291	28	2.14	1071.8	0.0770	44	3.91	1954.7	0.0707	60	8.11	4053.8	0.1067
13	1.51	755.0	0.0624	29	3.46	1730.1	0.0327	45	3.93	1965.1	0.0618	61	8.11	4055.9	0.1047
14	1.52	758.1	0.0664	30	3.47	1737.4	0.0672	46	3.95	1975.2	0.0212	62	8.12	4057.7	0.1124
15	1.53	766.9	0.0680	31	3.49	1745.7	0.0887	47	4.00	1999.0	0.0202				
16	1.54	770.0	0.0595	32	3.51	1753.3	0.1398	48	4.02	2010.3	0.1033				

No.	(ppm)	Value	Absolute Value
1	[1.15 .. 1.44]	3.113	2.05846e+3
2	[1.44 .. 1.61]	1.043	6.89926e+2
3	[1.67 .. 1.86]	3.229	2.13542e+3
4	[1.86 .. 1.93]	2.898	1.91621e+3
5	[1.94 .. 2.02]	3.102	2.05170e+3
6	[2.07 .. 2.23]	1.093	7.22986e+2
7	[3.39 .. 3.64]	2.052	1.35711e+3
8	[3.64 .. 3.79]	1.061	7.01892e+2
9	[3.82 .. 3.97]	1.051	6.95234e+2
10	[3.97 .. 4.13]	2.005	1.32598e+3
11	[5.84 .. 6.08]	1.001	6.61679e+2
12	[7.60 .. 7.71]	1.077	7.12517e+2
13	[7.71 .. 7.81]	1.945	1.28624e+3
14	[8.02 .. 8.18]	1.000	6.61314e+2

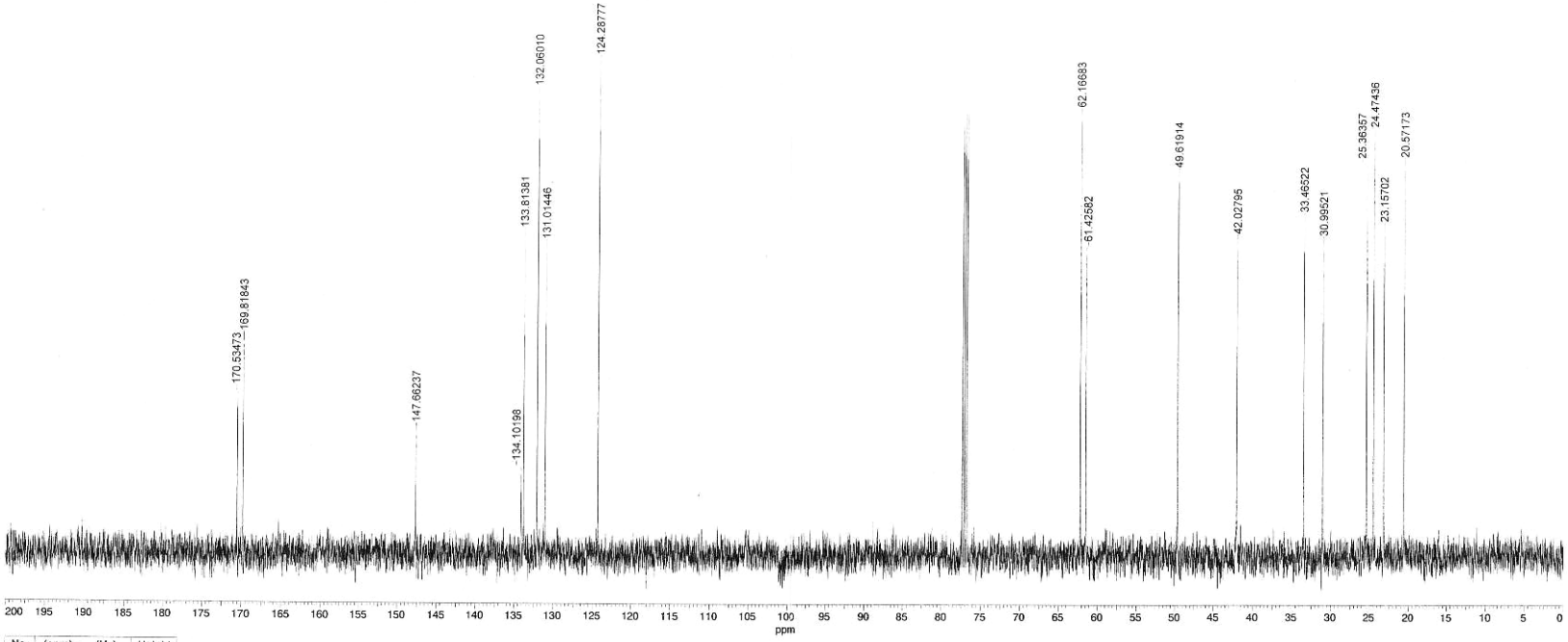


10

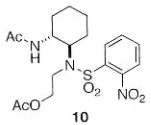
C:\Documents and Settings\Owner\My Documents\ R‰®\YD2-H\YD2-H.nmdata

24 May 2006
noe

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Wed May 24 04:19:01 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD2-C\YD2-C.nmdata
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	20	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height
1	20.57	2584.8	0.7939
2	23.16	2909.7	0.6604
3	24.47	3075.2	0.8553
4	25.36	3186.9	0.7912
5	31.00	3894.5	0.6315
6	33.47	4204.9	0.6800
7	42.03	5280.8	0.6357
8	49.62	6234.6	0.7721
9	61.43	7718.2	0.6204
10	62.17	7811.3	0.8955
11	124.29	15616.8	1.0000
12	131.01	16462.0	0.6212
13	132.06	16593.4	0.9353
14	133.81	16813.7	0.6444
15	134.10	16849.9	0.1654
16	147.66	18553.8	0.2434
17	169.82	21337.7	0.4293
18	170.53	21427.7	0.3190

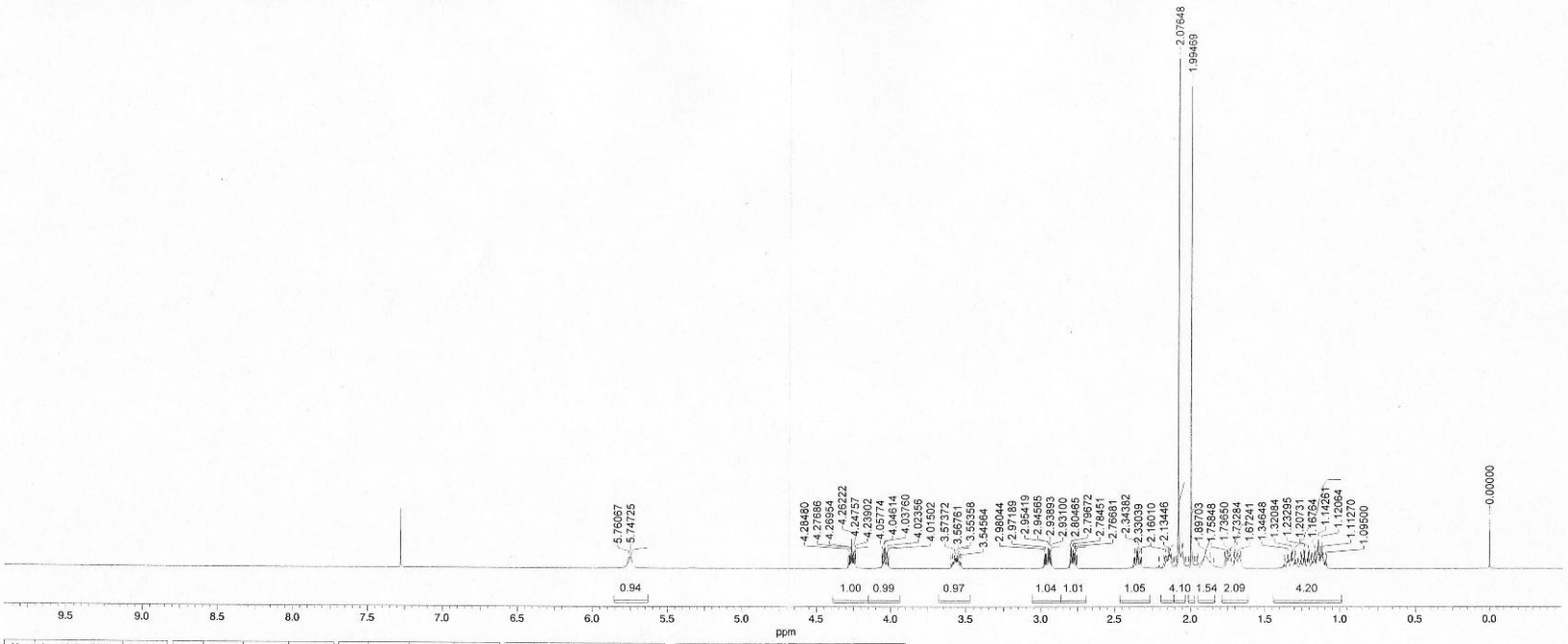


10

C:\Documents and Settings\Owner\My Documents\ R‰ª\YD2-C\YD2-C.nmdata

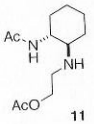
20 May 2006
1H Line

Acquisition Time (sec)	3.2768	*Comment*	1H Line	*Date*	Fri May 26 19:04:58 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R%*%YD3H\YD3H.nmdata
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000					*Solvent*	CHLOROFORM-D



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	-0.00	-0.0	0.0988	27	1.30	647.6	0.0181	53	1.77	884.4	0.0158	79	2.13	1067.2	0.0279
2	1.09	543.5	0.0118	28	1.30	651.0	0.0118	54	1.84	920.7	0.0048	80	2.14	1069.1	0.0268
3	1.10	547.5	0.0205	29	1.31	657.1	0.0206	55	1.87	932.6	0.0152	81	2.14	1070.9	0.0241
4	1.10	551.2	0.0131	30	1.32	660.4	0.0334	56	1.90	948.5	0.0259	82	2.15	1074.6	0.0186
5	1.11	556.4	0.0328	31	1.33	663.8	0.0181	57	1.95	972.6	0.0126	83	2.16	1078.2	0.0238
6	1.12	560.3	0.0524	32	1.34	669.9	0.0175	58	1.95	976.9	0.0070	84	2.16	1080.0	0.0253
7	1.13	564.0	0.0283	33	1.35	673.2	0.0279	59	1.96	981.2	0.0076	85	2.16	1082.2	0.0241
8	1.14	567.6	0.0334	34	1.35	676.6	0.0146	60	1.97	983.3	0.0075	86	2.17	1083.7	0.0220
9	1.14	569.2	0.0295	35	1.36	682.4	0.0063	61	1.97	986.4	0.0071	87	2.17	1087.4	0.0084
10	1.14	571.3	0.0578	36	1.37	686.1	0.0100	62	1.99	997.3	0.9459	88	2.20	1102.3	0.0066
11	1.16	580.2	0.0198	37	1.38	689.4	0.0053	63	2.01	1004.1	0.0070	89	2.32	1161.5	0.0229
12	1.17	583.8	0.0341	38	1.66	831.3	0.0170	64	2.01	1006.5	0.0069	90	2.33	1165.2	0.0240
13	1.17	586.3	0.0189	39	1.67	834.7	0.0256	65	2.02	1009.6	0.0048	91	2.34	1171.9	0.0428
14	1.18	591.1	0.0145	40	1.67	836.2	0.0258	66	2.03	1012.9	0.0068	92	2.35	1175.6	0.0405
15	1.19	594.5	0.0103	41	1.68	839.6	0.0188	67	2.03	1016.0	0.0060	93	2.36	1182.3	0.0226
16	1.20	600.6	0.0199	42	1.69	844.4	0.0163	68	2.05	1024.5	0.0342	94	2.37	1186.3	0.0213
17	1.21	603.7	0.0337	43	1.70	848.1	0.0217	69	2.05	1026.6	0.0306	95	2.76	1379.4	0.0268
18	1.21	607.0	0.0213	44	1.70	849.6	0.0225	70	2.06	1028.5	0.0291	96	2.77	1383.4	0.0327
19	1.23	613.1	0.0202	45	1.71	853.0	0.0158	71	2.08	1038.2	1.0000	97	2.77	1385.2	0.0316
20	1.23	616.5	0.0364	46	1.73	863.4	0.0203	72	2.10	1047.7	0.0075	98	2.78	1389.2	0.0298
21	1.24	619.8	0.0211	47	1.73	866.4	0.0281	73	2.10	1050.4	0.0049	99	2.78	1392.3	0.0369
22	1.25	625.9	0.0115	48	1.74	868.3	0.0276	74	2.11	1053.2	0.0058	100	2.79	1396.5	0.0423

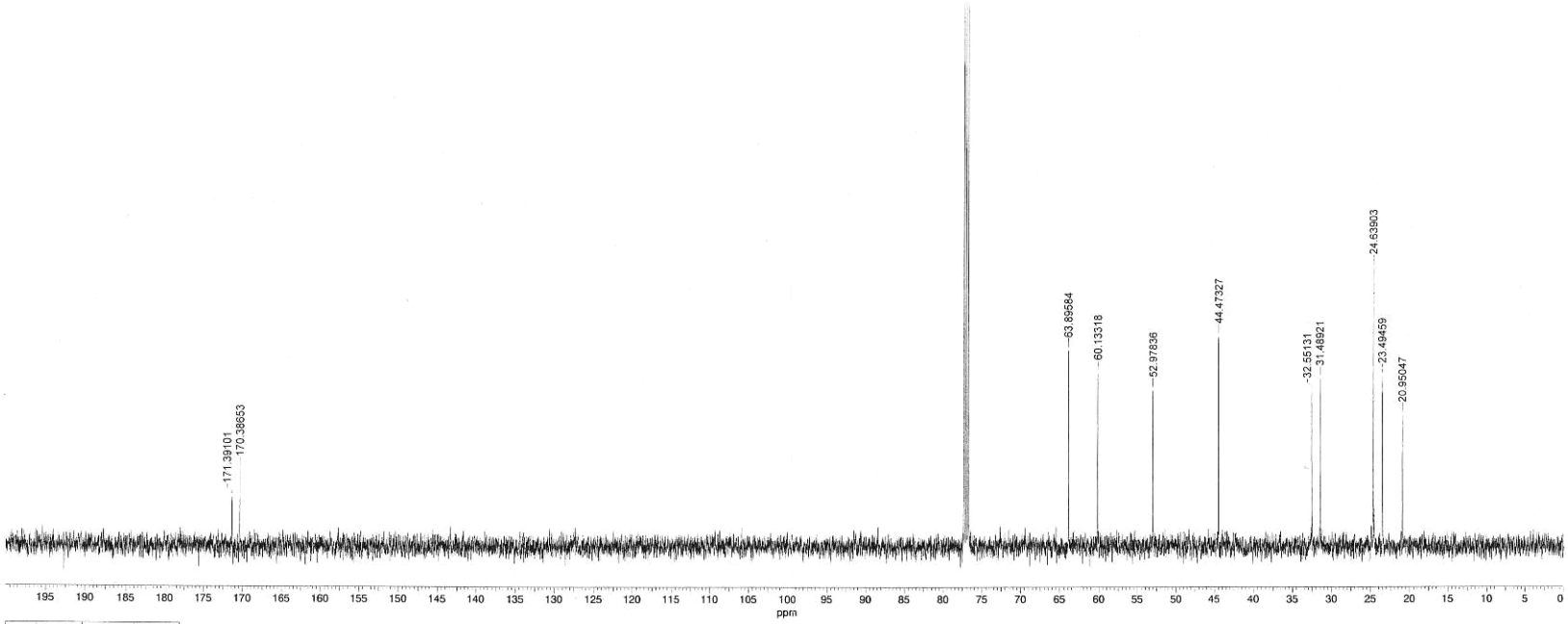
No.	(ppm)	Value	Absolute Value
1	[0.99 .. 1.44]	4.202	2.76646e+3
2	[1.62 .. 1.79]	2.086	1.37326e+3
3	[1.84 .. 1.94]	1.536	1.01146e+3
4	[1.97 .. 2.01]	2.867	1.88726e+3
5	[2.03 .. 2.10]	4.100	2.69920e+3
6	[2.11 .. 2.19]	1.125	7.40929e+2
7	[2.27 .. 2.46]	1.053	6.93215e+2
8	[2.69 .. 2.86]	1.008	6.63370e+2
9	[2.87 .. 3.06]	1.035	6.81628e+2
10	[3.47 .. 3.68]	0.975	6.41727e+2
11	[3.94 .. 4.15]	0.991	6.52675e+2
12	[4.15 .. 4.39]	1.000	6.58386e+2
13	[5.63 .. 5.86]	0.938	6.17437e+2



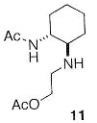
11

26 May 2006
1H Line

Acquisition Time (sec)	0.9667	*Comment*	1H Line	*Date*	Fri May 26 19:09:37 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD3C\YD3C.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	71	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height
1	20.95	2632.4	0.2385
2	23.49	2952.1	0.3103
3	24.64	3095.9	0.5107
4	31.49	3956.6	0.3061
5	32.55	4090.1	0.2833
6	44.47	5588.1	0.3837
7	52.98	6656.7	0.2850
8	60.13	7555.7	0.3171
9	63.90	8028.5	0.3586
10	170.39	21409.1	0.1385
11	171.39	21535.3	0.0889

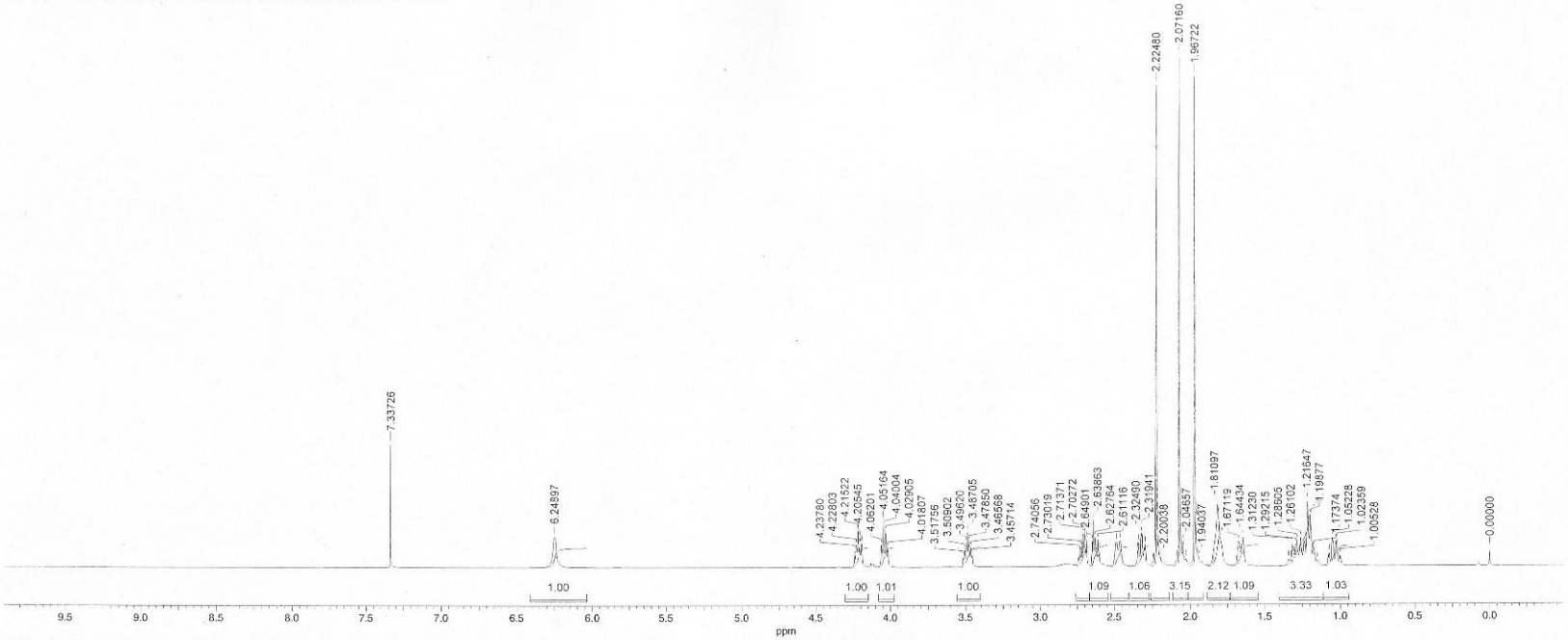


11

C:\Documents and Settings\Owner\My Documents\ R‰ª\YD3C\YD3C.nmdata

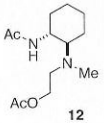
12 Jun 2006
noe

Acquisition Time (sec)	3.2768	*Comment*	noe	*Date*	Mon Jun 12 18:46:15 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\new1H\new1H.nmdata		
Frequency (MHz)	500.00	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	10000.00	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.0306	22	1.32	659.2	0.0319	43	2.32	1159.7	0.0793	64	3.48	1739.2	0.0506
2	1.00	499.0	0.0197	23	1.33	665.9	0.0109	44	2.32	1162.5	0.0649	65	3.49	1743.5	0.0697
3	1.01	502.6	0.0215	24	1.34	669.0	0.0137	45	2.34	1170.7	0.0464	66	3.50	1748.1	0.0476
4	1.02	511.8	0.0518	25	1.64	822.2	0.0569	46	2.35	1173.4	0.0314	67	3.51	1754.5	0.0338
5	1.03	515.5	0.0485	26	1.67	835.6	0.0487	47	2.46	1232.0	0.0509	68	3.52	1758.8	0.0196
6	1.05	522.8	0.0485	27	1.81	905.5	0.1225	48	2.49	1244.2	0.0484	69	4.02	2009.0	0.0387
7	1.05	526.1	0.0550	28	1.81	907.0	0.1215	49	2.60	1300.4	0.0299	70	4.03	2014.5	0.0704
8	1.07	535.6	0.0258	29	1.94	970.2	0.0183	50	2.61	1305.6	0.0528	71	4.04	2020.0	0.0798
9	1.08	539.0	0.0245	30	1.97	983.6	0.9603	51	2.62	1311.1	0.0378	72	4.05	2025.8	0.0877
10	1.15	574.7	0.0113	31	2.02	1010.8	0.0102	52	2.63	1313.8	0.0571	73	4.06	2031.0	0.0445
11	1.17	586.9	0.0371	32	2.03	1013.2	0.0146	53	2.64	1319.3	0.0914	74	4.19	2095.7	0.0466
12	1.18	589.9	0.0297	33	2.05	1023.3	0.0499	54	2.65	1324.5	0.0503	75	4.20	2100.6	0.0550
13	1.20	599.4	0.0991	34	2.05	1026.3	0.0273	55	2.69	1344.3	0.0529	76	4.21	2102.7	0.0603
14	1.22	608.2	0.1253	35	2.07	1035.8	1.0000	56	2.70	1349.8	0.0659	77	4.22	2107.6	0.0730
15	1.23	617.1	0.0533	36	2.09	1046.2	0.0134	57	2.70	1351.4	0.0689	78	4.22	2111.9	0.0429
16	1.24	620.4	0.0502	37	2.19	1096.2	0.0103	58	2.71	1356.9	0.0651	79	4.23	2114.0	0.0444
17	1.25	623.5	0.0286	38	2.20	1100.2	0.0187	59	2.73	1363.3	0.0365	80	4.24	2118.9	0.0321
18	1.26	630.5	0.0563	39	2.22	1112.4	0.9438	60	2.73	1365.1	0.0389	81	6.25	3124.5	0.0603
19	1.29	643.0	0.0513	40	2.24	1122.2	0.0100	61	2.74	1370.3	0.0307	82	7.34	3668.6	0.2414
20	1.29	646.1	0.0431	41	2.30	1148.7	0.0428	62	3.46	1728.6	0.0238				
21	1.31	656.1	0.0422	42	2.30	1151.8	0.0386	63	3.47	1732.8	0.0389				

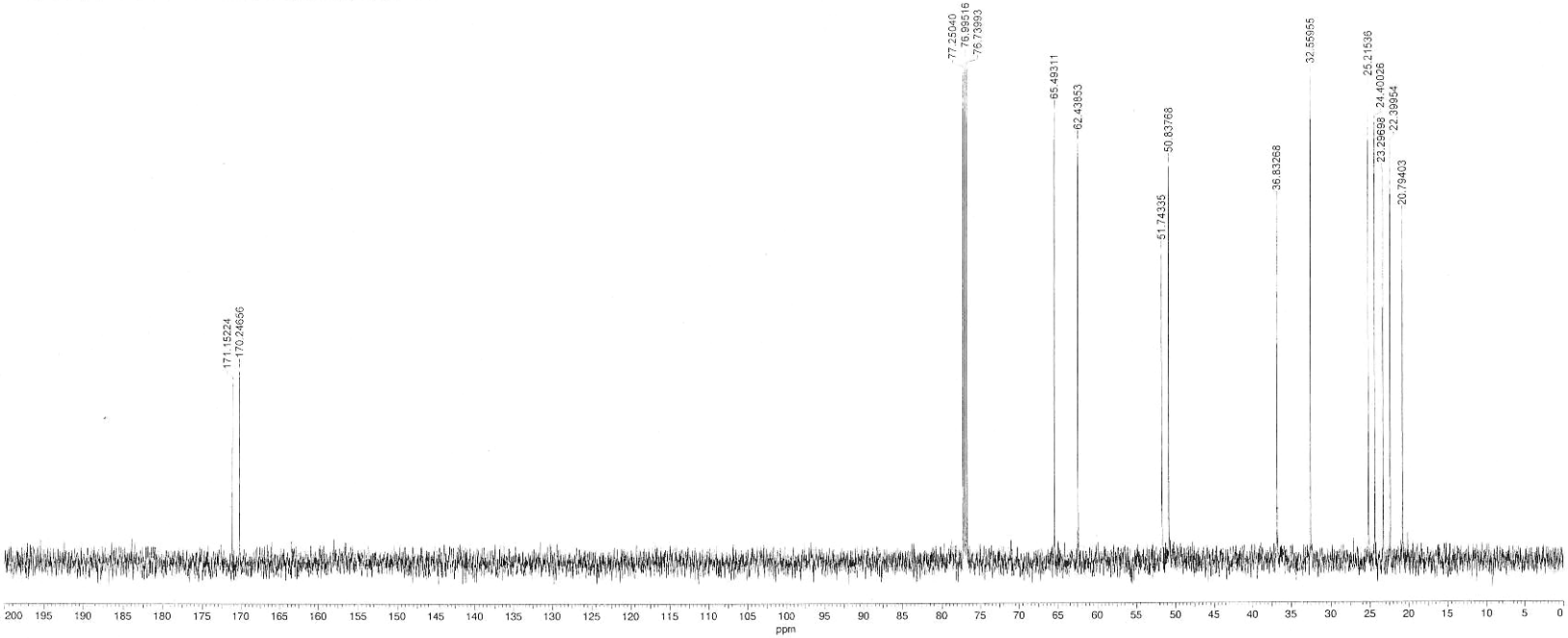
No.	(ppm)	Value	Absolute Value
1	[0.94 .. 1.11]	1.035	6.86635e+2
2	[1.11 .. 1.41]	3.331	2.21023e+3
3	[1.54 .. 1.73]	1.088	7.22255e+2
4	[1.73 .. 1.88]	2.119	1.40629e+3
5	[1.91 .. 2.01]	3.050	2.02371e+3
6	[2.02 .. 2.12]	3.152	2.09122e+3
7	[2.14 .. 2.27]	3.058	2.02881e+3
8	[2.27 .. 2.40]	1.057	7.01476e+2
9	[2.41 .. 2.53]	1.006	6.67698e+2
10	[2.54 .. 2.67]	1.089	7.22631e+2
11	[2.67 .. 2.76]	1.026	6.80854e+2
12	[3.41 .. 3.56]	1.000	6.63512e+2
13	[3.98 .. 4.08]	1.008	6.68770e+2
14	[4.15 .. 4.30]	1.000	6.63336e+2
15	[6.04 .. 6.41]	0.997	6.61854e+2



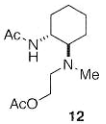
12

12 Jun 2006
noe

Acquisition Time (sec)	0.9667	*Comment*	noe	*Date*	Mon Jun 12 18:48:57 2006			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\13C\13C.nmdata		
Frequency (MHz)	125.65	*Nucleus*	13C	*Number of Transients*	34	*Original Points Count*	32768	*Points Count*	32768	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	33898.30	*Temperature (degree C)*	0.000								



No.	(ppm)	(Hz)	Height
1	20.79	2612.8	0.6825
2	22.40	2814.5	0.8312
3	23.30	2927.3	0.7683
4	24.40	3065.9	0.8768
5	25.22	3168.3	0.9415
6	32.56	4091.1	0.9668
7	36.83	4628.0	0.7131
8	50.84	6387.8	0.7895
9	51.74	6501.6	0.6145
10	62.44	7845.4	0.8363
11	65.49	8229.2	0.8976
12	76.74	9642.4	0.9861
13	77.00	9674.4	1.0000
14	77.25	9706.5	0.9780
15	170.25	21391.5	0.3797
16	171.15	21505.3	0.3573

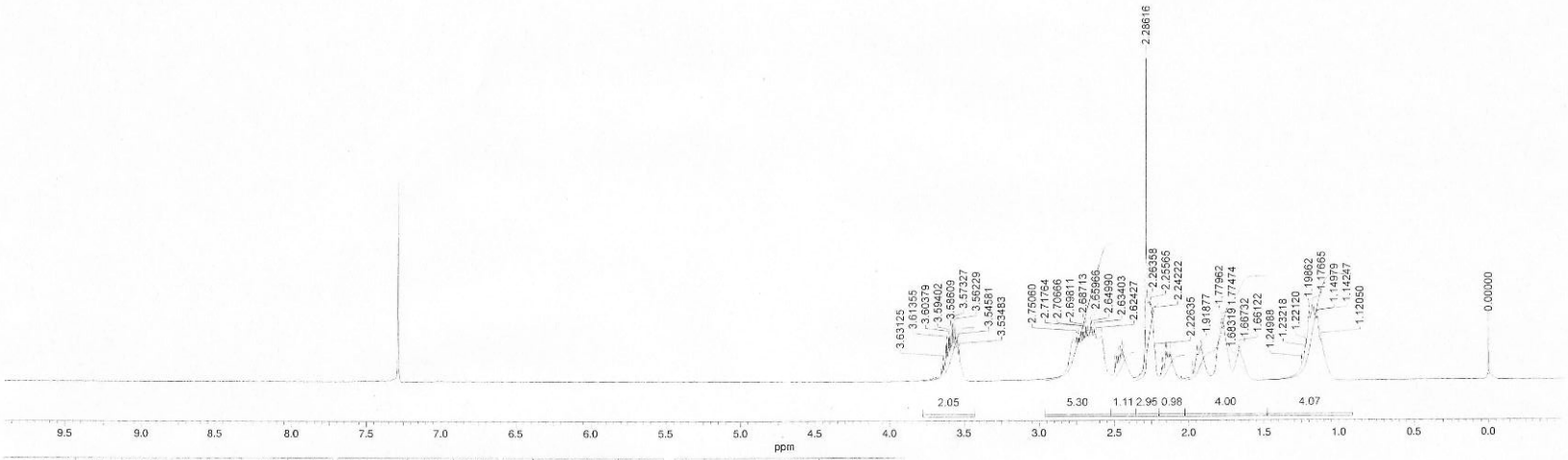


12

C:\Documents and Settings\Owner\My Documents\ R‰ª\13C\13C.nmdata

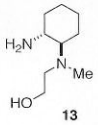
5 Jul 2006

Acquisition Time (sec)	4.1001	*Date*	05 Jul 2006 12:34:20			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD51NON_E101_FT.als			*Frequency (MHz)*	399.65
Nucleus	1H	*Number of Transients*	8	*Original Points Count*	32768	*Points Count*	32768	*Pulse Sequence*	NON	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	7992.01	*Temperature (degree C)*	20.500								



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.0975	18	1.91	764.2	0.0543	35	2.44	976.6	0.0527	52	2.74	1094.9	0.0781
2	1.12	447.8	0.0738	19	1.92	766.8	0.0608	36	2.45	980.3	0.0569	53	2.75	1099.3	0.0796
3	1.14	456.6	0.1153	20	1.94	773.4	0.0466	37	2.47	985.4	0.0474	54	3.53	1412.7	0.0569
4	1.15	459.5	0.1140	21	1.94	776.3	0.0475	38	2.48	989.5	0.0456	55	3.55	1417.1	0.0739
5	1.18	470.2	0.1363	22	1.97	787.8	0.0183	39	2.49	993.4	0.0452	56	3.56	1422.2	0.0795
6	1.18	471.5	0.1351	23	2.12	848.1	0.0478	40	2.50	998.5	0.0323	57	3.56	1423.7	0.1011
7	1.20	479.0	0.1235	24	2.13	851.0	0.0522	41	2.59	1034.2	0.0801	58	3.57	1428.1	0.1059
8	1.22	488.1	0.0645	25	2.15	858.3	0.0519	42	2.62	1048.8	0.0848	59	3.59	1433.2	0.0870
9	1.23	492.4	0.0516	26	2.15	861.2	0.0526	43	2.63	1052.7	0.0934	60	3.59	1436.4	0.0811
10	1.25	498.3	0.0316	27	2.18	869.3	0.0265	44	2.65	1059.0	0.0971	61	3.60	1440.3	0.0786
11	1.25	499.5	0.0321	28	2.18	872.2	0.0250	45	2.66	1062.9	0.1039	62	3.61	1444.2	0.0692
12	1.66	663.9	0.0608	29	2.23	889.8	0.0552	46	2.67	1069.0	0.0835	63	3.62	1447.8	0.0660
13	1.67	666.3	0.0526	30	2.24	896.1	0.1198	47	2.69	1073.9	0.0979	64	3.63	1451.2	0.0343
14	1.68	672.7	0.0349	31	2.26	901.5	0.1383	48	2.70	1078.3	0.0898	65	3.64	1455.1	0.0301
15	1.77	706.6	0.1000	32	2.26	904.6	0.1425	49	2.71	1081.7	0.0881	66	3.65	1458.8	0.0237
16	1.77	709.3	0.1093	33	2.27	906.1	0.1424	50	2.72	1086.1	0.0882				
17	1.78	711.2	0.1113	34	2.29	913.7	0.5800	51	2.73	1091.5	0.0773				

No.	(ppm)	Value	Absolute Value
1	[0.91 .. 1.48]	4.068	1.26068e+3
2	[1.48 .. 2.02]	4.000	1.23970e+3
3	[2.02 .. 2.20]	0.976	3.02449e+2
4	[2.20 .. 2.36]	2.949	9.13922e+2
5	[2.36 .. 2.53]	1.111	3.44267e+2
6	[2.53 .. 2.96]	5.299	1.64229e+3
7	[3.43 .. 3.78]	2.047	6.34359e+2

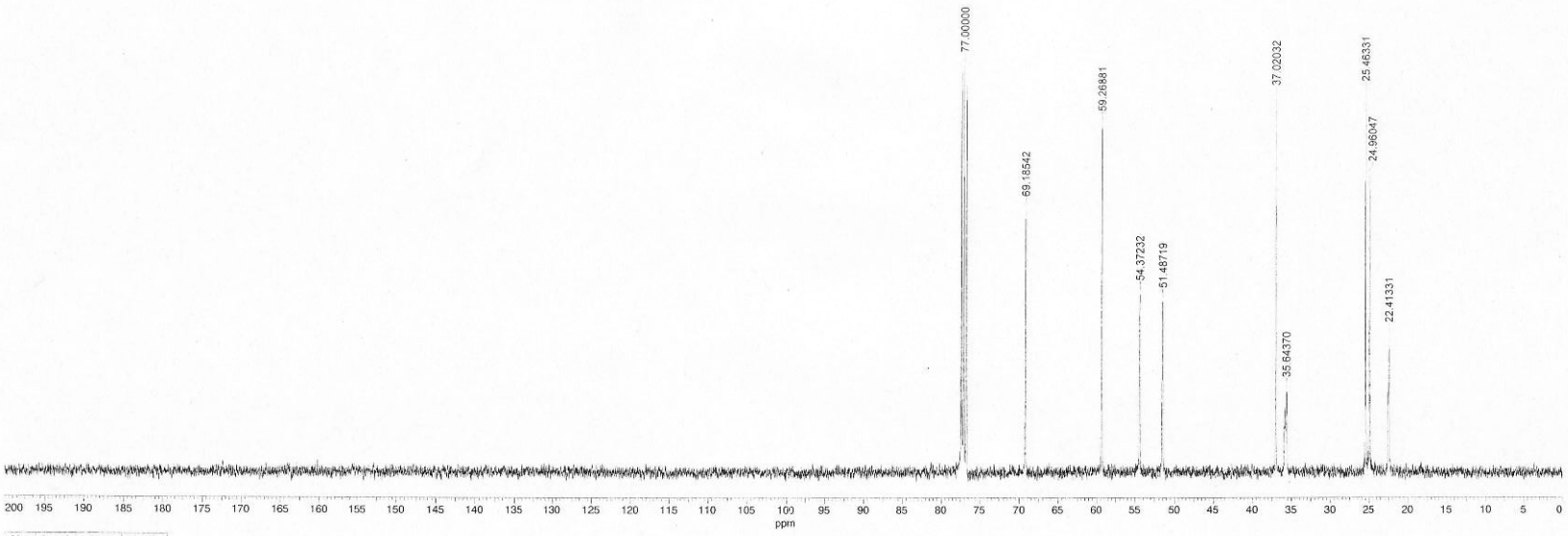


13

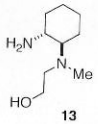
C:\Documents and Settings\Owner\My Documents\ R‰ª\YD51NON_E101_FT.als

5 Jul 2006

Acquisition Time (sec)	1.2083	*Date*	05 Jul 2006 12:32:22			*File Name*	C:\Documents and Settings\Owner\My Documents\ R‰ª\YD5CC1BCM_E107_FT.als			*Frequency (MHz)*	100.40
Nucleus	13C	*Number of Transients*	512	*Original Points Count*	32768	*Points Count*	32768	*Pulse Sequence*	BCM	*Solvent*	CHLOROFORM-D
Sweep Width (Hz)	27118.64	*Temperature (degree C)*	20.500								



No.	(ppm)	(Hz)	Height
1	22.41	2250.3	0.2347
2	24.96	2506.0	0.5194
3	25.46	2556.5	0.6616
4	35.64	3578.6	0.1391
5	37.02	3716.8	0.6545
6	51.49	5169.3	0.2961
7	54.37	5459.0	0.3084
8	59.27	5950.6	0.6085
9	69.19	6946.2	0.4578
10	77.00	7730.8	0.7137



13

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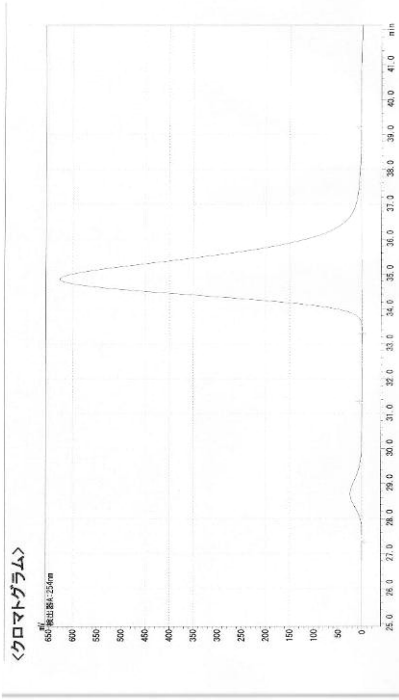
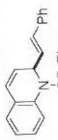
Copies of HPLC of 5a-6aF.



〈ピークレポート〉

検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	23.705	1459059	24049	2.954	3.700	S
2	34.851	47928281	626009	97.046	96.300	
合計		49387341	650058	100.000	100.000	



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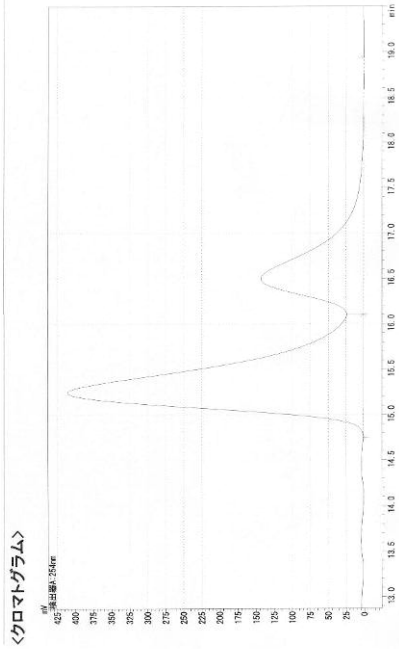
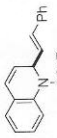


〈ピークレポート〉

検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	15.240	12846028	409074	71.178	74.214	
2	16.493	5201818	142131	28.822	25.786	V
合計		18047846	551205	100.000	100.000	



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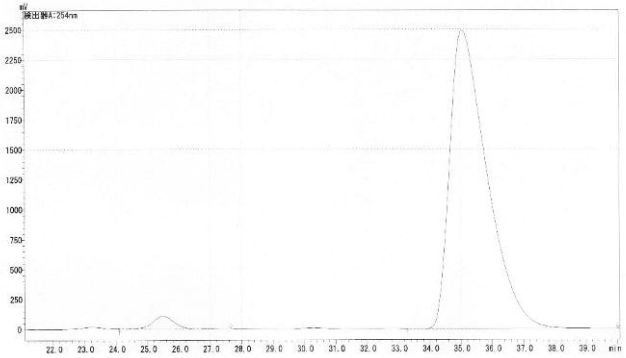

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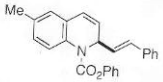
検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	25.483	5201913	107111	2.471	4.122	
2	35.066	205291732	2491121	97.529	95.878	
合計		210493645	2598232	100.000	100.000	



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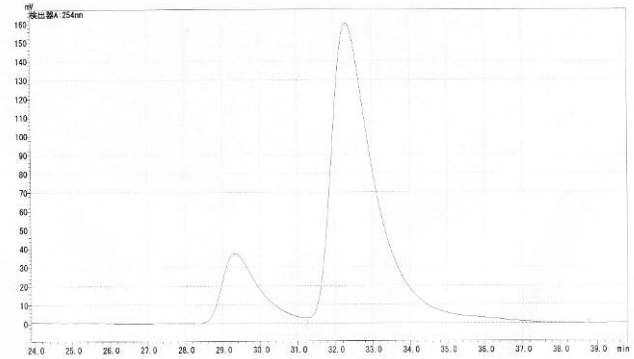

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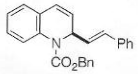
検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	29.330	2589248	37165	16.558	18.837	
2	32.304	13047996	160135	83.442	81.163	V
合計		15637244	197299	100.000	100.000	



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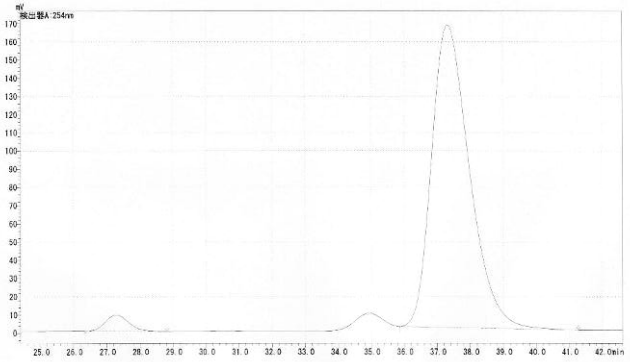

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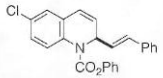
検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	27.279	431911	8914	3.165	5.088	
2	37.317	13213285	166270	96.835	94.912	
合計		13645196	175184	100.000	100.000	



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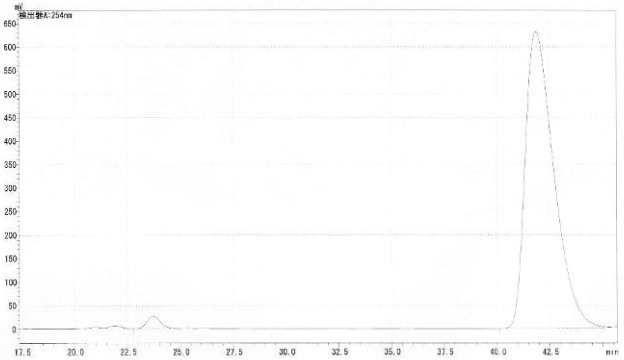

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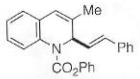
検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	23.706	1209185	27115	1.993	4.119	
2	41.869	59473143	631224	98.007	95.881	
合計		60682328	658339	100.000	100.000	



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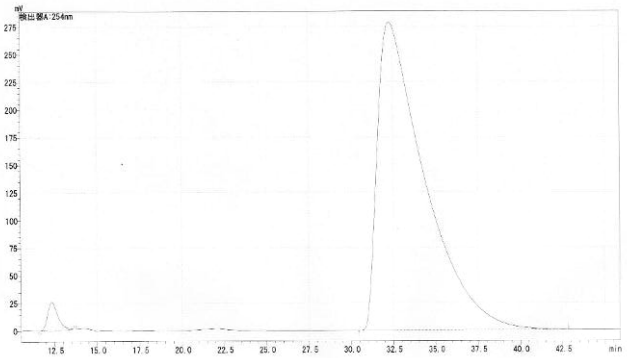

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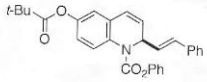
検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	12.325	1064550	25529	1.939	8.389	
2	32.283	53830413	278793	98.061	91.611	
合計		54894963	304321	100.000	100.000	



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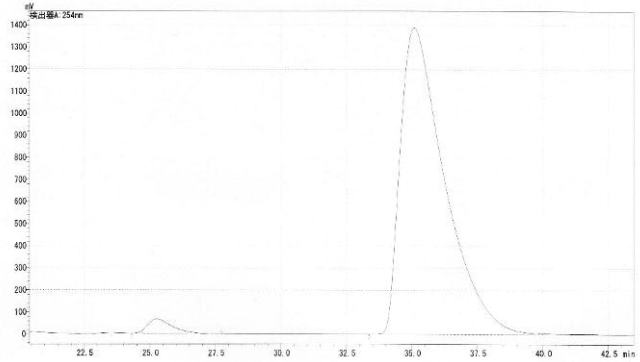

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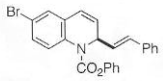
検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	25.257	4237555	66050	2.532	4.544	S
2	35.088	163147565	1387384	97.468	95.456	SV
合計		167385120	1453434	100.000	100.000	



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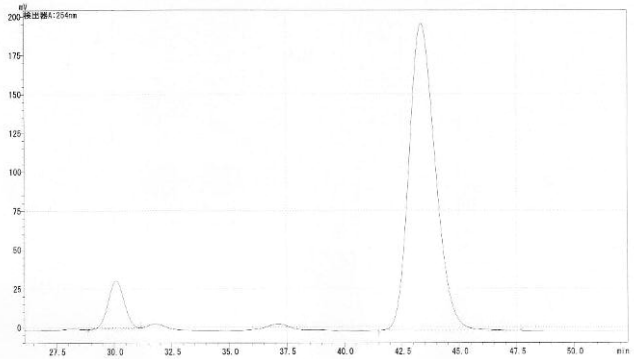

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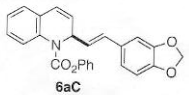
検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	30.084	1491870	30909	8.679	13.529	
2	43.372	15697226	197545	91.321	86.471	
合計		17189096	228453	100.000	100.000	



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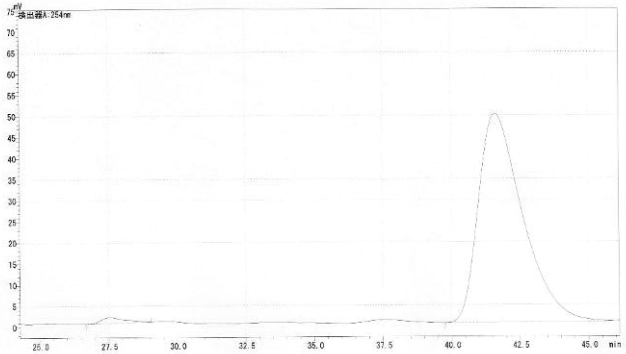

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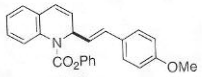
検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	27.543	81186	1363	1.441	2.676	
2	41.611	5554408	49559	98.559	97.324	
合計		5635594	50921	100.000	100.000	



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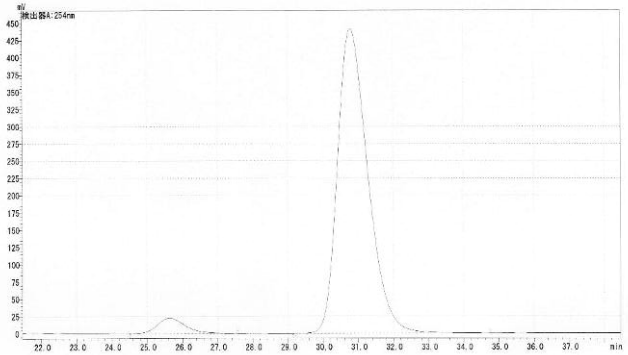

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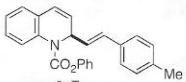
検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	25.631	1195256	22180	4.323	4.784	
2	30.785	26454838	441462	95.677	95.216	
合計		27650094	463642	100.000	100.000	



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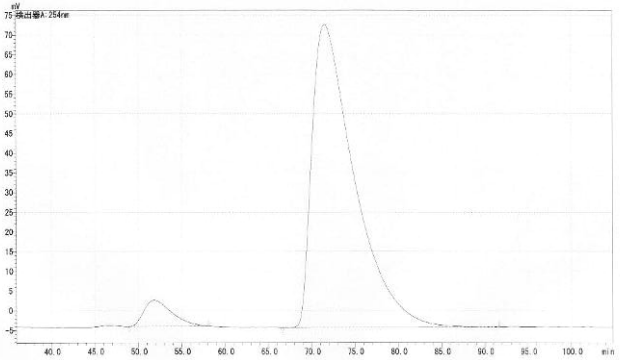

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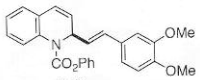
検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	51.775	1479452	6667	5.379	7.979	
2	71.543	26024434	76893	94.621	92.021	
合計		27503886	83560	100.000	100.000	



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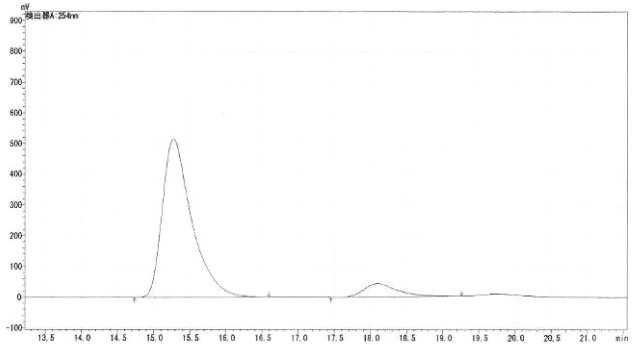

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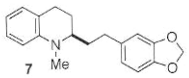
検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	15.271	14432183	513646	91.489	92.345	
2	18.092	1342556	42579	8.511	7.655	
合計		15774740	556226	100.000	100.000	



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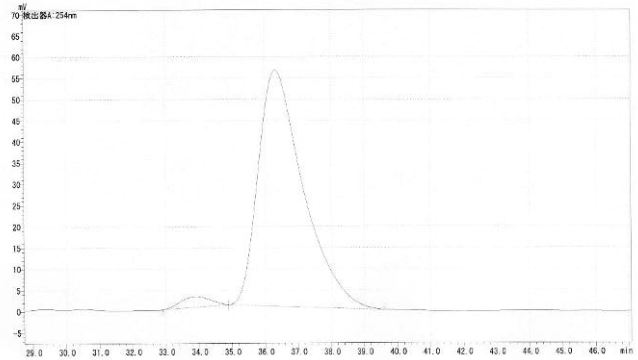

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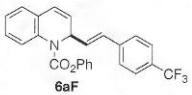
検出器A Ch1 254nm

ピーク#	保持時間	面積	高さ	面積%	高さ%	マーク
1	33.898	132326	2355	2.502	4.093	
2	36.321	5157195	55192	97.498	95.907	
合計		5289520	57547	100.000	100.000	



6aF