Supporting Information

Catalytic Enantioselective Boron Conjugate Addition to Cyclic Carbonyl Compounds: A New Approach to Cyclic β-Hydroxy Carbonyls.

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TABLE OF CONTENTS

General Methods. All reactions were performed in oven-dried Schlenk tubes under a positive pressure of nitrogen and run two or more times. THF was distilled from sodium benzophenone ketyl under nitrogen. CuCl, NaO*t*-Bu, bis(pinacolato)diboron and other commercial substrates were purchased and used as received. Flash chromatography was performed on silica gel from Merck (70–230 mesh). All ^{1}H NMR spectra were obtained on Varian Mercury 300 systems and reported in parts per million (ppm) downfield from tetramethylsilane. ^{13}C NMR spectra are reported in ppm referenced to deuteriochloroform (77.16 ppm). Infrared spectra (IR) were obtained on a Nicolet FT-IR instrument. HPLC and GC analysis was performed on a Younglin Acme 9000 series. High resolution mass spectra (HRMS) were obtained at Korea Basic Science Institute (Daegu, Korea) and reported in the form of m/z (intensity relative to base peak = 100).

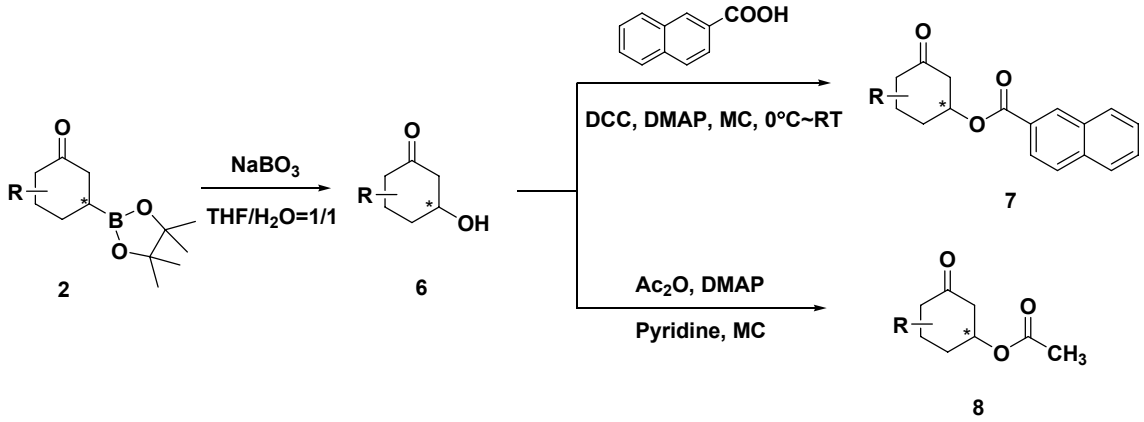
Cyclic carbonyl compounds such as **1f**, **1g**, and 3-methyl-2-cyclohexenone were purchased from Aldrich and used as received. 2-Cyclohexenone and **3** were purified by Kugelrohr distillation before use. **1a**–**1e** were prepared according to published procedures.[1]

General Procedure for the Asymmetric β-Boration of Cyclic Enones with (*R*,*S*)-Taniaphos (Table 2): To a oven dried schlenk tube equipped with a stir bar were added CuCl (0.010 mmol, 1.5 mg), NaO*t*-Bu (0.015 mmol, 1.4 mg), (*R*,*S*)-Taniaphos ligand (0.020 mmol, 13.8 mg) and THF (0.4 mL) under nitrogen. After the mixture was stirred at room temperature for 30 min, bis(pinacolato)diboron (0.11 mmol, 140 mg) dissolved in THF (0.30 mL) was added. The reaction mixture was stirred for 10 min. Then, cyclic enone (0.5 mmol) was added followed by MeOH (1 mmol, 0.04 mL). The reaction tube was washed with THF (0.3 mL), sealed, and stirred for 24 h. The reaction mixture was filtered through a pad of Celite and concentrated. The product was purified by silica gel chromatography.

General Procedure for the Sequential Boration/Oxidation: When the β-boration reaction proceeded to completion, the reaction mixture was filtered through a pad of Celite and concentrated. To the crude product in THF (2.5 mL) and water (2.5 mL) was added sodium perborate (2.5 mmol, 204.6 mg). The reaction mixture was stirred vigorously for 0.5−1 h at room temperature. The reaction mixture was quenched with water and then, extracted with

ethyl acetate (3 x 20 mL). The combined organic layers were washed with brine (10 mL), dried over $MgSO_4$, and concentrated. The β-hydroxy ketone product was purified by silica gel chromatography.

Methods for the Determination of ee:



1) **2g**, **4** and **5**: the ee was determined by chiral GC analysis of the β-borylated product (**2**) itself.

2) **2a**: the ee was determined by HPLC analysis of the corresponding hydroxy compound (**6a**).

3) β-Borylated cyclohexanone (Table 1), **2b**, **2c** and **2f**: the ee was determined by HPLC analysis of the corresponding naphthoate derivative obtained by naphthylation.[2a]

4) Diastereomeric **2e**: the ee was determined by HPLC analysis of the corresponding acetate derivative obtained by acetylation.[2b]

To make sure that there is no significant change in the oxidation step, the ee of **2a** was double-checked with both **2a** and hydroxy derivative **6a**. See below.

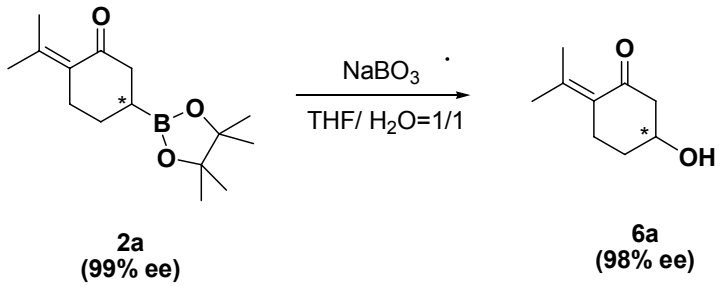
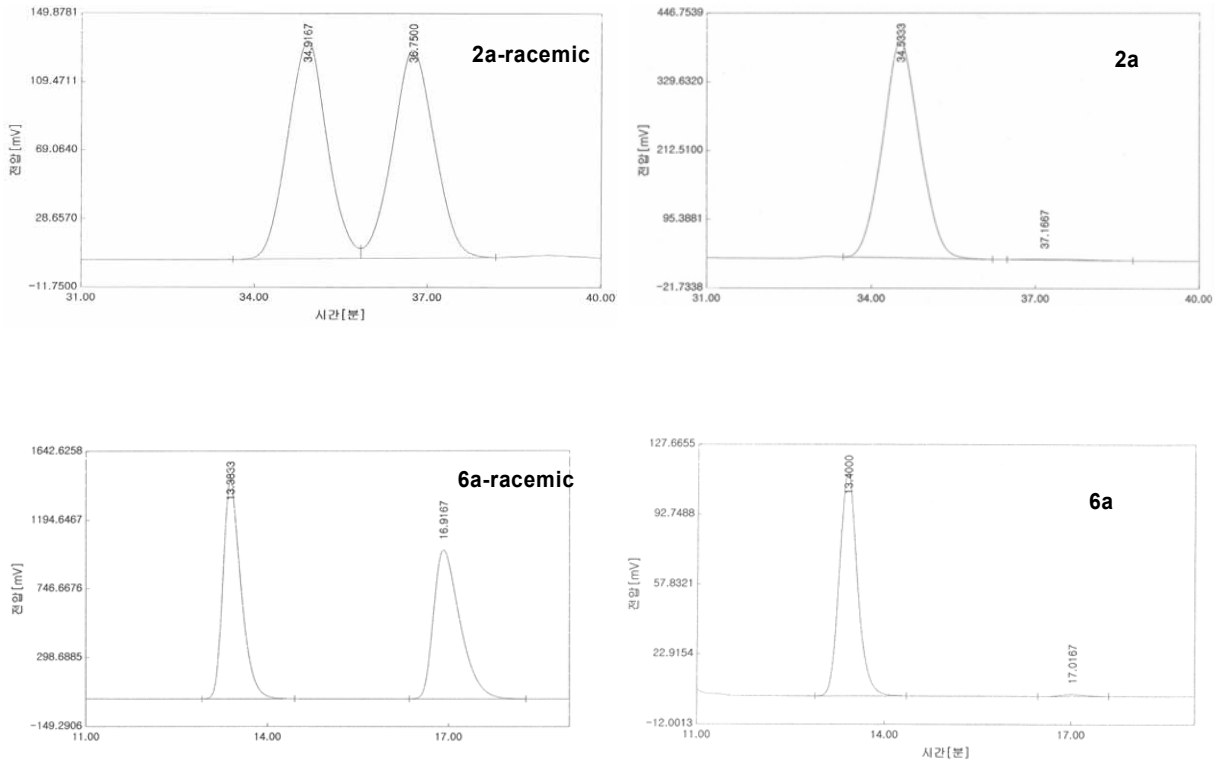
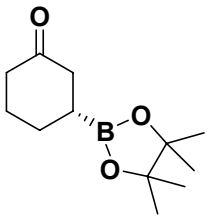


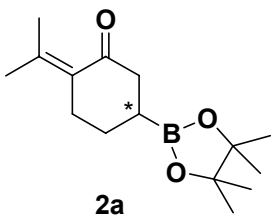
Figure 1 HPLC spectra of **2a** and **6a**



Characterization Data



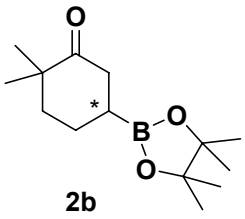
(*R*)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cyclohexanone (Table 1, entry 8). Using the general procedure, the title compound was obtained as a colorless oil in 92% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.50–2.24 (m, 4H), 2.16–2.02 (m, 1H), 1.95–1.55 (m, 3H), 1.55–1.39 (m, 1H), 1.24 (s, 12H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ 212.5, 83.5, 42.7, 42.0, 28.5, 26.6, 24.83, 24.78. The spectroscopic data match those reported previously.[3] The ee (98% ee) was obtained by chiral HPLC analysis of the corresponding naphthoate derivative using an AD-H column (*i*-PrOH/hexanes = 10/90, 0.5 mL/min, UV detection at 254 nm); (*S*)-isomer t_r = 22.8 min and (*R*)-isomer t_r = 28.0 min. The absolute configuration was assigned by comparison of optical rotation of the corresponding TBS-protected hydroxy compound of the boronate product, $[\alpha]_D^{23}$ +4.8º (*c* 0.86 in $CDCl_3$) (lit.[4] $[\alpha]_D^{25}$ –5.6º (*c* 1.02 in $CDCl_3$), nature compound (*S*)).



2a

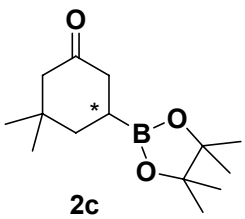
2-(propan-2-ylidene)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-

yl)cyclohexanone (2a) (Table 2, entry 1). Using the general procedure, the title compound was obtained as a colorless oil in 93% yield. $[\alpha]_D^{23}$ +12.7º (*c* 1.0 in $CDCl_3$); ^1H NMR (300 MHz, $CDCl_3$): δ 2.69 (dt, *J* = 15.4, 4.4 Hz, 1H), 2.53–2.24 (m, 3H), 1.97 (s, 3H), 1.94–1.84 (m, 1H), 1.76 (s, 3H), 1.73–1.56 (m, 1H), 1.56–1.42 (m, 1H), 1.23 (s, 12H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ 204.9, 141.8, 132.4, 83.4, 43.3, 30.6, 30.0, 24.74, 24.72, 23.0, 22.0, 20.4 (C–B); IR (neat): 2978, 1683, 1381 cm^{-1}; HRMS (EI) calcd for $C_{15}H_{25}BO_3$: 264.1897; found 264.1900. The ee (98% ee) was obtained by chiral HPLC analysis of the corresponding hydroxy cycloketone **6a** using an AS-H column (*i*-PrOH/hexanes = 10/90, 0.5 mL/min, UV detection at 254 nm); major isomer t_r = 13.4 min and minor isomer t_r = 17.0 min.



2b

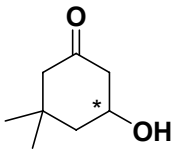
2,2-dimethyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) cyclohexanone (2b) (Table 2, entry 2). Using the general procedure, the title compound was obtained as a colorless oil in 78% yield (conversion 83 %). $[\alpha]_D^{23}$ -2.4º (*c* 1.0 in $CDCl_3$); ^1H NMR (300 MHz, $CDCl_3$): δ 2.50 (dd , *J* = 14.4, 12.3 Hz, 1H), 2.29 (dd, *J* = 14.5, 4.3 Hz, 1H), 1.94–1.71 (m, 3H), 1.71–1.55 (m, 1H), 1.55–1.36 (m, 1H), 1.24 (s, 12H), 1.15 (s, 3H), 1.06 (s, 3H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ 216.6, 83.5, 45.2, 42.7, 39.1, 25.6, 25.2, 24.83, 24.79, 23.1; IR (neat): 2977, 1707, 1382 cm^{-1}; HRMS (EI) Calcd for $C_{14}H_{25}BO_3$: 252.1897; found 252.1899. The ee (95% ee) was obtained by chiral HPLC analysis of the corresponding naphthoate derivative **7b** using an AS-H column (*i*-PrOH/hexanes = 10/90, 0.6 mL/min, UV detection at 254 nm); minor isomer t_r = 11.0 min and major isomer t_r = 12.2 min. The spectroscopic data of the corresponding hydroxy ketone **6b** match those reported previously.[5]



2c

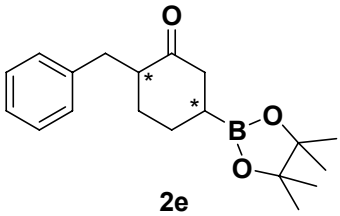
3,3-dimethyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cyclohexa -none (2c) (Table 2, entry 4). Using the general procedure, the title compound was prepared as a colorless oil in 92% yield. $[\alpha]_D^{23}$ +9.7º (*c* 2.1 in $CDCl_3$); ^1H NMR (300 MHz, $CDCl_3$): δ 2.42–2.14 (m, 3H), 2.14–2.01 (m, 1H), 1.67–1.54 (m, 3H), 1.25 (s, 12H), 1.05 (s, 3H), 0.89 (s, 3H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ 212.7, 83.6, 54.9, 41.6, 39.5, 37.5, 32.0, 25.2, 24.9, 24.8, 19.3 (C–B); IR (neat):

2957, 1709, 1380 cm^{-1}; HRMS (EI) Calcd for $C_{14}H_{25}BO_3$: 252.1897; found 252.1899. The ee (>99% ee) was obtained by chiral HPLC analysis of the corresponding naphthoate derivative **7c** using an AS-H column (*i*-PrOH/hexanes = 10/90, 0.6 mL/min, UV detection at 254 nm); minor isomer t_r = 15.1 min and major isomer t_r = 17.9 min.



6c

5-hydroxy-3,3-dimethylcyclohexanone (6c)[6] ^{1}H NMR (300 MHz, $CDCl_3$): δ 4.11 (sept, 1H), 2.88 (br s, 1H), 2.71 (ddt, *J* = 13.5, 5.1, 1.8 Hz, 1H), 2.31 (ddd, *J* = 13.4, 10.4, 1.0 Hz, 1H), 2.23 (d, *J* = 13.6 Hz, 1H), 2.10 (dt, *J* = 13.6, 2.1 Hz, 1H), 1.96 (ddt, *J* = 13.1, 4.4, 1.9 Hz, 1H), 1.62 (dd, *J* = 12.9, 10.9 Hz, 1H), 1.11 (s, 3H), 0.87 (s, 3H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ 210.1, 67.2, 53.9, 50.5, 47.1, 33.1, 31.7, 26.6.

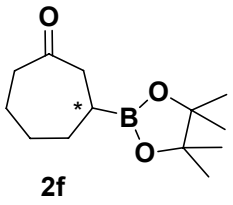


2e

2-benzyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cyclohexanone (2e) (diasteromeric mixture, Table 2, entry 6). Using the general procedure, the title compound was prepared as a colorless oil in 90% yield. The diasteroisomeric ratio (43:57) was determined by GC analysis of the crude reaction mixture and its spectrum is shown in the following. IR (neat): 2978, 1709, 1382 cm^{-1}; HRMS (EI) Calcd for $C_{19}H_{27}BO_3$: 314.2053; found 314.2057. The corresponding acetate derivative **8e** of the diastereomers can be separated by silica gel chromatography, and the ee was determined by chiral HPLC using an OD-H column (*i*-PrOH/hexanes = 10/90, 0.3 mL/min, UV detection at 254 nm). Minor diastereomer (96% ee): major isomer t_r = 24.2 min and minor isomer t_r = 27.5 min ; Major diastereomer(>99% ee): minor isomer t_r = 25.0 min and major isomer t_r = 27.5 min.

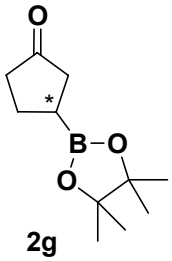
8e: Minor diastereomer (96% ee) was isolated as a colorless oil in 30% yield from **1e**. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.40–7.14 (m, 5H), 4.97 (sept, 1H), 3.23 (dd, *J* = 12.9, 3.5 Hz, 1H), 2.82 (ddd, *J* = 13.4, 5.0, 1.9 Hz, 1H), 2.38–2.55 (m, 3H), 2.27–2.12 (m, 1H) 2.04 (s, 3H), 2.02–1.92 (m, 1H), 1.80–1.56 (m, 1H), 1.42–1.18 (m, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ 207.8, 170.1, 139.8, 129.2, 128.5, 126.3, 71.6, 51.4, 47.3, 35.1, 30.2, 26.4, 21.3. **Major diastereomer** (>99% ee) was isolated as a colorless oil in 33% yield from **1e**. ^{1}H NMR (300

MHz, $CDCl_3$): δ 7.35–7.12 (m, 5H), 5.41 (br s, 1H). 3.30 (dd, *J* = 13.6, 4.3 Hz, 1H), 2.74–2.51 (m, 3H), 2.45 (dd, *J* = 13.6, 9.1 Hz, 1H), 2.04 (s, 3H), 1.96–1.60 (m, 4H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ 209.1, 170.1, 140.1, 129.2, 128.5, 126.3, 72.6, 52.2, 46.2, 35.2, 29.1, 27.4, 21.3.



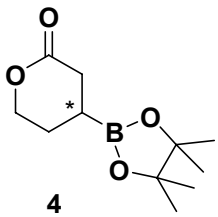
2f

3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cycloheptanone (2f) (Table 2, entry 7). Using the general procedure, the title compound was prepared as a colorless oil in 95% yield. $[\alpha]_D^{23}$ +26.3º (*c* 0.77 in $CDCl_3$); ^1H NMR (300 MHz, $CDCl_3$): δ 2.68–2.42 (m, 4H), 2.08–1.90 (m, 2H), 1.90–1.74 (m, 2H),1.74–1.52 (m, 1H), 1.52–1.41 (m, 2H), 1.24 (s, 12H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ 215.6, 83.5, 44.9, 43.8, 31.9, 31.1, 24.8, 24.7, 24.4, 21.7 (C–B); The spectroscopic data match those reported previously.[7] The ee (90% ee) was obtained by chiral HPLC analysis of the corresponding naphthoate derivative **7f** using an OD-H column (*i*-PrOH/hexane, 15:85, 0.7 mL/min, UV detection at 254 nm); major isomer t_r = 13.7 min and minor isomer t_r = 17.1 min.



2g

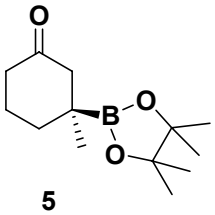
3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cyclopentanone (2g) (Table 2, entry 8). Using the general procedure, the title compound was prepared as a colorless oil in 82% yield. $[\alpha]_D^{23}$ +11.6º (*c* 1.6 in $CDCl_3$); ^1H NMR (300 MHz, $CDCl_3$): δ 2.42–2.02 (m, 5H), 1.94–1.76 (m, 1H), 1.74–1.56 (m, 1H), 1.26 (s, 12H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ 221.4, 83.7, 40.4, 39.1, 25.4, 24.9. The spectroscopic data match those reported previously.[8] The ee (74% ee) was obtained by chiral GC analysis of the boration compound **2g** using a CHIRASIL DEX CB column (120 ℃ constant temperature); major isomer t_r = 49.9 min and minor isomer t_r = 50.9 min.



4

4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)tetrahydropyran-2-one (4) (Scheme 1). Using the general procedure, the title compound was prepared as a colorless oil in 96% yield. ^1H NMR (300 MHz, $CDCl_3$): δ 4.50–4.20 (m, 2H), 2.64 (dd, *J* = 17.8, 6.9 Hz, 1H), 2.51 (dd, *J* = 17.8, 10.1 Hz, 1H), 2.14–1.90 (m, 1H), 1.90–1.74 (m, 1H), 1.66–1.44 (m, 1H), 1.25 (s, 12H); ^{13}C NMR

(75.4 MHz, $CDCl_3$): δ 171.8, 84.0, 70.1, 31.0, 24.9, 24.8, 24.1, 17.7 (C–B); The spectroscopic data match those reported previously.[8] The ee (97% ee) was obtained by chiral GC analysis of **4** using a CHIRASIL DEX CB column (140 ℃ constant temperature); minor isomer t_r = 57.1 min and major isomer t_r = 57.8 min.



5

3-methyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cyclohexanone (5) (Scheme 1). Using the general procedure with (*S,S,R,R*)-Tangphos, the title compound was obtained as a colorless oil in 96% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.51 (dt, *J* = 13.8, 1.3 Hz, 1H), 2.40–2.14 (m, 2H), 2.10–1.89 (m, 3H), 1.87–1.66 (m, 1H), 1.52–1.36 (m, 1H), 1.21 (s, 12H), 1.03 (s, 3H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ 212.2, 83.6, 50.8, 41.3, 34.3, 24.8, 24.7, 24.3, 24.0. The spectroscopic data match those reported previously.[9] The ee (64% ee) was obtained by chiral GC analysis of **5** using a CHIRASIL DEX CB column (120℃ constant temperature); major isomer t_r = 48.2 min and minor isomer t_r = 49.5 min. $[\alpha]_D^{23}$ +7.9º (*c* 5.0 in $CDCl_3$) (lit.[10] $[\alpha]_D^{25}$ +9.2º (*c* 0.5 in $CDCl_3$, 81% ee)).

References

(1) (*a*) F. A. Marques, C. A. Lenz, F. Simonelli, B. H. L. N. S. Maia, A. P. Vellasco and M. N. Eberlin, *J. Nat. Prod.*, 2004, **67**, 1939–1941; (*b*) L. M. Urbaneja and N. Krause, *Eur. J. Org. Chem.*, 2004, 4467–4470; (*c*) W. F. Gannon and H. O. House, *Organic Syntheses*, 1960, **40**, 41–42; W. F. Gannon and H. O. House, *Organic Syntheses*, 1960, **40**, 14–16; (*d*) H. Hopf, J. Kämpen, P. Bubenitschek and P. G. Jones, *Eur. J. Org. Chem.*, 2002, 1708–1721.

(2) (*a*) B.-Z. Ahn, K.-U. Baik, G.-R. Kweon, K. Lim and B.-D. Hwang, *J. Med. Chem.*, 1995, **38**, 1044–1047; (*b*) M. Sodeoka, T. Iimori and M. Shibasaki, *Tetrahedron Lett.*, 1985, **26**, 6497–6500.

(3) G. W. Kabalka, Z. Z. Wu, M.-L. Yao and N. Natarajan, *Appl. Radiat. Isot.*, 2004, **61**, 1111–1115.

(4) M. A. Arai, R. Tsutsumi, H. Hara, T. C. Chen, T. Sakaki, N. Urushino, K. Inouye and A. Kittaka, *Heterocycles*, 2005, **66**, 469–479.

(5) M. D. Keränen, K. Kot, C. Hollmann and P. Elibracht, *Org. Biomol. Chem*., 2004, **2**, 3379–3384.

(6) R. Semet and R. Longeray, *Bull. Soc. Chim. France*, 1978, **3**–**4**, 185–192.

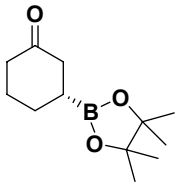
(7) H. A. Ali, I. Goldberg and M. Srebnik, *Organometallics*, 2001, **20**, 3962–3965.

(8) K. Lee, A. R. Zhugralin and A. H. Hoveyda, *J. Am. Chem. Soc.*, 2009, **131**, 7253–7255.

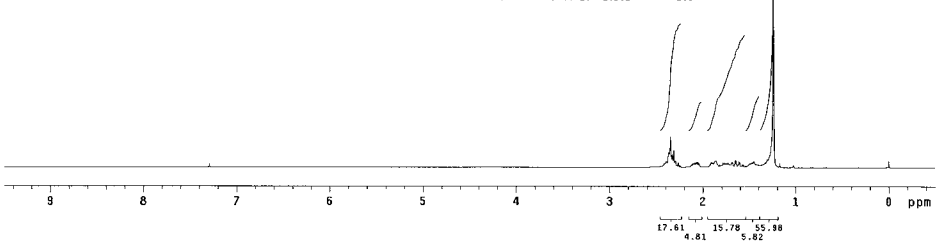
(9) S. Mun, J.-E. Lee and J. Yun, *Org. Lett.*, 2006, **8**, 4887–4889.

(10) I.-H. Chen, L. Yin, W. Itano, M. Kanai and M. Shibasaki, *J. Am. Chem. Soc.*, ASAP, 10.1021/ja9045839.

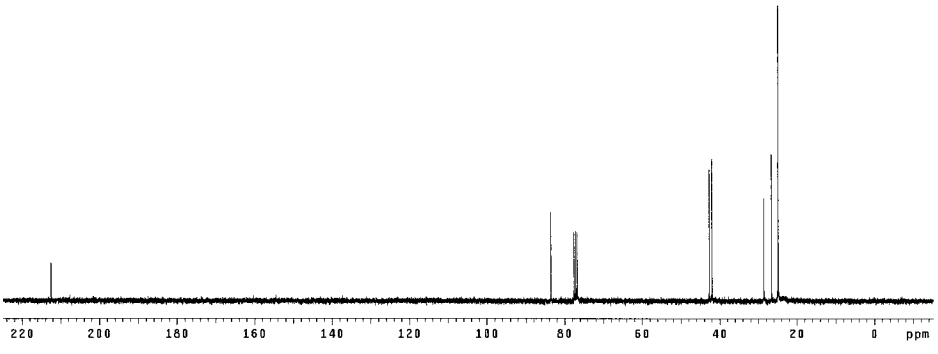
NMR Spectra

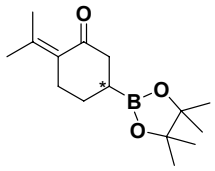


INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2186.408	7.290	0.9	40	503.353	1.678	1.5	78	389.833	1.300	2.0
2	723.912	2.414	1.0	41	495.764	1.653	1.6	80	389.099	1.297	2.1
3	722.738	2.410	1.0	42	494.003	1.647	1.4	81	388.366	1.295	2.2
4	718.484	2.396	1.5	43	492.536	1.642	2.0	82	387.779	1.293	2.3
5	717.310	2.392	1.6	44	490.775	1.636	1.0	83	387.045	1.291	2.4
6	708.653	2.363	4.0	45	484.613	1.616	1.1	84	386.458	1.289	2.5
7	703.958	2.347	8.4	46	482.998	1.610	1.7	85	385.725	1.286	2.7
8	697.356	2.325	3.5	47	481.826	1.607	1.3	86	384.404	1.282	3.0
9	692.808	2.310	4.7	48	479.625	1.599	1.3	87	378.625	1.263	8.1
10	687.526	2.292	1.7	49	472.142	1.574	0.9	88	371.640	1.239	144.8
11	686.792	2.290	1.8	50	451.748	1.506	0.9	89	366.211	1.221	1.3
12	678.868	2.264	1.4	51	447.053	1.491	1.1	90	365.477	1.218	1.0
13	632.853	2.109	1.1	52	441.038	1.471	1.4	91	351.686	1.173	1.1
14	629.572	2.099	1.2	53	435.022	1.451	1.6	92	-0.000	-0.000	1.8
15	628.545	2.096	1.1	54	434.582	1.449	1.6				
16	624.290	2.082	1.3	55	432.528	1.442	1.2				
17	619.742	2.066	1.4	56	429.887	1.433	0.8				
18	615.780	2.053	1.4	57	405.825	1.353	0.8				
19	611.819	2.040	1.0	58	405.092	1.351	0.9				
20	572.791	1.910	1.4	59	404.505	1.349	0.9				
21	571.911	1.907	1.4	60	403.771	1.346	0.9				
22	569.417	1.899	1.4	61	403.184	1.344	0.8				
23	568.243	1.895	1.4	62	402.451	1.342	1.0				
24	564.428	1.882	1.2	63	401.717	1.339	1.0				
25	563.255	1.878	1.4	64	401.130	1.338	1.0				
26	562.081	1.874	1.4	65	400.396	1.335	1.1				
27	558.706	1.863	1.9	66	399.810	1.333	1.1				
28	556.799	1.857	1.9	67	399.076	1.331	1.1				
29	555.772	1.853	1.8	68	398.489	1.329	1.2				
30	552.104	1.841	0.9	69	397.756	1.326	1.2				
31	535.085	1.784	1.2	70	397.022	1.324	1.3				
32	531.857	1.773	1.2	71	396.435	1.322	1.3				
33	529.803	1.767	1.3	72	395.701	1.319	1.4				
34	526.428	1.755	1.1	73	395.115	1.317	1.4				
35	524.227	1.748	1.0	74	394.381	1.315	1.5				
36	521.293	1.738	1.1	75	393.794	1.313	1.6				
37	519.092	1.731	1.2	76	393.061	1.311	1.7				
38	516.011	1.721	1.1	77	391.740	1.306	2.2				
39	505.741	1.686	1.4	78	390.420	1.302	2.0				



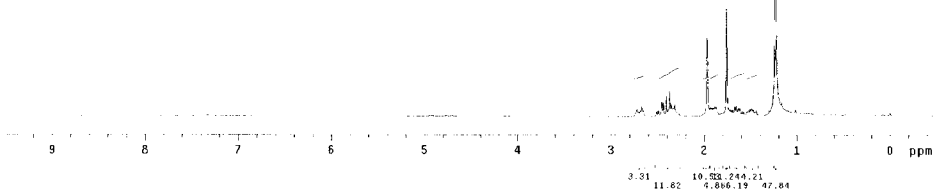
INDEX	FREQUENCY	PPM	HEIGHT
1	16022.818	212.471	10.1
2	6299.210	83.531	23.7
3	5850.292	77.578	18.3
4	5818.226	77.153	18.6
5	5786.714	76.735	18.2
6	3215.938	42.645	34.9
7	3163.418	41.948	37.6
8	2150.568	28.518	27.5
9	2003.523	26.568	38.8
10	1871.950	24.823	78.5
11	1868.080	24.772	69.5



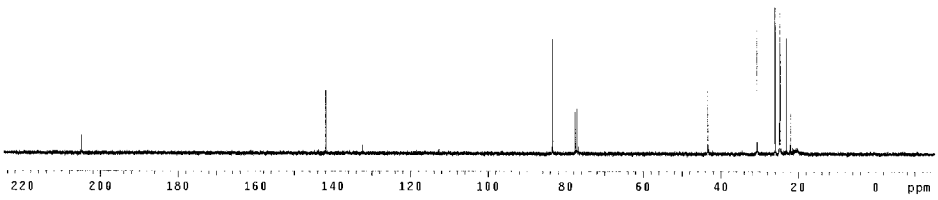


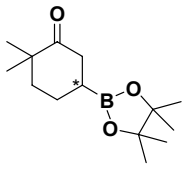
2a

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	815.171	2.718	1.8	40	494.003	1.647	1.4
2	810.330	2.702	1.1	41	490.775	1.636	1.8
3	804.161	2.682	1.3	42	487.588	1.627	2.1
4	799.766	2.667	2.4	43	485.334	1.620	1.9
5	795.071	2.651	1.3	44	483.293	1.611	1.8
6	753.109	2.511	1.0	45	477.571	1.592	1.3
7	752.062	2.508	1.1	46	472.725	1.576	1.2
8	747.534	2.493	1.3	47	461.578	1.539	1.2
9	746.507	2.489	1.4	48	458.057	1.527	1.3
10	735.786	2.453	3.7	49	456.288	1.521	1.4
11	731.395	2.439	3.3	50	451.161	1.504	1.9
12	730.221	2.435	3.6	51	447.493	1.492	1.9
13	721.125	2.406	5.3	52	445.732	1.486	1.9
14	710.414	2.368	6.4	53	442.065	1.474	1.7
15	704.839	2.350	3.8	54	436.930	1.457	1.0
16	698.916	2.324	2.1	55	435.022	1.451	1.0
17	694.275	2.315	3.3	56	431.794	1.440	1.4
18	684.685	2.284	1.0	57	389.539	1.299	1.1
19	683.271	2.278	1.0	58	369.282	1.231	151.9
20	589.811	1.967	21.4	59	349.632	1.166	8.6
21	578.100	1.931	2.3	60	330.265	1.101	1.3
22	575.579	1.918	2.0	61	329.678	1.099	1.3
23	574.112	1.914	2.2	62	329.091	1.097	1.3
24	570.737	1.903	2.0	63	317.647	1.059	1.0
25	569.554	1.899	2.1	64	317.060	1.057	1.0
26	565.896	1.887	2.5	65	312.365	1.042	0.9
27	564.859	1.883	2.3	66	311.831	1.039	0.9
28	562.524	1.876	2.2	67	311.045	1.037	0.9
29	561.054	1.871	2.4	68	305.463	1.018	1.6
30	557.973	1.860	1.3				
31	556.212	1.855	1.1				
32	543.301	1.812	0.9				
33	527.309	1.758	28.5				
34	516.451	1.722	1.7				
35	511.903	1.707	1.7				
36	507.061	1.691	1.7				
37	501.193	1.671	2.6				
38	498.698	1.663	1.6				
39	496.351	1.655	2.8				



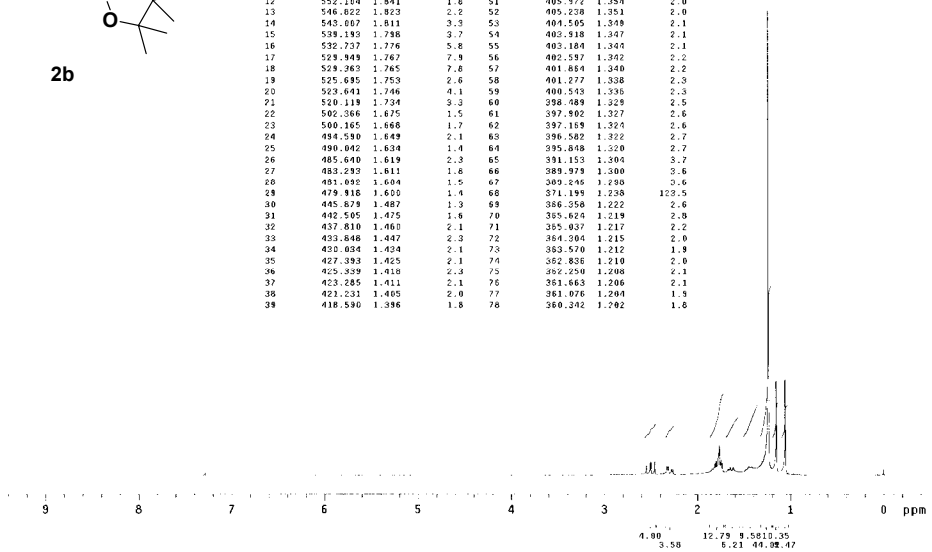
INDEX	FREQUENCY	PPM	HEIGHT
1	15452.772	204.905	11.8
2	10696.816	141.845	18.9
3	9885.845	132.415	14.4
4	6286.494	83.362	30.6
5	5850.845	77.585	11.1
6	5816.779	77.160	11.9
7	5786.714	76.735	11.2
8	3266.249	43.312	36.0
9	2308.152	30.607	33.0
10	1958.748	25.974	39.0
11	1865.316	24.735	94.5
12	1864.210	24.720	90.0
13	1737.606	23.042	31.0
14	1658.548	21.993	24.0



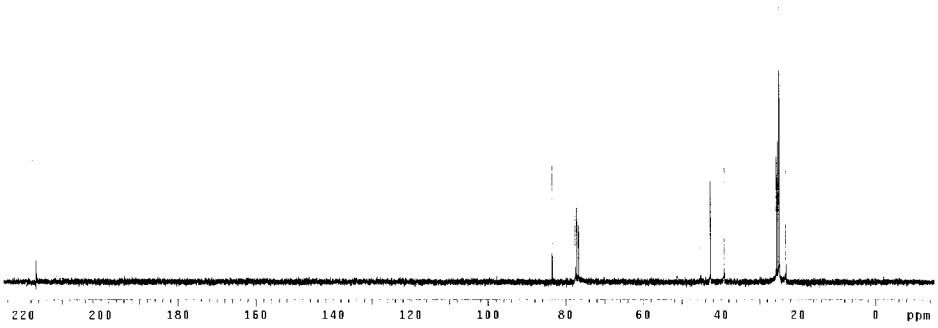


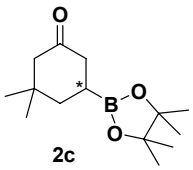
2b

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	763.966	2.547	2.4	40	418.003	1.394	1.8	79	359.609	1.199	1.8
2	751.642	2.506	3.1	41	415.362	1.385	2.0	80	358.022	1.197	1.8
3	749.588	2.499	3.5	42	413.895	1.380	1.9	81	358.288	1.195	1.8
4	737.264	2.458	3.7	43	413.308	1.378	1.9	82	357.555	1.192	1.8
5	697.643	2.326	2.5	44	412.574	1.376	1.9	83	356.968	1.190	1.9
6	696.622	2.323	2.3	45	411.841	1.373	2.0	84	356.234	1.188	1.9
7	692.808	2.310	2.5	46	410.667	1.369	2.1	85	355.500	1.185	2.0
8	683.271	2.278	1.6	47	409.200	1.364	2.0	86	351.099	1.171	3.9
9	682.244	2.275	1.5	48	408.813	1.362	2.0	87	345.817	1.153	27.2
10	678.283	2.262	1.5	49	407.292	1.358	1.9	88	317.353	1.058	28.5
11	554.011	1.847	1.5	50	406.559	1.356	2.0	89	0.000	0.000	2.1
12	552.104	1.841	1.8	51	405.972	1.354	2.0				
13	546.822	1.823	2.2	52	405.238	1.351	2.0				
14	543.067	1.811	3.3	53	404.505	1.348	2.1				
15	539.193	1.798	3.7	54	403.918	1.347	2.1				
16	532.737	1.776	5.8	55	403.184	1.344	2.1				
17	529.949	1.767	7.9	56	402.597	1.342	2.2				
18	528.363	1.765	7.8	57	401.864	1.340	2.2				
19	525.695	1.753	2.6	58	401.277	1.338	2.3				
20	523.641	1.746	4.1	59	400.543	1.336	2.3				
21	520.118	1.734	9.3	60	398.489	1.329	2.5				
22	502.366	1.675	1.5	61	397.902	1.327	2.6				
23	500.165	1.668	1.7	62	397.169	1.324	2.6				
24	494.590	1.649	2.1	63	396.582	1.322	2.7				
25	490.042	1.634	1.4	64	395.848	1.320	2.7				
26	485.640	1.619	2.3	65	391.153	1.304	3.7				
27	483.293	1.611	1.8	66	389.979	1.300	3.6				
28	481.092	1.604	1.5	67	389.246	1.298	3.6				
29	479.918	1.600	1.4	68	371.199	1.238	123.5				
30	445.879	1.487	1.3	69	386.358	1.222	2.6				
31	442.505	1.475	1.6	70	365.624	1.219	2.8				
32	437.810	1.460	2.1	71	365.037	1.217	2.2				
33	433.848	1.447	2.3	72	364.304	1.215	2.0				
34	430.034	1.434	2.1	73	363.570	1.212	1.9				
35	427.393	1.425	2.1	74	362.836	1.210	2.0				
36	425.339	1.418	2.3	75	362.250	1.208	2.1				
37	423.285	1.411	2.1	76	361.663	1.206	2.1				
38	421.231	1.405	2.0	77	361.076	1.204	1.9				
39	418.590	1.396	1.8	78	360.342	1.202	1.8				



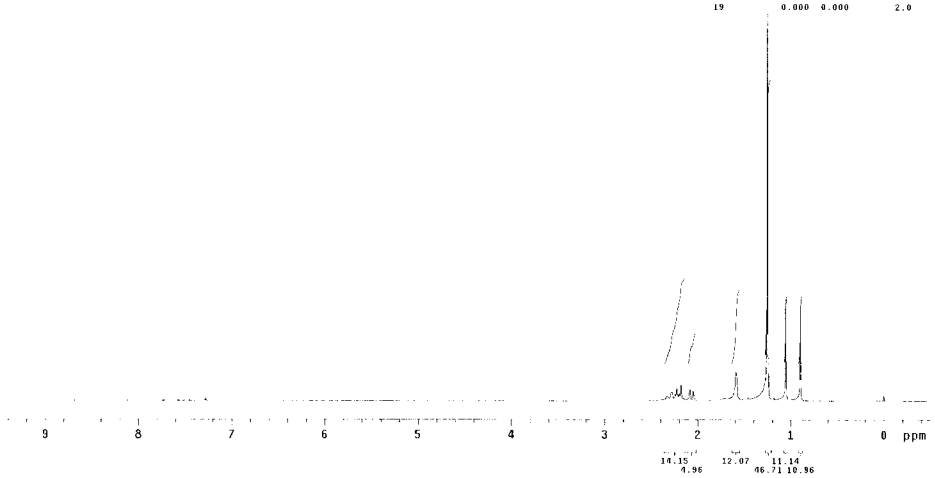
INDEX	FREQUENCY	PPM	HEIGHT
1	16336.286	216.628	5.8
2	6295.893	83.487	31.1
3	5850.845	77.585	18.0
4	5818.779	77.160	19.7
5	5786.713	76.735	19.9
6	3406.874	45.174	16.8
7	3217.045	42.660	27.0
8	2951.122	39.133	30.9
9	1927.788	25.563	33.3
10	1902.356	25.226	37.4
11	1873.055	24.838	75.2
12	1868.738	24.794	72.3
13	1745.346	23.144	30.5



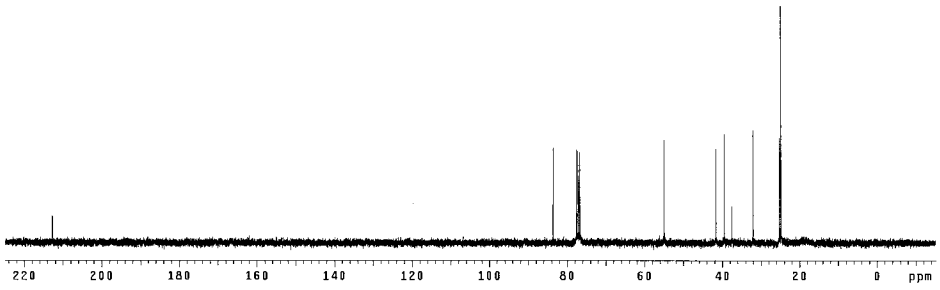


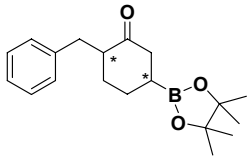
2c

INDEX	FREQUENCY	PPM	HEIGHT
1	684.151	2.281	2.4
2	682.584	2.276	2.3
3	681.369	2.272	2.3
4	671.533	2.239	1.9
5	666.838	2.223	3.5
6	658.916	2.197	2.0
7	653.487	2.179	4.4
8	625.170	2.085	3.1
9	614.753	2.050	2.7
10	484.613	1.616	1.9
11	477.277	1.591	7.7
12	474.930	1.584	7.4
13	393.207	1.311	2.4
14	385.431	1.285	4.3
15	384.844	1.283	4.3
16	374.427	1.248	104.2
17	315.740	1.053	25.3
18	267.909	0.893	22.3
19	0.000	0.000	2.0



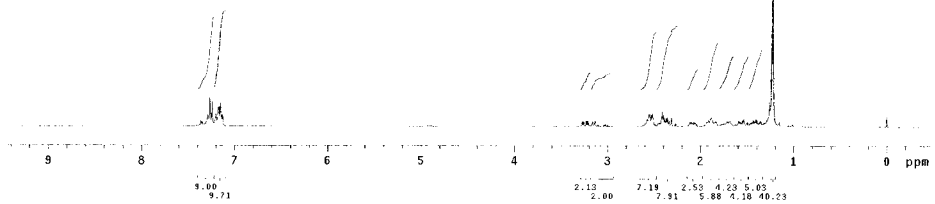
INDEX	FREQUENCY	PPM	HEIGHT
1	16042.168	212.727	7.2
2	6303.632	83.589	25.6
3	5850.845	77.585	25.0
4	5816.779	77.160	24.5
5	5787.286	76.769	24.3
6	4143.629	54.947	27.5
7	3137.987	41.611	25.2
8	2979.870	39.515	29.1
9	2828.941	37.513	9.6
10	2416.511	32.044	30.1
11	1902.909	25.234	28.2
12	1875.819	24.874	63.0
13	1870.844	24.808	62.4



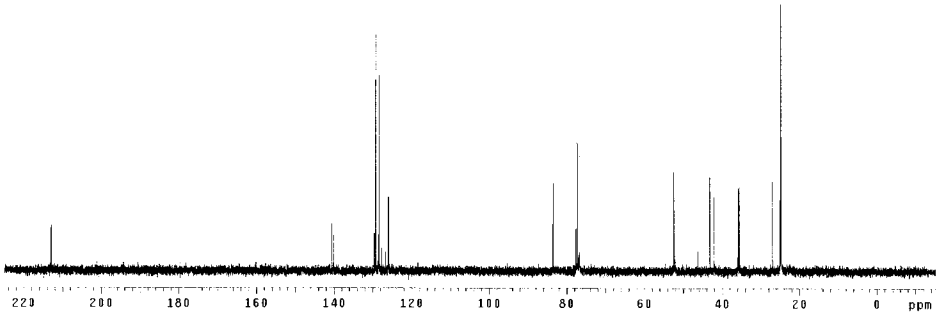


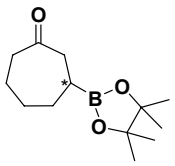
2e

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2207.829	7.367	1.6	40	692.661	2.310	2.4
2	2150.517	7.304	1.3	41	628.105	2.094	1.3
3	2187.142	7.293	2.1	42	574.699	1.916	1.7
4	2185.675	7.288	3.1	43	572.845	1.909	1.0
5	2184.208	7.283	2.1	44	568.243	1.895	2.1
6	2182.300	7.277	2.0	45	564.575	1.882	2.4
7	2178.926	7.265	7.5	46	563.108	1.878	2.2
8	2177.605	7.261	6.0	47	552.384	1.840	1.3
9	2171.443	7.240	6.5	48	551.224	1.838	1.9
10	2163.667	7.214	1.4	49	550.197	1.835	1.9
11	2158.972	7.199	3.2	50	513.664	1.713	1.5
12	2150.902	7.172	5.1	51	507.061	1.691	1.5
13	2149.142	7.166	4.9	52	503.540	1.679	1.4
14	2146.061	7.156	5.3	53	476.690	1.589	1.6
15	2144.947	7.150	6.1	54	473.463	1.579	1.4
16	2142.686	7.144	3.8	55	463.632	1.546	1.8
17	2137.640	7.128	5.0	56	460.698	1.536	2.0
18	980.964	3.271	1.4	57	429.740	1.433	1.8
19	976.259	3.255	1.5	58	425.192	1.418	1.5
20	967.026	3.224	1.6	59	420.937	1.404	2.1
21	962.477	3.209	1.6	60	417.416	1.392	1.8
22	947.806	3.160	1.5	61	408.319	1.361	1.7
23	938.149	3.131	1.5	62	404.798	1.350	1.5
24	770.716	2.570	2.0	63	386.752	1.290	1.7
25	767.634	2.560	1.7	64	377.948	1.260	7.3
26	764.700	2.550	3.3	65	366.651	1.223	151.2
27	762.206	2.541	3.4	66	-0.000	-0.000	3.0
28	757.071	2.524	3.1				
29	753.843	2.514	3.4				
30	723.472	2.412	4.0				
31	721.565	2.406	2.6				
32	719.217	2.398	3.1				
33	717.457	2.392	2.4				
34	714.962	2.384	2.0				
35	709.827	2.367	2.5				
36	706.746	2.357	2.2				
37	705.866	2.354	2.5				
38	701.024	2.337	1.6				
39	693.395	2.312	2.3				



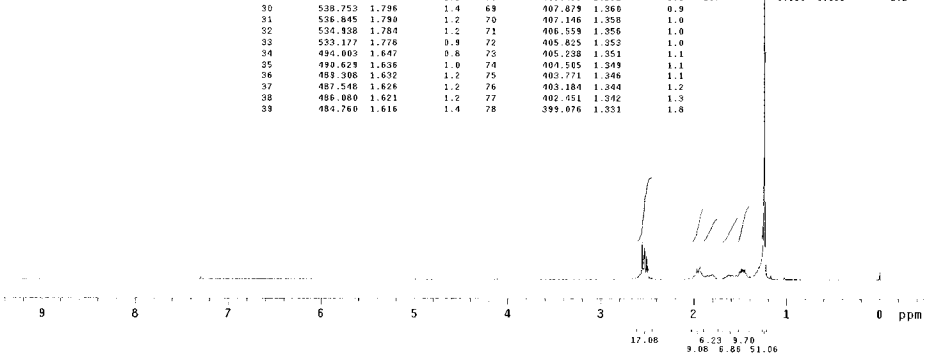
INDEX	FREQUENCY	PPM	HEIGHT
1	10864.835	213.028	11.4
2	10851.568	212.852	11.9
3	10802.078	140.589	12.7
4	10567.801	140.131	9.4
5	9773.992	129.607	10.0
6	9748.470	129.270	50.9
7	9744.600	129.218	65.1
8	9697.608	128.595	8.2
9	9690.420	128.500	9.6
10	9681.575	128.382	52.4
11	9678.811	128.346	52.0
12	9509.837	126.103	19.7
13	9501.897	126.000	11.0
14	9499.686	125.971	26.6
15	6306.397	83.626	22.2
16	6298.104	83.516	23.6
17	5850.292	77.578	34.2
18	5818.779	77.160	34.0
19	5786.714	76.735	33.6
20	3950.683	52.388	26.5
21	3930.780	52.124	20.6
22	3249.664	43.092	25.2
23	3170.605	42.044	20.1
24	2705.655	35.878	22.4
25	2699.820	35.760	22.1
26	2677.459	35.504	22.7
27	2408.219	31.934	20.2
28	2036.359	27.030	24.3
29	1887.982	25.036	18.9
30	1874.161	24.852	55.5
31	1871.397	24.816	71.1
32	1868.974	24.752	61.2



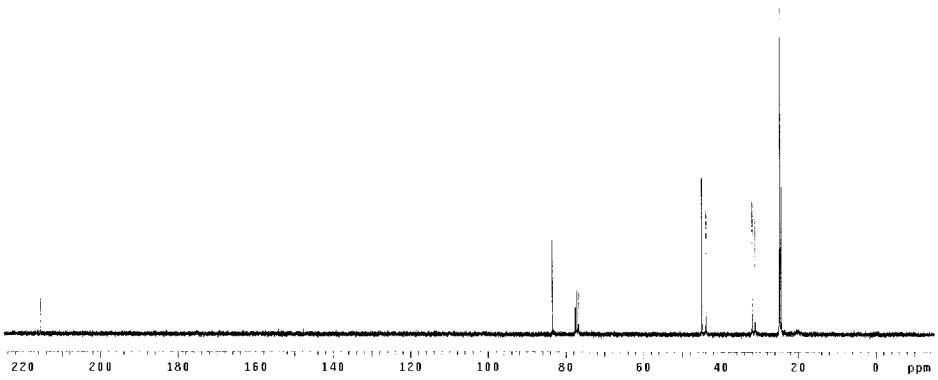


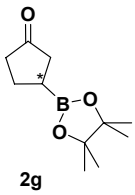
2f

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	775.411	2.585	1.0	40	483.146	1.611	1.1	79	398.489	1.329	1.9
2	774.384	2.582	1.1	41	480.065	1.601	1.2	80	397.902	1.327	2.0
3	771.743	2.573	1.5	42	477.864	1.593	1.1	81	397.169	1.324	2.0
4	764.847	2.550	11.0	43	477.131	1.591	1.1	82	396.582	1.322	2.0
5	759.858	2.534	5.2	44	475.223	1.585	1.3	83	395.848	1.320	2.0
6	758.685	2.530	6.7	45	473.463	1.579	1.2	84	395.115	1.317	2.1
7	757.071	2.524	8.4	46	471.849	1.573	0.9	85	393.713	1.313	3.2
8	751.055	2.504	6.1	47	469.795	1.566	1.0	86	389.833	1.300	3.1
9	746.654	2.490	3.6	48	468.474	1.562	0.9	87	389.099	1.297	3.1
10	745.186	2.485	2.8	49	466.273	1.555	0.9	88	388.512	1.295	3.2
11	597.000	1.991	1.1	50	462.752	1.543	1.2	89	387.779	1.293	3.3
12	593.772	1.980	1.2	51	461.138	1.538	1.1	90	387.192	1.291	3.4
13	589.077	1.964	3.0	52	459.818	1.533	1.1	91	386.458	1.289	3.6
14	584.089	1.948	2.0	53	457.910	1.527	1.0	92	385.725	1.286	3.8
15	581.888	1.940	2.7	54	452.775	1.510	2.2	93	385.138	1.284	3.9
16	578.660	1.929	3.5	55	451.181	1.504	2.3	94	384.404	1.282	4.0
17	573.378	1.912	1.8	56	449.547	1.499	1.9	95	383.817	1.280	4.2
18	572.058	1.907	1.6	57	446.026	1.487	3.2	96	383.084	1.277	4.4
19	567.069	1.891	1.0	58	443.385	1.478	2.3	97	382.497	1.275	4.6
20	565.686	1.887	0.9	59	441.771	1.473	2.8	98	380.443	1.269	5.7
21	565.309	1.885	0.9	60	439.884	1.467	2.6	99	378.535	1.262	7.1
22	559.147	1.864	1.0	61	436.489	1.455	2.5	100	371.053	1.237	150.9
23	554.745	1.850	1.3	62	435.189	1.451	3.0	101	365.624	1.219	1.6
24	551.077	1.837	1.0	63	431.961	1.437	1.8	102	364.890	1.217	1.4
25	548.023	1.831	1.0	64	429.887	1.433	1.6	103	364.304	1.215	1.2
26	546.822	1.823	1.2	65	426.512	1.422	0.9	104	363.570	1.212	1.0
27	545.355	1.818	1.1	66	409.787	1.366	0.8	105	362.836	1.210	0.9
28	542.567	1.809	1.2	67	409.200	1.364	0.9	106	351.098	1.171	1.1
29	540.953	1.804	1.3	68	408.686	1.362	0.9	107	0.000	0.000	2.2
30	538.753	1.796	1.4	69	407.879	1.360	0.9				
31	536.845	1.790	1.2	70	407.146	1.358	1.0				
32	534.938	1.784	1.2	71	406.559	1.356	1.0				
33	533.177	1.778	0.9	72	405.825	1.353	1.0				
34	494.003	1.647	0.8	73	405.238	1.351	1.1				
35	490.629	1.636	1.0	74	404.505	1.349	1.1				
36	489.308	1.632	1.2	75	403.771	1.346	1.1				
37	487.546	1.626	1.2	76	403.184	1.344	1.2				
38	486.080	1.621	1.2	77	402.451	1.342	1.3				
39	484.760	1.616	1.4	78	399.076	1.331	1.8				



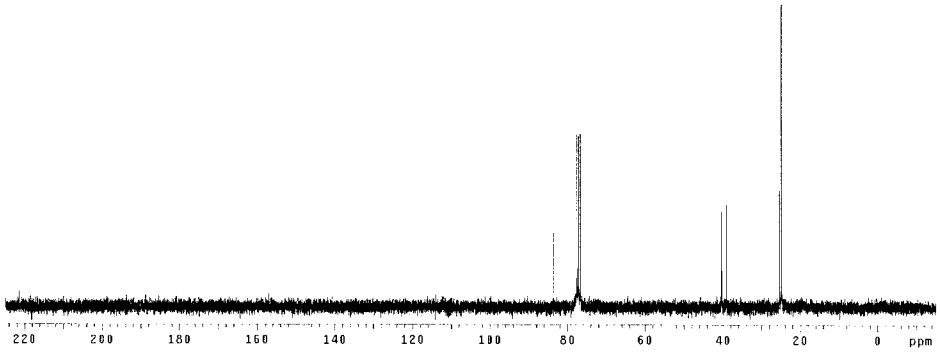
INDEX	FREQUENCY	PPM	HEIGHT
1	16255.570	215.557	9.1
2	6295.340	83.479	25.2
3	5850.845	77.585	10.7
4	5818.779	77.160	11.5
5	5787.267	76.742	11.2
6	3384.807	44.874	41.6
7	3302.738	43.786	35.1
8	2406.807	31.905	35.5
9	2345.746	31.106	31.0
10	1869.185	24.786	86.8
11	1864.210	24.720	78.8
12	1837.120	24.361	39.2

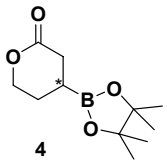




2g

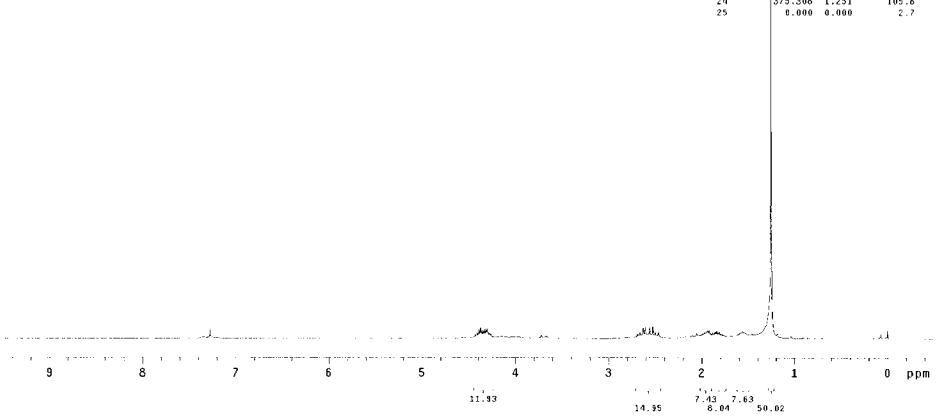
INDEX	FREQUENCY	PPM	HEIGHT
1	16655.642	221.393	4.0
2	16446.304	218.606	-3.9
3	6308.655	83.848	19.6
4	5850.292	77.578	46.0
5	5818.779	77.160	45.8
6	5786.713	76.735	46.3
7	3041.790	40.336	25.7
8	2947.805	39.089	27.4
9	1915.872	25.395	31.3
10	1874.161	24.852	80.8



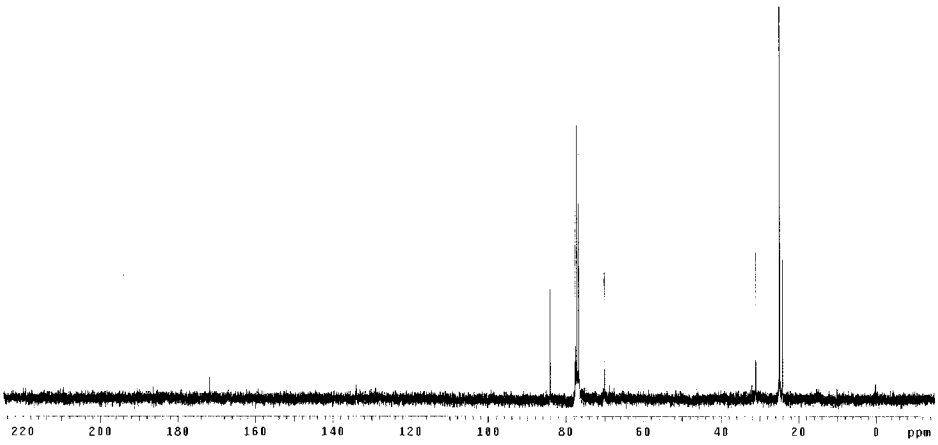


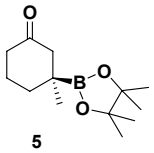
4

INDEX	FREQUENCY	PPM	HEIGHT
1	2182.154	7.276	2.7
2	1316.951	4.391	2.4
3	1311.522	4.373	2.9
4	1306.536	4.356	2.2
5	1301.545	4.340	2.3
6	1297.291	4.326	2.5
7	1293.182	4.312	2.5
8	1290.395	4.303	2.0
9	1288.928	4.298	2.5
10	787.001	2.624	2.9
11	780.106	2.601	3.0
12	766.754	2.557	3.2
13	756.631	2.523	3.3
14	749.001	2.497	1.7
15	738.878	2.464	1.8
16	585.996	1.954	1.7
17	581.446	1.939	2.2
18	576.166	1.921	2.1
19	555.625	1.853	1.9
20	550.637	1.836	2.0
21	542.127	1.808	1.8
22	467.154	1.558	1.8
23	395.115	1.317	3.3
24	375.308	1.251	105.8
25	0.000	0.000	2.7



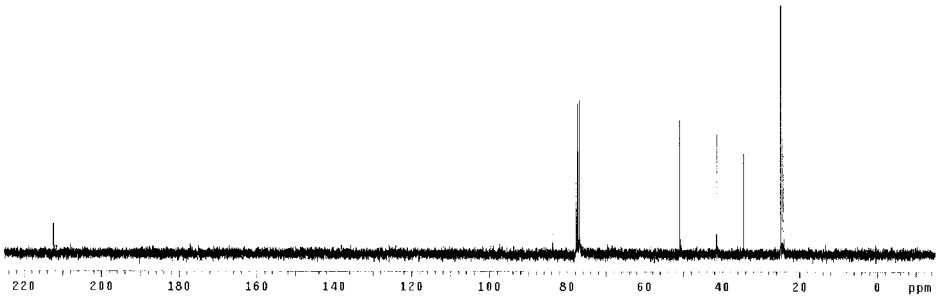
INDEX	FREQUENCY	PPM	HEIGHT
1	12956.133	171.805	5.8
2	6337.910	84.044	29.5
3	5850.845	77.585	68.8
4	5818.779	77.160	73.0
5	5786.713	76.735	69.2
6	5284.169	70.071	33.7
7	2338.559	31.010	39.5
8	1874.181	24.852	104.7
9	1872.502	24.830	92.5
10	1814.453	24.061	37.1

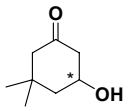




5

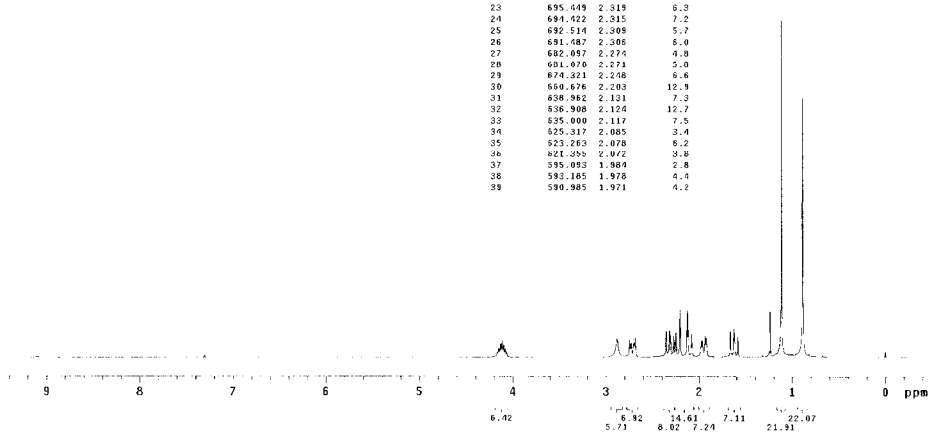
INDEX	FREQUENCY	PPM	HEIGHT
1	16012.608	217.335	8.0
2	6312.773	83.711	18.7
3	5858.879	77.692	38.9
4	5827.366	77.274	40.2
5	5795.301	76.849	40.9
6	3838.195	50.896	35.7
7	3122.248	41.403	32.1
8	2597.589	34.445	26.9
9	1876.114	24.878	66.3
10	1871.138	24.812	58.5
11	1841.837	24.424	31.3
12	1816.406	24.086	32.5



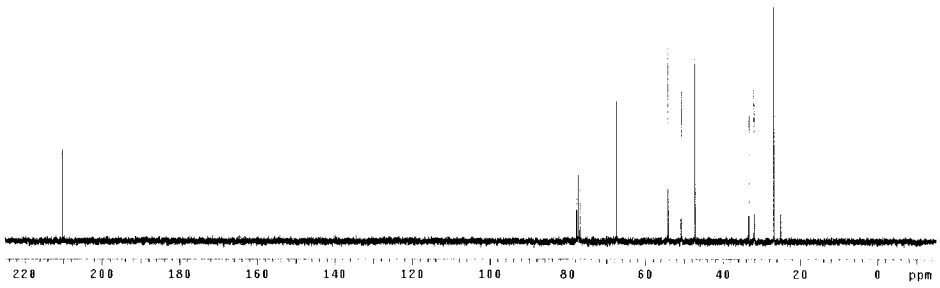


6c

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	1249.460	4.166	1.5	40	588.784	1.963	4.4
2	1244.765	4.150	2.5	41	586.877	1.957	2.7
3	1239.190	4.132	3.5	42	582.181	1.941	3.5
4	1234.201	4.115	4.6	43	580.274	1.935	5.6
5	1229.056	4.098	3.4	44	577.927	1.927	5.2
6	1223.638	4.080	2.5	45	575.726	1.920	5.3
7	1218.796	4.064	1.4	46	573.819	1.913	3.0
8	863.589	2.880	5.0	47	498.405	1.662	7.3
9	824.551	2.749	2.7	48	487.548	1.626	7.7
10	822.801	2.744	4.6	49	485.494	1.619	6.5
11	820.747	2.737	3.3	50	474.636	1.583	5.4
12	819.573	2.733	3.2	51	375.601	1.252	1.5
13	817.666	2.726	4.5	52	372.667	1.243	1.6
14	815.758	2.720	2.9	53	371.053	1.237	12.4
15	811.210	2.705	3.3	54	334.078	1.114	89.8
16	809.303	2.699	5.6	55	265.708	0.886	70.3
17	807.395	2.692	3.9	56	0.000	0.000	2.0
18	806.222	2.688	3.7				
19	804.168	2.681	5.2				
20	802.407	2.676	3.1				
21	705.856	2.354	6.2				
22	704.839	2.350	7.0				
23	695.649	2.319	6.3				
24	694.422	2.315	7.2				
25	692.514	2.308	5.7				
26	691.687	2.306	6.0				
27	682.057	2.274	4.8				
28	681.070	2.271	5.0				
29	674.321	2.248	6.6				
30	660.676	2.203	12.9				
31	638.962	2.131	7.3				
32	636.908	2.124	12.7				
33	635.000	2.117	7.5				
34	625.317	2.085	3.4				
35	623.263	2.078	6.2				
36	621.355	2.072	3.8				
37	595.083	1.984	2.8				
38	593.185	1.978	4.4				
39	590.985	1.971	4.2				

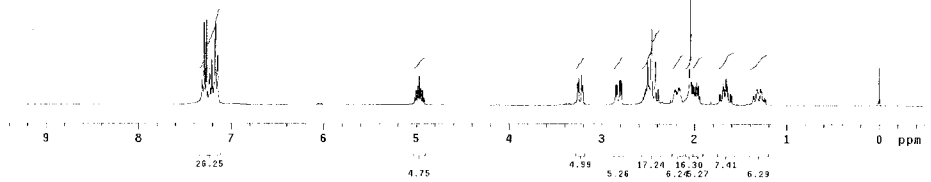


INDEX	FREQUENCY	PPM	HEIGHT
1	15852.833	210.217	24.5
2	5862.749	77.743	15.8
3	5830.683	77.318	17.7
4	5798.618	76.893	16.8
5	5081.565	67.384	37.4
6	4080.898	54.115	61.2
7	3821.610	50.677	51.4
8	3560.109	47.209	49.5
9	2506.580	33.235	33.8
10	2405.749	31.901	80.3
11	2015.303	26.727	62.5

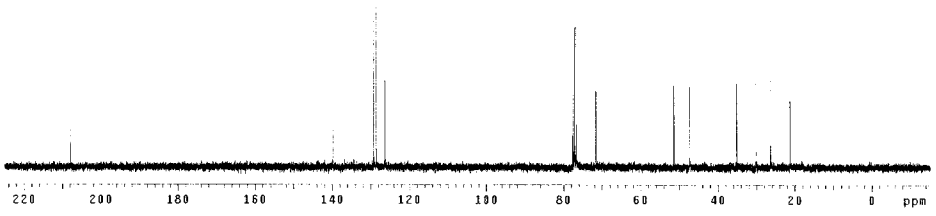


8e (Minor diastereomer)

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2194.038	7.316	6.0	40	756.044	2.521	4.6	79	504.420	1.682	4.5
2	2192.571	7.311	8.8	41	751.055	2.504	12.4	80	502.220	1.675	5.5
3	2190.957	7.305	4.9	42	747.387	2.492	5.5	81	495.911	1.654	7.9
4	2187.582	7.294	8.5	43	746.067	2.488	5.3	82	493.270	1.645	5.1
5	2185.822	7.288	22.7	44	744.159	2.481	4.9	83	491.803	1.640	5.5
6	2184.208	7.283	13.8	45	740.198	2.468	13.8	84	489.455	1.632	3.4
7	2179.659	7.268	11.3	46	737.704	2.460	20.6	85	482.853	1.610	3.3
8	2177.899	7.262	25.0	47	728.901	2.430	5.1	86	479.038	1.597	2.8
9	2169.242	7.233	6.0	48	726.847	2.424	8.3	87	410.227	1.368	2.7
10	2167.775	7.228	10.8	49	724.792	2.417	12.1	88	406.852	1.357	2.9
11	2166.308	7.223	8.0	50	715.686	2.386	6.2	89	398.049	1.327	4.3
12	2162.933	7.212	4.5	51	666.398	2.222	2.5	90	396.435	1.322	5.0
13	2160.586	7.204	12.4	52	664.344	2.215	4.1	91	395.115	1.317	4.4
14	2157.851	7.194	5.1	53	662.290	2.208	4.2	92	393.061	1.311	3.9
15	2154.570	7.184	4.4	54	660.676	2.203	4.4	93	384.404	1.282	4.7
16	2153.250	7.180	6.0	55	658.622	2.196	4.2	94	382.790	1.276	3.8
17	2149.875	7.168	20.6	56	655.881	2.187	3.8	95	381.176	1.271	3.8
18	2148.261	7.163	22.8	57	653.927	2.180	3.6	96	0.000	0.000	10.4
19	2146.207	7.156	6.4	58	651.286	2.172	4.8				
20	2141.512	7.141	15.5	59	649.232	2.165	4.7				
21	1500.056	5.002	4.1	60	647.765	2.160	4.7				
22	1494.188	4.982	5.2	61	645.711	2.153	4.5				
23	1489.491	4.967	7.7	62	643.510	2.146	2.7				
24	1484.798	4.951	4.9	63	620.515	2.070	2.9				
25	1478.928	4.931	4.0	64	611.819	2.040	151.2				
26	977.296	3.259	6.1	65	608.591	2.029	5.3				
27	973.775	3.247	7.4	66	607.124	2.024	3.2				
28	964.985	3.218	8.2	67	606.537	2.022	3.2				
29	960.423	3.202	5.4	68	604.776	2.017	5.7				
30	855.666	2.853	5.4	69	600.228	2.001	5.1				
31	853.759	2.847	5.6	70	599.788	2.000	5.1				
32	850.677	2.836	5.8	71	595.388	1.985	5.4				
33	848.623	2.830	5.5	72	591.572	1.973	5.4				
34	842.315	2.809	6.8	73	585.996	1.954	5.9				
35	840.260	2.802	7.0	74	581.595	1.939	2.8				
36	837.326	2.792	6.9	75	518.652	1.729	3.2				
37	835.272	2.785	6.4	76	514.837	1.717	3.1				
38	760.945	2.536	3.6	77	508.235	1.695	4.0				
39	759.271	2.532	3.5	78	506.181	1.688	8.0				

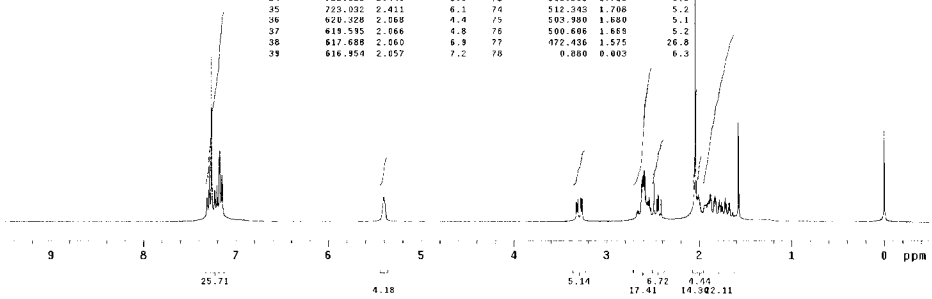


INDEX	FREQUENCY	PPM	HEIGHT
1	15676.178	207.874	10.9
2	12828.976	170.119	8.9
3	10542.370	139.797	10.1
4	9743.494	129.204	44.7
5	9653.738	128.544	45.8
6	9528.775	126.330	23.5
7	5850.292	77.578	35.9
8	5818.779	77.160	37.6
9	5786.714	76.735	37.8
10	5402.480	71.640	20.8
11	3871.942	51.334	22.2
12	3563.343	47.278	22.0
13	2646.498	35.094	22.8
14	2274.981	30.167	24.3
15	1980.261	26.392	23.7
16	1605.474	21.289	17.8



8e (Major diastereomer)

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2194.185	7.316	4.4	40	616.367	2.055	7.9	79	-0.000	-0.000	40.3
2	2192.864	7.312	6.7	41	615.633	2.053	9.0				
3	2191.397	7.307	4.4	42	614.313	2.048	11.7				
4	2185.868	7.289	16.7	43	613.726	2.046	12.8				
5	2184.648	7.284	12.1	44	611.379	2.039	111.3				
6	2182.154	7.276	4.8	45	608.004	2.027	7.8				
7	2180.099	7.269	9.1	46	607.417	2.025	7.2				
8	2178.045	7.262	44.3	47	606.830	2.023	6.4				
9	2167.482	7.227	8.6	48	606.097	2.021	5.9				
10	2166.014	7.222	7.4	49	605.363	2.018	6.2				
11	2162.640	7.211	4.5	50	604.776	2.017	6.3				
12	2160.292	7.203	10.1	51	604.043	2.014	6.5				
13	2157.505	7.194	5.1	52	603.309	2.012	6.7				
14	2152.663	7.178	17.6	53	601.255	2.005	7.4				
15	2151.196	7.173	19.4	54	598.761	1.996	8.1				
16	2144.300	7.150	13.1	55	582.768	1.943	9.5				
17	1624.327	5.416	4.9	56	581.448	1.939	9.7				
18	1623.953	5.405	7.1	57	579.394	1.932	9.6				
19	1618.752	5.397	5.8	58	578.073	1.928	9.6				
20	996.516	3.323	5.9	59	572.645	1.909	9.1				
21	992.261	3.309	6.2	60	570.004	1.901	9.1				
22	982.871	3.277	6.6	61	567.950	1.894	8.0				
23	978.617	3.263	6.4	62	566.629	1.889	8.0				
24	786.415	2.622	10.4	63	563.401	1.879	7.7				
25	784.380	2.615	11.6	64	561.934	1.874	7.5				
26	783.187	2.611	12.3	65	551.664	1.839	5.6				
27	780.986	2.604	12.5	66	549.170	1.831	6.7				
28	778.638	2.596	14.6	67	547.996	1.827	7.0				
29	774.970	2.584	14.6	68	545.502	1.819	5.7				
30	765.434	2.552	5.6	69	537.432	1.792	4.3				
31	760.739	2.537	6.8	70	534.791	1.783	6.1				
32	745.773	2.487	10.8	71	532.590	1.776	6.6				
33	736.677	2.456	6.3	72	527.745	1.760	5.3				
34	732.128	2.441	8.9	73	516.305	1.722	6.6				
35	723.032	2.411	6.1	74	512.348	1.708	5.2				
36	620.328	2.068	4.4	75	503.980	1.680	5.1				
37	619.595	2.066	4.8	76	500.606	1.669	5.2				
38	617.688	2.060	6.9	77	472.436	1.575	26.8				
39	616.954	2.057	7.2	78	0.880	0.003	6.3				



INDEX	FREQUENCY	PPM	HEIGHT
1	15713.480	208.164	3.7
2	10563.378	140.076	3.7
3	9748.811	129.248	16.5
4	9692.632	128.529	17.0
5	9522.352	126.271	6.7
6	5850.844	77.585	49.2
7	5818.779	77.160	50.9
8	5786.713	76.735	49.6
9	5475.456	72.607	7.9
10	3936.862	52.205	7.4
11	3486.838	46.237	8.5
12	2657.556	35.241	7.7
13	2185.369	29.112	7.2
14	2066.554	27.404	7.1
15	1605.896	21.348	6.7