**Supporting Information**

# Experimental Entropy (ΔH) and Enthalpy (ΔS) for π-Stacking Interactions in near-Sandwich Configurations

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Table of Contents

Experimentals·····S2

General Synthetic Procedure for the preparation of compound **3** ·····S2

General Synthetic Procedure for the preparation of compound **4** ·····S3

General Synthetic Procedure for the preparation of compound **5** ·····S5

Preparation of model compounds **6-14**·····S7

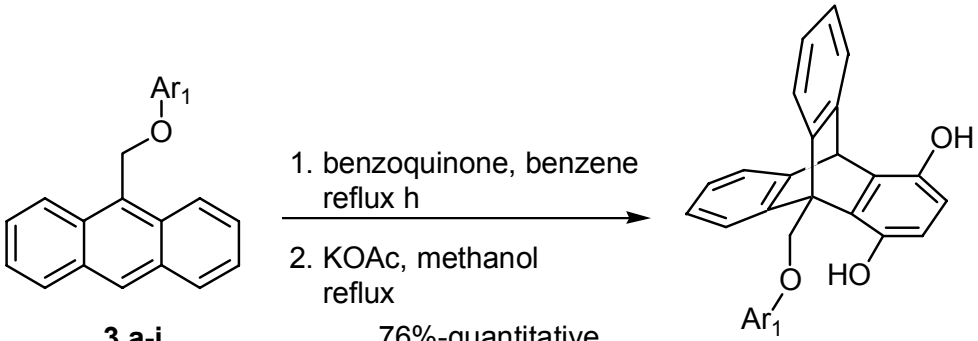
Variable Temperature NMR Experimental Procedure·····S10

References·····S10

$^{1}$H NMR spectra of compounds **4-12**----------S11

**Experimentals**

All reactions were carried out under an atmosphere of nitrogen in oven-dried glassware. Reagents were purchased from commercial sources and used without further purification. Compounds **3a**-**3i** were prepared according to the literature procedures.[1,2] Flash column chromatographic separations were performed using silica gel 40 –63 μm. Reactions were monitored with TLC and UV light. NMR spectra ($^{1}H$, $^{13}C$) were recorded on Bruker 200 and 300 spectrometers with $CDCl_3$ or DMSO-$d_6$ as the solvents. Melting points are not corrected.




**3 a-i** 76%-quantitative **4 a-i**

$Ar_1$ = 4-dimethylaminophenyl, phenyl
4-nitrophenyl, 4-methylphenyl
4-methoxyphenyl, 3,5-dimethyl
3,4,5-trimethyl

**General Synthetic Procedure for 9-(4-Substituted phenoxymethyl)-1,4–Dihydroxyl triptycene (4)**.[3,4] The 9-(aryloxymethyl)anthracene (**3**) (0.8 mmol) and p-benzoquinone (0.26 g, 2.4 mmol) in 4 ml of benzene were refluxed under a nitrogen atmosphere for 1-2 days. After cooling, the solvent was removed under reduced pressure and the formed Diels-Alder adduct was used directly for the aromatization without purification.

To the residue from the last step, KOAc (0.10 g, 0.96 mmol) and methnol (10 ml) were added. The mixture was allowed to reflux for 1-2 days. After cooling to room temperature, most methanol was removed under reduced pressure and to the residue water was added. The precipitate was collected by filtration. Further purification via recrystallization or flash column chromatography afforded 9-substituted-1,4–dihydroxytriptycene (**4**) as a solid.

**9-(4-Dimethylaminophenoxymethyl)-1,4-dihydroxytriptycene (4a):** Yield 91%; white solid; m.p. 299-301 °C; $^{1}H$ NMR (300 MHz, $CDCl_3$) δ 8.16 (1H, s), 7.41-7.44 (3H, m), 7.24-7.26 (3H, m), 6.97-7.04 (4H, m), 6.84 (2H, d, J = 8.9 Hz), 6.50 (1H, d, J = 8.6 Hz), 6.42 (1H, d, J = 8.6 Hz), 5.84 (1H, s), 5.41-5.74 (2H, m), 4.44 (1H, s), 2.96 (6H, s); $^{13}C$ NMR (75 MHz, DMSO) δ 150.85, 146.05, 145.15, 144.70, 134.39, 130.04, 124.65, 124.38, 123.32, 115.23, 114.84,

114.13,113.68, 66.80, 54.89, 54.70, 46.49, 41.35; HRMS calcd for $C_{29}H_{25}NO_3$ + Na 458.1732, found 458.1730.

**9-(Phenoxymethyl)-1,4-dihydroxytriptycene (4b):** Yield 85%; white solid; m.p. 255-257 °C; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.70 (1H, s), 7.42-7.50 (5H, m), 7.31-7.34 (3H, m), 7.20-7.24 (1H, m), 6.98-7.05 (4H, m), 6.50 (1H, d, J = 8.5 Hz), 6.43 (1H, d, J = 8.5 Hz), 5.85 (1H, s), 5.52-5.80 (2H, m), 4.41 (1H, s); HRMS calcd for $C_{27}H_{20}O_3$ + Na 415.1310, found 415.1319.

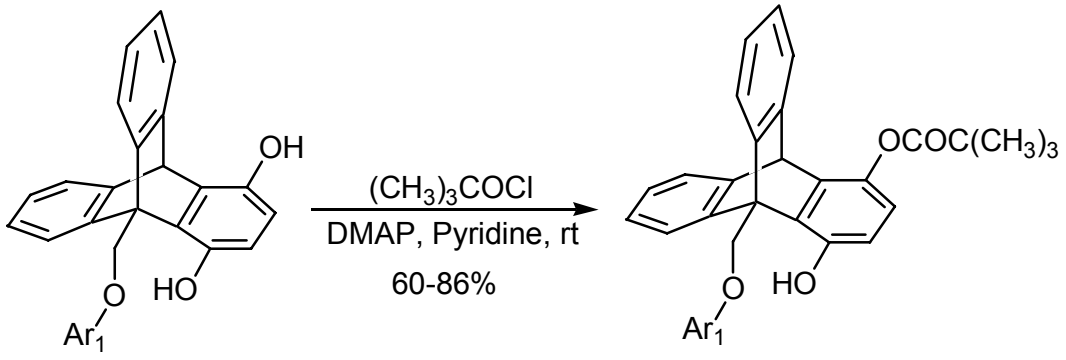
**9-(4-Nitrophenoxymethyl)-1,4-dihydroxytriptycene (4c):** Yield quantitative; brown solid; m.p. >300 °C; $^1$H NMR (300 MHz, DMSO-$d_6$) δ 8.91 (2H,br), 8.35 (2H, d, J = 9.1 Hz), 7.35-7.45 (6H, m), 6.97-7.04 (4H, m), 6.36 (1H, d, J = 8.6 Hz), 6.29 (1 H, d, J = 8.6 Hz), 5.83-5.90 (3H, m); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 164.02, 149.63, 146.03, 145.53, 145.01, 144.72, 141.10, 134.10, 129.48, 126.15, 124.85, 124.52, 123.91, 123.48, 123.04, 115.32, 114.12, 113.82, 67.40, 53.80, 46.49; HRMS calcd for $C_{27}H_{19}NO_5$ + Na 460.1161, found 460.1159.

**9-(4-Methylphenoxymethyl)-1,4-dihydroxytriptycene (4d):** Yield 93%; $^1$H NMR (200 MHz, $CDCl_3$) δ 7.87 (1H, s), 7.41-7.45 (3H, m), 7.24-7.41 (5H, m), 6.96-7.06 (4H, m), 6.49 (1H, d, J = 8.8 Hz), 6.41 (1H, d, J = 8.8 Hz), 5.49-5.86 (3H, m), 4.64 (1H, s), 2.38 (3H, s); HRMS calcd for $C_{28}H_{22}O_3$ + Na 429.1467, found 429.1464.

**9-(4-Methoxyphenoxymethyl)-1,4-dihydroxytriptycene (4e):** Yield 92%; brown solid; m.p. >300 °C; $^1$H NMR (300 MHz, DMSO-$d_6$) δ 8.83-8.88 (2H, m), 7.37-7.43 (4H, m), 6.98-7.09 (8H, m), 6.34 (1H, d, J = 8.6 Hz), 6.27 (1H, d, J = 8.6 Hz), 5.81 (1H, s), 5.64 (2H, br), 3.73 (3H, s); HRMS calcd for $C_{28}H_{22}O_4$ + Na 445.1416, found 445.1417.

**9-(3,5-Dimethylphenoxymethyl)-1,4-dihydroxytriptycene (4f):** Yield 94%; brown solid; m.p. 262-264 °C; $^1$H NMR (200 MHz, $CDCl_3$) δ 7.84 (1H, s), 7.31-7.45 (4H, m), 6.99-7.03 (4H, m), 6.93 (2H, s), 6.83 (1H,s), 6.49 (1H, d, J = 8.6 Hz), 6.42 (1H, d, J = 8.6 Hz), 5.85 (1H, s), 5.51-5.73 (2H, m), 4.52 (1H, s), 2.39 (6H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 156.61, 145.89, 145.37, 144.75, 144.26, 143.59, 140.07, 139.51, 133.74, 130.62, 125.41, 125.17, 124.95, 124.26, 123.81, 122.77, 120.54, 116.93, 114.64, 113.09, 112.38, 67.75, 52.60, 47.13, 21.46; HRMS calcd for $C_{29}H_{24}O_3$ + Na 443.1623, found 443.1626.

**9-(3,4,5-Trimethylphenoxymethyl)-1,4-dihydroxytriptycene (4g):** Yield 80%; brown solid; m.p. 284-286 °C; $^1$H NMR (200 MHz, $CDCl_3$) δ 7.95 (1H, s), 7.30-7.45 (4H, m), 6.98-7.05 (6H, m), 6.49 (1H, d, J = 8.6 Hz), 6.42 (1H, d, J = 8.6 Hz), 5.85 (1H, s), 5.49-5.71 (2H, m), 4.52 (1H, s), 2.35 (6H, s), 2.18 (3H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 155.74, 153.91, 145.96, 145.29, 144.78, 144.31, 143.62, 138.40, 137.85, 133.74, 130.60, 130.16, 125.55, 125.38, 124.93, 124.24, 123.80, 122.78, 120.46, 116.89, 114.65, 114.39, 113.94, 113.68, 52.62, 47.12, 20.88, 14.76; HRMS calcd for $C_{30}H_{26}O_3$ + Na 457.1780, found 457.1783.




**4 a-i** **5 a-i**

$Ar_1$ = 4-dimethylaminophenyl, phenyl
4-nitrophenyl, 4-methylphenyl
4-methoxyphenyl, 3,5-dimethyl
3,4,5-trimethyl

**General Synthetic Procedure for 9-(4-Substituted phenoxymethyl)-1-hydroxy-4-pivaloyloxy triptycene (5).**[5] 9-Substituted-1,4-dihydroxytriptycene (**4**) (1.27 mmol) was treated with pivaloyl chloride (0.19 g, 1.53 mmol) and 4-(dimethylamino)pyridine (50 mg, 0.42 mmol) in pyridine (5 ml) at ambient temperature for ~20 h. Then 15 ml of 1N HCl was added to quench the reaction. The mixture was extracted with methylene chloride and the extract was washed with aqueous HCl solution two times and dried over $MgSO_4$. The solvent was removed under reduced pressure and a residue was left. Further purification of the crude via flash column chromatography provided compound **5** as a solid.

**9-(4-Dimethylaminophenoxymethyl)-1-hydroxy-4-pivaloyloxytriptycene (5a):** Yield 64%; brown solid; m.p. 233-235 °C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.59 (1H, s), 7.29-7.47 (6H, m), 7.03-7.08 (4H, m), 6.88-6.91 (2H, m), 6.40-6.70 (2H, m), 5.42-5.80 (3H, m), 2.97 (6H, s), 1.56 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.93, 149.32, 148.30, 147.47, 144.91, 144.54, 139.32, 139.08, 130.19, 125.43, 125.13, 123.77, 120.24, 117.19, 116.47, 114.34, 68.68, 52.61, 48.43, 41.23, 39.21, 27.41. HRMS calcd for $C_{34}H_{33}NO_4$ + Na 542.2307, found 542.2309.

**9-phenoxymethyl-1-hydroxy-4-pivaloyloxytriptycene (5b):** Yield 74%; white solid; m.p. 251-253 °C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.05 (1H, s), 7.46-7.49 (3H, m), 7.30-7.35 (5H, m), 7.21 (1H, m), 6.97-7.05 (4H, m), 6.68 (1H, d, J = 8.4 Hz), 6.62 (1H, d, J = 8.4 Hz), 5.56-5.77 (2H, m), 5.38 (1H, s), 1.52 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.94, 156.60, 149.20, 144.45, 139.50, 139.15, 130.15, 125.55, 125.21, 123.88, 123.49, 120.37, 117.36, 115.46, 67.86, 52.56, 48.47, 39.28, 27.47; HRMS calcd for $C_{32}H_{28}O_4$ + Na 499.1885, found 499.1883.

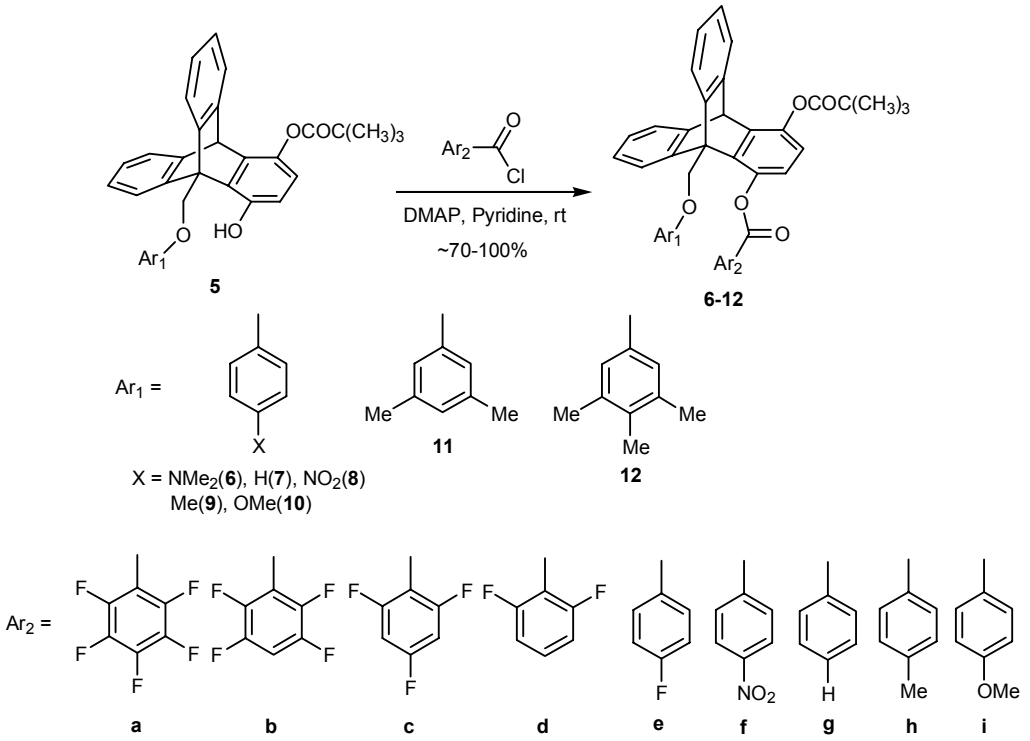
**9-(4-Nitrophenoxymethyl)-1-hydroxy-4-pivaloyloxytriptycene (5c):** Yield 80%; yellow solid; m.p. 287-289 °C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.32 (2H, d, J = 8.2 Hz), 7.32-7.34 (6H, m), 7.01-7.03 (4H, m), 5.84-6.41 (4H, m), 5.35 (1H, s), 5.10 (1H, br), 1.52 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 177.29, 148.45, 144.68, 144.24, 139.52, 130.56, 126.18, 125.55, 125.25, 123.93, 123.10, 120.02, 115.02, 67.42, 50.86, 48.54, 39.35, 27.47; HRMS calcd for $C_{32}H_{27}NO_6$ + Na 544.1736, found 544.1732.

**9-(4-Methylphenoxymethyl)-1-hydroxy-4-pivaloyloxytriptycene (5d):** Yield 83%; white solid; m.p. 239-241°C; $^{1}$H NMR (300 MHz, $CDCl_3$) δ 8.16 (1H, s), 7.26-7.32 (6H, m), 7.20-7.24 (2H, m), 6.97-7.04 (4H, m), 6.67 (1H, d, J = 8.7 Hz), 6.61 (1H, d, J = 8.7 Hz), 5.51-5.74 (2H, m), 5.37 (1H, s), 2.38 (3H, s), 1.51 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.88, 154.53, 149.28, 144.51, 139.51, 139.12, 133.06, 130.59, 130.21, 125.57, 125.23, 123.92, 122.84, 120.38, 117.36, 115.35, 114.48, 68.06, 53.39, 52.60, 48.48, 39.30, 27.49, 20.63; HRMS calcd for $C_{33}H_{30}O_4$ + Na 513.2042, found 513.2043.

**9-(4-Methoxyphenoxymethyl)-1-hydroxy-4-pivaloyloxytriptycene (5e):** Yield 60%; white solid; m.p. 243-245 °C; $^{1}$H NMR (300 MHz, $CDCl_3$) δ 8.33 (1H, s), 7.29-7.36 (6H, m), 7.01-7.07 (6H, m), 6.71 (1H, d, J = 8.5 Hz), 6.66 (1H, d, J = 8.5 Hz), 5.48-5.73 (2H, m), 5.40 (1H, s), 3.85 (3H, s), 1.55 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.94, 155.79, 150.59, 149.27, 144.49, 139.46, 139.13, 130.22, 125.54, 125.20, 123.87, 120.36, 117.30, 116.56, 115.19, 55.75, 52.62, 48.47, 39.28, 27.47; HRMS calcd for $C_{33}H_{30}O_5$ + Na 529.1991, found 529.1993.

**9-(3,5-Dimethylphenoxymethyl)-1-hydroxy-4-pivaloyloxytriptycene (5f):** Yield 63%; white solid; m.p. 266-268°C; $^{1}$H NMR (200 MHz, $CDCl_3$) δ 8.16 (1H, s), 7.26-7.33 (4H, m), 6.99-7.04 (4H, m), 6.94 (2H, s), 6.84 (1H, s), 6.67 (1H, d, J = 8.7 Hz), 6.61 (1H, d, J = 8.7 Hz), 5.55-5.71 (2H, m), 5.37 (1H, s), 2.40 (6H, s), 1.51 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.91, 156.57, 149.28, 144.53, 140.09, 139.47, 139.13, 130.23, 125.53, 125.22, 123.86, 122.70, 120.34, 117.32, 113.94, 113.12, 67.66, 55.15, 52.59, 48.49, 39.28, 27.48, 21.48; HRMS calcd for $C_{34}H_{32}O_4$ + Na 527.2198, found 527.2199.

**9-(3,4,5-Trimethylphenoxymethyl)-1-hydroxy-4-pivaloyloxytriptycene (5g):** Yield 85%; white solid; m.p. 285-287 °C; $^{1}$H NMR (200 MHz, $CDCl_3$) δ 8.27 (1H, s), 7.28-7.32 (4H, m), 6.99-7.03 (6H, m), 6.67 (1H, d, J = 8.7 Hz), 6.60 (1H, d, J = 8.7 Hz), 5.50-5.70 (2H, m), 5.36 (1H, s), 2.36 (6H, s), 2.19 (3H, s), 1.51 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.83, 153.89, 149.35, 144.57, 139.47, 139.09, 138.44, 130.26, 125.54, 125.23, 123.89, 120.34, 117.33, 114.44, 67.72, 52.60, 48.47, 39.19, 27.49, 21.03, 20.94; HRMS calcd for $C_{35}H_{34}O_4$ + Na 541.2355, found 541.2354.




**General Synthetic Procedure for 9-(4-Substituted phenoxymethyl)-1-(substituted benzoyloxy)-4-pivaloyloxytriptycene (6-12).**[5,6] 9-(4-Substituted phenoxymethyl)-1-hydroxy-4-pivaloyloxy triptycene (**5**) (0.15 mmol) was treated with corresponding benzoyl chloride (0.19 mmol) and 4-(dimethylamino)pyridine (50 mg, 0.42 mmol) in pyridine (1 ml) at ambient temperature for 0.5-1 d. Then 5 ml of 1N HCl was added to quench the reaction. The mixture was extracted with methylene chloride and the extract was washed with aqueous HCl solution two times and dried over $MgSO_4$. The solvent was removed under reduced pressure and a residue was left. Further purification of the crude via flash column chromatography provided compound **6-12** as a solid.

**9-(4-Dimethylaminophenoxymethyl)-1-pentafluorobenzoyloxy-4-pivaloyloxytriptycene (6a):** Yield 77%; yellow solid; m.p. 237-240 °C; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.47-7.49 (1H, m), 7.29-7.34 (3H, m), 7.04 (4H, m), 6.82-6.89 (4H, m), 6.57 (2H, d, J = 8.8 Hz), 5.56-5.59 (1H, m), 5.43 (1H, s), 5.13-5.16 (1H, m), 2.86 (6H, s), 1.53 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.30, 157.41, 149.97, 147.90, 145.95, 145.65, 144.95, 144.24, 143.63, 142.55, 141.52, 140.74, 139.05, 136.42, 135.65,125.64, 125.64, 125.54, 124.56, 124.04, 123.55, 121.24, 120.92, 120.11, 114.48, 113.77, 106.74, 65.93, 53.20, 48.48, 41.19, 39.39, 27.42; HRMS calcd for $C_{41}H_{32}F_5NO_5$ + H 714.2279, found 714.2297.

**9-(4-Dimethylaminophenoxymethyl)-1-(2,3,5,6-tetrafluorobenzoyloxy)-4-pivaloyloxytriptycene (6b):** Yield quantitative; yellow solid; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.33-7.50 (4H, m), 7.04 (5H, m), 6.83-6.90 (4H, m), 6.60 (2H, br), 5.19-5.61 (3H, m), 2.87 (6H, s), 1.54 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.27, 157.95, 157.91, 157.87, 150.21, 147.46, 146.96, 145.59, 144.23, 143.59, 142.61, 140.66, 136.42, 125.59, 125.48, 124.54, 123.97, 123.54,

121.20, 120.91, 120.10, 114.36, 109.58, 109.27, 108.99, 65.87, 53.16, 48.46, 41.50, 39.36, 27.40; HRMS calcd for $C_{41}H_{33}F_4NO_5$ + H 696.2373, found 696.2371.

**9-(4-Dimethylaminophenoxymethyl)-1-(2,4,6-trifluorobenzoyloxy)-4-pivaloyloxytriptycene (6c):** Yield 71%; brown solid; m.p. 203-204°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.31-7.45 (4H, m), 7.03 (5H, m), 6.59-6.89 (6H, m), 6.41 (1H, br), 5.12-5.62 (3H, m), 2.85 (6H, s), 1.53 (9H, s); HRMS calcd for $C_{41}H_{34}F_3NO_5$ + H 678.2467, found 678.2460.

**9-(4-Dimethylaminophenoxymethyl)-1-(2,6-difluorobenzoyloxy)-4-pivaloyloxytriptycene (6d):** Yield 73%; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.33-7.66 (5H, m), 6.43-7.16 (12H, m), 5.16-5.69 (3H, m), 2.86 (6H, s), 1.54 (9H, s); HRMS calcd for $C_{41}H_{35}F_2NO_5$ + Na 682.2381, found 682.2380.

**9-(4-Dimethylaminophenoxymethyl)-1-(4-fluorobenzoyloxy)-4-pivaloyloxytriptycene (6e):** Yield 96%; white solid; m.p. 249-251°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.78-8.36 (2H, m), 7.31-7.42 (5H, m), 6.73-7.03 (7H, m), 6.50-6.52 (4H, m), 5.08-5.62 (3H, m), 2.83 (6H, s), 1.53 (9H, m); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.35, 164.05, 162.23, 144.34, 143.44, 133.24, 125.72, 125.65, 125.41, 124.56, 123.89, 121.23, 120.34, 116.48, 115.18, 66.30, 55.0, 48.50, 39.39, 32.62, 27.43. HRMS calcd for $C_{41}H_{36}FNO_5$ + H, 642.2656, found 642.2642

**9-(4-Dimethylaminophenoxymethyl)-1-benzoyloxy-4-pivaloyloxytriptycene (6g):** Yield 64%; brown solid; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.58-8.35 (4H, m), 7.31-7.42 (5H, m), 7.00-7.05 (4H, m), 6.82 (1H, d, J = 8.8 Hz), 6.76 (1H, d, J = 8.8 Hz), 6.51-6.55 (4H, m), 5.45 (3H, m), 2.83 (6H, s), 1.53 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.27, 165.03, 150.71, 145.74, 144.37, 143.88, 143.32, 142.71, 141.42, 137.48, 133.98, 130.53, 129.30, 128.97, 125.45, 125.34, 124.08, 123.68, 121.25, 120.09, 114.90, 66.09, 55.18, 48.49, 41.78, 39.34, 27.39; ; HRMS calcd for $C_{41}H_{37}NO_5$ + H 624.2750, found 624.2762.

**9-Phenoxymethyl-1-(pentafluorobenzoyloxy)-4-pivaloyloxytriptycene (7a):** Yield 77%; ligh yellow solid; m.p. 240-242°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.26-7.43 (5H, m), 7.21-7.24 (1H, m), 7.07 (4H, m), 6.86-6.97 (5H, m), 5.27-5.67 (3H, m), 1.56 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.31, 157.99, 157.29, 147.83, 145.92, 145.15, 144.24, 144.07, 143.67, 142.49, 141.81, 140.73, 139.12, 136.19, 135.75, 129.34, 125.74, 125.54, 124.29, 124.12, 123.69, 121.18, 120.22, 114.02, 106.69, 65.88, 53.06, 48.49, 39.41, 29.69, 27.44; HRMS calcd for $C_{39}H_{27}F_5O_5$ + Na 693.1676, found 693.1686.

**9-Phenoxymethyl-1-(4-fluorobenzoyloxy)-4-pivaloyloxytriptycene (7e):** Yield 78%; light yellow solid; m.p. 203-205°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.78-8.40 (2H, m), 7.34-7.36 (5H, m), 7.03-7.11 97H, m), 6.75-6.86 (4H, m), 6.63 (1H, m), 5.18-5.68 (3H, m), 1.54 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.31, 164.06, 158.16, 144.30, 143.70, 143.41, 142.55, 141.41, 137.31, 133.20, 132.47, 129.31, 125.57, 125.39, 123.80, 121.07, 120.22, 116.06, 115.19, 114.30, 65.80, 55.01, 48.49, 39.35, 27.39; HRMS calcd for $C_{39}H_{31}FO_5$ + Na 621.2053, found 621.2046.

**9-Phenoxymethyl-1-(4-nitrobenzoyloxy)-4-pivaloyloxytriptycene (7f):** Yield 71%; white solid; m.p. 253-255°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.51 (1H, br), 7.93 (3H, m), 7.34-7.36 (4H, m), 7.01-7.05 (6H, m), 6.75-6.89 (5H, m), 5.17-5.66 (3H, m), 1.55 (9H, s); $^{13}$C NMR (75

MHz, $CDCl_3$) δ 176.30, 163.10, 157.86, 150.07, 146.04, 144.16, 143.58, 143.27, 140.48, 136.44, 134.67, 130.73, 129.29, 125.66, 125.43, 124.13, 123.66, 123.01, 121.43, 121.12, 120.69, 120.31, 114.20, 65.85, 53.22, 48.46, 39.36, 27.38; HRMS calcd for $C_{39}H_{31}NO_7$ + Na 648.1998, found 648.2018.

**9-Phenoxymethyl-1-benzoyloxy-4-pivaloyloxytriptycene (7g):** Yield quantitative; white solid; m.p. 205-207°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.39 (1H, br), 7.70-7.84 (3H, m), 7.36-7.43 (4H, m), 7.04-7.06 (7H, m), 6.62-6.91 (5H, m), 5.21-5.74 (3H, m), 1.56 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.33, 165.07, 158.26, 144.41, 143.79, 143.42, 142.71, 141.46, 137.39, 134.20, 130.59, 129.37, 129.30, 129.06, 125.58, 125.41, 123.80, 121.31, 120.96, 120.23, 114.42, 65.86, 55.12, 48.55, 39.40, 27.45; HRMS calcd for $C_{39}H_{32}O_5$ + Na 603.2147, found 603.2141.

**9-Phenoxymethyl-1-(4-methylbenzoyloxy)-4-pivaloyloxytriptycene (7h):** Yield 78%; white solid; m.p. 221-223°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.33-8.27 (8H, m), 7.02-7.06 (6H, m), 6.75-6.91 (3H, m), 6.61 (2H, m), 5.18-5.69 (3H, m), 2.32-2.59 (3H, m), 1.53 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.29, 165.11, 158.27, 145.16, 144.41, 143.81, 143.33, 142.74, 141.36, 137.36, 130.63, 129.69, 129.26, 126.51, 125.52, 125.36, 123.92, 123.76, 121.36, 120.91, 120.15, 114.45, 65.86, 55.06, 48.52, 39.35, 27.42, 21.79; HRMS calcd for $C_{40}H_{34}O_5$ + Na 617.2304, found 617.2309.

**9-Phenoxymethyl-1-(4-methoxybenzoyloxy)-4-pivaloyloxytriptycene (7i):** Yield 89%;white solid; m.p. 213-214°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.76-8.35 (2H, m), 7.35-7.42 (4H, m), 7.04-7.15 (8H, m), 6.76-6.93 (3H, m), 6.67 (2H, m), 5.47-5.53 (3H, m), 3.81-3.99 (3H, m), 1.55 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.32, 164.78, 164.44, 158.31, 144.43, 143.85, 143.30, 142.82, 141.28, 137.41, 132.78, 129.32, 125.53, 125.37, 123.92, 123.76, 121.52, 120.95, 120.14, 114.48, 114.26, 65.87, 55.66, 55.04, 48.53, 39.37, 27.43; HRMS calcd for $C_{40}H_{34}O_6$ + Na 633.2253, found 633.2233.

**9-(4-Nitrophenoxymethyl)-1-pentafluorobenzoyloxy-4-pivaloyloxytriptycene (8a):** Yield 26%; white solid; m.p. 253-255°C; $^1$H NMR (200 MHz, $CDCl_3$) δ 8.16 (2H, d, J = 9.1 Hz), 7.28-7.35 (4H, m), 7.04-7.07 (6H, m), 6.87(2H, m), 5.71 (1H, m), 5.39-5.46 (2H, m), 1.54 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.31, 162.77, 157.16, 147.71, 145.69, 144.19, 143.85, 143.41, 142.42, 142.05, 140.75, 139.21, 135.72, 126.03, 125.62, 124.06, 123.57, 121.01, 120.63, 114.42, 67.09, 52.95, 48.46, 39.44, 27.43; HRMS calcd for $C_{39}H_{26}F_5NO_7$ + Na 738.1527, found 738.1525.

**9-(4-Nitrophenoxymethyl)-1-(4-fluorobenzoyloxy)-4-pivaloyloxytriptycene (8e):** Yield 86%; yellow solid; m.p. 298-299°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.40 (1H, br), 8.00 (2H, d, J = 9.2 Hz), 7.78 (1H, br), 7.27-7.38 (4H, m), 7.04-7.24 (5H, m), 6.75-6.87 (4H, m), 6.66 (1H, m), 5.33-5.78 (3H, m), 1.52 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.34, 163.92, 162.96, 144.29, 143.52, 142.41, 141.86, 133.13, 132.44, 125.86, 125.70, 125.45, 124.08, 123.39, 121.46, 120.50, 116.24, 115.40, 114.43, 66.92, 52.97, 48.48, 39.39, 27.41; HRMS calcd for $C_{39}H_{30}FNO_7$ + Na 666.1904, found 666.1882.

**9-(4-Nitrophenoxymethyl)-1-(4-nitrobenzoyloxy)-4-pivaloyloxytriptycene (8f):** Yield 55%; yellow solid; m.p. >307°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.95-8.51 (6H, m), 7.18-7.37 (4H, m),

7.05-7.10 (4H, m), 6.77-6.90 (4H, m), 5.33-5.77 (3H, m), 1.55 (9H, s); HRMS calcd for $C_{39}H_{30}N2O_9$ + Na 693.1849, found 693.1873.

**9-(4-Nitrophenoxymethyl)-1-benzoyloxy-4-pivaloyloxytriptycene (8g):** Yield 75%; white solid; m.p. 295-296°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.39 (1H, br), 7.73-7.94 (5H, m), 7.27-7.38 (4H, m), 7.04-7.24 (5H, m), 6.48-6.89 (4H, m), 5.30-5.83 (3H, m), 1.53 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.34, 164.90, 162.99, 144.33, 143.48, 141.78, 134.60, 130.48, 129.13, 128.21, 125.84, 125.44, 124.03, 123.37, 121.43, 120.46, 114.48, 66.99, 54.66, 48.50, 39.40, 27.43; HRMS calcd for $C_{39}H_{31}NO_7$ + Na 648.1998, found 648.1976.

**9-(4-Nitrophenoxymethyl)-1-(4-methylbenzoyloxy)-4-pivaloyloxytriptycene (8h):** Yield 92%; white solid; m.p. 296-298°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.26 (1H, br), 7.93 (2H, d, J = 9.2 Hz), 7.27-7.53 (6H, m), 7.04-7.09 (5H, m), 6.63-6.86 (4H, m), 5.31-5.83 (3H, m), 2.30-2.64 (3H, m), 1.54 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.33, 164.91, 163.08, 145.67, 144.36, 143.42, 141.72, 130.52, 129.88, 128.92, 126.39, 125.81, 125.65, 125.42, 124.04, 123.42, 121.52, 120.41, 114.52, 67.01, 54.67, 48.50, 39.38, 27.42, 21.81; HRMS calcd for $C_{40}H_{33}NO_7$ + Na 662.2155, found 662.2139.

**9-(4-Nitrophenoxymethyl)-1-(4-methoxybenzoyloxy)-4-pivaloyloxtriptycene (8i):** Yield 60%; white solid; m.p. 295-296°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.32 (1H, br), 7.96 (2H, d, J = 9.0 Hz), 7.68 (1H, br), 7.27-7.37 (4H, m), 7.04-7.17 (5H, m), 6.66-6.85 (5H, m), 5.30-5.82 (3H, m), 3.76-4.03 (3H, m), 1.53 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.32, 164.53, 163.11, 144.35, 143.35, 142.72, 141.02, 136.83, 132.65, 125.78, 125.69, 125.39, 124.00, 123.35, 121.59, 121.29, 120.36, 114.52, 113.48, 67.00, 55.67, 54.70, 48.48, 39.36, 27.40; HRMS calcd for $C_{40}H_{33}NO_8$ + Na 678.2104, found 678.2086.

**9-(4-Methylphenoxymethyl)-1-pentafluorobenzoyloxy-4-pivaloyloxytriptycene (9a):** Yield 88%; %; white solid; m.p. 259-260°C; $^1$H NMR (300 MHz, $CDCl_3$) δ7.32-7.43 (4H, m), 6.98-7.04 (6H, m), 6.79-6.90 (4H, m), 5.19-5.58 (3H, m), 2,26 (3H, s), 1.53 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.30, 157.28, 155.88, 147.82, 145.91, 144.13, 143.65, 142.50, 140.738, 136.23, 135.79, 130.70, 129.64, 125.71, 125.53, 124.39, 124.10, 123.64, 121.16, 120.91, 120.17, 113.79, 65.85, 53.13, 48.48, 39.41, 27.44, 20.12; HRMS calcd for $C_{40}H_{29}F_5O_5$ + Na 707.1833, found 707.1848.

**9-(4-Methoxyphenoxymethyl)-1-pentafluorobenzoyloxy-4-pivaloyloxytriptycene (10a):** Yield 89%; white solid; m.p. 240-241°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.32-7.44 (4H, m), 7.04 (4H, m), 6.84-6.89 (4H, m), 6.73 (2H, d, J = 8.9 Hz), 5.17-5.57 (3H, m), 3.76 (3H, s), 1.53 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.31, 157.34, 154.17, 152.09, 147.87, 145.87, 144.12, 143.68, 142.52, 140.73, 139.12, 136.30, 135.75, 125.72, 125.54, 124.37, 124.10, 123.66, 121.18, 120.84, 120.21, 114.67, 114.31, 106.82, 66.19, 55.59, 53.15, 48.48, 39.41, 27.44; HRMS calcd for $C_{40}H_{29}F_5O_6$ + Na 723.1782, found 723.1771.

**9-(3,5-Dimethylphenoxymethyl)-1-pentafluorobenzoyloxy-4-pivaloyloxytriptycene (11a):** Yield 89%; white solid; m.p. 246-248°C; $^1$H NMR (300 MHz, $CDCl_3$) δ 7.32-7.43 (4H, m), 7.01-7.05 (4H, m), 6.90 (1H, d, J = 8.8 Hz), 6.84 (1H, d, J = 8.8 Hz), 6.52 (3H, m), 5.60-5.62 (1H, m), 5.43 (1H, s), 5.14-5.17 (1H, m), 2.25 (6H, s), 1.53 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$)

δ 176.33, 158.03, 157.23, 148.06, 145.94, 144.18, 143.61, 142.50, 140.73, 139.52, 136.18, 125.70, 125.57, 124.42, 124.09, 123.62, 122.74, 121.20, 120.13, 111.64, 106.77, 65.63, 53.10, 48.49, 39.43, 27.46, 21.10; HRMS calcd for $C_{41}H_{31}F_5O_5$ + Na 721.1989, found 721.2000.

**9-(3,4,5-Trimethylphenoxymethyl)-1-pentafluorobenzoyloxy-4-pivaloyloxytriptycene (12a):** Yield 91%; white solid; m.p. 243-245°C; $^1$H NMR (300 MHz, $CDCl_3$) δ7.32-7.45 (4H, m), 6.98-7.05 (4H, m), 6.90 (1H, d, J = 8.9 Hz), 6.84 (1H, d, J = 8.9 Hz), 6.56 (2H, s), 5.57-5.60 (1H, m), 5.43 (1H, s), 5.12-5.15 (1H, m), 2.22 (6H, s), 2.07 (3H, s), 1.53 (9H, s); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 176.32, 157.20, 155.35, 147.85, 145.95, 145.17, 144.23, 143.60, 142.51, 140.72, 139.21, 137.71, 136.24, 135.89, 127.71, 125.67, 125.57, 125.47, 124.521, 124.08, 123.57, 121.20, 120.96,120.08, 112.90, 106.93, 106.78, 65.45, 53.12, 48.49, 39.41, 27.45, 20.75, 20.45; HRMS calcd for $C_{42}H_{33}F_5O_5$ + Na 735.2146, found 735.2137.

## Variable Temperature NMR Experimental Procedure

The $^1$H NMR spectra were recorded on a Bruker 300 MHz instrument with a variable temperature probe. A 0.05 M solution of the sample in a deuterated solvent such as chloroform was placed in a high quality NMR tube. All samples were degassed using a needle to bubble nitrogen through the sample for ~1 minute. The NMR tube was then capped with a cap and sealed with parafilm. The sample tube was placed into the NMR probe and the air line to the probe was replaced with liquid nitrogen transfer line. The desired temperature was set on the variable temperature unit and the sample was allowed to equilibrate for 10 ~ 15 minutes at each set temperature. Then the $^1$H NMR spectrum at each temperature was recorded. The ratios of rotamers were obtained through the integrations of selected peaks.

## References


(1) Tamura, Y.; Yamamoto, G.; Oki, M. *Bull. Chem. Soc. Jpn.* **1987**, *60*, 1781-8. "CH3-O hydrogen bond. Implications of its presence from the substituent effects on the populations of rotamers in 4-substituted 9-ethyl-1-methoxytriptycenes and 9-(substituted phenoxymethyl)-1,4-dimethyltriptycenes"

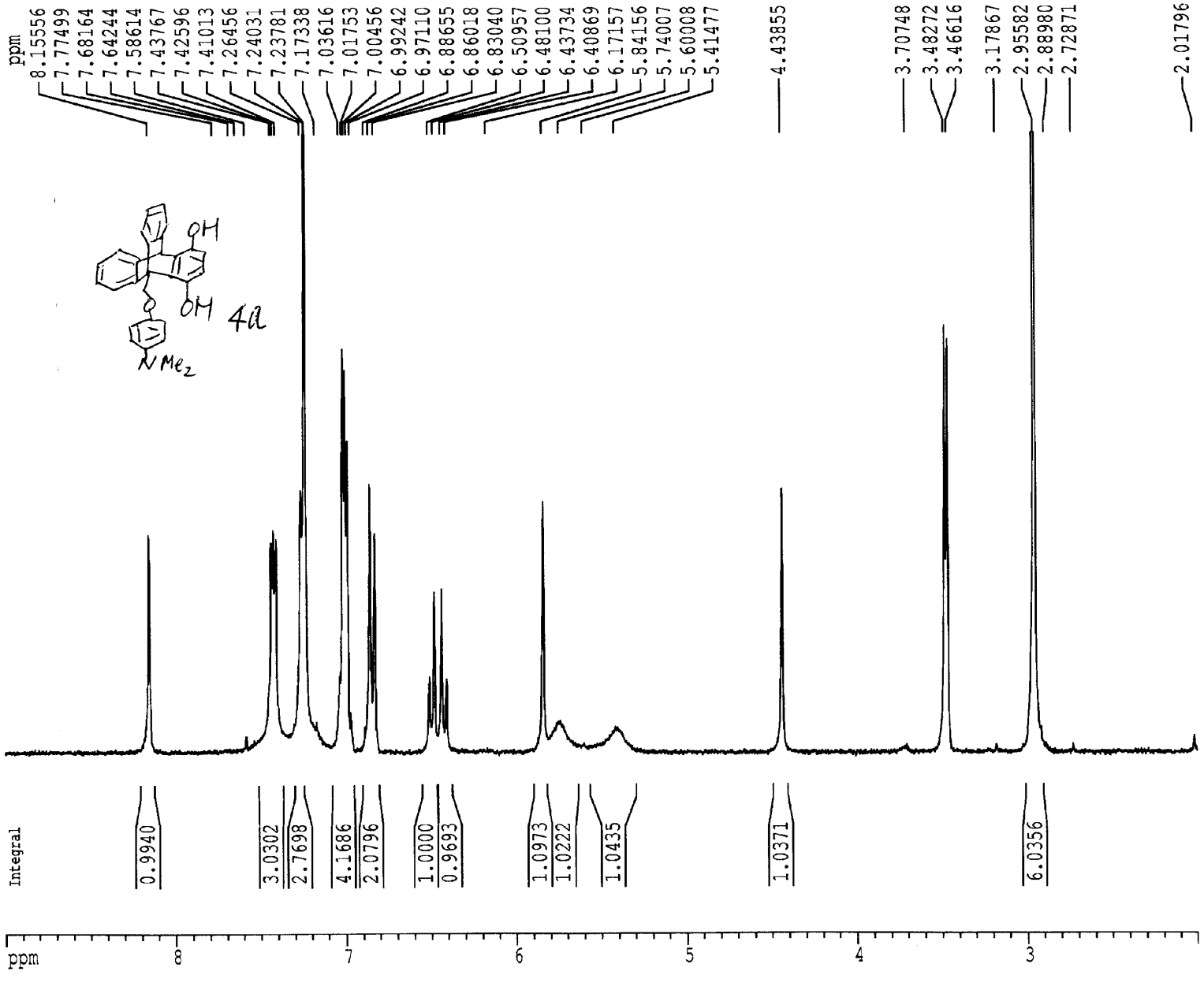
(2) Kimura, N. *J. Am. Chem. Soc.* **2001**, *123*, 3824-3825. "The Role of the Leaving Group in the Dissociation of Radical Anions of 9-(Aryloxymethyl)anthracenes"

(3) Oki, M.; Izumi, G.; Yamamoto, G.; Nakamura, N. *Bull. Chem. Soc. Jpn.* **1982**, *55*, 159-66. "Attractive interactions between carbonyls and groups bearing lone-pair electrons in triptycene systems"

(4) Smith, J. G.; Dibble, P. W.; Sandborn, R. E. *Journal of Organic Chemistry* **1986**, *51*, 3762-3768. "The Preparation and Reactions of Naphtho 1,2-C Furan and Naphtho 2,3-C Furan"

(5) Cunningham, B. D. M.; Lowe, P. R.; Threadgill, M. D. *Journal of the Chemical Society-Perkin Transactions 2* **1989**, 1275-1283. "Structural Studies on Bio-Active Compounds .12. Tautomerism and Conformation of Aryl-Substituted 1-(2-Hydroxyphenyl)-3- Phenylpropane-1,3-Diones in the Solid-Phase and in Solution"

(6) Gung Benjamin, W.; Xue, X.; Reich Hans, J. *J. Org. Chem.* **2005**, *70*, 3641-4. "The strength of parallel-displaced arene-arene interactions in chloroform"

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1D NMR plot parameters

| | |
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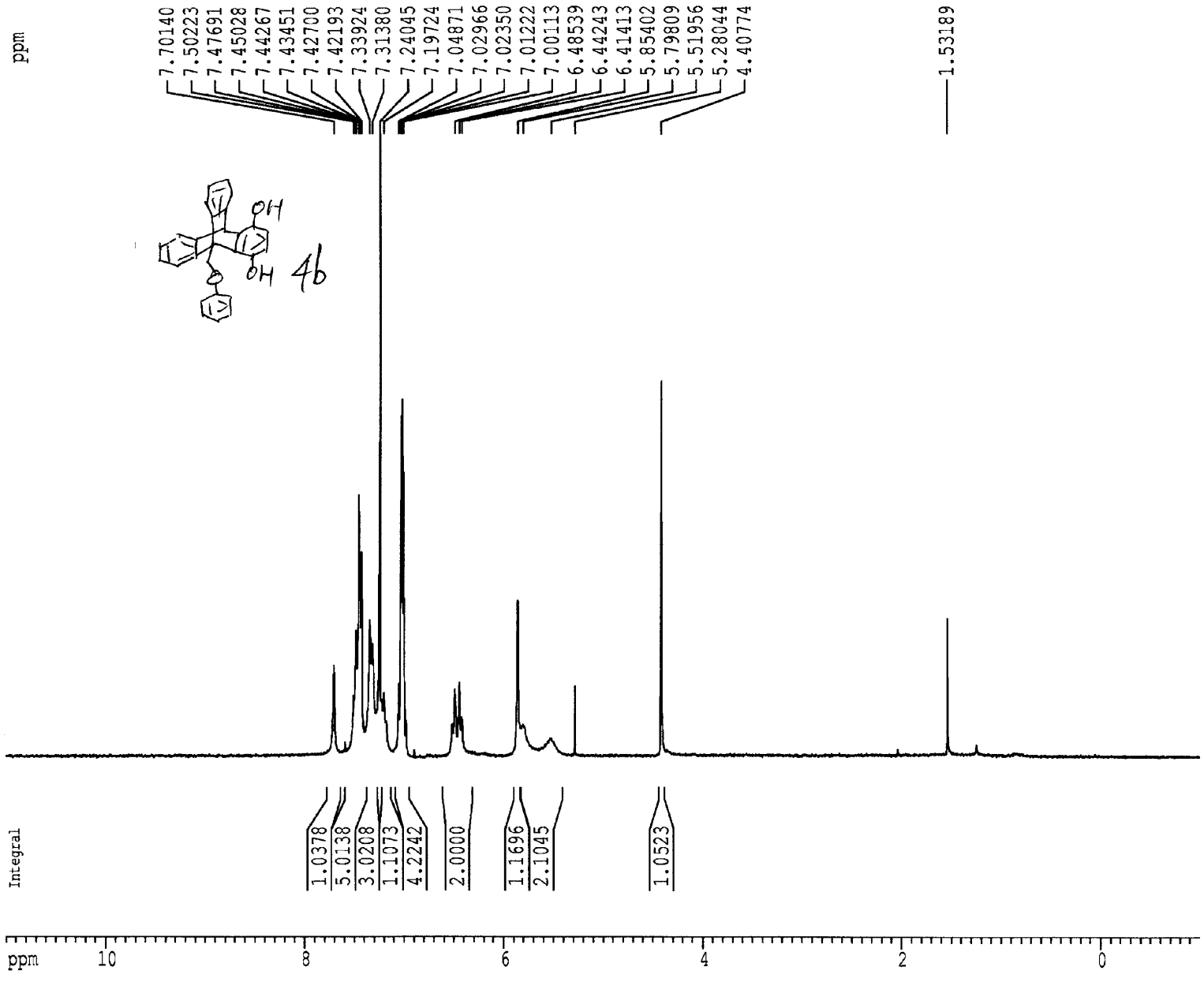


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1D NMR plot parameters

| | |
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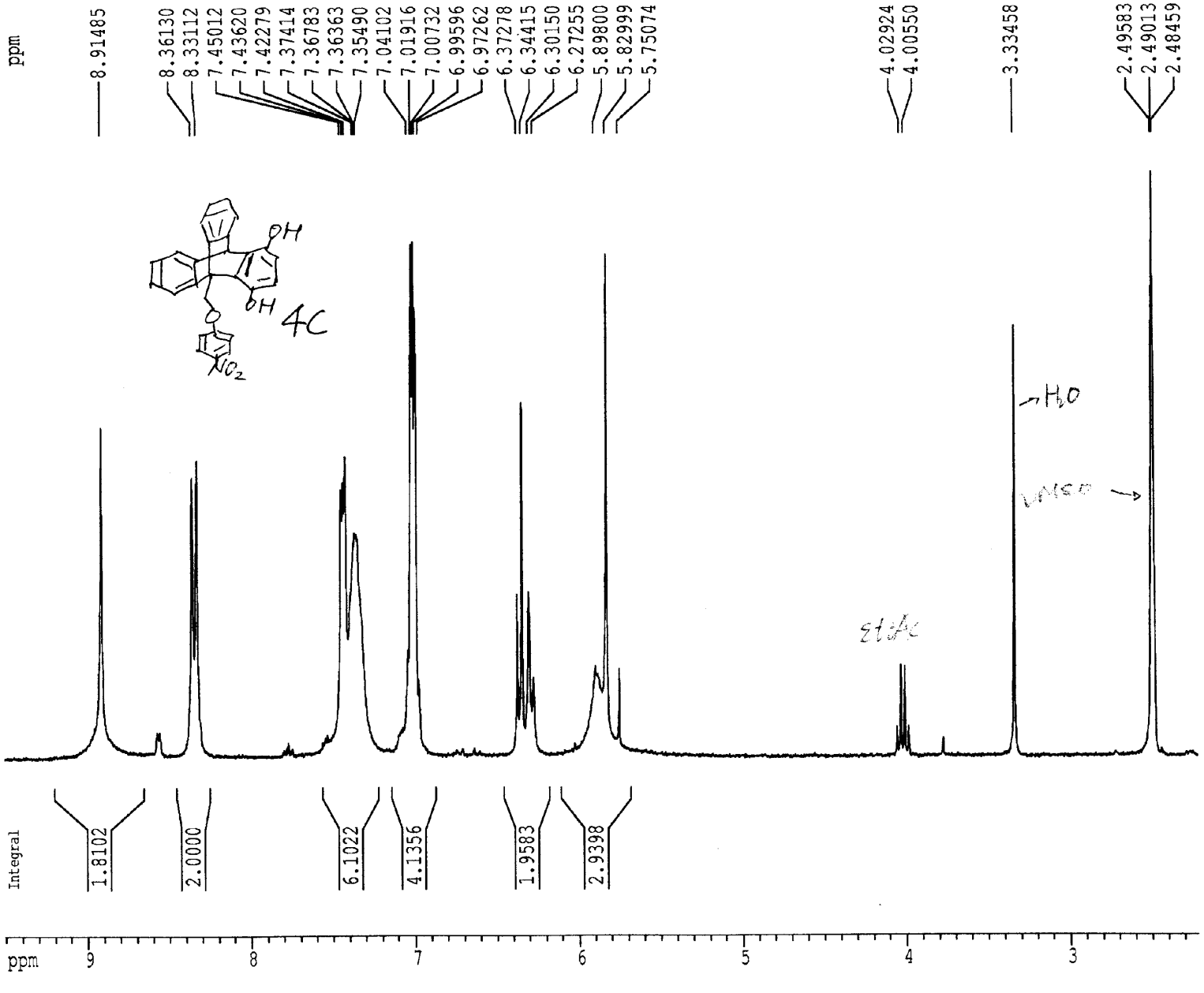


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1D NMR plot parameters

| | |
|---|---|
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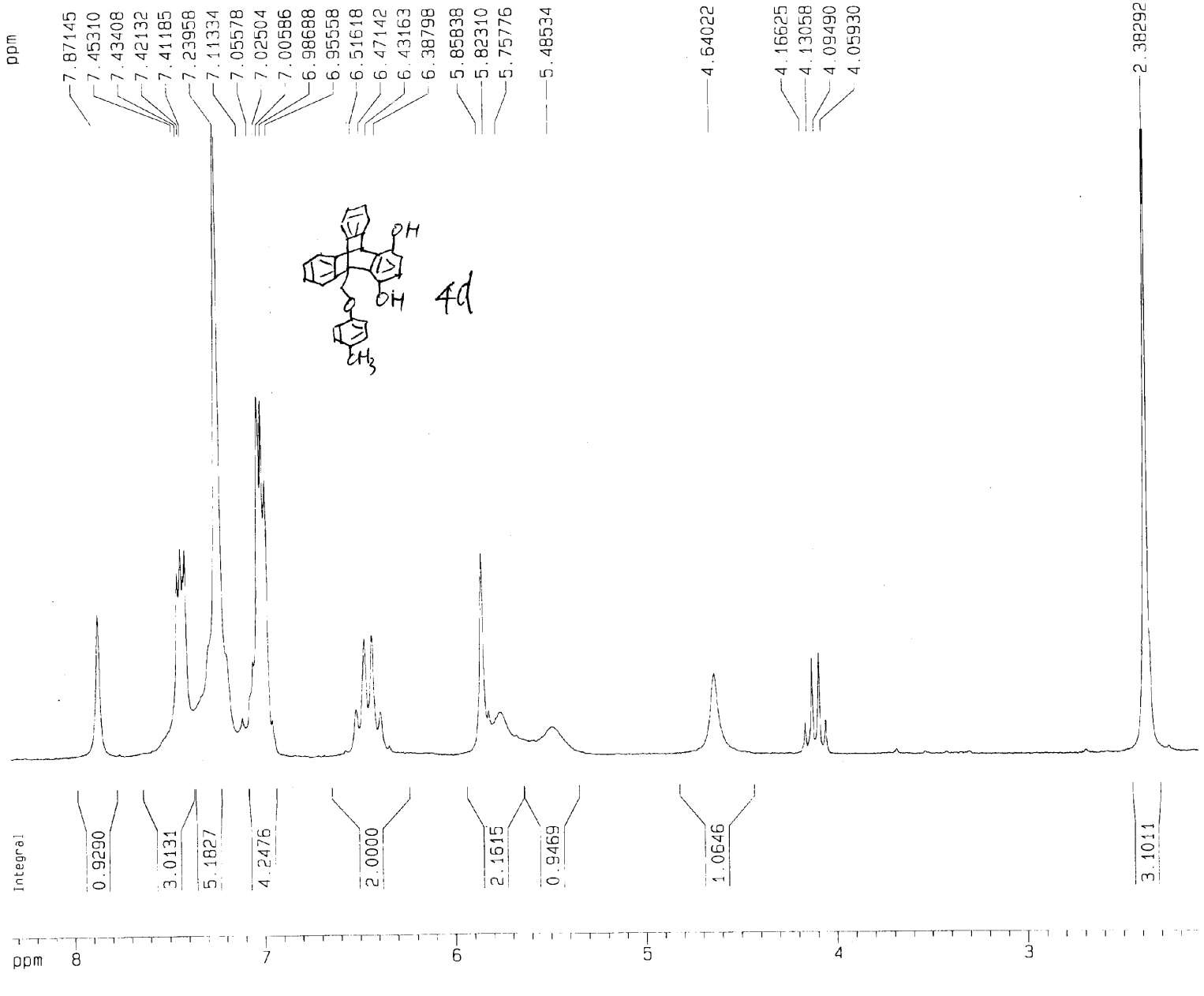


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| GB | 0 |
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1D NMR plot parameters

| | |
|---|---|
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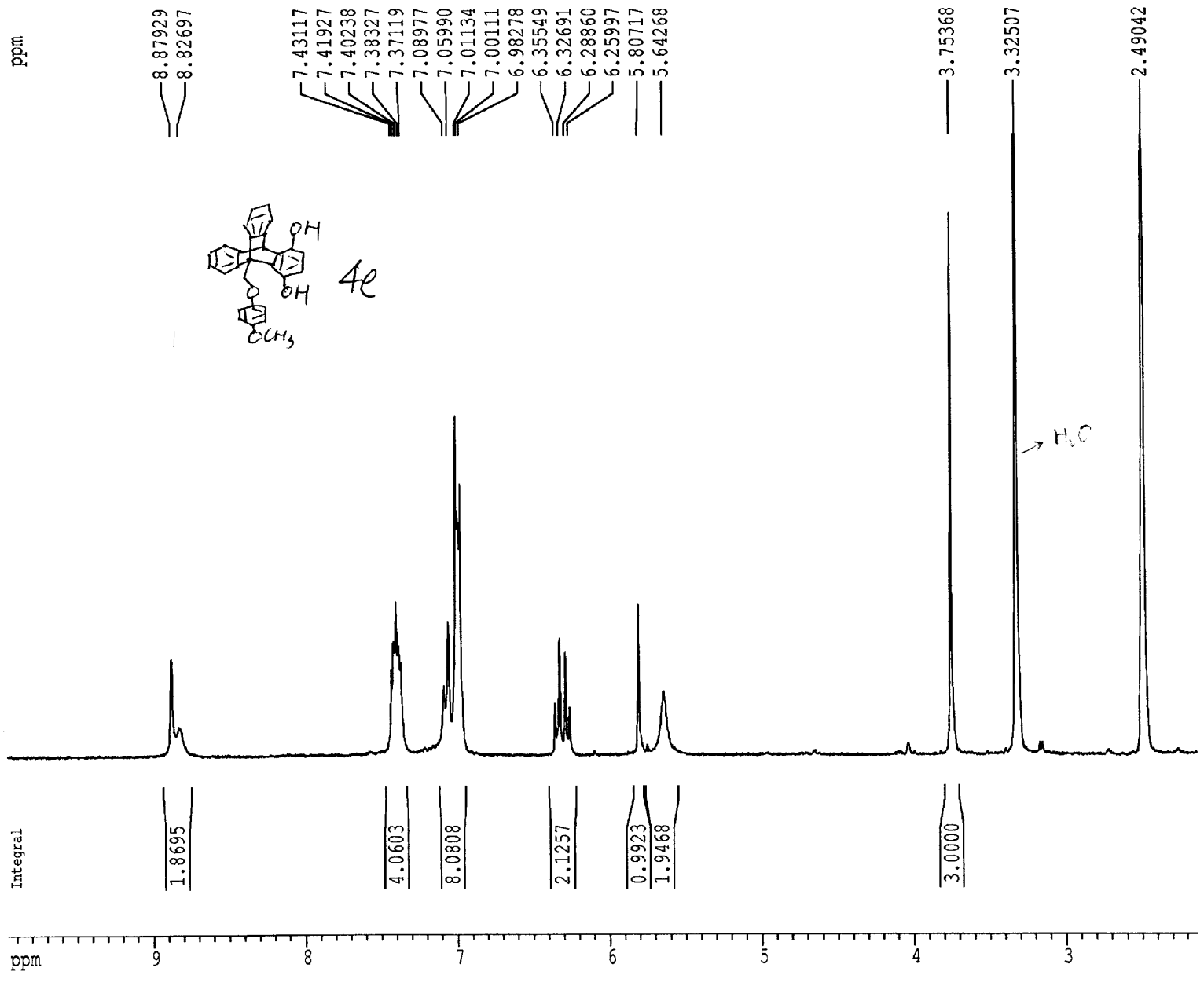


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| PULPROG | zg30 |
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| SWH | 6188.119 Hz |
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1D NMR plot parameters

| | |
|---|---|
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| F1P | 9.958 ppm |
| F1 | 2988.62 Hz |
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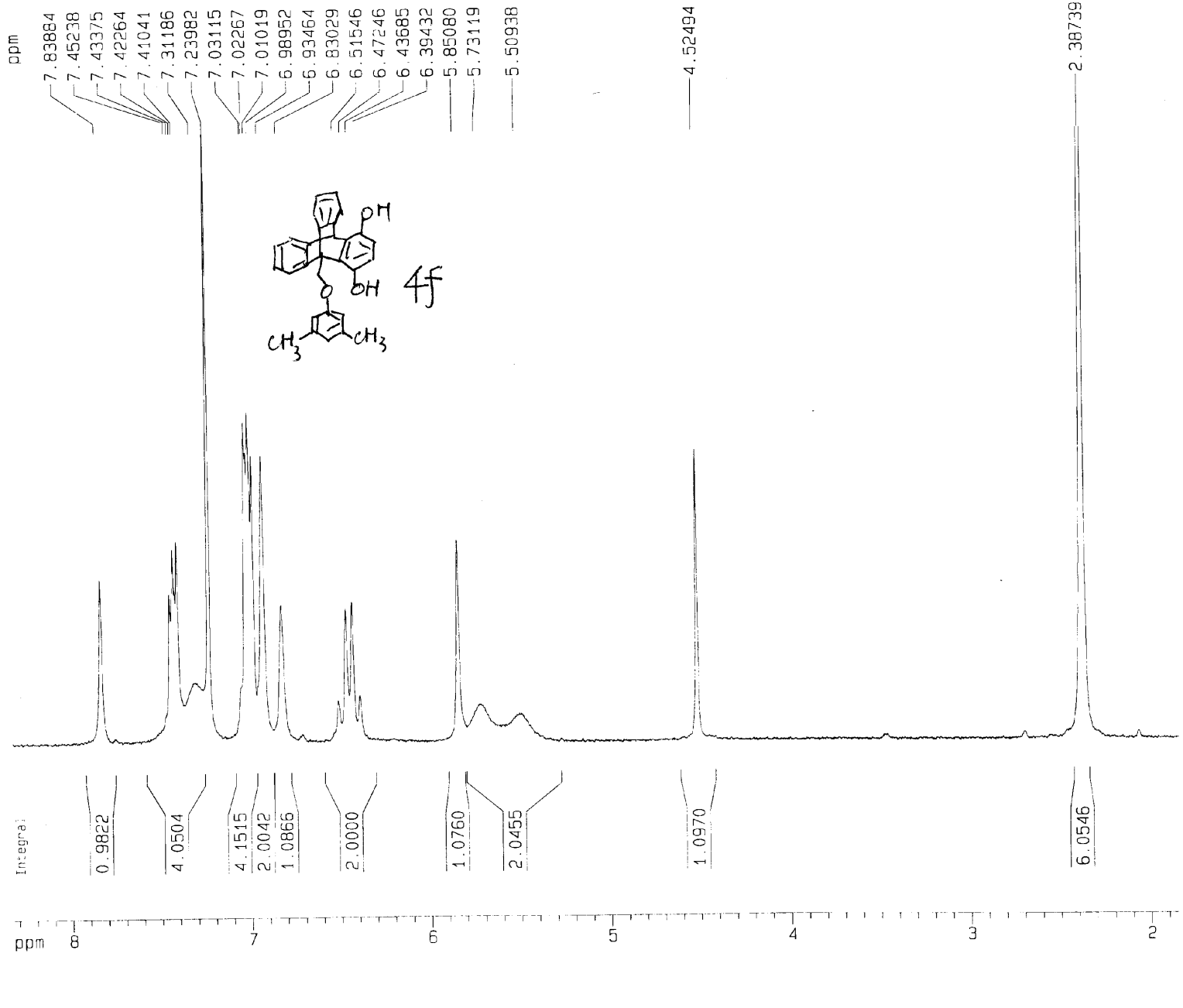


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| PROCNO | 1 |

F2 - Acquisition Parameters

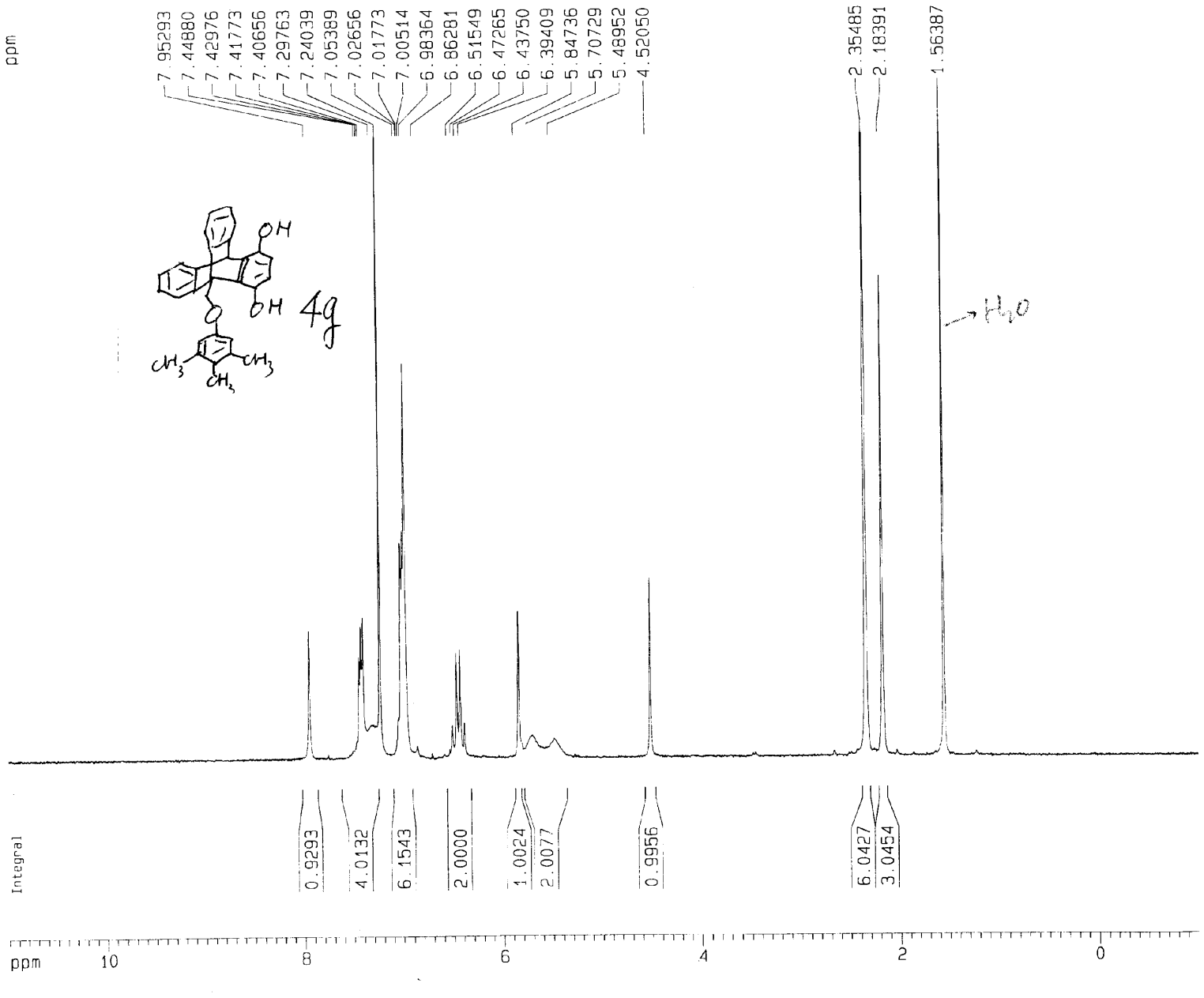
| | |
|---|---|
| Date_ | 20060525 |
| Time | 14.45 |
| INSTRUM | spect |
| PROBHD | 5 mm QNP 1H |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 32 |
| DS | 2 |
| SWH | 4111.842 Hz |
| FIDRES | 0.125483 Hz |
| AQ | 3.9846387 sec |
| RG | 8192 |
| DW | 121.600 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 6.30 usec |
| SFO1 | 200.1312359 MHz |
| NUC1 | 1H |
| PL1 | -6.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 200.1300131 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 8.333 ppm |
| F1 | 1667.63 Hz |
| F2P | 1.848 ppm |
| F2 | 369.93 Hz |
| PPMCM | 0.32421 ppm/cm |
| HZCM | 64.88506 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | trimephendiol3 |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

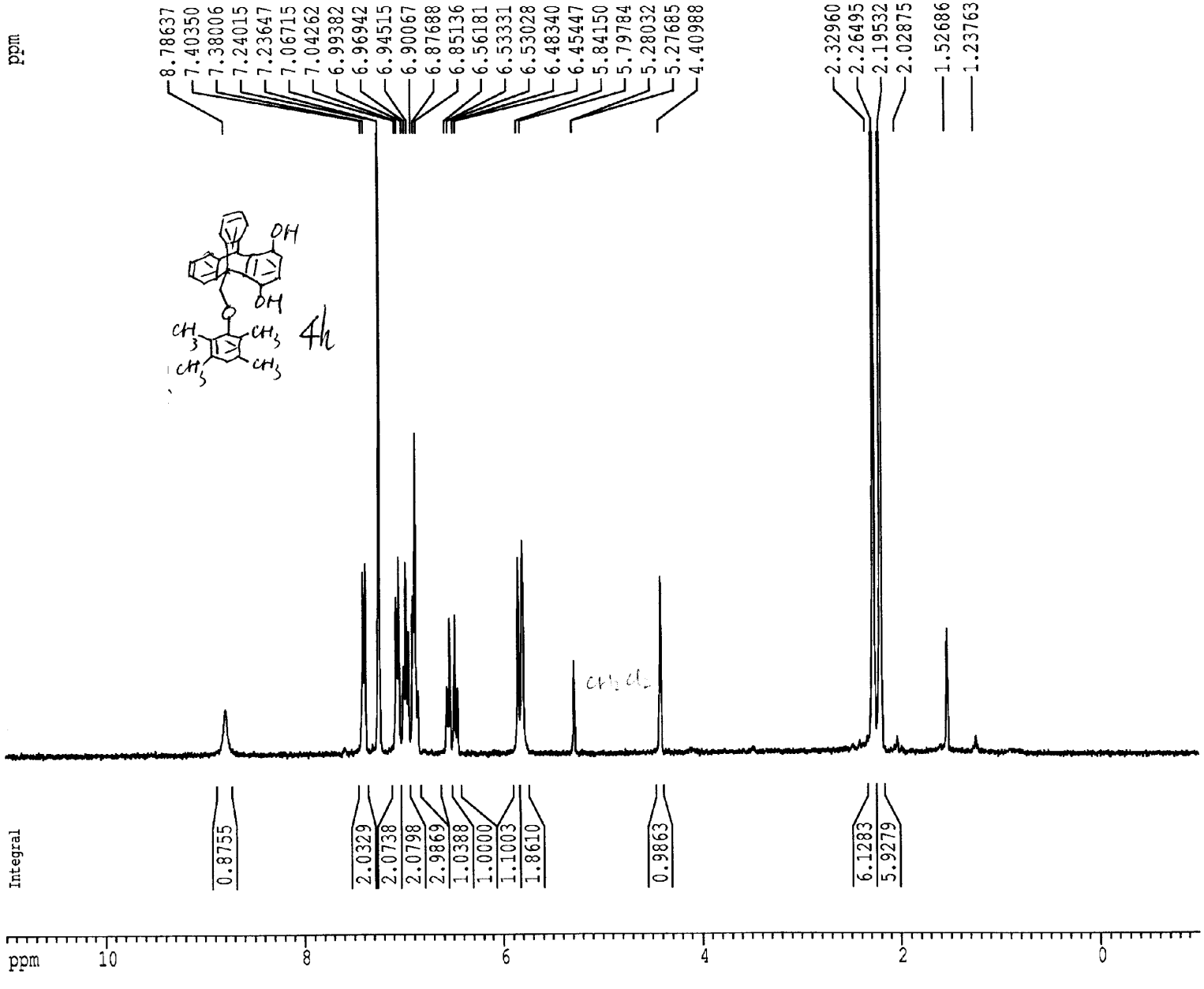
| | |
|---|---|
| Date_ | 20060525 |
| Time | 14.00 |
| INSTRUM | spect |
| PROBHD | 5 mm QNP 1H |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 32 |
| DS | 2 |
| SWH | 4111.842 Hz |
| FIDRES | 0.125483 Hz |
| AQ | 3.9846387 sec |
| RG | 8192 |
| DW | 121.600 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 6.30 usec |
| SFO1 | 200.1312359 MHz |
| NUC1 | 1H |
| PL1 | -6.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 200.1300128 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 2201.43 Hz |
| F2P | -1.000 ppm |
| F2 | -200.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 120.07801 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | tetramediol4 |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

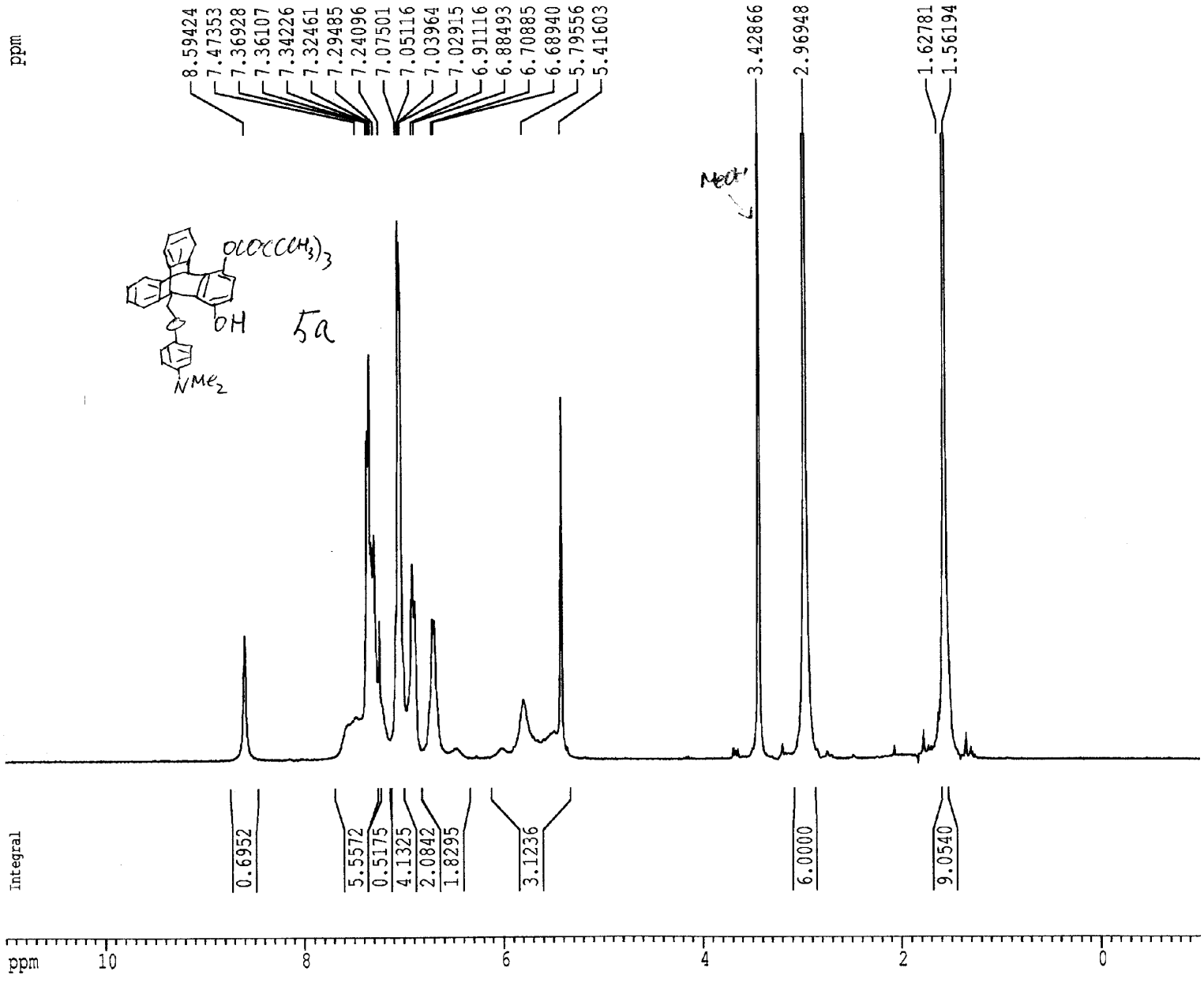
| | |
|---|---|
| Date_ | 20060525 |
| Time | 11.14 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 32 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 1290.2 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300125 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | dimentbu |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

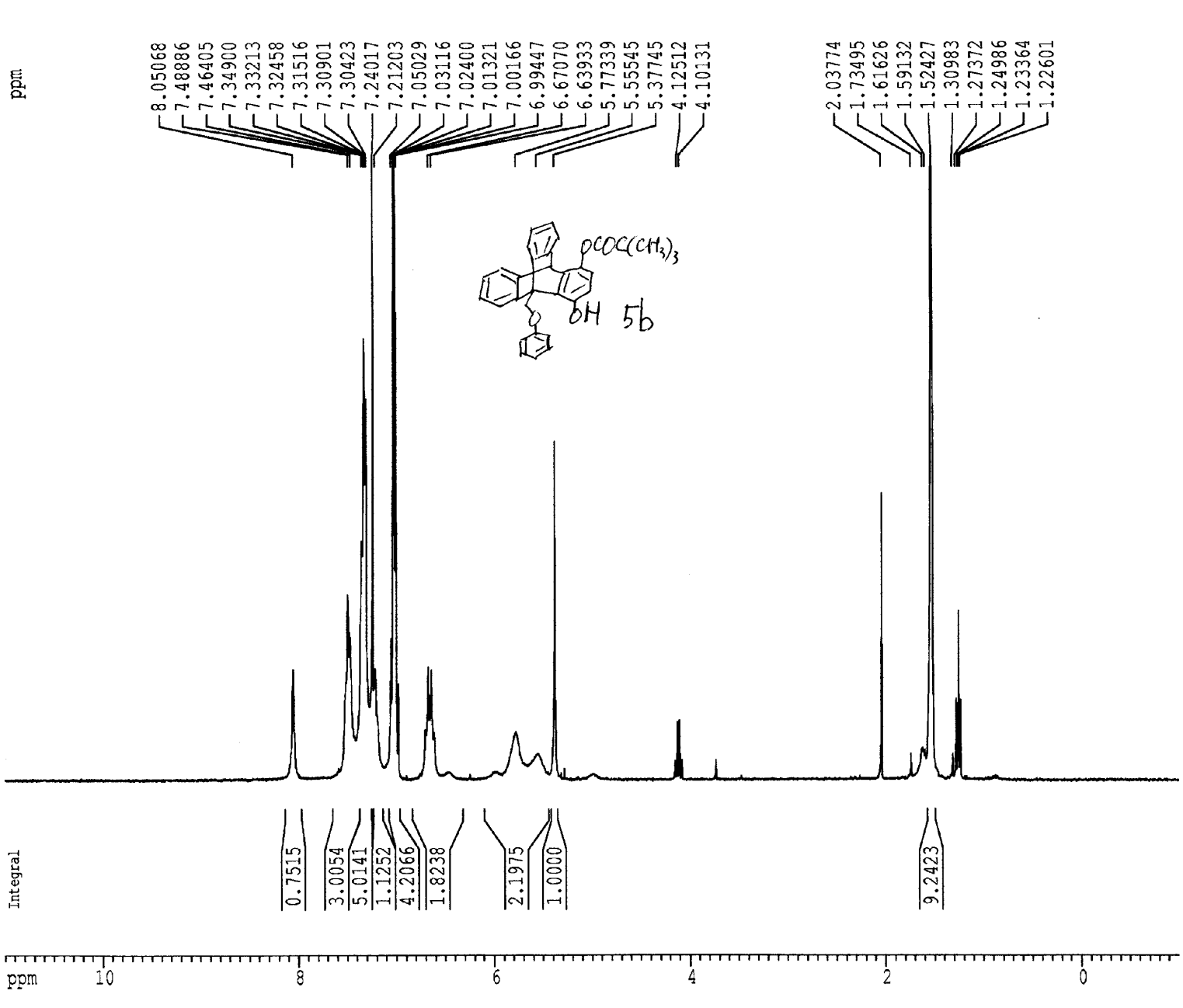
| | |
|---|---|
| Date_ | 20051226 |
| Time | 19.15 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 90.5 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300117 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | hphenoltbu6 |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

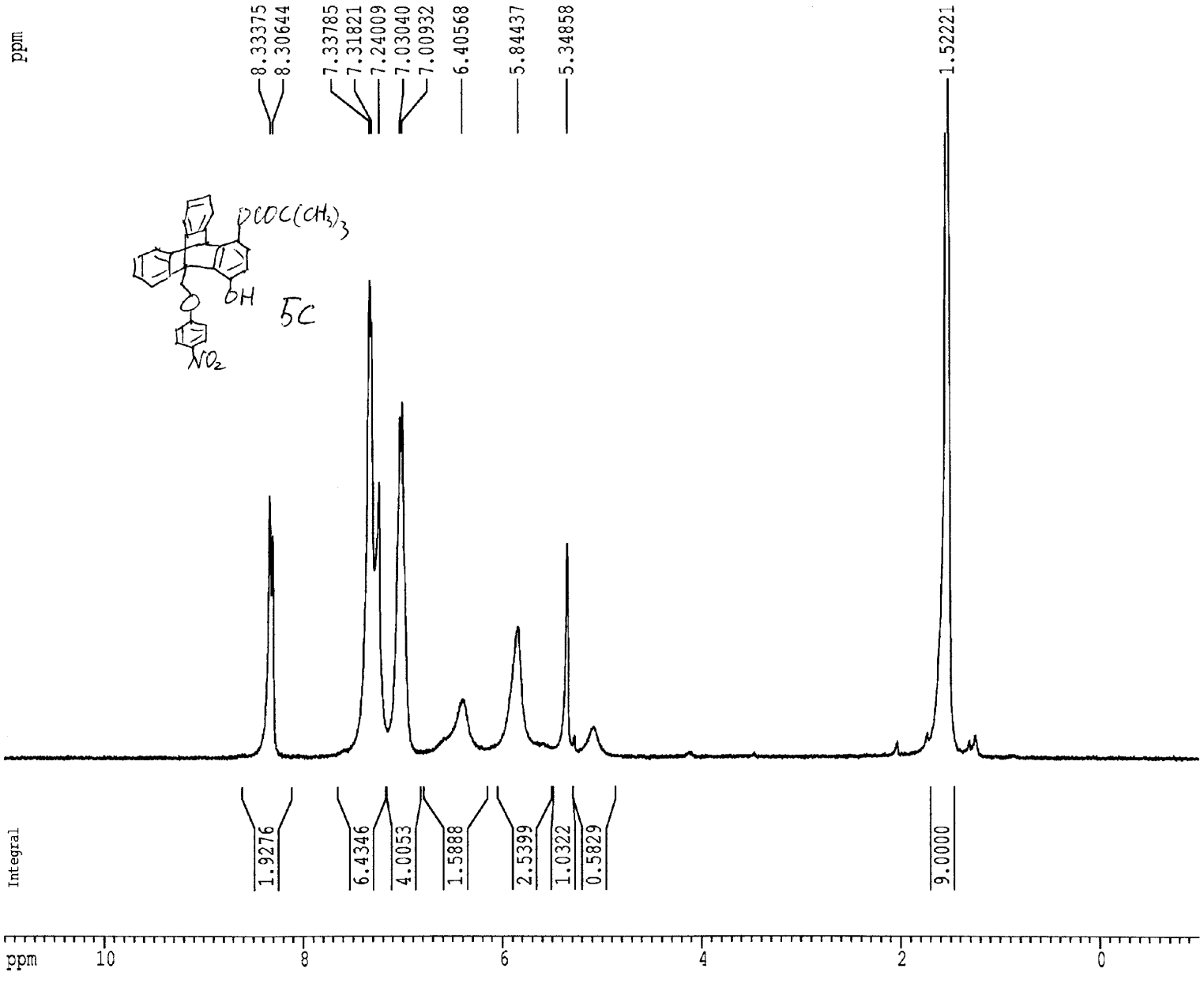
| | |
|---|---|
| Date_ | 20060102 |
| Time | 13.48 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 362 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300121 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | no2phenoltnu3 |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

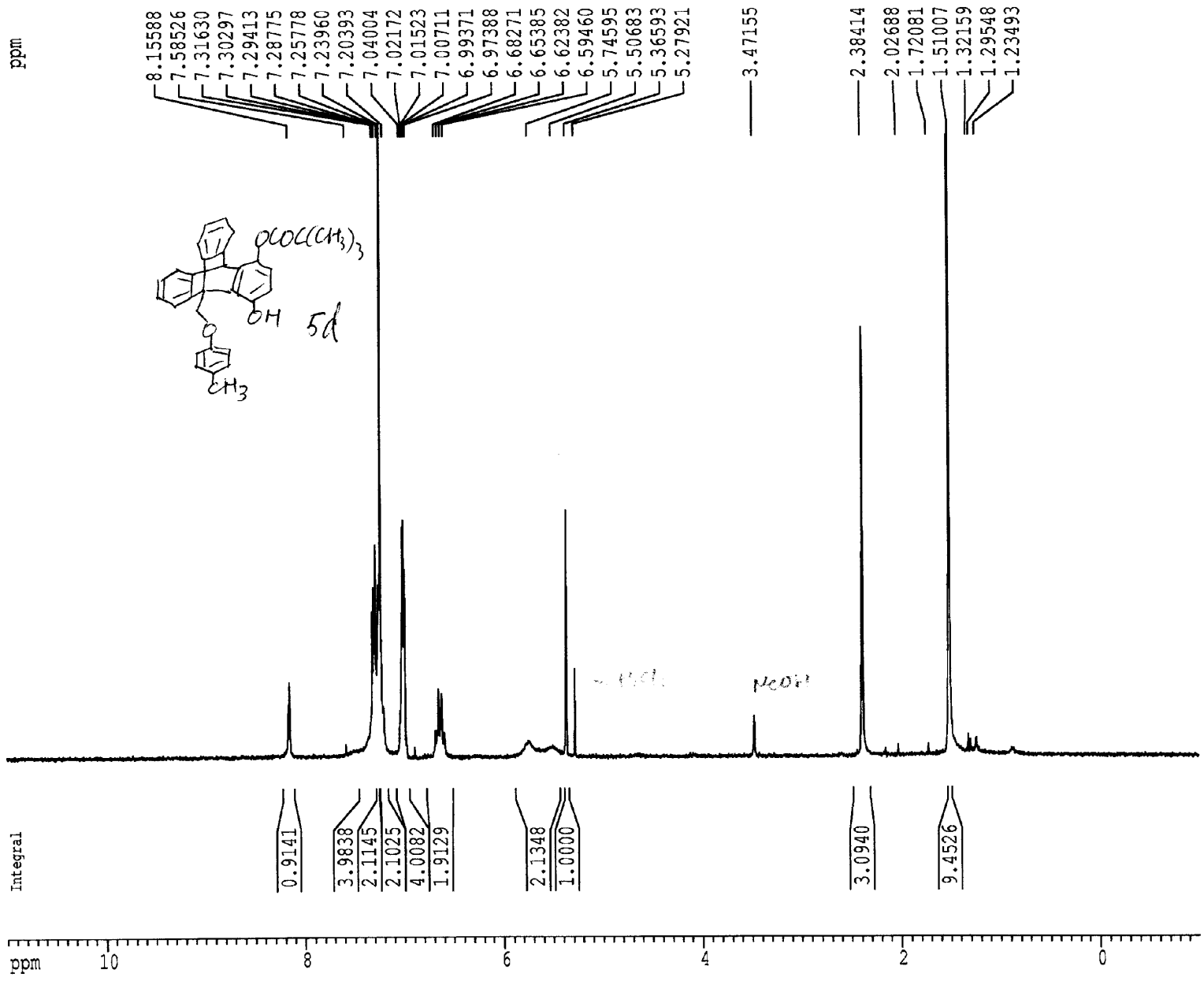
| | |
|---|---|
| Date_ | 20060103 |
| Time | 16.55 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 406.4 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300117 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | metriptbu2 |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

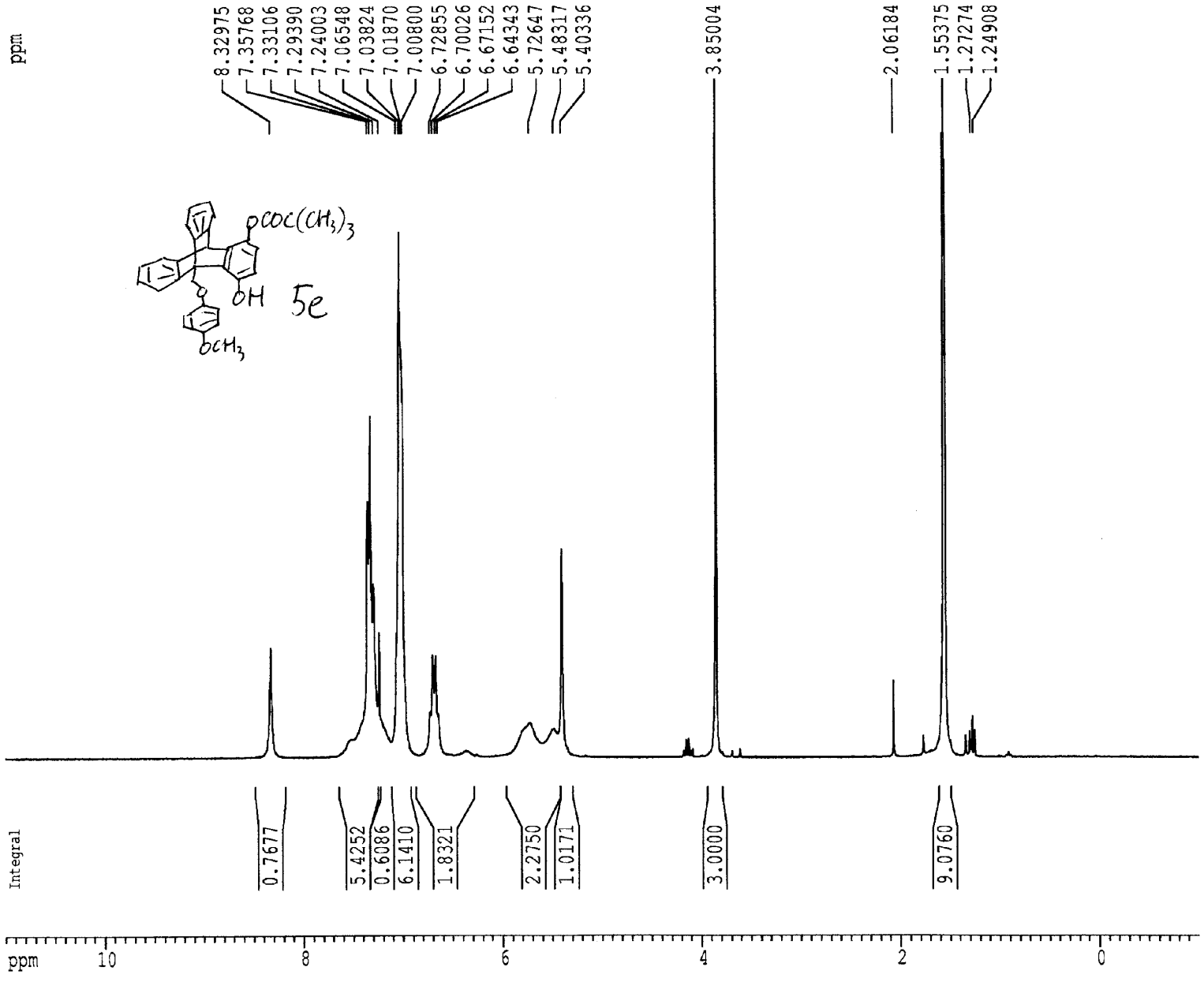
| | |
|---|---|
| Date_ | 20060525 |
| Time | 16.22 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 32 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 1448.2 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300125 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | dimeotbu |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

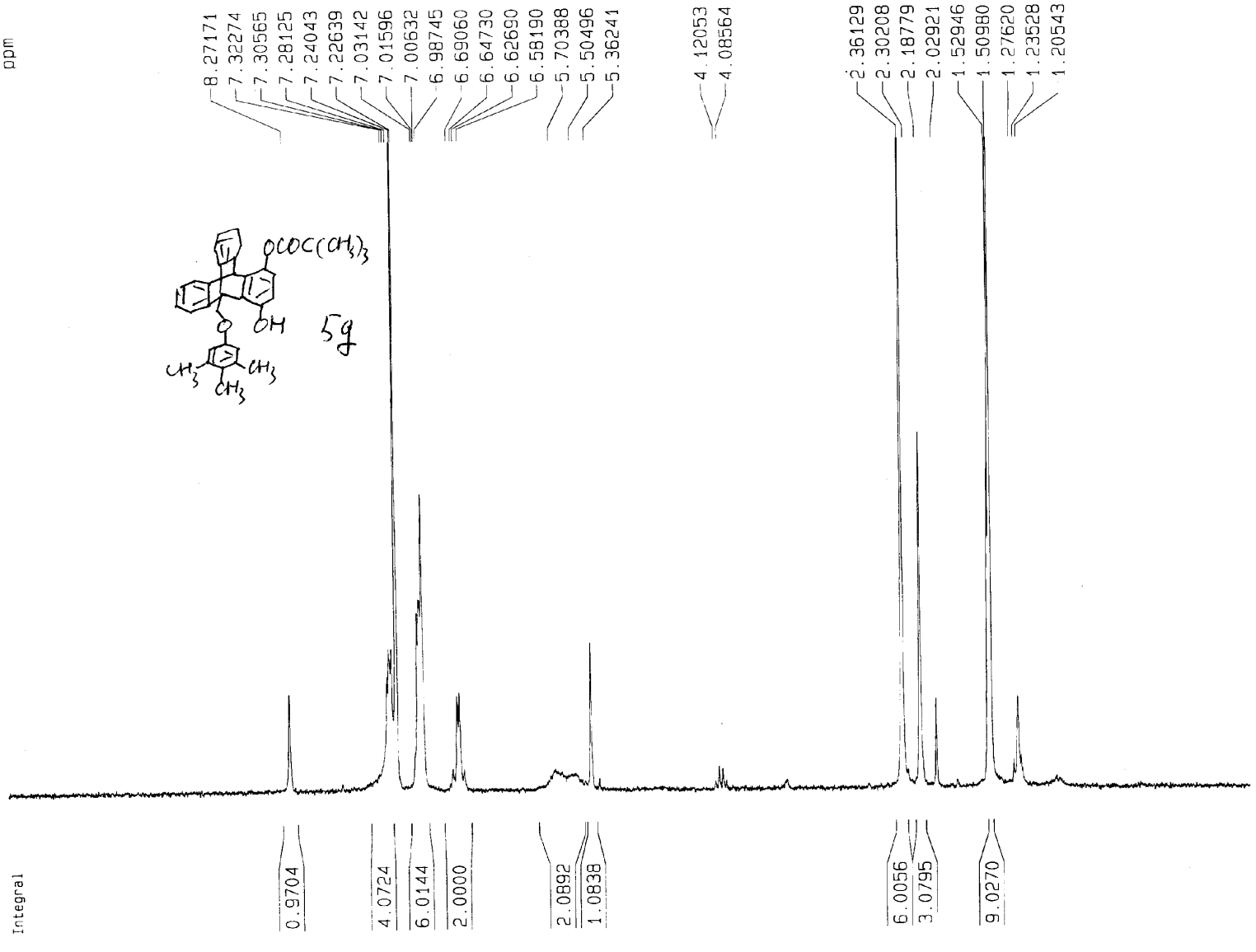
| | |
|---|---|
| Date_ | 20051226 |
| Time | 16.27 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 143.7 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300121 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | trimephenoltbu |
| EXPNO | 3 |
| PROCNO | 1 |

F2 - Acquisition Parameters

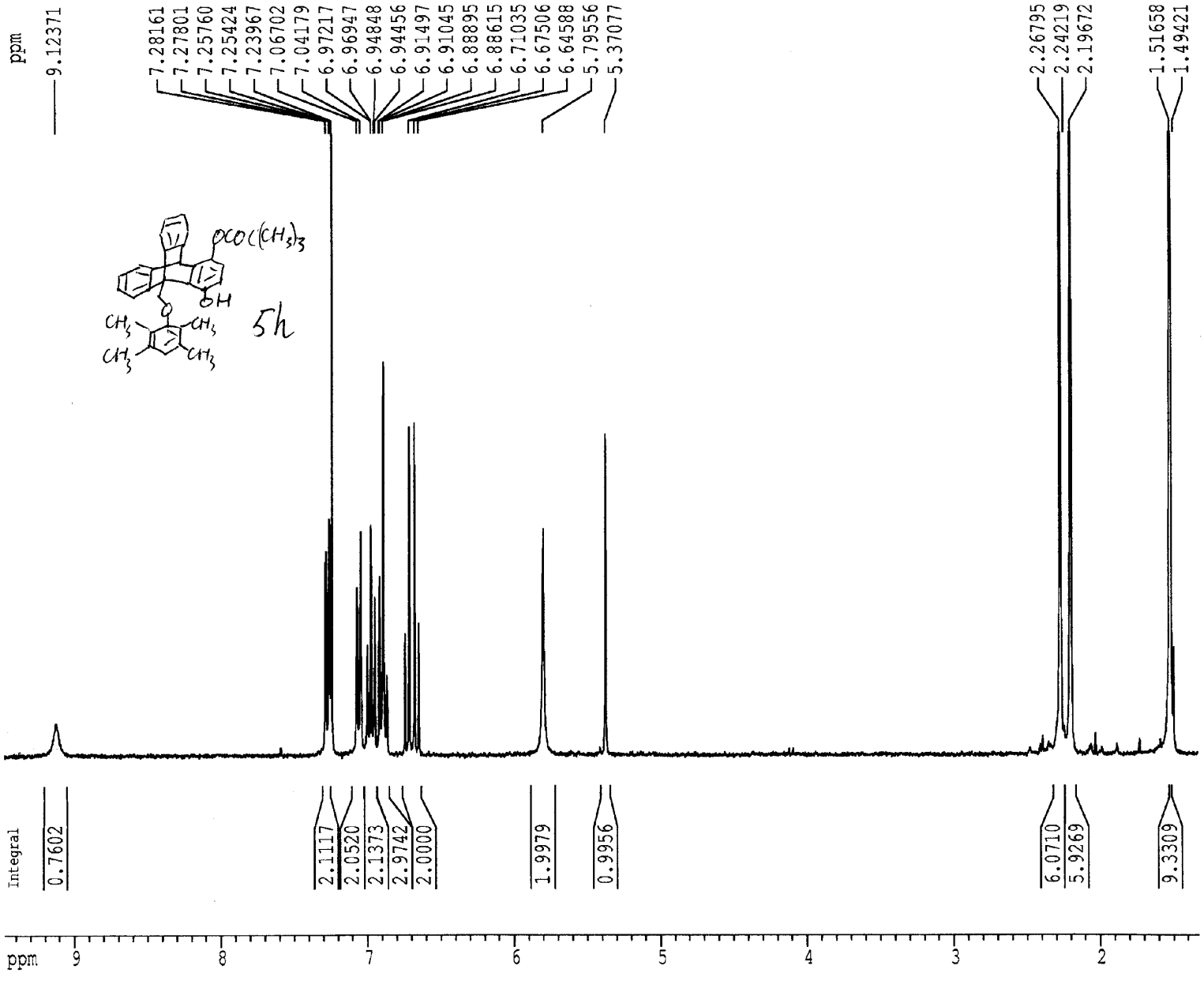
| | |
|---|---|
| Date_ | 20060526 |
| Time | 16.38 |
| INSTRUM | spect |
| PROBHD | 5 mm GNP 1H |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 32 |
| DS | 2 |
| SWH | 4111.842 Hz |
| FIDRES | 0.125483 Hz |
| AQ | 3.9846387 sec |
| RG | 13004 |
| DW | 121.600 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 6.30 usec |
| SFO1 | 200.1312359 MHz |
| NUC1 | 1H |
| PL1 | -6.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 200.1300126 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 2201.43 Hz |
| F2P | -1.000 ppm |
| F2 | -200.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 120.07801 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | tetrametbu |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

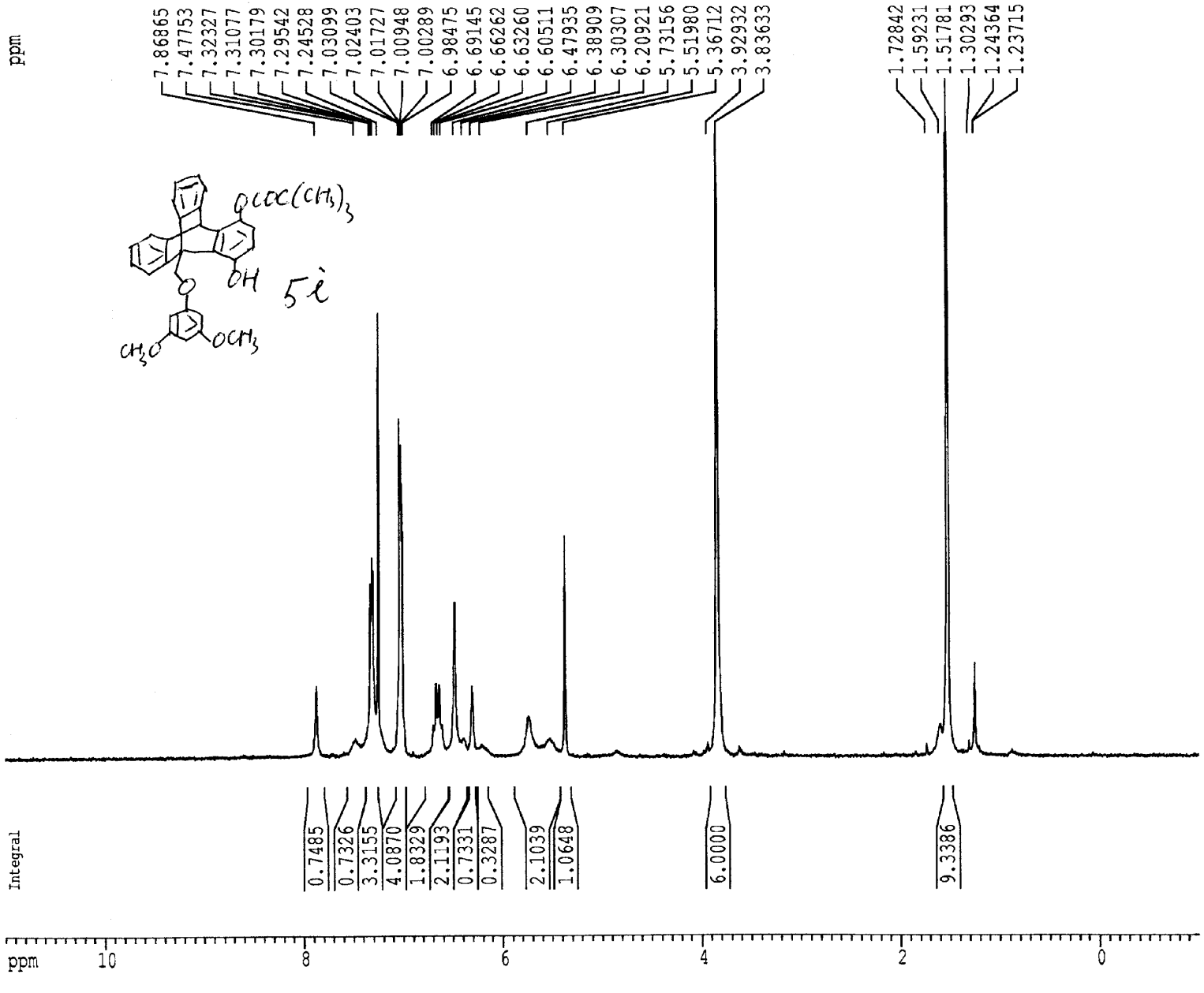
| | |
|---|---|
| Date_ | 20060310 |
| Time | 9.25 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 912.3 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300125 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 9.474 ppm |
| F1 | 2843.53 Hz |
| F2P | 1.326 ppm |
| F2 | 397.94 Hz |
| PPMCM | 0.40742 ppm/cm |
| HZCM | 122.27941 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | dimeotbuoh4 |
| EXPNO | 4 |
| PROCNO | 1 |

F2 - Acquisition Parameters

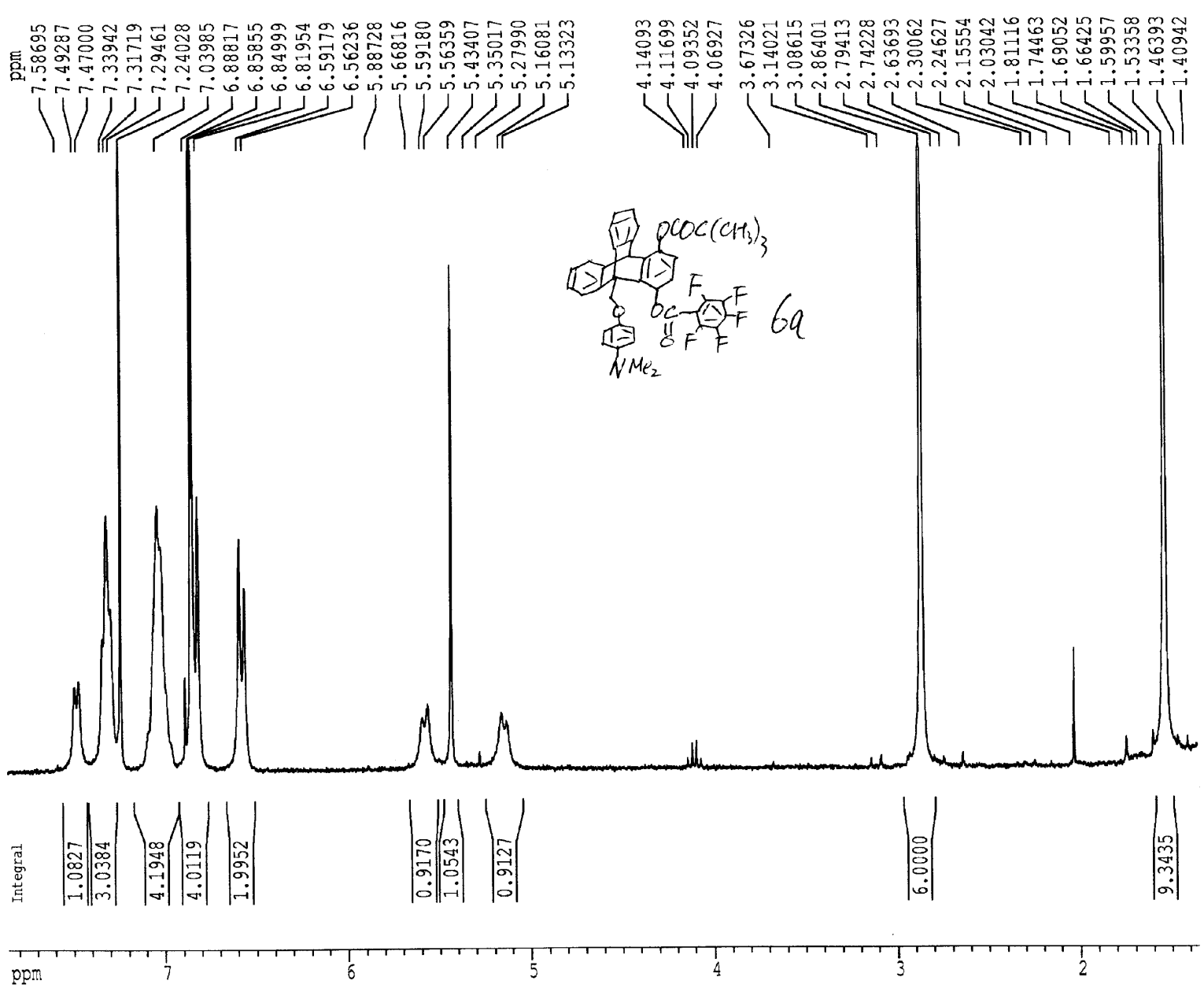
| | |
|---|---|
| Date_ | 20060105 |
| Time | 17.19 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 724.1 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300106 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |







6a

Current Data Parameters

| | |
|---|---|
| NAME | dimeamino5fben |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

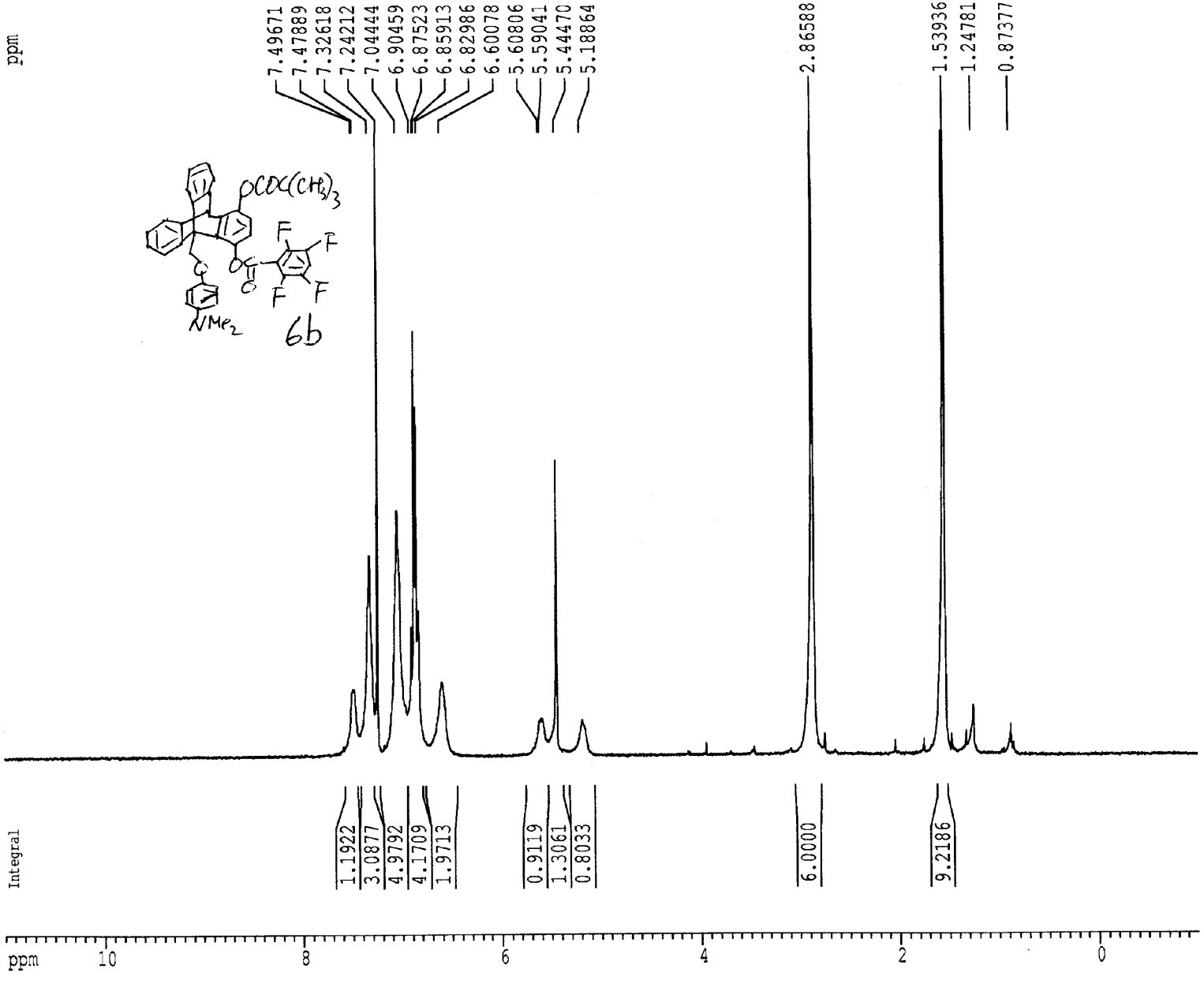
| | |
|---|---|
| Date_ | 20051122 |
| Time | 15.17 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 512 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300121 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 7.859 ppm |
| F1 | 2358.81 Hz |
| F2P | 1.354 ppm |
| F2 | 406.35 Hz |
| PPMCM | 0.32527 ppm/cm |
| HZCM | 97.62309 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | nmephenol4f2 |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

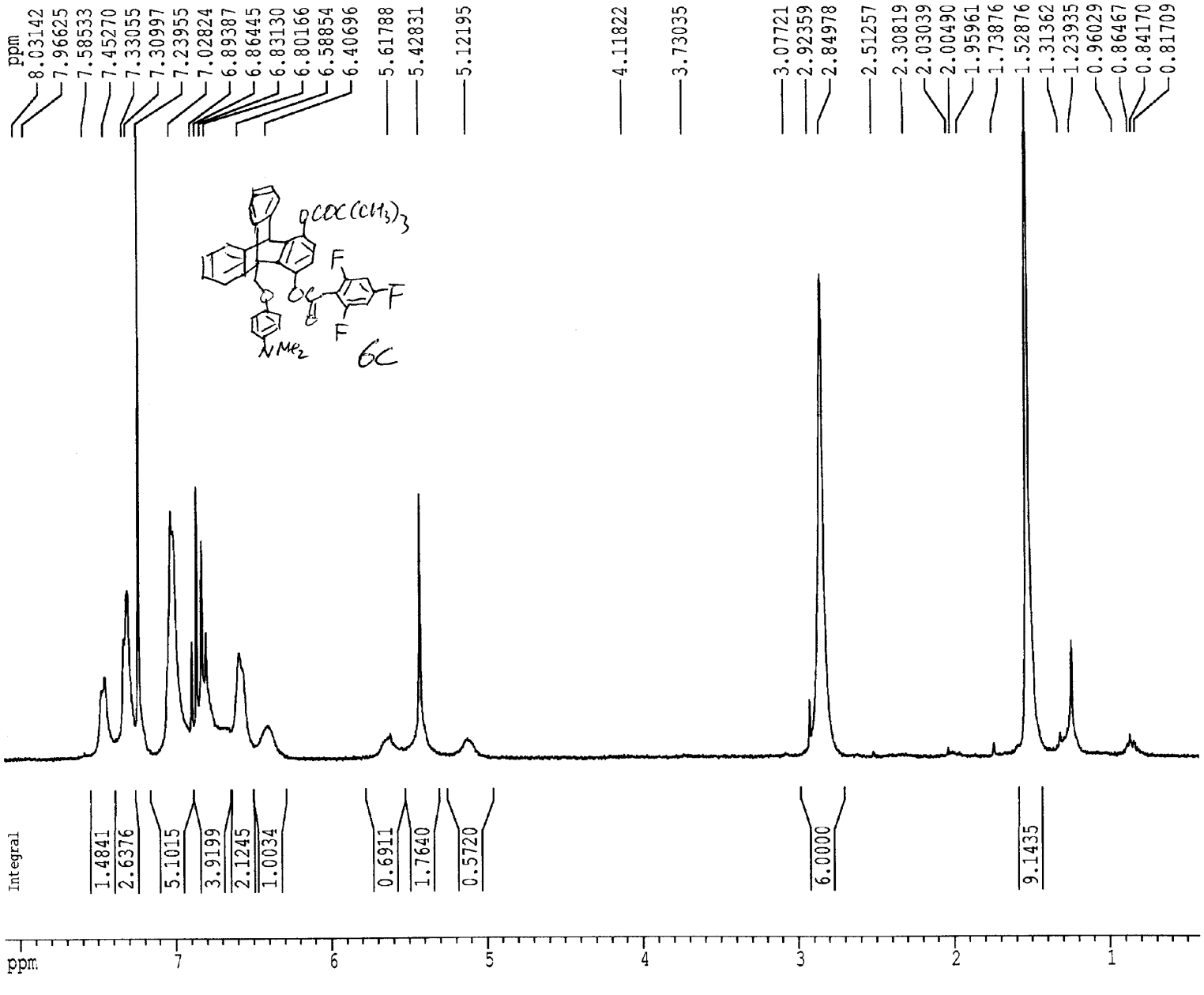
| | |
|---|---|
| Date_ | 20051214 |
| Time | 12.33 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 512 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300113 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | nme2f3 |
| EXPNO | 2 |
| PROCNO | 1 |

F2 - Acquisition Parameters

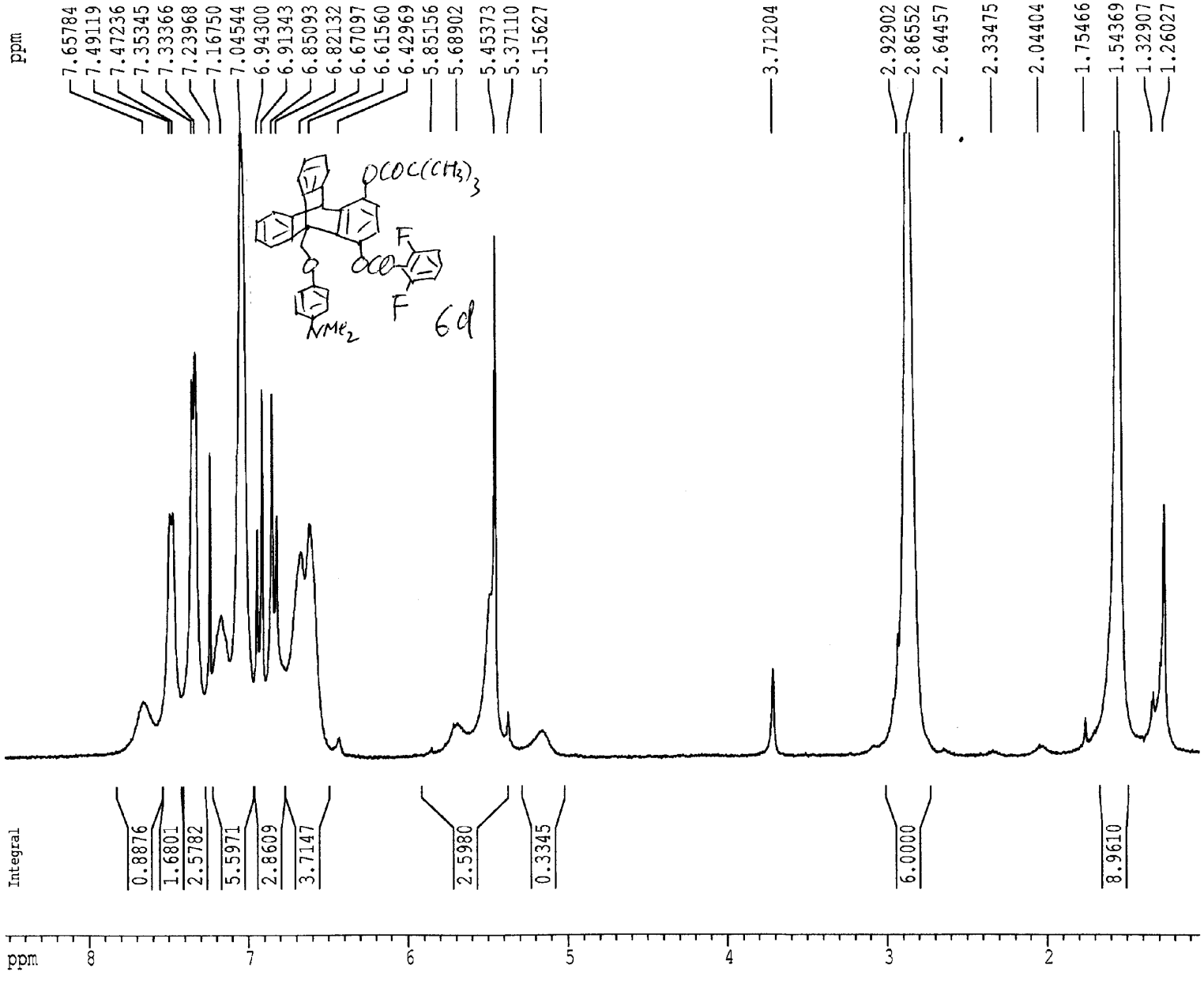
| | |
|---|---|
| Date_ | 20051208 |
| Time | 15.25 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 645.1 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300129 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 8.099 ppm |
| F1 | 2430.66 Hz |
| F2P | 0.422 ppm |
| F2 | 126.51 Hz |
| PPMCM | 0.38386 ppm/cm |
| HZCM | 115.20766 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | nme2phe2f |
| EXPNO | 2 |
| PROCNO | 1 |

F2 - Acquisition Parameters

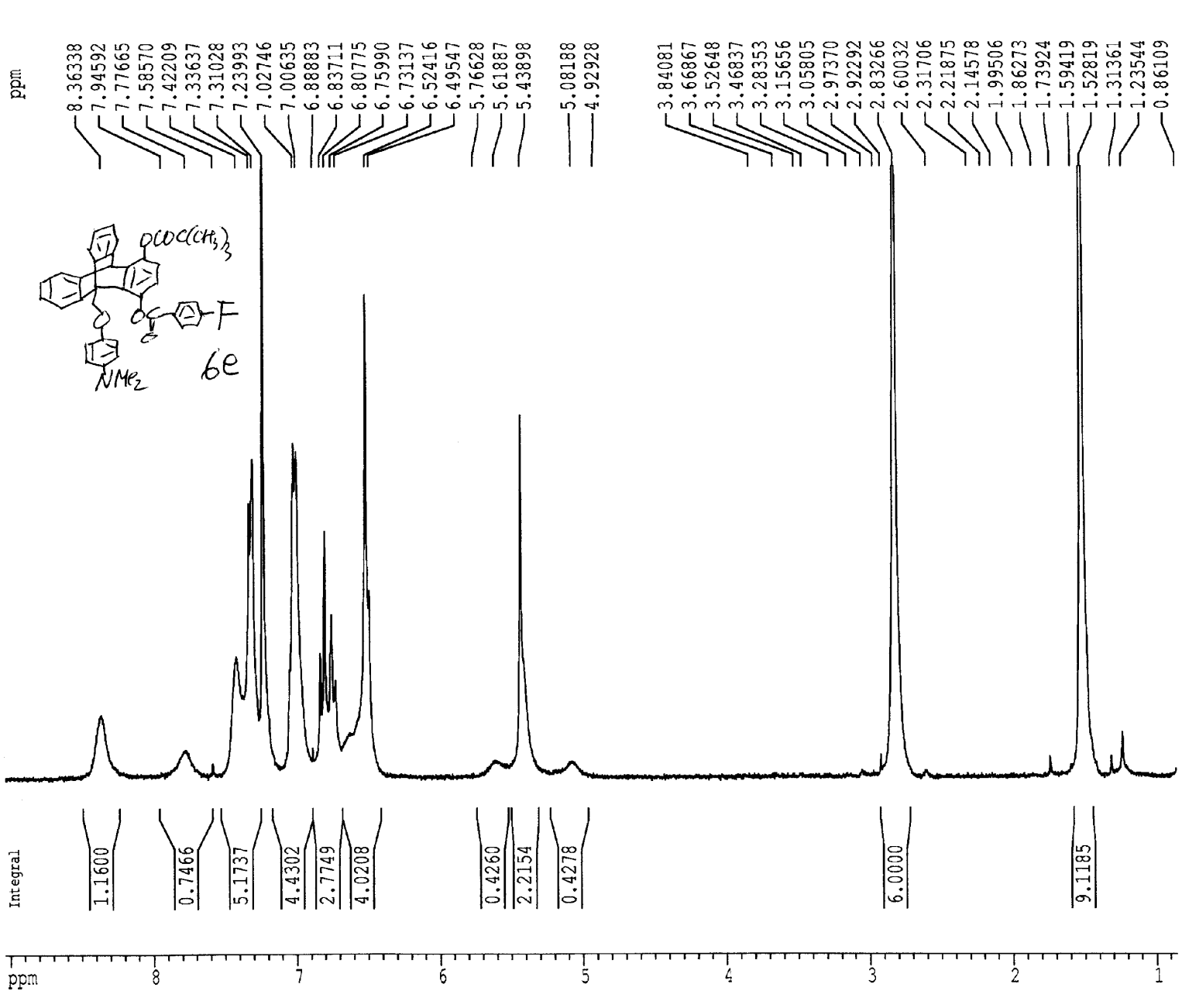
| | |
|---|---|
| Date_ | 20051209 |
| Time | 15.30 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 256 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300121 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 8.525 ppm |
| F1 | 2558.49 Hz |
| F2P | 1.042 ppm |
| F2 | 312.63 Hz |
| PPMCM | 0.37415 ppm/cm |
| HZCM | 112.29282 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | nme2f |
| EXPNO | 2 |
| PROCNO | 1 |

F2 - Acquisition Parameters

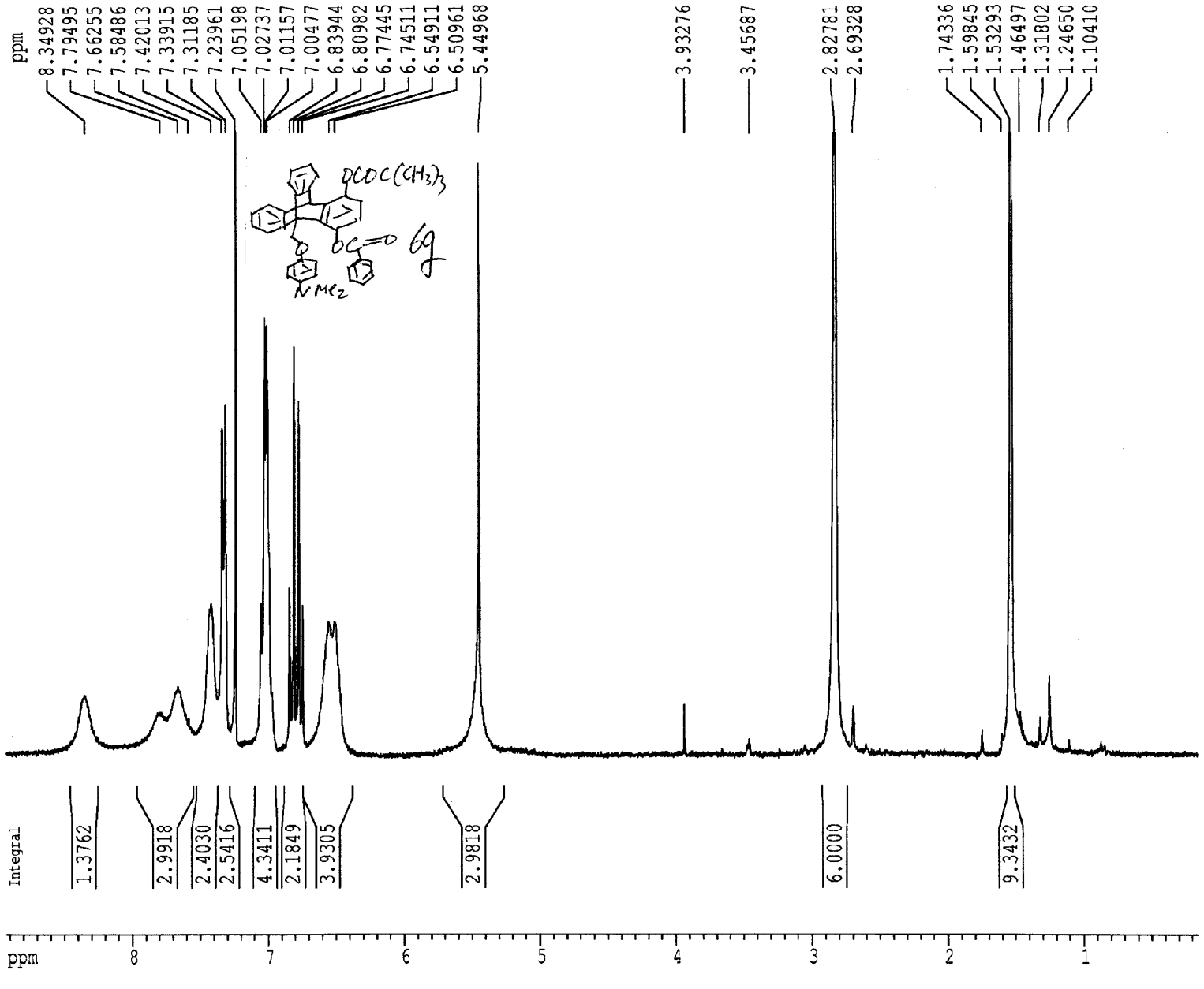
| | |
|---|---|
| Date_ | 20051208 |
| Time | 15.46 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 64 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 1024 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300125 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 9.036 ppm |
| F1 | 2712.03 Hz |
| F2P | 0.860 ppm |
| F2 | 258.01 Hz |
| PPMCM | 0.40883 ppm/cm |
| HZCM | 122.70084 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | nme-hben_20 |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

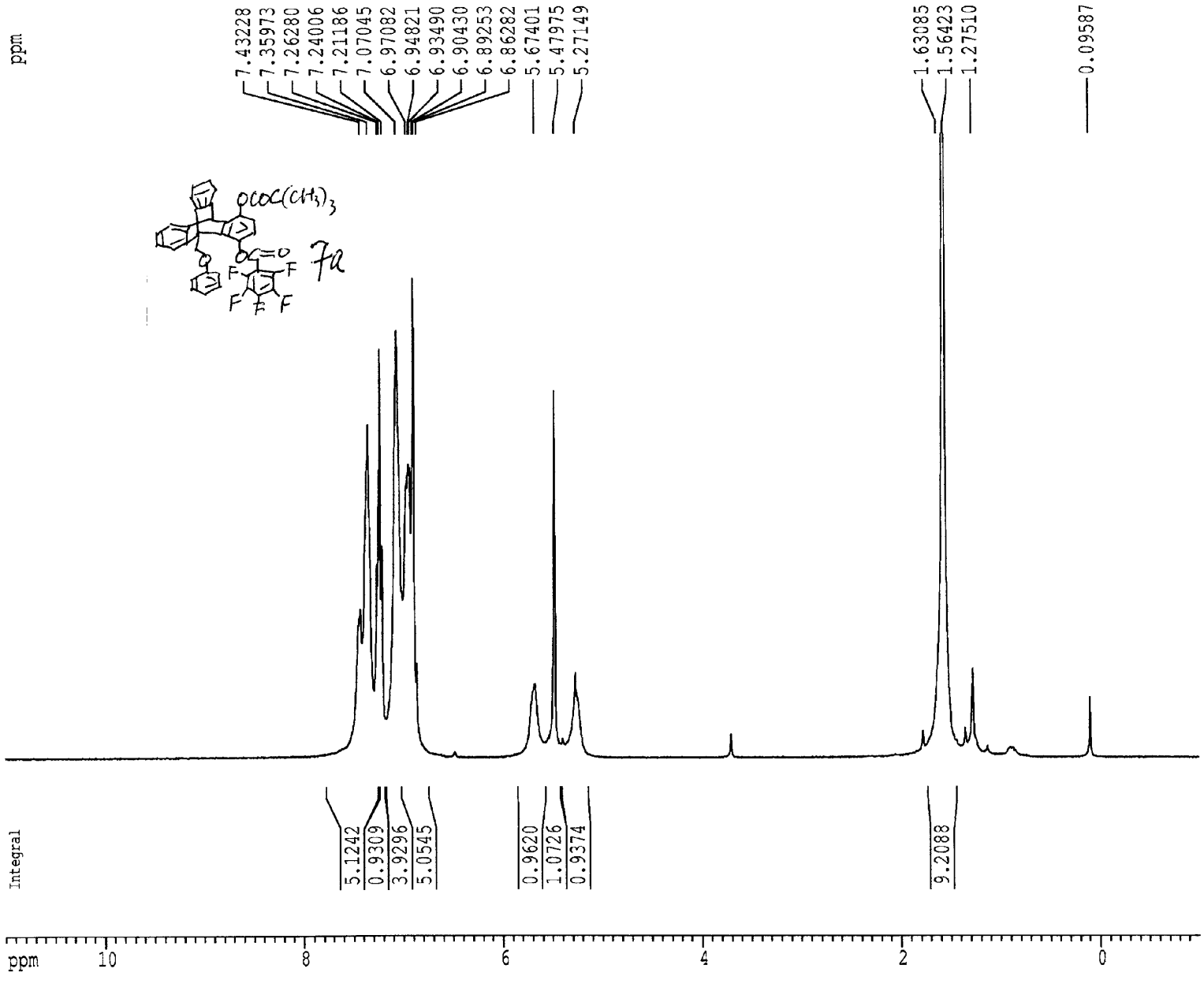
| | |
|---|---|
| Date_ | 20051209 |
| Time | 18.48 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 812.7 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300125 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 8.932 ppm |
| F1 | 2680.81 Hz |
| F2P | 0.152 ppm |
| F2 | 45.71 Hz |
| PPMCM | 0.43899 ppm/cm |
| HZCM | 131.75510 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | phenol5f3 |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

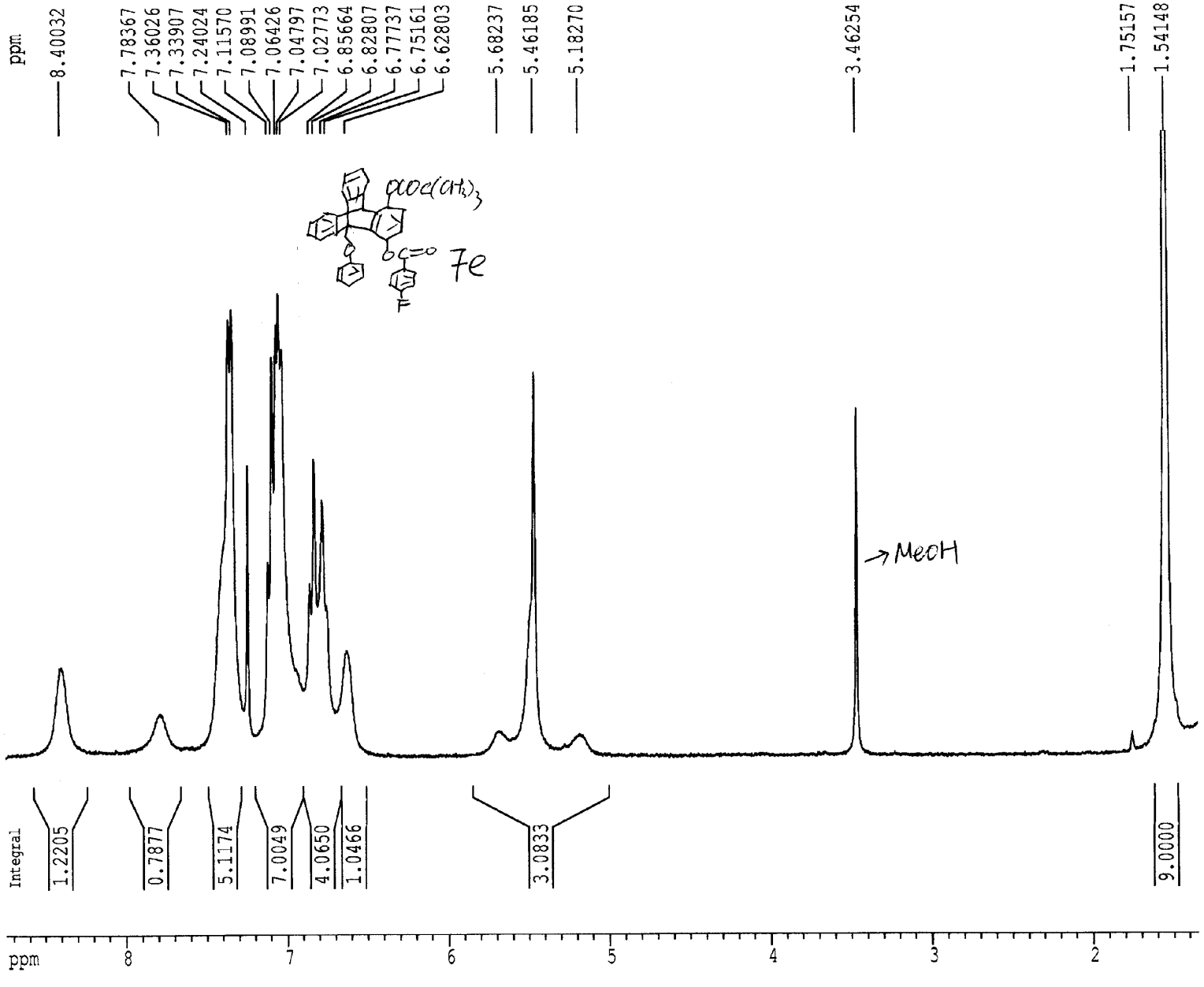
| | |
|---|---|
| Date_ | 20060605 |
| Time | 15.30 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 25 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 203.2 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300117 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | hphenoltripf |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

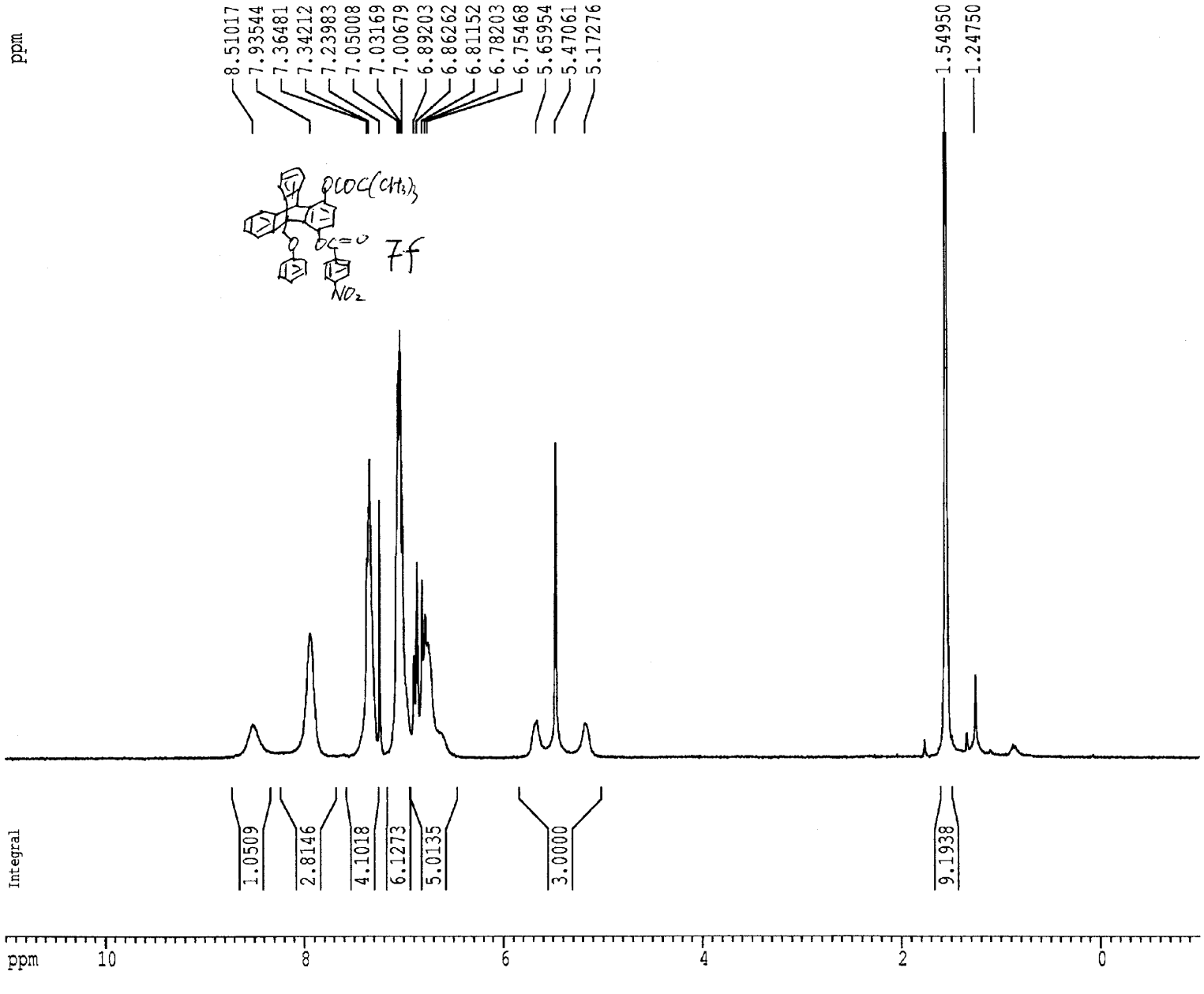
| | |
|---|---|
| Date_ | 20051231 |
| Time | 11.42 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 362 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300121 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 8.744 ppm |
| F1 | 2624.37 Hz |
| F2P | 1.347 ppm |
| F2 | 404.37 Hz |
| PPMCM | 0.36984 ppm/cm |
| HZCM | 110.99999 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | hphenolnitro |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

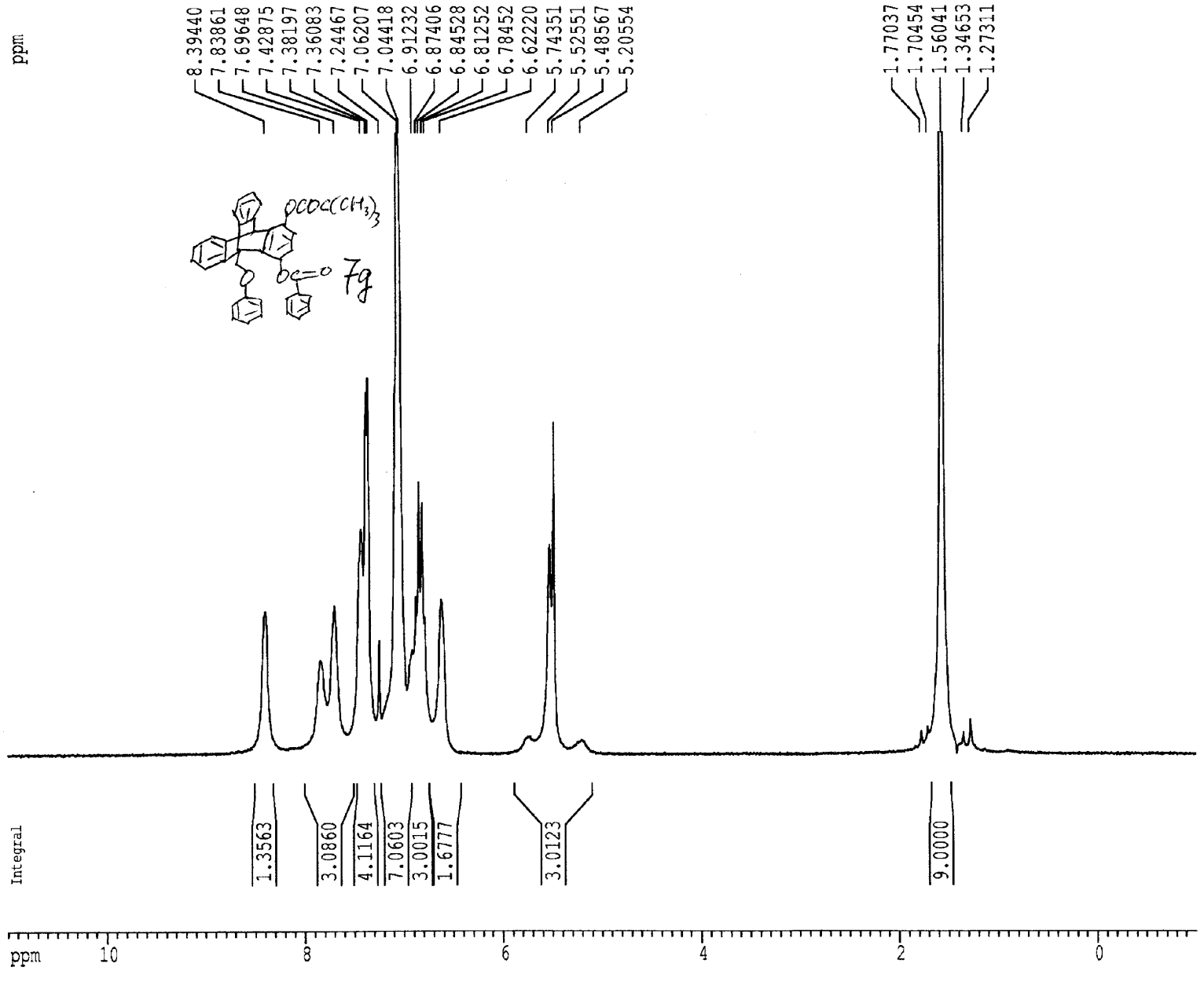
| | |
|---|---|
| Date_ | 20051226 |
| Time | 10.27 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 362 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300125 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | hphenolh |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

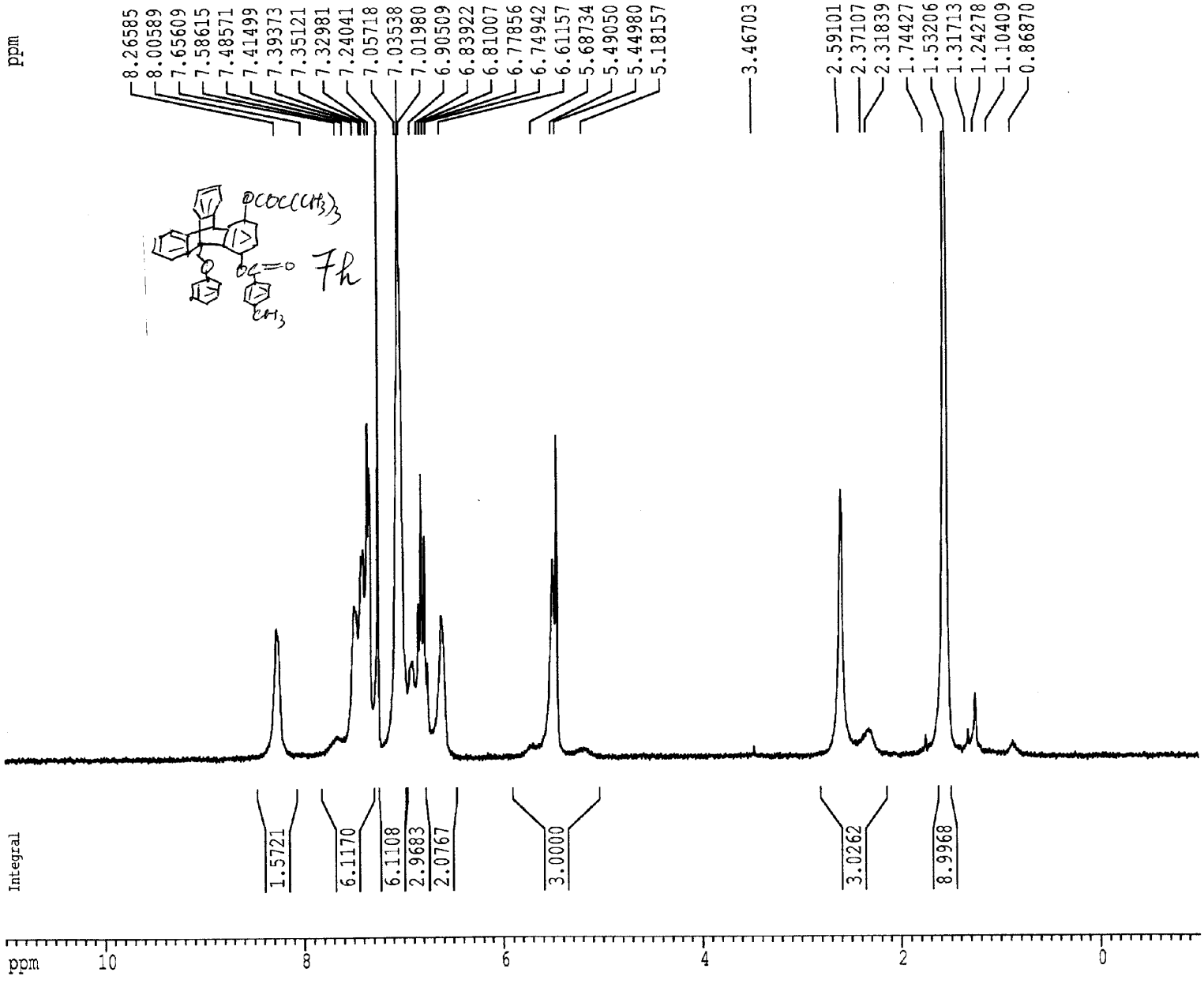
| | |
|---|---|
| Date_ | 20051225 |
| Time | 12.03 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 203.2 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300110 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | phenoltripme |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

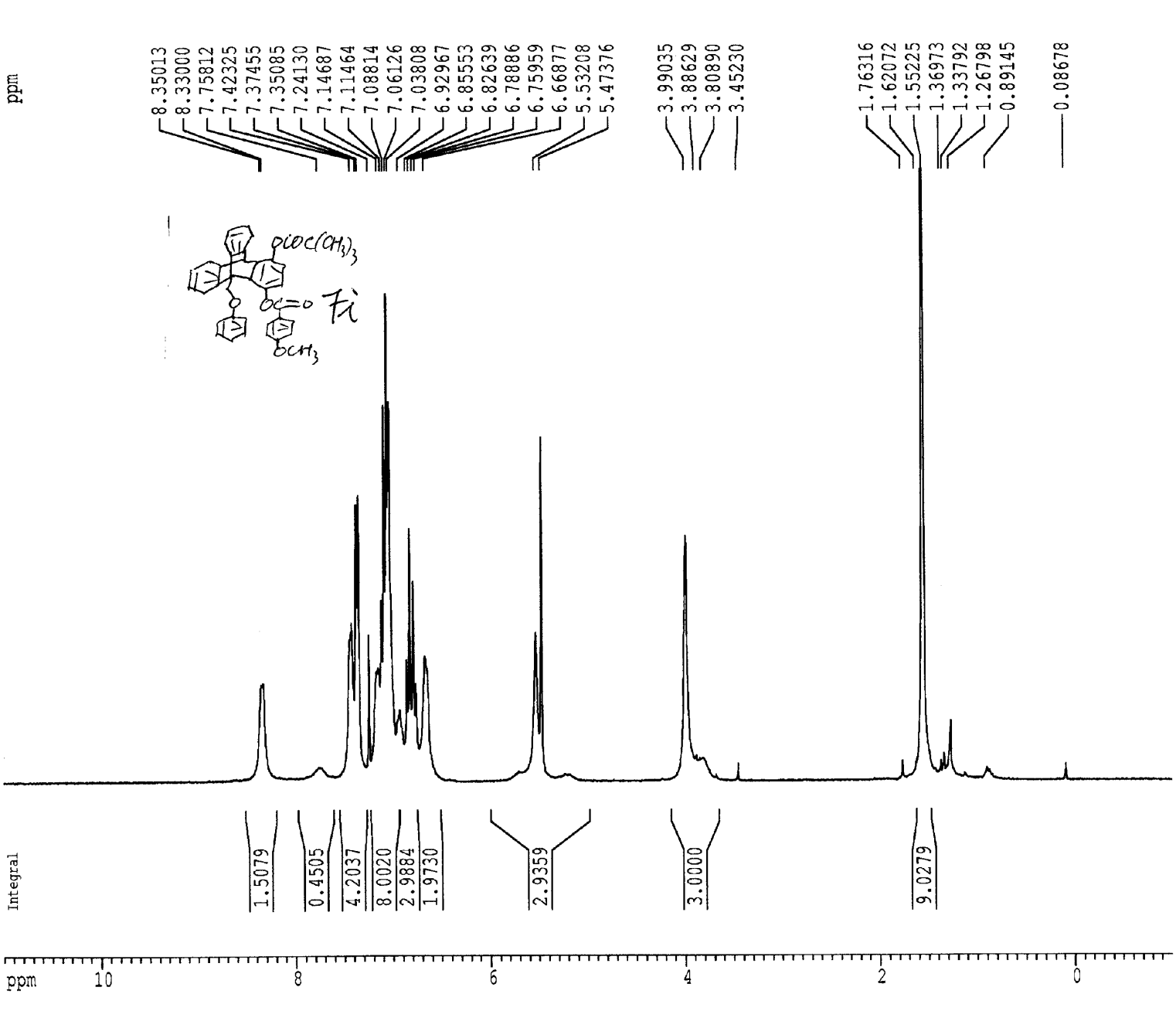
| | |
|---|---|
| Date_ | 20051227 |
| Time | 15.46 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 32 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 812.7 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300113 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | hphenolmeo |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

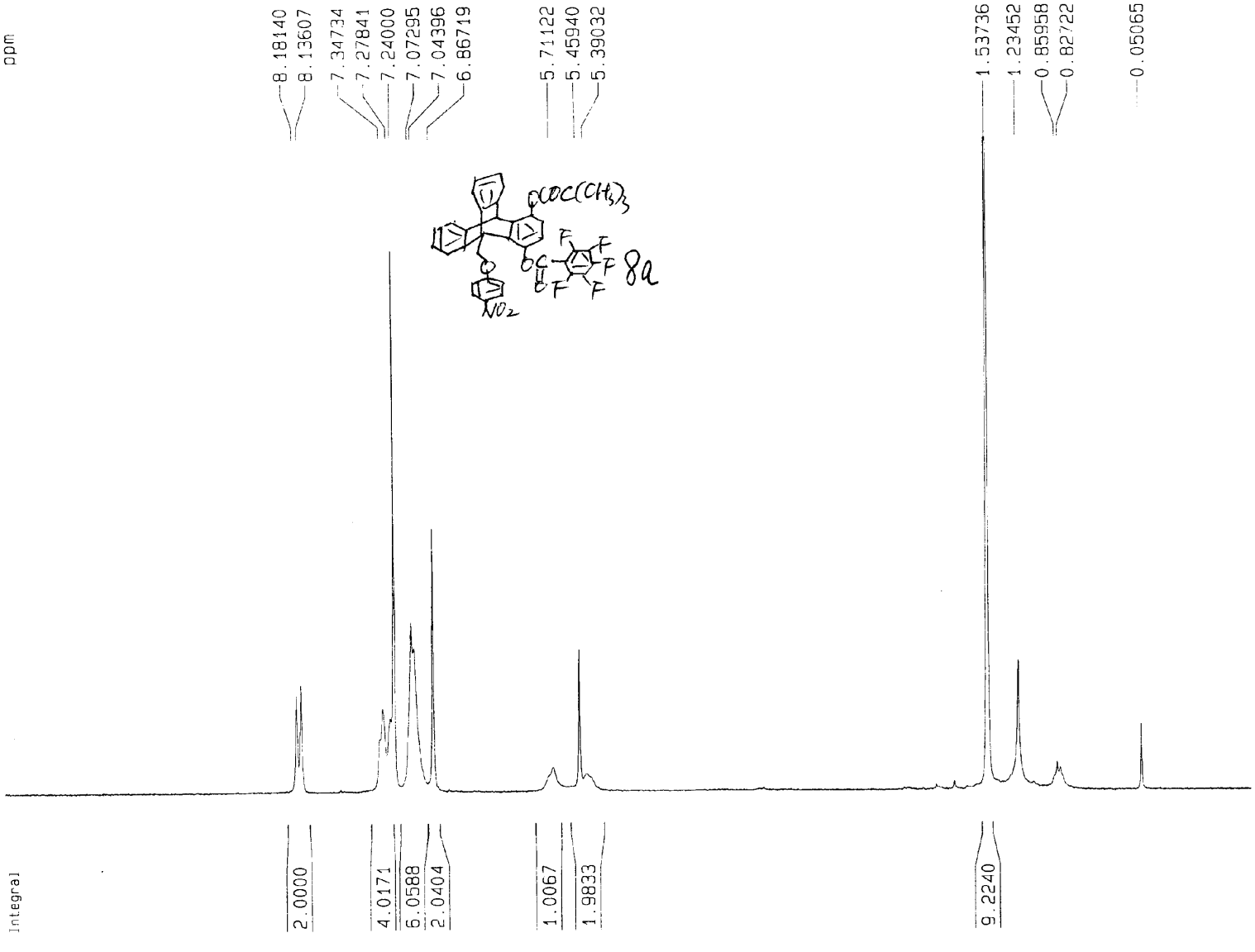
| | |
|---|---|
| Date_ | 20051227 |
| Time | 21.39 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 228.1 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300117 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | nitrophenoSf |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

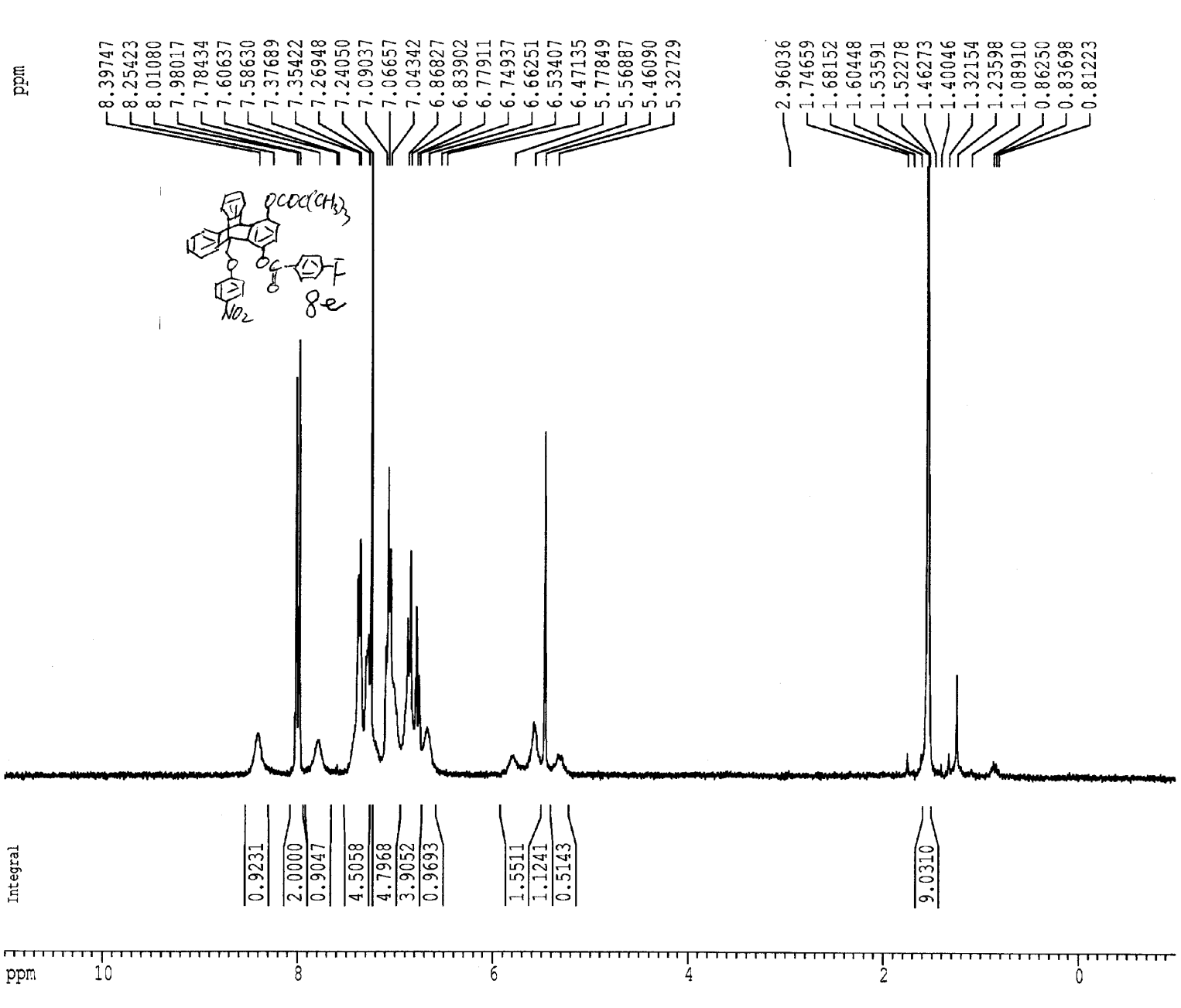
| | |
|---|---|
| Date_ | 20060524 |
| Time | 9.38 |
| INSTRUM | spect |
| PROBHD | 5 mm QNP 1H |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 64 |
| DS | 2 |
| SWH | 4111.842 Hz |
| FIDRES | 0.125483 Hz |
| AQ | 3.9846387 sec |
| RG | 8192 |
| DW | 121.600 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 6.30 usec |
| SFO1 | 200.1312359 MHz |
| NUC1 | 1H |
| PL1 | -6.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 200.1300128 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 2201.43 Hz |
| F2P | -1.000 ppm |
| F2 | -200.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 120.07801 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | nitrophenolf |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

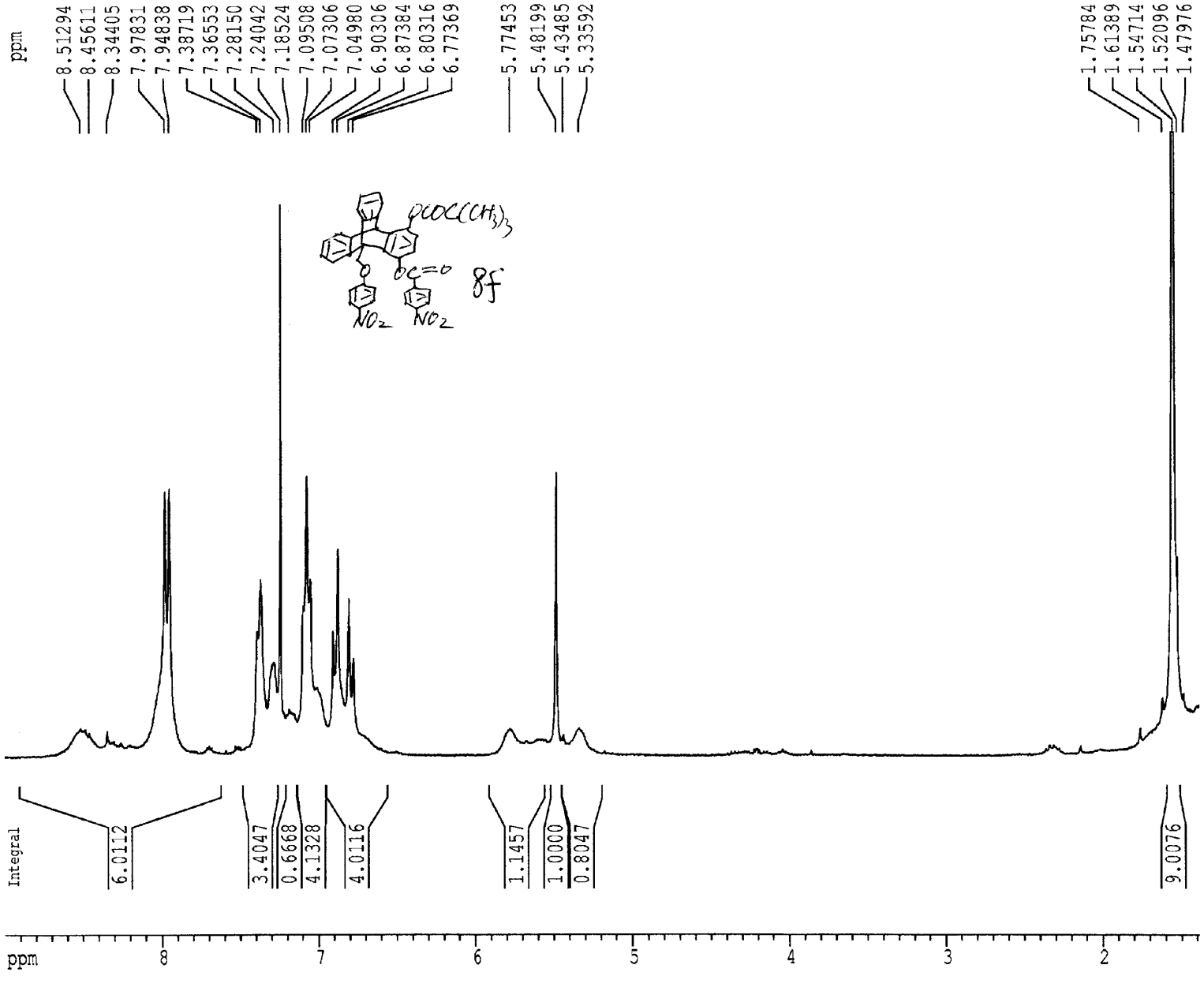
| | |
|---|---|
| Date_ | 20051114 |
| Time | 14.58 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 1024 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300121 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | nitrophenolno2 |
| EXPNO | 4 |
| PROCNO | 1 |

F2 - Acquisition Parameters

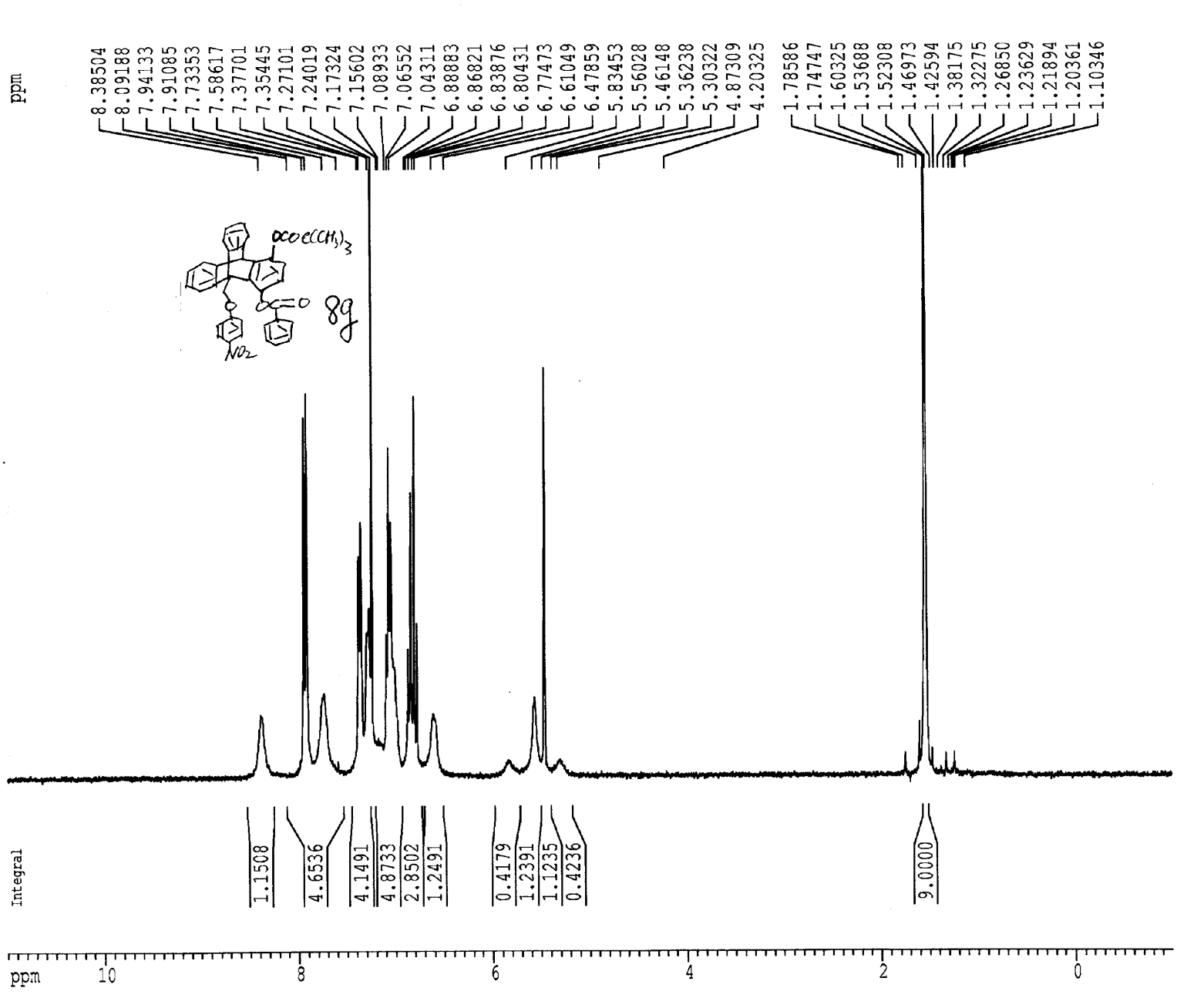
| | |
|---|---|
| Date_ | 20060605 |
| Time | 20.40 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 64 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 362 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300121 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 8.998 ppm |
| F1 | 2700.46 Hz |
| F2P | 1.385 ppm |
| F2 | 415.72 Hz |
| PPMCM | 0.38062 ppm/cm |
| HZCM | 114.23696 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | nitrophenol-h |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

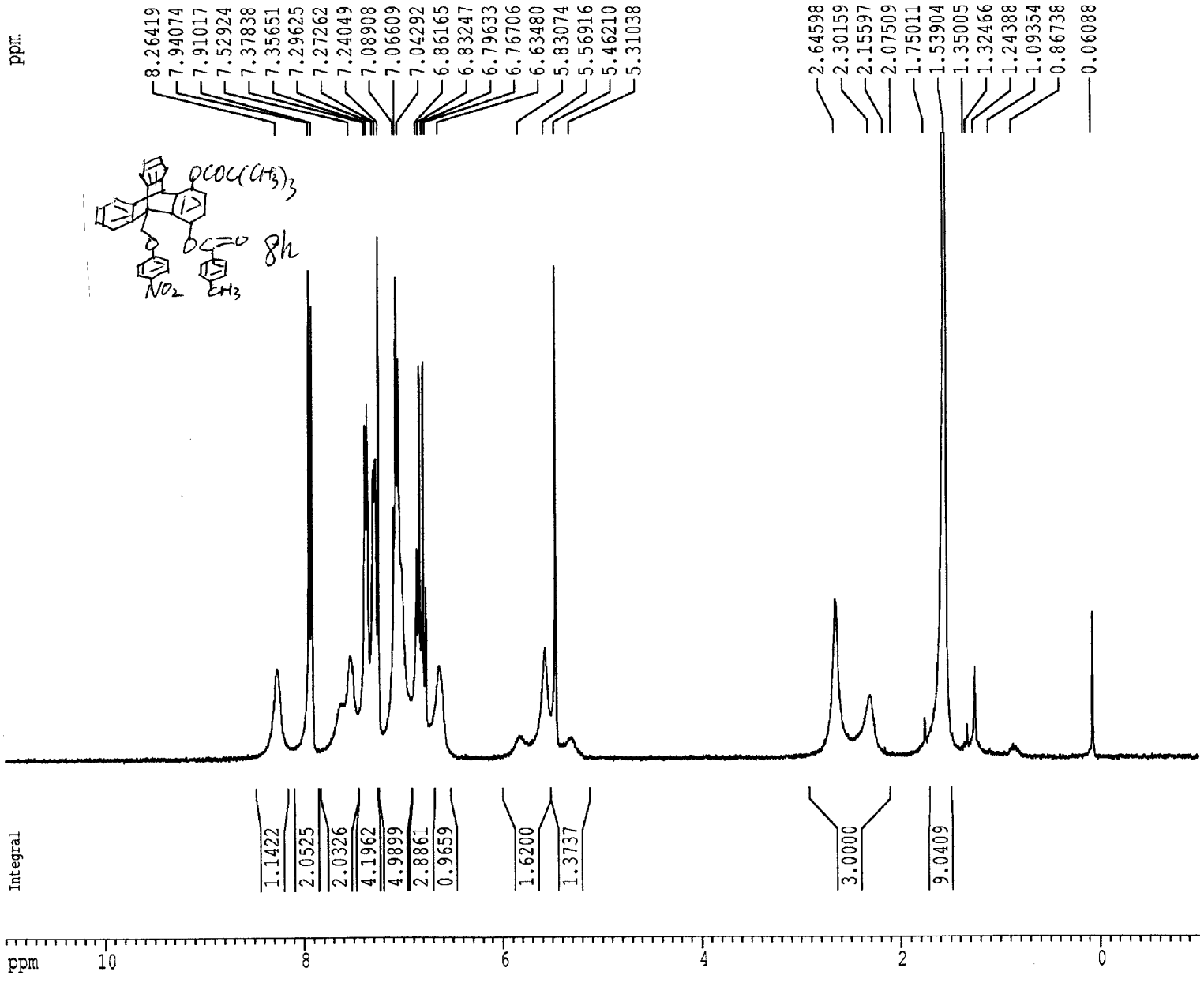
| | |
|---|---|
| Date_ | 20051108 |
| Time | 16.16 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 912.3 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300121 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | nitrophenolme |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

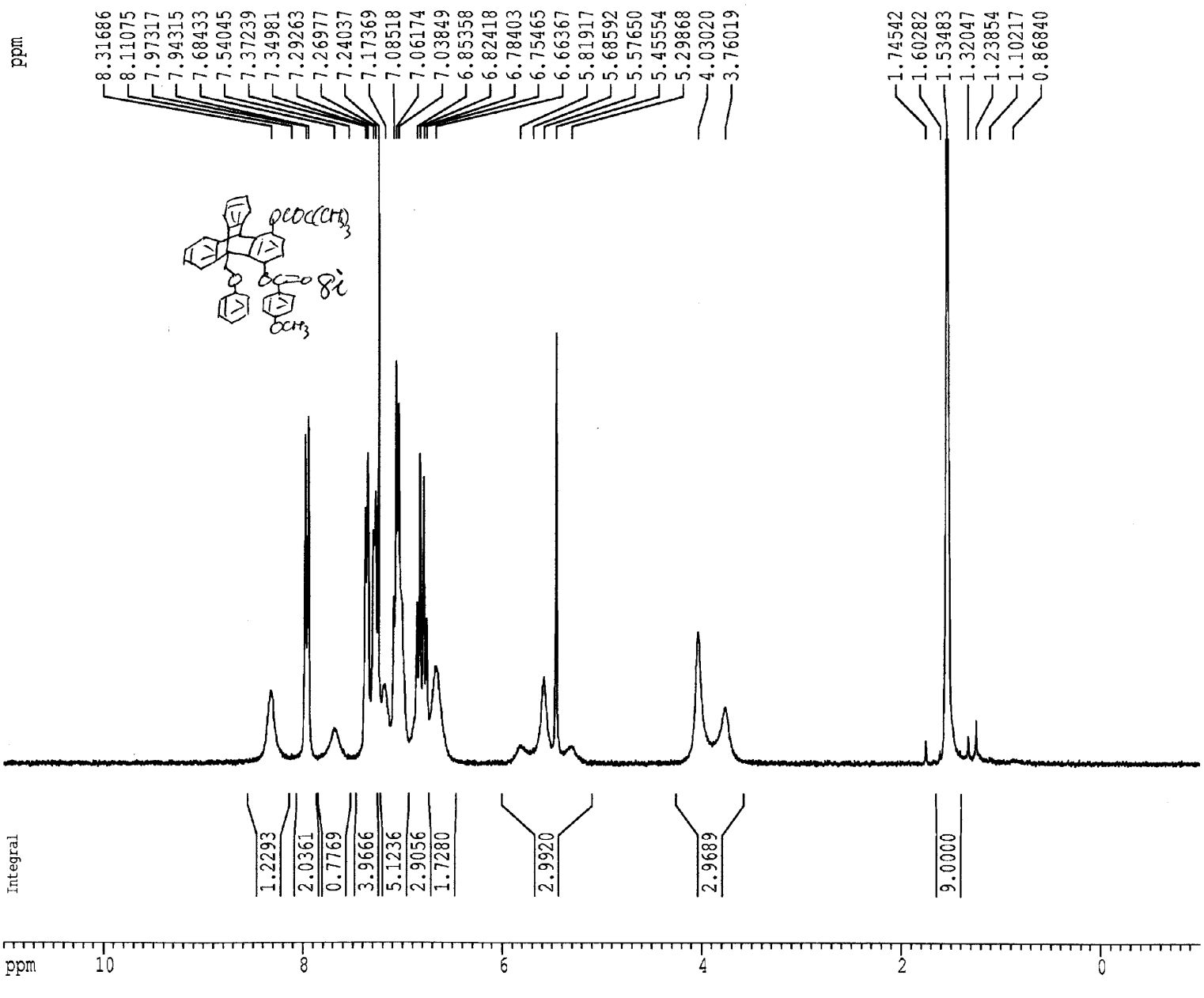
| | |
|---|---|
| Date_ | 20051213 |
| Time | 17.17 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 512 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300117 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | nitrophenomeo2 |
| EXPNO | 2 |
| PROCNO | 1 |

F2 - Acquisition Parameters

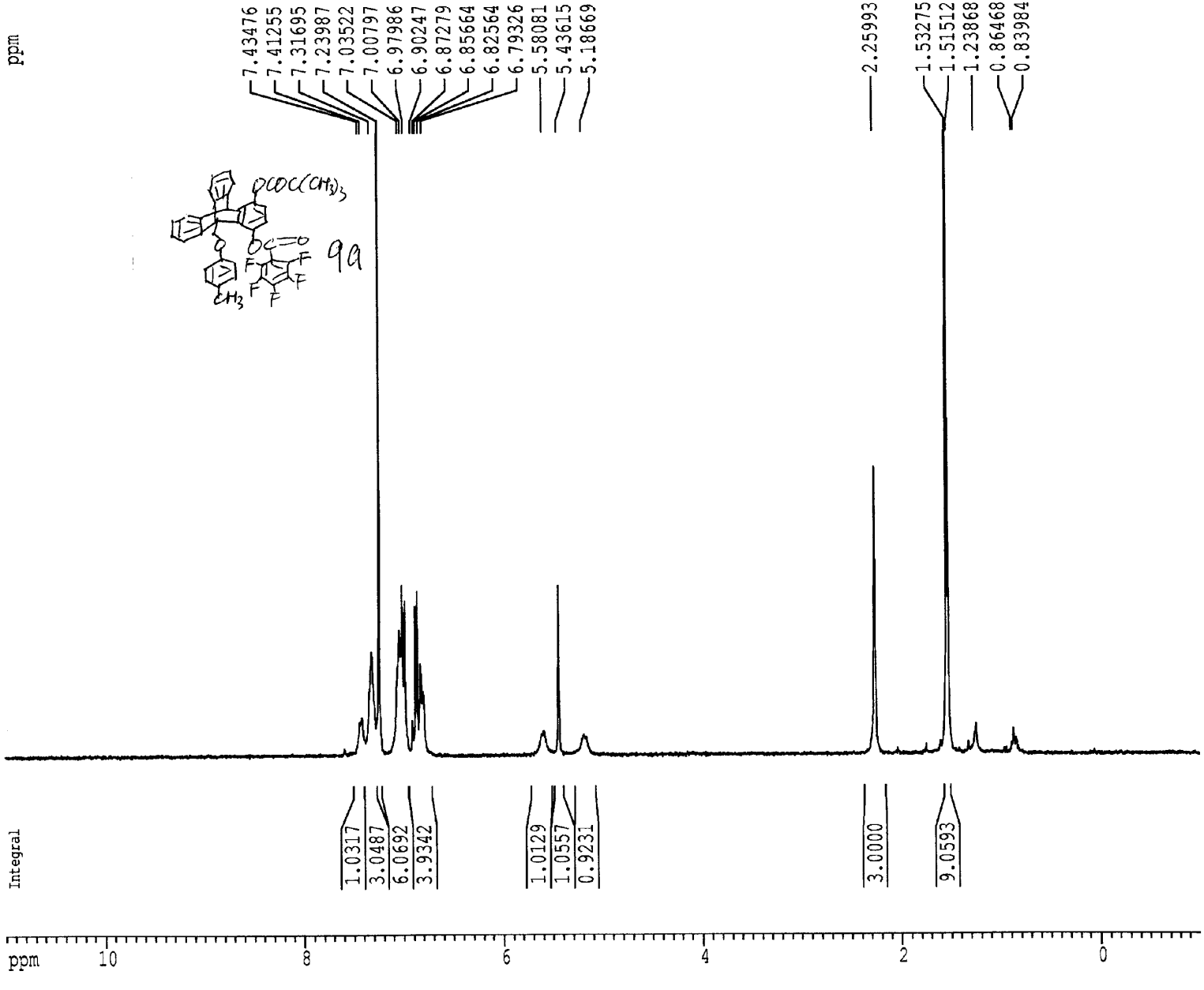
| | |
|---|---|
| Date_ | 20051104 |
| Time | 13.05 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 512 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300121 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | trimepheno5f2 |
| EXPNO | 2 |
| PROCNO | 1 |

F2 - Acquisition Parameters

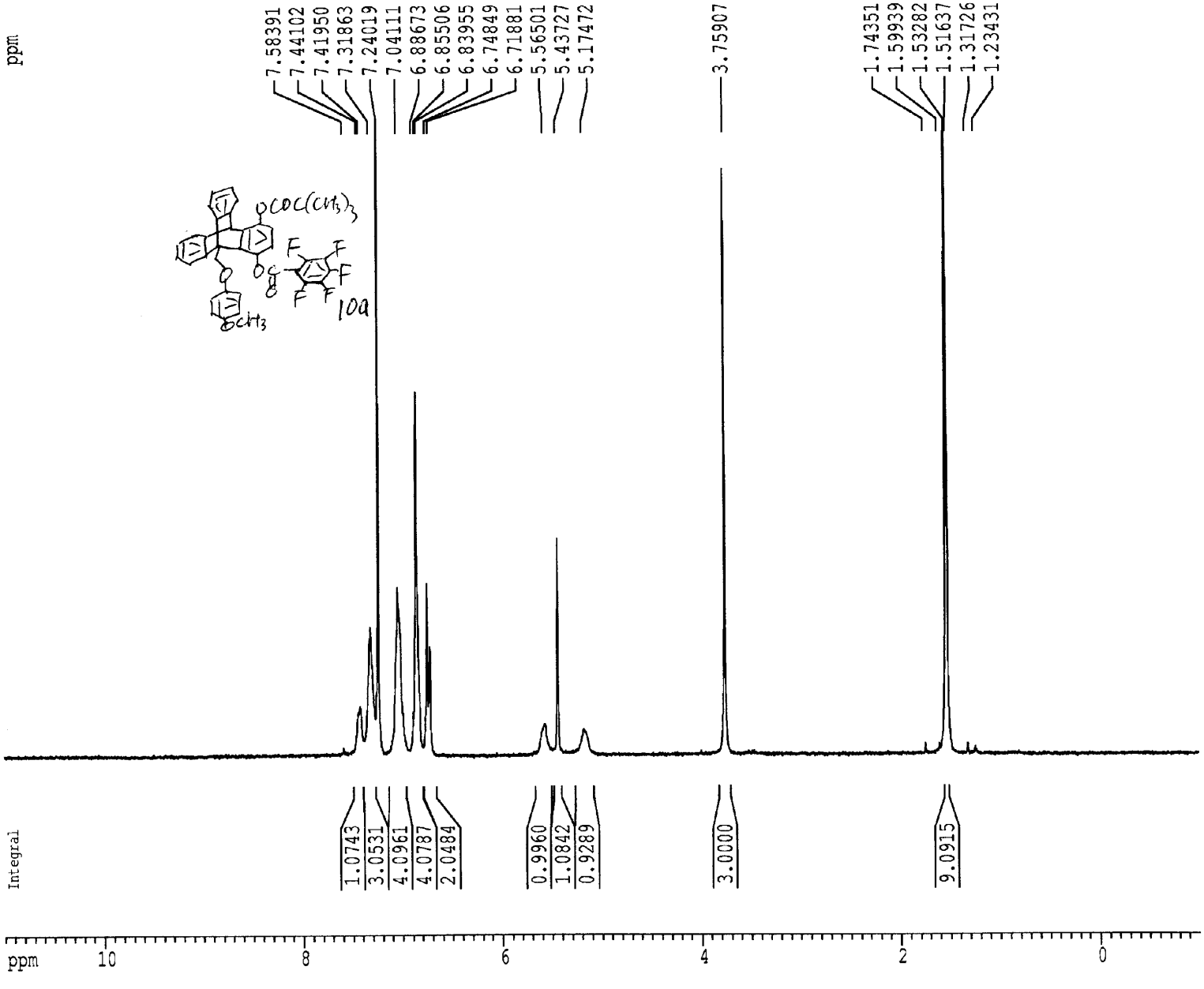
| | |
|---|---|
| Date_ | 20060527 |
| Time | 14.31 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 39 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 1149.4 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300125 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | meophenol5f3 |
| EXPNO | 3 |
| PROCNO | 1 |

F2 - Acquisition Parameters

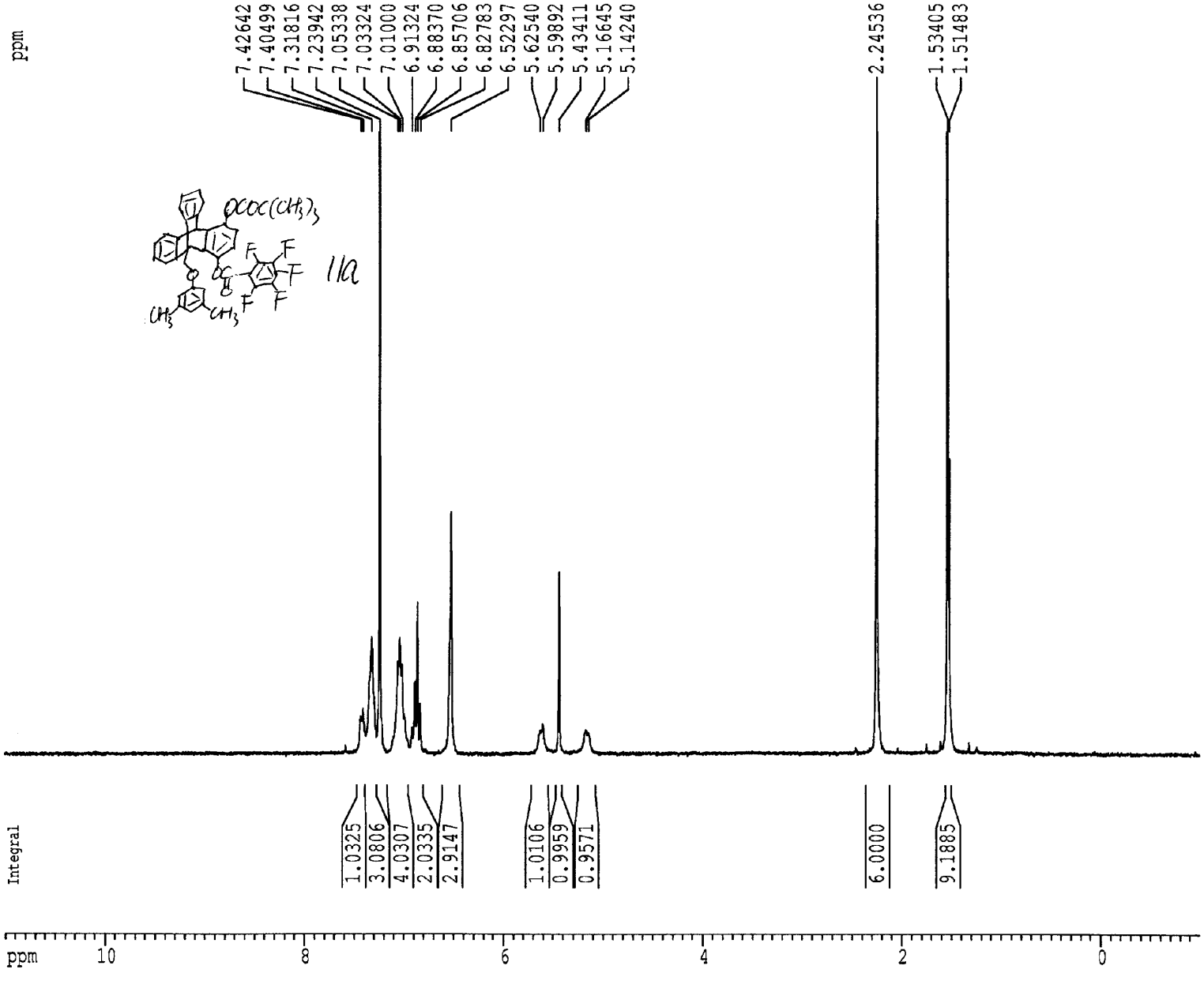
| | |
|---|---|
| Date_ | 20060529 |
| Time | 14.09 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 64 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 1149.4 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300125 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | dimepheno5f2 |
| EXPNO | 2 |
| PROCNO | 1 |

F2 - Acquisition Parameters

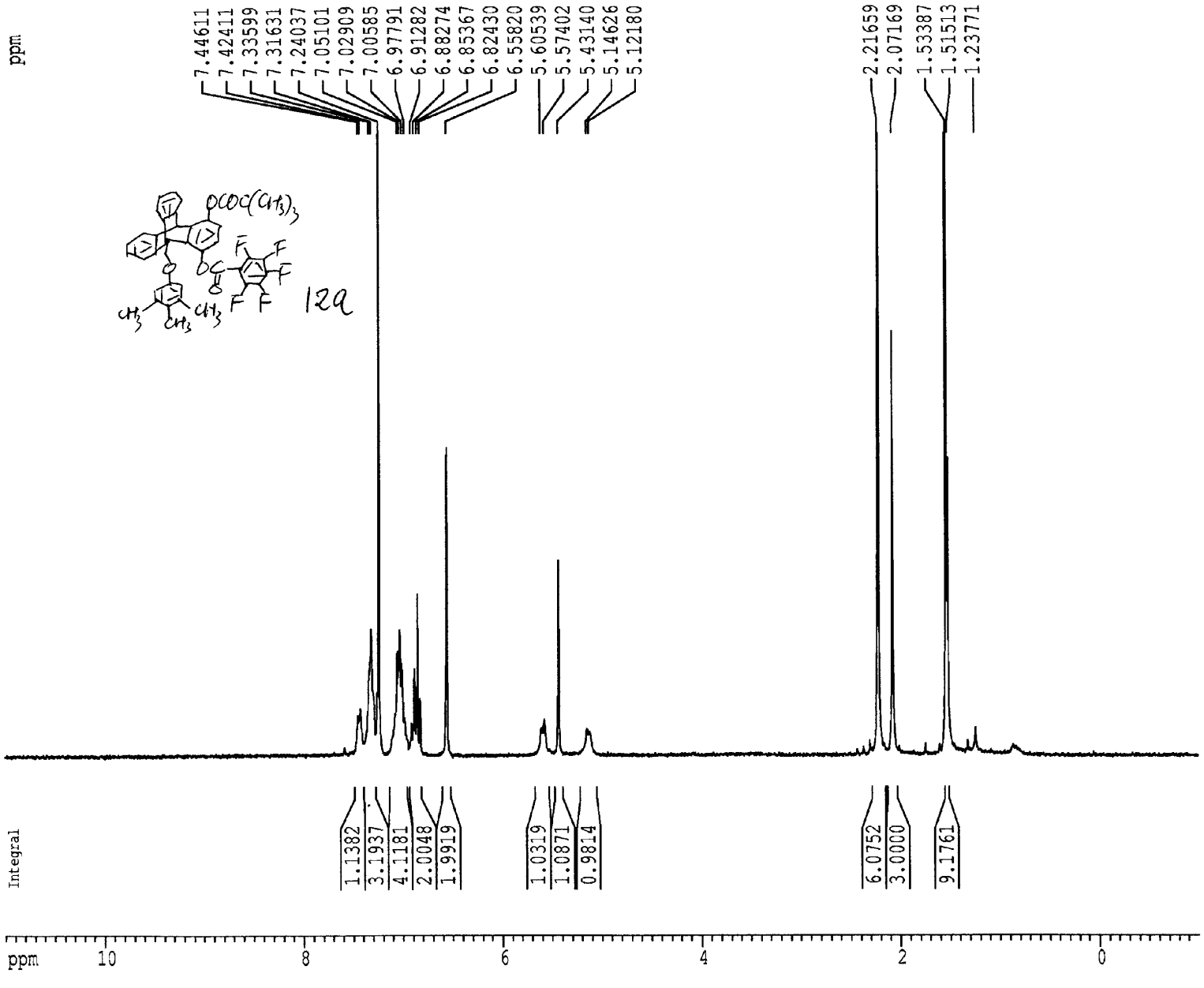
| | |
|---|---|
| Date_ | 20060527 |
| Time | 20.52 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 64 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 1290.2 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300125 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | triimepheno5f3 |
| EXPNO | 3 |
| PROCNO | 1 |

F2 - Acquisition Parameters

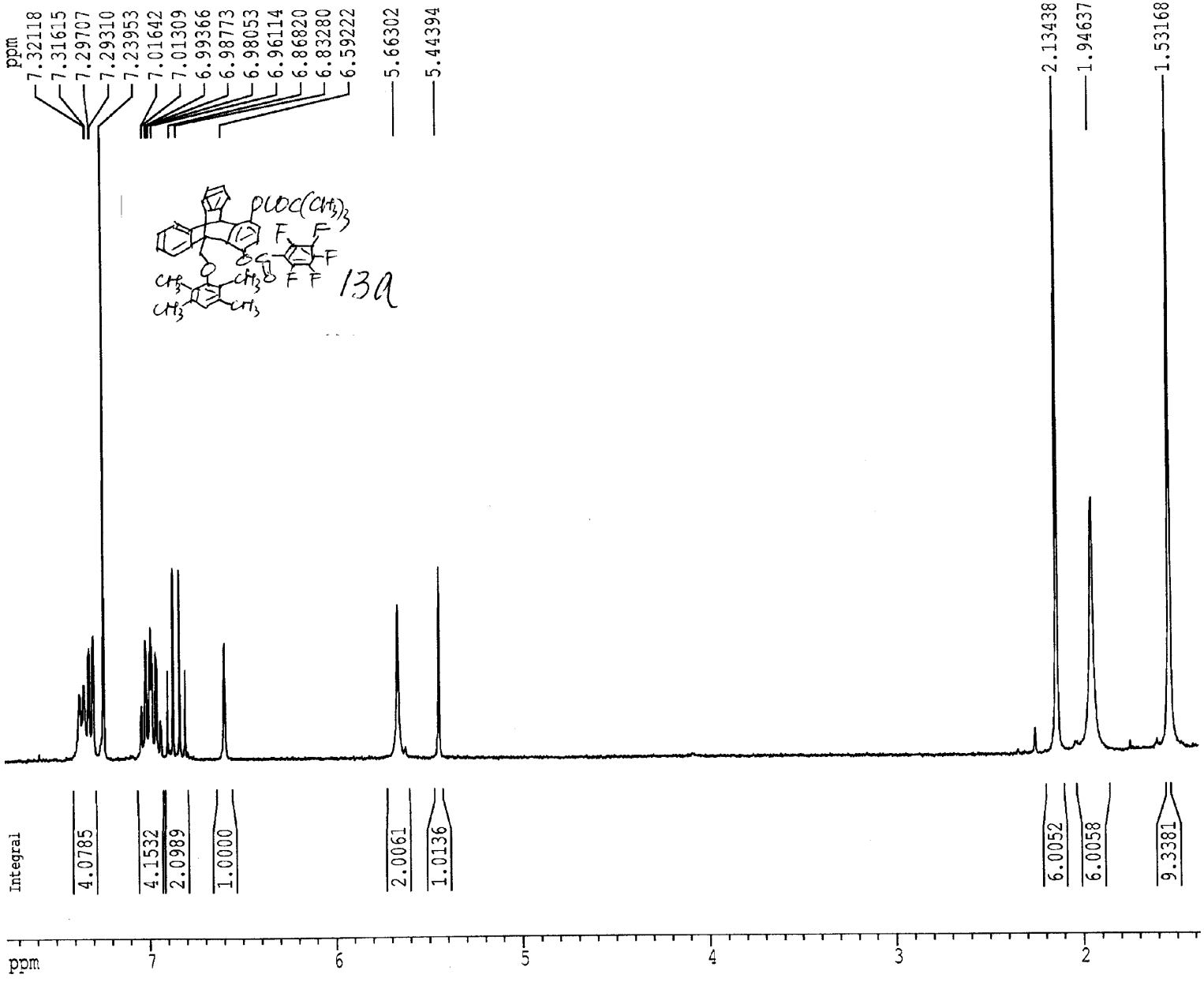
| | |
|---|---|
| Date_ | 20060529 |
| Time | 10.10 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 64 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 1149.4 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300125 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 11.000 ppm |
| F1 | 3301.43 Hz |
| F2P | -1.000 ppm |
| F2 | -300.13 Hz |
| PPMCM | 0.60000 ppm/cm |
| HZCM | 180.07800 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | tetramepheno5f |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

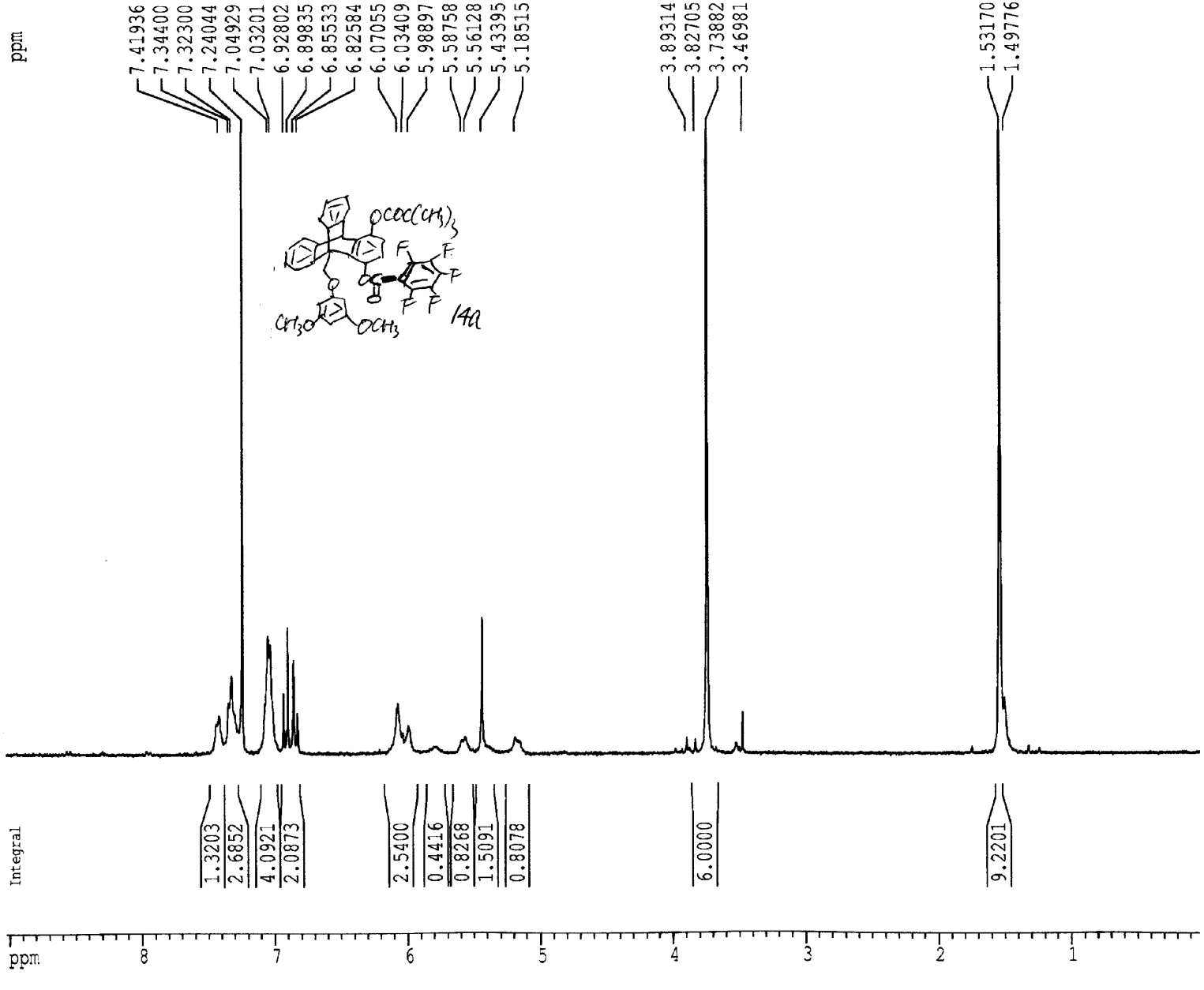
| | |
|---|---|
| Date_ | 20060311 |
| Time | 10.44 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 912.3 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300125 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 7.768 ppm |
| F1 | 2331.42 Hz |
| F2P | 1.376 ppm |
| F2 | 413.10 Hz |
| PPMCM | 0.31958 ppm/cm |
| HZCM | 95.91605 Hz/cm |




Current Data Parameters

| | |
|---|---|
| NAME | dimeotrip5f2 |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

| | |
|---|---|
| Date_ | 20060103 |
| Time | 15.37 |
| INSTRUM | spect |
| PROBHD | 5 mm Multinu |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | DMSO |
| NS | 16 |
| DS | 2 |
| SWH | 6188.119 Hz |
| FIDRES | 0.188846 Hz |
| AQ | 2.6477044 sec |
| RG | 724.1 |
| DW | 80.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| D1 | 1.00000000 sec |
| P1 | 14.10 usec |
| SFO1 | 300.1318534 MHz |
| NUC1 | 1H |
| PL1 | 3.00 dB |

F2 - Processing parameters

| | |
|---|---|
| SI | 16384 |
| SF | 300.1300121 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

1D NMR plot parameters

| | |
|---|---|
| CX | 20.00 cm |
| F1P | 9.021 ppm |
| F1 | 2707.58 Hz |
| F2P | 0.029 ppm |
| F2 | 8.74 Hz |
| PPMCM | 0.44961 ppm/cm |
| HZCM | 134.94189 Hz/cm |