Supporting Information

Ruthenium-Catalyzed Direct Arylation of C-H Bonds in Aromatic Amides Containing a Bidentate Directing Group: Significant Electronic Effects on Arylation

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Contents

I. General Information.

^{1}H NMR and ^{13}C NMR spectra were recorded on a JEOL ECS-400 spectrometer in $CDCl_3$ or DMSO-d_6 with tetramethylsilane as the internal standard. Data are reported as follows: chemical shift in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, bs = broad singlet, and m = multiplet), coupling constant (Hz), and integration. Infrared spectra (IR) were obtained using a Horiba FT-720 spectrometer; absorptions are reported in reciprocal centimeters with the following relative intensities: s (strong), m (medium), or w (weak). Mass spectra were ob tained using Shimadzu GCMS-QP 2014 and Shimadzu GCMS-QP 5000 instruments instrument with ionization voltages of 70 eV. High resolution mass spectra (HRMS) were obtained on a JEOL JMS -DX303 instrument. Analytical gas chromatography (GC) was carried out on S himadzu GC-14B, Shimadzu GC-2014 and Shimadzu GC-8A gas chromatographs, equipped with a flame ionization detector. Melting points were determined using a Yamato melting point apparatus. Column chromatography was performed with SiO_2 (Silicycle SiliaFlash F60 (230-400 mesh)). Some compounds were purified by LC-908 HPLC (GPC).

II. Materials.

$[RuCl_2(p\text{-cymene})]_2$ (CAS 52462-29-0) was purchased from Sigma-Aldrich. Bromobenzene (CAS 108-86-1) and Na_2CO_3 (CAS 497-19-8) was purchased from Nacalai Tesque, Inc. 8-Aminoquinoline (CAS 578-66-5), 2-methylbenzoic acid (CAS 118-90-1) and methyl 2-methylbenzoate (CAS 89-71-4) were purchased from Tokyo Kasei Kogyo Co., Ltd. PPh_3 (CAS 603-35-0) was purchased from Wako Pure Chemicals. These reagents were used as received. Toluene was dried on a Glass Contour solvent dispensing system (Nikko Hansen & Co., Ltd.). $[Ru(OAc)_2(p\text{-cymene})]_2$ (CAS 111409-79-1) was prepared by following procedure [1]

III. Synthesis of the Starting Amides.

All amides bearing 8-aminoquinoline moiety were prepared by the reaction of the corresponding acid chlorides with 8-aminoquinoline. 2-Methyl-*N*-phenylbenzamide (CAS 7055-03-0) was also prepared using the same procedure. 2-Methyl-*N*-(8-quinolinyl)benzamide **1** (CAS 1182669-71-1), 3-methyl-*N*-(8-quinolinyl)benzamide (CAS 443638-87-7), *N*-(8-quinolinyl)-1-naphthamide (CAS 443735-56-6), was prepared by previously reported procedure. [2] 2-Methyl-*N*-(2-pyridinylmethyl)benzamide was prepared by our previously reported procedure.[3]

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[1] Bennett, M. A.; Smith, A. K. *J. C. S. Dalton* **1974**, 233.
[2] Gou, F.-R.; Wang, X.-C.; Huo, P.-F.; Bi, H.-P.; Guan, Z.-H.; Liang, Y.-M. *Org. Lett.* **2009**, *11*, 5726.
[3] Inoue, S.; Shiota, H.; Fukumoto, Y.; Chatani, N. *J. Am. Chem. Soc.* **2009**, *131*, 6898.

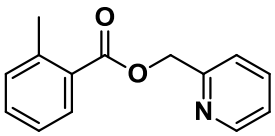
N-(8-Quinolinyl)-3-(trifluoromethyl)benzamide (28) (CAS 331627-96-4), 3-(Dimethylamino)-*N*-(8-quinolinyl)benzamide (CAS 1090409-09-8), 3-(*tert*-Butyldimethylsilyloxy)-*N*-(8-quinolinyl)benzamide (CAS 1351067-35-0), 2-Methyl-3-(8-quinolinylcarbamoyl)phenyl acetate (CAS 1351067-39-4), 7a-d_7 (CAS 1351066-84-6) was prepared by our previously reported procedure.[4]The representative procedure and spectroscopic data for new amides are shown below.

General Procedure for the Preparation of Starting Amide (7e).

To an oven-dried 100 mL three-necked flask, 3-phenylbenzoic acid (3.0 g, 15 mmol), DMF (5 drops) and DCM (30 mL) were added under a N_2 atmosphere. Oxalyl chloride (1.5 mL, 18 mmol, 1.2 equiv.) was added dropwise at 0 °C resulting in vigorous bubbling. The mixture was stirred for 5 h at room temperature, and the solvent was then removed *in vacuo*. The resulting acid chloride was used immediately without further purification.

To another oven-dried 100 mL three-necked flask, 8-aminoquinoline (2.9 g, 20 mmol, 1.3 equiv.), Et_3N (4.1 mL, 30 mmol, 2 equiv.) and DCM (30 mL) were added. A solution of the acid chloride in DCM (10 mL) was added dropwise to the solution at 0 °C, and the solution was then warmed to room temperature. After stirring overnight, the reaction system was quenched with sat. aq. $NaHCO_3$ (30 mL) and the organic layer was separated. The aqueous layer was extracted with DCM (2 x 15 mL). The combined organic layers were washed with 1 M HCl aq. (30 mL) and brine (30 mL), dried over $MgSO_4$, filtered and evaporated *in vacuo*. The obtained crude amide was purified by column chromatography on silica gel (eluant: hexane/EtOAc = 3/1) to afford the desired amide **7e** as a white solid (3.8 g, 78%).

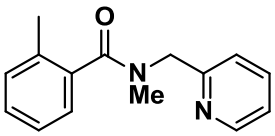
Pyridin-2-ylmethyl 2-methylbenzoate(4) [CAS: 77934-68-0].



R_f 0.57 (EtOAc). Colorless Oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.63 (s, 3H), 5.47 (s, 3H), 7.23-7.28(m, 3H), 7.41-7.46 (m , 2H), 7.72 (dt, J = 8.0, 2.0 Hz, 1H), 8.03 (d, J = 7.2 Hz), 8.62 (d, J = 4.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.84, 67.00, 121.62, 122.79, 125.73, 129.00, 130.74, 131.74, 132.22, 136.75, 140.60, 149.44, 156.04, 166.96; HRMS Calcd for $C_{14}H_{13}NO_2$: 227.0946; Found: 227.0949.

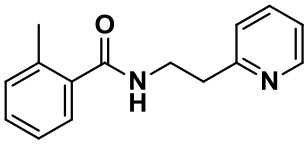
***N*,2-Dimethyl-*N*-(pyridin-2-ylmethyl)benzamide(5)**

[4] Ano, Y.; Tobisu, M.; Chatani, N. *Org. Lett.* **2012**, *14*, 354.



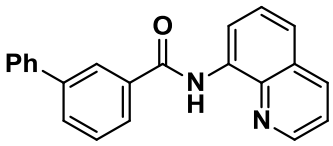
Spectroscopic data indicated that the title compound exists as a mixture of two rotational isomers. R_f 0.26 (EtOAc). Yellow Oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ [2.30, 2.32 (s, 3H)], [2.83, 3.12 (s, 3H)], [4.46, 4.89 (two broad singlet peaks, 2H)], 7.06-7.28 (m, 6H), 7.65, 7.70 (td, J = 7.2, 1.6 Hz, 1H), 8.52, 8.55 (d, J = 4.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ [18.79, 18.96], [32.85, 36.55], [52.09, 56.08], 120.87, [122.16, 122.34], [125.63, 125.72, 125.77 (two overlapping peaks)], [128.71, 128.78], [130.24, 130.34], [133.89, 134.27], [135.98, 136.19], [136.64, 136.79], [149.09, 149.53], [156.29, 156.92], [171.50, 172.10]; IR (neat) 3014 w, 2925w, 1637s, 1594 m, 1477 m, 1436 m, 1398 m, 1307 w, 1259 w, 1066 m, 754 m; MS *m/z* (relative intensity, %) 393 (M^+, 14), 121 (25), 119 (23), 94 (10), 93 (100), 92 (10), 91 (39), 65 (23). HRMS Calcd for $C_{15}H_{16}N_2O$: 240.1263; Found:240.1261.

2-Methyl-*N*-(2-(pyridin-2-yl)ethyl)benzamide (6)[CAS: 1089584-90-6].



R_f 0.17 (EtOAc). Yellow Oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.40 (s, 3H), 3.10 (t, J = 6 Hz, 2H), 3.87 (q, J = 6 Hz), 6.80 (brs, 1H), 7.14-7.22 (m, 4H), 7.27-7.33 (m, 2H), 7.63 (dd, J = 7.6, 1.6 Hz, 1H), 8.50 (d, J = 4.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 19.78, 36.86, 38.85, 121.61, 123.50, 125.66, 126.81, 129.66, 130.90, 135.97, 136.65 (two overlapping peaks), 149.21, 159.59, 169.91; HRMS Calcd for $C_{15}H_{16}N_2O$: 240.1203; Found: 240.1265

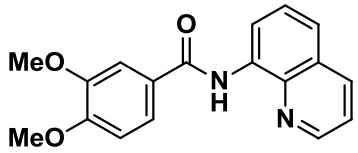
***N*-(quinolin-8-yl)-[1,1'-biphenyl]-3-carboxamide (7e).**



R_f 0.26 (hexane/EtOAc = 5/1). White solid. Mp = 86-87 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.41 (t, J = 11.6 Hz, 1H), 7.46-7.69 (m, 6H), 7.71-7.72 (m, 2H), 7.81 (d, J = 7.6 Hz, 1H), 7.05 (d, J = 7.0 Hz, 1H), 8.19 (dd, J = 8.4, 2.0 Hz, 1H), 8.31 (s, 1H), 8.85 (dd, J = 4.2, 2.0 Hz,1H), 8.97 (dd, J = 7.4, 1.6 Hz, 1H), 10.80 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 116.54, 121.67, 121.74, 125.84. 126.21, 127.26, 127.43, 127.76, 127.93, 128.92, 129.19, 130.52, 134.51, 135.75, 13 6.37, 138.70, 140.24, 141.85, 148.32, 165.45; IR (KBr) 3359 w, 3054 w, 3029 w, 1668 m, 1538 s,

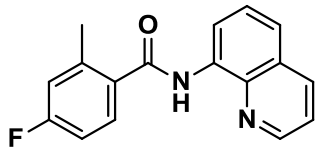
1479 m, 1429 m, 1384 m, 1330 m, 1243 m, 1222 m, 790 m, 725 m, 690 m; MS *m/z* (relative intensity, %) 325 (14), 324 (M^+, 57), 182 (14), 181 (100), 153 (36), 152 (37). HRMS Calcd for $C_{14}H_{14}N_2O$: 324.1263; Found:324.1266.

3,4-Dimethoxy-*N*-(quinolin-8-yl)benzamide [CAS: 443730-38-9].



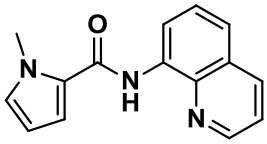
R_f 0.14 (hexane/EtOAc = 5/1). White solid. Mp = 139-140°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.98 (s, 3H), 4.02 (s, 3H), 7.00 (d, J = 9.2 Hz, 2H),7.48 (dd, J = 8.0, 4.0 Hz, 1H), 7.53-7.62 (m, 2H), 7.66-7.69 (m, 2 H), 8.19 (dd, J = 8.0 , 1.6 Hz, 1H), 8.85 (dd, J = 4.4, 0.8 Hz, 1H), 8.92 (dd, J = 8.0, 1.6 Hz, 1H), 10.72 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 56.04 (two overlapping peaks), 110.32, 110.74, 116.26, 119.76, 121.43, 121.64, 127.49, 127.76, 127.96, 134.66, 136.38, 138.70, 148.21, 149.09, 151.99, 165.03; IR (KBr) 3365 w, 2997 w, 1657 m, 1535 s, 1513 s, 1487 m, 1332 m, 1272 m, 1027 w; MS *m/z* (relative intensity, %) 308 (M^+, 31), 165 (100). HRMS Calcd for $C_{18}H_{16}N_2O_3$: 308.1161; Found:308.1158.

4-Fluoro-2-methyl-*N*-(quinolin-8-yl)benzamide.



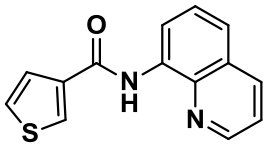
R_f 0.31 (hexane/EtOAc = 5/1). White solid. Mp = 105-106 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.61 (s, 3H), 6.99-7.03 (m, 2H), 7.47 (dd, J = 7.6, 4.0 Hz, 1H), 7.55-7.63 (m, 2 H), 7.69 (dd, J = 9.2, 5.6 Hz, 1H), 8.29 (dd, J = 8.4, 1.6 Hz, 1H), 8.79 (dd, J = 4.8, 1.6 Hz, 1H), 8.91 (dd, J = 7.2, 1.6 Hz, 1H), 10.20 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 20.40, 112.88 (d, J = 21.9 Hz), 116.45, 118.81 (d, J = 21.0 Hz), 121.78 (d, J = 15.2 Hz), 127.39, 127.95, 129.40 (d, J = 9.6 Hz), 132.73, 134.53, 136.40, 138.50, 140.03 (d, J = 8.6 Hz), 148.29, 162.25, 164.74, 167.19; IR (KBr) 3365 m, 3342 w, 3045 w, 2927 w, 2856 w, 1679 s, 1589 w, 1535 s, 1484 m, 1425 w, 1384 w, 1328 w, 1261 w, 1238 w, 958 w, 821 w, 788 w; MS *m/z* (relative intensity, %) 280 (M^+, 27), 263 (22), 144 (13), 137 (100), 136 (12), 109 (35). HRMS Calcd for $C_{17}H_{13}FN_2O$: 280.1012; Found: 280.1013.

1-Methyl-*N*-(quinolin-8-yl)-1H-pyrrole-2-carboxamide.



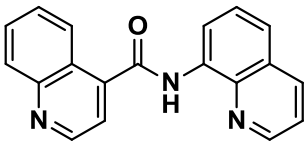
R_f 0.24 (hexane/EtOAc = 5/1). White solid. Mp = 110-111 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.06 (s, 3H), 6.21 (dd, J = 3.6, 2.0 Hz, 1H), 6.82 (t, J = 2.0 Hz, 1H), 7.02 (dd, J = 4.0, 1.6 Hz, 1H), 7.44-7.50 (m, 2H), 7.55 (t, J = 8.0 Hz, 1H), 8.16 (dd, J = 8.0, 1.6 Hz, 1H), 8.78-8.84 (m, 2H), 10.44 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 36.96, 107.53, 112.98, 115.72, 120.91, 121.58, 126.19, 127.38, 127.98, 128.81, 134.98, 136.27, 138.53, 148.13, 160.02; IR (KBr) 3367w, 3102 w, 1758w, 1668 s, 1536 s, 1481 s, 1419 m, 1382 m, 1328 m, 1247 m, 1122 m, 1068 w, 869 w, 825 m, 721 s; MS *m/z* (relative intensity, %) 251 (M^+, 42), 108 (100). HRMS Calcd for $C_{15}H_{13}N_3O$: 251.1059; Found: 251.1056.

_N_-(Quinolin-8-yl)thiophene-3-carboxamide [CAS: 930053-64-8].



R_f 0.31 (hexane/EtOAc = 5/1). White solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.43-7.49 (m, 2H), 7.52-7.58 (m, 2H), 7.79 (d, J = 5.2 Hz, 1H), 8.16-8.19 (m, 2H), 8.83-8.90 (m, 2H), 10.54 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 116.44, 121.56, 121.66, 126.33, 126.69, 127.43, 127.93, 128.92, 128.92, 134.44, 136.36, 138.30, 138.54, 148.24, 160.99; IR (neat) 3353 w, 3116 w, 1666 m, 1533 s, 1483 m, 1423 w, 1384 w, 1328 w, 1263 w, 1120 w, 856 m, 823 m; MS *m/z* (relative intensity, %) 255 (11), 254 (M^+, 67), 111 (100). HRMS Calcd for $C_{14}H_{10}N_2OS$: 254.0514; Found: 524.0515.

_N_-(Quinolin-8-yl)quinoline-4-carboxamide.



R_f 0.66 (EtOAc). Pale Yellow solid. Mp = 206-207 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.48 (dd, J = 8.4, 4.0 Hz, 1H), 7.61-7.68 (m, 3H), 7.76 (d, J = 4.0 Hz, 1H), 7.81 (t, J = 7.2 Hz, 1H), 8.21 (d, J = 8.4 Hz, 2H), 8.46 (d, J = 8.4 Hz, 1H), 8.76 (dd, J = 8.0 , 1.6 Hz, 1H), 9.02 (dd, J = 7.6, 1.6 Hz, 1H), 9.09 (d, J = 4.0 Hz, 1H), 10.48 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 116.97, 118.70, 121.88, 122.57, 124.49, 125.39, 127.34, 127.8, 127.95, 129.96, 130.09, 134.13, 136.44, 138.44, 141.85, 148.49, 148.89, 150.04, 165.39; IR (KBr) 3328 m, 3060 w, 3039 w, 3004 w, 1666 s, 1579 w, 1523 s,

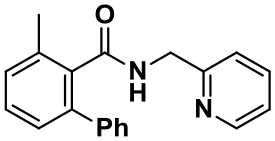
1482 m, 1459 m, 1423 m, 1380 m, 1324 m, 1270 m, 1141 w, 831 m, 755 m; MS *m/z* (relative intensity, %) 300 (18), 299 (M^+, 84), 271 (16), 270 (16), 255 (20), 171 (76), 156 (57), 149 (11), 130 (18), 129 (19), 128 (100), 101 (30). HRMS Calcd for $C_{19}H_{13}N_3O$: 299.1059; Found: 299.1060.

V. General Procedure for the Ru-Catalyzed Arylation: Ru-Catalyzed Reaction of Amide 7a with PhBr.

To an oven-dried 5 mL screw-capped vial, 2-methyl-*N*-(8-quinolinyl)benzamide **7a** (79 mg, 0.3 mmol), bromobenzene (56 mg, 0.36 mmol), $[RuCl_2(p\text{-cymene})]_2$ (9 mg, 0.015 mmol), PPh_3 (31 mg, 0.12 mmol), Na_2CO_3 (64 mg, 0.6 mmol) and toluene (2 mL) were added under a gentle stream of nitrogen. The mixture was stirred for 15 h at 130 °C followed by cooling. The mixture was filtered through a celite pad and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (eluent: hexane/EtOAc= 20/1) to afford the desired arylated product **3** (72 mg, 80%) as a colorless oil.

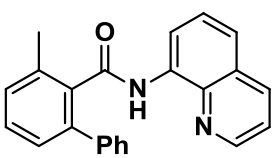
VI. Spectroscopic Data for Arylated Products

3-Methyl-*N*-(pyridin-2-ylmethyl)-[1,1'-biphenyl]-2-carboxamide (2a).



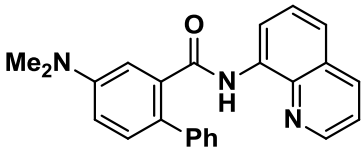
R_f 0.34 (EtOAc). White solid. Mp = 246-247 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.43 (s, 3H), 4.44 (d, J = 5.2 Hz, 2H), 6.53 (brs, 1H), 6.84 (d, 7.6 Hz, 1H), 7.08 (t, J = 6.2 Hz, 1H), 7.18-7.34 (m, 6H), 7.38-7.41 (m, 2H), 7.50 (dt, J = 8.0, 2.0 Hz, 1H), 8.29 (d, J = 4.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 19.51, 44.48, 121.72, 122.05, 127.16, 127.25, 128.14, 128.56, 128.85, 129.21, 135.54, 136.29, 136.60, 139.25, 140.39, 156.15, 169.77; 3056 w, 2919 w, 1714 w, 1654 s, 1592 m, 1442 m, 1415 m, 1355 w, 1229 m, 1157 w, 993 w, 796 w, 767 s, 703 m; MS *m/z* (relative intensity, %) 303 (11), 302 (M^+, 50), 301 (36), 195 (55), 194 (100), 166 (15), 165 (46), 152 (26), 107 (51). HRMS Calcd for $C_{20}H_{18}N_2O$: 302.1419; Found: 302.1420.

3-Methyl-*N*-(quinolin-8-yl)-[1,1'-biphenyl]-2-carboxamide (7a).



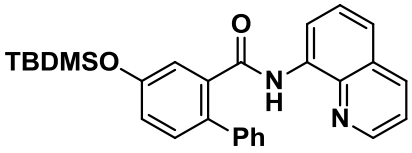
R_f 0.29 (hexane/EtOAc = 5/1). Colorless Oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.54 (s, 3H), 7.09 (t, J = 6.4 Hz, 1H), 7.20-7.257 (m, 2H), 7.32-7.35 (m, 2H), 7.36 (dd, J = 4.4, 1.6 Hz, 1H), 7.40-7.53 (m, 5H), 8.08 (d, J = 8.4 Hz, 1H), 8.61 (dd, J = 4.0, 1.6 Hz, 1H), 8.77 (d, J = 7.2 Hz, 1H), 9.64 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 19.80, 116.42, 121.44, 121.64, 127.73, 128.14, 128.61, 129.18, 129.47, 134.34, 135.82, 136.08, 136.81, 138.33, 139.64, 140.34, 147.95, 168.28; IR (neat) 3342 s, 3058 m, 3012 m, 1673 s, 1592 m, 1523 s, 1482 s, 1425 s, 1384 s, 1326 s, 1265 s, 1218 m, 1132 m, 1074 w, 898 m, 827 s, 757 s; MS *m/z* (relative intensity, %) 338 (M^+, 33), 196 (15), 195 (100), 165 (17), 152 (15). HRMS Calcd for $C_{23}H_{18}N_2O$: 338.1419; Found: 338.1422.

4-(Dimethylamino)-*N*-(quinolin-8-yl)-[1,1'-biphenyl]-2-carboxamide (8b).



R_f 0.20 (hexane/EtOAc = 5/1). Pale yellow solid. Mp = 164-165 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.91 (brs, 1H), 7.07 (t, J = 7.6 Hz, 1H), 7.22 (t, J = 7.6 Hz, 1H), 7.30 (dd, J = 7.6, 3.6 Hz, 1H), 7.36 (d, J = 8.8 Hz, 1H), 7.42 (dd, J = 8.0, 1.6 Hz, 1H), 7.47-7.52 (m, 3H), 8.02 (dd, J = 8.4, 1.6 Hz, 1H), 4.0, 2.0 Hz, 1H), 8.83 (dd, J = 8.0, 1.6 Hz, 1H), 9.77 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 40.54, 121.75, 114.37, 116.04, 121.27, 121.30, 126.62, 126.80, 127.16, 127.58, 127.91, 128.16, 128.92, 131.47, 134.57, 135.81, 136.54, 138.32, 140.08, 147.61, 149.63, 168.59; IR (KBr) 3315 w, 3043 w, 2996 w, 2884 w, 2809 w, 1664 m, 1604 m, 1523 s, 1482 s, 1442m, 1421 m, 1363m, 1322 m, 1259 w, 1224 m, 1108 w, 1068 w, 908 w, 821 m, 790 w, 761 w, 742 w, 698 m; MS *m/z* (relative intensity, %) 368 (16), 367 (M^+, 55), 225 (16), 224 (100), 196 (10), 153 (10), 152 (10). HRMS Calcd for $C_{24}H_{21}N_3O_2$: 367.1685; Found: 367.1687.

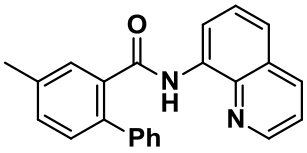
4-(*tert*-Butyldimethylsilyloxy)-*N*-(quinolin-8-yl)-[1,1'-biphenyl]-2-carboxamide (8c).



R_f 0.43 (hexane/EtOAc = 5/1). Clorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.28 (s, 6H), 1.02 (s, 9H), 7.03 (dd, J = 4.4, 2.8 Hz, 1H), 7.12 (t, J = 7.2 Hz, 1H), 7.23-7.27 (m, 2H), 7.32-7.36 (m, 2H), 7.39 (d, J = 2.8 Hz, 1H), 7.44-7.53 (m, 4H), 8.06 (dd, J = 8.4, 1.2 Hz, 1H), 8.51 (dd, J = 4.4,1.2 Hz, 1H), 8.80 (dd, J = 7.2, 1.2 Hz, 1H), 9.80 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ -4.38, 18.19, 25.64, 116.14, 120.54, 121.36, 121.45, 122.26, 127.16, 127.21, 127,62, 128.25, 128.99, 131.92, 133.28, 134.45, 135.92, 136.94, 138.32, 139.73, 147.68, 155.18, 167.42; IR (neat) 3052 w, 2956 m, 2857 w, 1668 s,

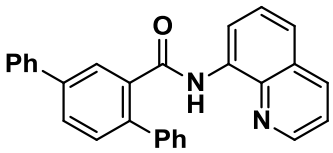
1602 w, 1527 s, 1481 s, 1425w, 1386 w, 1326 w, 1297 m, 1257 m, 1222 m, 971 m, 889 s, 833 s, 759 s; MS *m/z* (relative intensity, %) 456 (17), 454 (M^+, 45), 313 (25), 311 (100), 253 (15), 198 (16), 73 (25). HRMS Calcd for $C_{28}H_{30}N_2O_2Si$: 454.2077; Found: 454.2075.

4-Methyl-*N*-(quinolin-8-yl)-[1,1'-biphenyl]-2-carboxamide (8d).



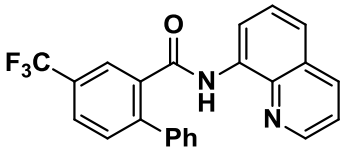
R_f 0.29 (hexane/EtOAc = 5/1). White solid. Mp = 156-157 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.46 (s, 3H), 7.13 (t, J = 3.2 Hz, 1H), 7.23-7.27 (m , 2H), 7.31(dd, J = 8.0, 4.4, 1H), 7.34-7.38 (m, 2H), 7.42 (dd, J = 8.0 , 1.2 Hz, 1H), 7.47-7.51 (m, 3H), 7.72 (s, 1H), 8.02 (dd, J = 8.0, 1.6 Hz, 1H), 8.49 (dd, J = 4.0, 1.6 Hz, 1H), 8.81 (dd, J = 7.6, 1.6 Hz,1H), 9.75 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.00, 116.13, 121.31, 121.38, 127.18, 127.32, 127.60, 128.27,128.93, 129.69, 13056, 131.22, 134.49, 135.84, 135.89, 137.32, 137.47, 138.30, 139.87, 147.65, 167.99; IR (KBr) 3307 m, 3054 w, 1660 s, 1608 w, 1523 s, 1481m, 1421 m, 1378 m, 1322 m, 1259w, 1197 w, 931 w, 898 w, 842 m, 703 m; MS *m/z* (relative intensity, %) 338 (M^+, 32), 196 (15), 195 (100), 165 (17), 152 (21). HRMS Calcd for $C_{23}H_{18}N_2O$: 338.1419; Found: 338.1420.

***N*-(quinolin-8-yl)-[1,1':4',1''-terphenyl]-2'-carboxamide (8e).**



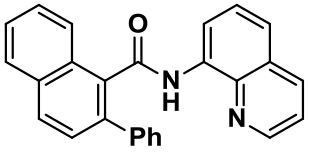
R_f 0.40 (hexane/EtOAc = 5/1). White solid. Mp = 72-73 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.16 (t, J = 7.6 Hz, 1H), 7.28-7.33 (m, 3H), 7.38 (dt, J = 8.0, 1.6 Hz, 1H), 7.4-7.57 (m, 7H), 7.69-7.71 (m , 2H), 7.78 (dd, J = 8.0, 1.6 Hz, 1H), 8.03 (dd, J = 8.0, 1.6 Hz, 1H), 8.15 (d, J = 2.0 Hz, 1H), 8.50 (dd, J = 4.0, 1.6 Hz, 1H), 8.84 (dd, J = 8.0, 1.2 Hz, 1H), 9.85(brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 116.20, 121.36, 121.53, 127.07, 127.19, 127.62, 127.71, 127.78, 128.37, 128.89, 28.91, 128.97, 131.17, 134.42, 135.91, 136.47, 138.29, 138.98, 139.53, 139.75, 140.44, 147.72, 167.74; IR (KBr) 3052 w, 3025 w, 1664 m, 1523 s, 1481 m, 1423 m, 1382 m, 1255w, 1220 w, 823 w, 788 w, 757 m, 698 m; MS *m/z* (relative intensity, %) 401 (10), 400(M^+, 33), 259 (20), 257 (100), 229 (15), 228 (22). HRMS Calcd for $C_{28}H_{20}N_2O$: 400.1576; Found: 400.1573.

***N*-(Quinolin-8-yl)-4-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxamide (8f).**



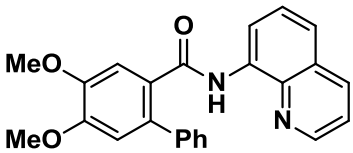
R_f 0.26 (hexane/EtOAc = 5/1). White solid. Mp = 121-122 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.21 (t, 3.2 Hz, 1H), 7.29-7.37 (m, 3H), 7.46-7.54 (m, 4H), 7.61 (d, J = 8.0 Hz, 1H), 7.81 (dd, J = 8.0, 1.2 Hz, 1H), 8.07 (dd, J = 8.4, 1.2 Hz, 1H), 8.20 (s, 1H), 8.50 (dd, J = 4.0, 2.0 Hz, 1H), 8.79 (dd, J = 8.0, 2.0 Hz, 1H), 9.79 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 116.3, 121.46, 121.87, 123.78 (q, J = 270 Hz), 126.48 (d, J = 3.9 Hz), 127.05 (d, J = 3.9 Hz), 127.14, 128.36, 128.59, 128.82, 129.80 (q, J = 33.4 Hz), 131.24, 134.03, 135.99, 136.50, 138.20, 138.51; IR (KBr) 3301 m, 3062 w, 1664 s, 1616 w, 1531s, 1482 s, 1425 w, 1384 m, 1328 s, 1255 s, 1224 m, 1260 s, 1126 s, 1078m, 921 w, 844 w, 78 m, 698 s; MS *m/z* (relative intensity, %) 393 (12), 392 (M^+, 46), 391 (26), 250 (14), 249 (100), 201 (31), 171 (13), 152 (20), 144 (20). HRMS Calcd for $C_{23}H_{15}F_3N_2O$: 392.1136; Found: 392.1134.

2-Phenyl-*N*-(quinolin-8-yl)-1-naphthamide (9).



R_f 0.26 (hexane/EtOAc = 5/1). White solid. Mp = 157-158 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.12 (t, J = 8.0 Hz, 1H), 7.23-7.32 (m, 4H), 7.45 (d, J = 8.0 Hz, 1H), 7.51-7.57 (m, 3 H), 7.59 (d, J = 8.0 Hz, 1H), 7.65 (d, J = 8.0 Hz, 2H), 7.89-7.93 (m, 1H), 7.99 (d, J = 8.0 Hz, 1H), 8.03 (dd, J = 8.0, 1.6 Hz, 1H), 8.23 (d, J = 8.0 Hz, 1H), 8.51 (dd, J = 4.0, 1.6 Hz, 1H), 8.92 (d, J = 8.0 Hz, 1H), 9.83 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 116.47, 121.42, 121.79, 125.57, 126.37, 127.18, 127.41, 127.47, 127.67, 127.71, 127.99, 128.29, 128.87, 129.67, 130.40, 132.49, 133.63, 134.42, 125.99, 136.90, 138.23, 140.21, 147.92, 167.84; IR (KBr) 3353 m, 3048 w, 2923 w, 1660 s, 1594 w, 1515 s, 1481 s, 1423 m, 1384 m, 1332 m, 1257 w, 1218 w, 896 w, 865 w, 821 m, 765 m, 647 m; MS *m/z* (relative intensity, %) 374 (M^+, 14), 245 (10), 232 (18), 231 (100), 203 (17), 202 (34). HRMS Calcd for $C_{26}H_{18}N_2O$: 374.1419; Found: 374.1418.

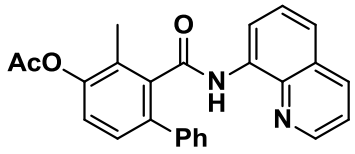
4,5-Dimethoxy-*N*-(quinolin-8-yl)-[1,1'-biphenyl]-2-carboxamide (10).



R_f 0.09 (hexane/EtOAc = 5/1). White solid. Mp = 159-160 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.98 (s,

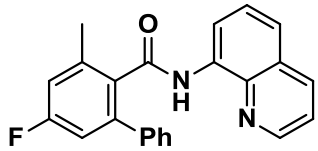
3H), 4.01 (s, 3H), 6.92 (s, 1H), 7.15 (t, J = 7.2 Hz, 1H), 7.26-7.33 (m, 3H), 7.43 (dd, J = 8.4, 0.8 Hz, 1H), 7.49-7.54 (m, 4 H), 8.04 (dd, J = 8.4, 1.6 Hz, 1H), 8.43 (dd, J = 4.0, 1.6 Hz, 1H), 8.82 (dd, J = 8.0, 0.8 Hz, 1H), 9.70 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 56.07, 56.11, 112.35, 113.13, 115.92, 121.26 (two overlapping peaks), 127.19, 127.50, 127.56, 127.81, 128.38, 129.25, 133.70, 134.53, 135.82, 138.30, 139.85, 147.49, 148.20, 150.40, 167.15; IR (KBr) 3309 m, 3010 m, 2967 w, 2935 w, 2846 w, 1662 s, 1600 m, 1529 s, 1482s, 1463 s, 1423 m, 1380 m, 1346 m, 1324 m, 1267 s, 1234 m, 1207 s, 1164 m, 1114 m, 1072 w, 1035 m, 825 w, 744 m, 903 m; MS *m/z* (relative intensity, %) 384 (M^+, 27), 242 (16), 241 (100). HRMS Calcd for $C_{24}H_{20}N_2O_3$: 384.1474; Found: 384.1469.

3-Methyl-2-(quinolin-8-ylcarbamoyl)-[1,1'-biphenyl]-4-yl acetate (11).



R_f 0.11 (hexane/EtOAc = 5/1). White solid. Mp = 179-180 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.34 (s, 3H), 2.38 (s, 3H), 7.08 (t, J = 7.2 Hz, 1H), 7.19-7.22 (m, 3H), 7.33 (d, J = 8.8 Hz, 1H), 7.43-7.53 (m, 4 H), 8.04 (dd, J = 8.4, 1.2 Hz, 1H), 8.60 (dd, J = 4.0, 1.2 Hz, 1H), 8.74 (dd, J = 7.2, 1.6 Hz, 1H), 9.68 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.31, 20.85, 116.36, 121.46, 122.98, 127.07, 127.34, 127.62, 128.09, 128.14, 128.55, 128.62, 134.10, 135.97, 137.51, 138.20, 138.32, 139.60, 147.99, 148.65, 167.16, 169.44; IR (KBr) 3334 m, 3062 w, 3025 w, 2931 w, 1756 m, 1670 s, 1594 w, 1517 s, 1481 s, 1423 m, 1371 m, 1321 m, 1255 w, 1197 s, 1164 m, 1014 m, 892 m, 827 m, 790 w, 759 m, 700 m; MS *m/z* (relative intensity, %) 397 (11), 396 (M^+, 38), 253 (57), 252 (11), 212 (15), 211 (100), 210 (13), 181 (10), 144 (11), 135 (10). HRMS Calcd for $C_{25}H_{20}N_2O_3$: 396.1474; Found: 396.1470.

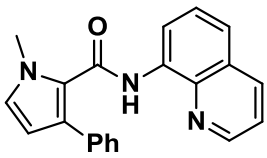
5-Fuoro-3-methyl-N-(quinolin-8-yl)-[1,1'-biphenyl]-2-carboxamide (12).



R_f 0.31 (hexane/EtOAc = 5/1). Colorless Oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.53 (s, 3H), 7.00 (dd, J = 8.8, 1.6 Hz, 1H), 7.11 (t, J = 7.6 Hz, 1H), 7.20-7.23 (m, 2H), 7.36 (dd, J = 8.8, 3.6 Hz, 1H), 7.45-7.52 (m, 4H), 8.07 (dd, J = 8.0, 1.6 Hz, 1H), 8.61 (dd, J = 4.4, 1.6 Hz, 1H), 8.75 (dd, J = 7.2, 1.6 Hz, 1H), 9.60 (brs,1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 19.98, 114.24 (d, J = 21.9 Hz), 116.15 (d, J = 21.0 Hz), 121.48, 121.77, 127.17, 127.69, 127.71, 128.33 (d, J = 10.5 Hz), 133.07 (d, J = 2.8 Hz), 134.17, 136.09, 138.3, 138.91 (d, J = 8.6 Hz), 139.28, 142.04 (d, J = 8.6 Hz), 147.99, 161.15, 163.62, 167.50; IR (neat) 3349 m, 1729 w, 1673 m, 1596 m, 1523 s, 1482 m, 1425 m, 1384 m, 1324 m, 1164

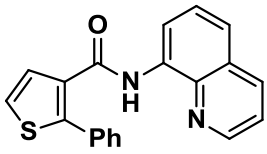
m, 757 m; MS *m/z* (relative intensity, %) 356 (M^+, 30), 214 (15), 213 (100), 183 (12). HRMS Calcd for $C_{23}H_{17}FN_2O$: 356.1325; Found: 356.1328.

1-Methyl-3-phenyl-*N*-(quinolin-8-yl)-1H-pyrrole-2-carboxamide (13).



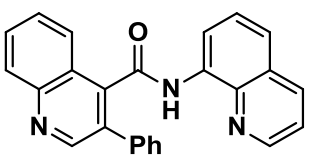
R_f 0.24 (hexane/EtOAc = 5/1). White solid. Mp = 107-108 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.05 (s, 3H), 6.22 (d, J = 2.8 Hz, 1H), 6.80 (d, J = 2.8 Hz, 1H), 7.23-7.30 (m, 4H), 7.40 (d, J = 8.0 Hz, 1H), 7.48-7.52 (m, 3H), 8.01 (dd, J = 8.0, 1.6 Hz, 1H), 8.22 (dd, J = 4.0, 1.6 Hz, 1H), 8.82 (dd, J = 8.0, 1.6 Hz, 1H), 9.86 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 37.23, 109.50, 115.57, 120.84, 121.14, 123.21, 126.97, 127.14 (two overlapping peaks), 127.68, 128.47, 129.61, 129.82, 134.94, 135.58, 135.65, 138.35, 147.36, 160.44; IR (KBr) 3295 m, 3045 w, 1656 s, 1598 w, 1525 s, 1481 s, 1400 s, 1324 s, 1274 m, 1209 m, 1116 m, 883 w, 825 m, 694s; MS *m/z* (relative intensity, %)327 (M^+, 37), 185 (13), 184 (100). HRMS Calcd for $C_{21}H_{17}N_3O$: 327.1372; Found: 327.1372.

2-Phenyl-*N*-(quinolin-8-yl)thiophene-3-carboxamide (14).



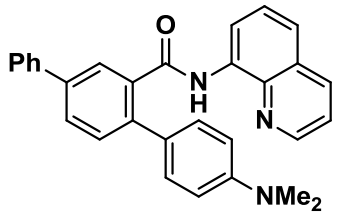
R_f 0.31 (hexane/EtOAc = 5/1). White solid. Mp = 101-102 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.29-7.39 (m, 5H), 7.44 (dd, J = 8.0, 2.0 Hz, 1H), 7.52 (t, J = 8.0 Hz, 1H), 7.59-7.62 (m, 2 H), 7.65 (d, J = 7.2 Hz, 1H), 8.06 (dd, J = 8.0, 2.0 Hz, 1H), 8.37 (dd, J = 4.0, 2.0 Hz, 1H), 8.85 (dd, J = 8.0, 1.6 Hz, 1H), 10.00 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 116.37, 121.30, 121.38, 124.64, 127.30, 127.71, 128.74, 128.76, 129.60, 129.99, 132.53, 132.53, 133.84, 134.46, 136.06, 138.24, 145.50, 147.50, 162.26; IR (KBr) 3299 m, 3126 w, 3043 w, 1654 s, 1529 s, 1428 m, 1425 m, 1384 m, 1324 m, 1265 m, 1076 w, 854 w, 829 w, 794 w, 755 m, 690 m; MS *m/z* (relative intensity, %) 330 (M^+, 23), 188 (12), 187 (100), 115 (28). HRMS Calcd for $C_{20}H_{14}N_2OS$: 330.0827; Found: 330.0828.

3-Phenyl-*N*-(quinolin-8-yl)quinoline-4-carboxamide (15).



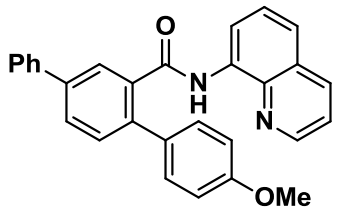
R_f 0.71 (EtOAc). Pale yellow solid. Mp = 77-78 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.23 (t, J = 7.6 Hz, 1H), 7.33-7.36 (m, 3H), 7.51-7.59 (m, 3H), 7.62 (t, J = 7.6 Hz, 1H), 7.67 (d, J = 8.0 Hz, 2H), 7.78 (t, J = 7.6 Hz, 1H), 8.08 (dd, J = 7.6 , 1.6Hz, 1H), 8.21 (t, J= 7.6 Hz, 2H), 8.54 (dd, J = 3.6, 1.6 Hz, 1H), 8.90 (dd, J = 7.6, 1.6 Hz, 1H), 9.11 (s, 1H), 9.90 (brs,1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 116.78, 121.61, 122.35, 124.30, 125.46, 127.14, 128.04, 128.27, 128.73, 129.65, 129.82, 130.80, 133.88, 136.14, 136.49, 138.17, 140.05, 147.41, 148.14, 151.72, 165.35; IR (KBr) 3326 w, 3054 w, 3008 w, 1671 m, 1596 w, 1577 w, 1523 s, 1481 s, 1423 m, 1384 m, 1322 m, 1255 m, 1203 m, 912 w, 877 w, 823 m, 754 w, 700 m; MS *m/z* (relative intensity, %) 376, (12), 375 (M^+, 43), 246 (12), 233 (17), 232 (100), 205 (15), 204 (64), 203 (12), 187 (13), 176 (20), 171 (12), 144 (11), 130 (21). HRMS Calcd for $C_{17}H_{14}N_2O_2$: 375.1372; Found: 375.1370.

4-(Dimethylamino)-*N*-(quinolin-8-yl)-[1,1':4',1''-terphenyl]-2'-carboxamide. (16a)



R_f 0.14 (hexane/EtOAc = 5/1). White solid. Mp = 174-175 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.81 (s, 6H), 6.63 (d, J = 8.8 Hz, 1H), 7.32 (dd, J = 8.0, 4.0 Hz, 1H), 7.37 (t, J = 7.6 Hz, 1H), 7.42-7.49 (m, 5H), 7.52-7.57 (m, 2H), 7.70 (d, J = 7.6 Hz, 2H), 7.75 (dd, J = 8.0, 1.6 Hz, 1H), 8.06 (dd, J = 8.0, 1.6 Hz, 1H), 8.12 (d, J = 2.0 Hz, 1H), 8.50 (dd, J = 4.0, 1.2 Hz, 1H), 8.87 (d, J = 8.0 Hz, 1H), 9.92 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 40.34, 112.39, 116.27, 121.24, 121.35, 127.02, 127.16, 127.25, 127.49, 127.66, 127.85, 128.84, 128.93, 129.72, 130.92, 134.73, 135.88, 135.92, 138.49, 139.30, 139.34, 140.03, 147.67, 150.11, 168.41; IR (KBr) 3297 m, 3054 w, 3023 w, 2956 w, 2883 w, 2846 w, 2794 w, 1662 s, 1606 m, 1517 s, 1479 s, 1421 m, 1380 m, 1348 m, 1322 m, 1255 m, 1216 m, 813 m, 788 m, 755 m, 696 m; MS *m/z* (relative intensity, %) 444 (22), 443 (M^+, 65), 301 (23), 300 (100), 221 (13). HRMS Calcd for $C_{30}H_{25}N_3O$: 443.1998; Found: 443.2000.

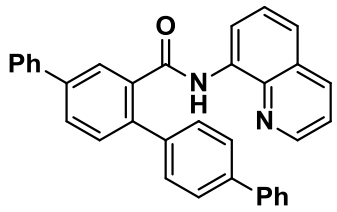
4-Methoxy-*N*-(quinolin-8-yl)-[1,1':4',1''-terphenyl]-2'-carboxamide (16b).



R_f 0.17 (hexane/EtOAc = 5/1). White solid. Mp = 134-135 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.63 (s, 3H), 6.82 (d, J = 8.0 Hz, 1H), 7.31-7.39 (m, 2H), 7.44-7.54 (m, 7H), 7.69 (d, J = 7.2 Hz, 1H), 7.76

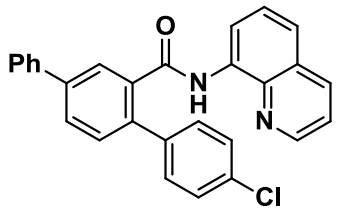
(dd, J = 8.0, 2.0 Hz, 1H), 8.05 (dd, J = 8.0, 1.6 Hz, 1H), 8.14 (d, J = 1.6 Hz, 1H), 8.51 (dd, J = 4.0, 2.0 Hz, 1H), 8.85 (dd, J = 8.0, 1.2 Hz, 1H), 9.88 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 55.07, 113.91, 116.25, 121.35, 121.52, 127.02, 127.20, 127.64, 127.81, 128.86, 128.95, 130.08, 131.07, 131.85, 134.48, 135.93, 136.21, 138.35, 138.62, 139.80, 140.01,147.69, 159.31, 167.93; IR (KBr) 3313 w, 3027 w, 2931 w, 2832 w, 1662 m, 1604 m, 1523 s, 1479 s, 1421 m, 1380 m, 1294 m, 1245 s, 1176 m, 1106w, 1033 m, 908 w, 825 m, 788 m, 759 m; MS *m/z* (relative intensity, %) 430 (M^+, 30), 288 (21), 287 (100), 215 (22). HRMS Calcd for $C_{29}H_{22}N_2O_2$: 430.1681; Found: 430.1684.

_N_-(quinolin-8-yl)-[1,1':4',1'':4'',1'''-quaterphenyl]-2''-carboxamide (16c).



R_f 0.20 (hexane/EtOAc = 5/1). White solid. Mp = 219-220 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.24-7.31 (m, 2H), 7.34-7.41 (m, 5H), 7.45-7.55 (m, 6H), 7.63 (t, J = 7.6 Hz, 3H), 7.72 (d, J = 7.6 Hz, 2H), 7.81 (dd, J = 7.6, 1.6 Hz, 1H), 8.03 (dd, J = 7.6, 1.6 Hz, 1H), 8.18 (d, J = 2.0 Hz, 1H), 8.45 (dd, J = 3.6, 1.6 Hz, 1H), 8.85 (d, J = 7.6 Hz, 1H), 9.93 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 116.36, 121.37, 121.63, 126.98, 127.12, 127.21, 127.24, 127.68, 127.78, 128.00, 128.62, 12 8.94, 129.12, 131.17, 134.47, 135.93, 136.39, 138.37, 138.49, 138.60, 139.80, 140.56 (three overlapping peaks), 147.78, 167.78; IR (KBr) 3311 m, 3050 w, 3025 w, 1658 s, 1521 s, 1477 s, 1421 m, 1382 m, 1322 m, 1255 m, 908 w, 825 m, 763 s, 692 m; MS *m/z* (relative intensity, %) 477 (15), 2476 (M^+, 39), 334 (27), 333 (100), 289 (10), 238 (14). HRMS Calcd for $C_{34}H_{24}N_2O$: 476.1889; Found: 476.1885.

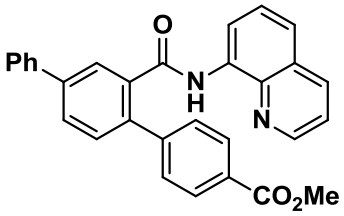
4-Chloro-_N_-(quinolin-8-yl)-[1,1':4',1''-terphenyl]-2'-carboxamide (16d).



R_f 0.29 (hexane/EtOAc = 5/1). White solid. Mp = 179-180 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.26 (d, J = 7.6 Hz, 2H), 7.33-7.40 (m, 2H), 7.50-7.54 (m, 7H), 7.68 (d, J = 7.6 Hz, 2H), 7.77 (dd , J = 8.4, 2.0 Hz, 1H), 8.06 (dd, J = 8.4, 1.6 Hz, 1H), 8.15 (d, J = 2.0 Hz, 1H), 8.53 (dd, J = 4.4, 2.0 Hz, 1H), 8.83 (dd, J = 7.6, 1.6 Hz, 1H), 9.87 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 116.35, 121.48, 121.76, 127.04, 127.16, 127.67, 127.83, 127.87, 128.60, 128.91, 129.08, 13

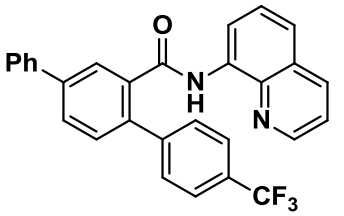
0.22, 131.02, 133.83, 134.24, 136.02, 136.29, 137.67, 138.02, 138.27, 139.54, 140.79, 147.82, 167.34; IR (KBr) 3361 m, 3060 w, 3029 w, 1677 s, 1590 w, 1529 s, 1481 s, 1423 m, 1384 m, 1328 m, 1259 w, 1240 w, 1220 w, 1091 m, 1000 w, 906 w, 821 m, 786 m, 759 m; MS *m/z* (relative intensity, %) 436 (15), 435 (15), 434 (M^+, 39), 293 (34), 292 (22), 291 (100), 256 (20), 228 (40), 226 (16), 200 (12). HRMS Calcd for $C_{28}H_{19}ClN_2O$: 434.1186; Found: 434.1181.

Methyl 2'-(quinolin-8-ylcarbamoyl)-[1,1':4',1''-terphenyl]-4-carboxylate (16e).



R_f 0.14 (hexane/EtOAc = 5/1). White solid. Mp = 166-167°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.25 (d, J = 1.6 Hz, 1H), 7.34 (dd, J = 8.0, 4.4 Hz, 1H), 7.41 (t, J = 8.0 Hz, 1H), 7.47-7.59 (m, 5H), 7.64 (d, J = 7.12 Hz, 2H), 7.71 (d, J = 8.0 Hz, 2H), 7.82 (d, J = 8.0 Hz, 1H), 7.98 (d, J = 8.0 Hz, 2H), 8.08 (d, J = 8.0 Hz, 1H), 8.15 (s, 1H), 8.52 (d, J = 4.8 Hz, 1H), 8.80 (d, J = 8.0 Hz, 1H), 9.87 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 52.05, 116.38, 121.47, 121.80, 127.13, 127.23, 127.71, 127.79, 127.94, 128.97 (two overlapping peaks), 129.12, 129.19, 129.72, 131.06, 134.24, 136.08, 136.63, 137.93, 138.29, 139.57, 141.20, 144.38, 147.87, 166.78, 167.35; IR (KBr) 34496 w, 3367 m, 3031 w, 2954 w, 1720 s, 1679 s, 1604 w, 1525 s, 1481 m, 1427 m, 1384 m, 1282 s, 1186 m, 1106 m, 908 w, 871 w, 827 m, 755 m; MS *m/z* (relative intensity, %) 459 (34), 458 (M^+, 100), 457 (24), 316 (16), 315 (69), 283 (18), 272 (22), 271 (86), 257 (12), 256 (55), 228 (27), 227 (14), 226 (25). HRMS Calcd for $C_{30}H_{22}N_2O_3$: 458.1630; Found: 458.1633.

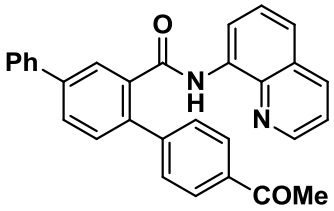
***N*-(Quinolin-8-yl)-4-(trifluoromethyl)-[1,1':4',1''-terphenyl]-2'-carboxamide. (16f)**



R_f 0.34 (hexane/EtOAc = 5/1). White solid. Mp = 169-170 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.34 (dd, J = 8.4, 4.0 Hz, 1H), 7.40 (t, J = 7.2 Hz, 1H), 7.47-7.56 (m, 7H), 7.65-7.72 (m, 4H), 7.81 (dd, J = 8.0, 1.6 Hz, 1H), 8.07 (dd, J = 8.0, 1.6 Hz, 1H), 8.18 (d, J = 1.6 Hz, 1H), 8.48 (dd, J = 4.0, 1.6 Hz, 1H), 8.81 (dd, J = 8.4, 0.8 Hz, 1H), 9.85 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 116.34, 121.45, 121.86, 123.99 (q, J = 270 Hz), 125.30 (d, J = 38 Hz), 127.08, 127.14, 127.65, 127.94, 128.95, 129.20, 129.30, 129.61 (q, J = 32.4 Hz), 131.08, 134.13, 136.05, 136.47, 137.50, 138.21, 139.43,

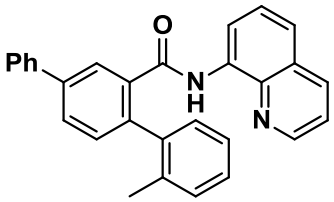
141.27, 143.28, 147.83, 167.12; IR (KBr) 3359 m, 3031 w, 2996 w, 1679 m, 1612 w, 1577 w, 1527 s, 1481 m, 1423 w, 1384 w, 1326 s, 1218 w, 1159 m, 1108 s, 1070 m, 906 w, 862 w, 825 m, 786 m, 759 m; MS *m/z* (relative intensity, %) 469 (13), 468 (M^+, 40), 326 (21), 325 (100), 228 (17). HRMS Calcd for $C_{29}H_{19}F_3N_2O$: 468.1449; Found: 468.1451.

4-Acetyl-*N*-(quinolin-8-yl)-[1,1':4',1''-terphenyl]-2'-carboxamide. (16g)



R_f 0.09 (hexane/EtOAc = 5/1). White solid. Mp =177-178 °C. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 2.46 (s, 1H), 7.34 (dd, J = 8.0, 4.0 Hz, 1H), 7.40 (t, J = 8.0 Hz, 1H), 7.47-7.58 (m, 5H), 7.65 (d, J = 8.0 Hz, 2H), 7.70 (d, J = 8.0 Hz, 2H), 7.82 (dd, J = 6.4, 2.0 Hz, 1H), 7.89 (d, J = 8.0 Hz, 2H), 8.08 (d, J = 8.0 Hz, 2H), 8.15 (d, J = 1.2 Hz, 1H), 8.51 (d, J = 4.0 Hz, 1H), 8.81 (d, J = 7.2 Hz, 1H), 9.90 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 26.53, 116.42, 121.46, 121.82, 127.10, 127.24, 127.70, 127.73, 127.95, 128.46, 128.96, 129.14 (two overlapping peaks), 130.99, 134.24, 136.01, 136.10, 136.62, 137.87, 138.27, 139.52, 141.25, 144.55, 147.82, 167.35, 197.65; IR 1679 s, 1604 m, 1523 s, 1484 m, 1424 m, 1384 w, 1326 m, 1265 m, 827 m, 756 s; MS *m/z* (relative intensity, %) 443 (23), 442 (M^+, 67), 441 (14), 299 (34), 258 (20), 257 (100), 228 (12), 43 (21); HRMS Calcd for $C_{30}H_{22}N_2O_2$: 442.1681; Found: 442.1679.

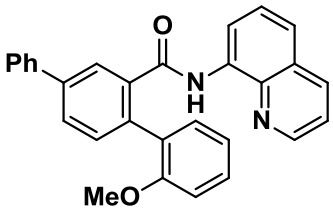
2-Methyl-*N*-(quinolin-8-yl)-[1,1':4',1''-terphenyl]-2'-carboxamide (17a).



R_f 0.26 (hexane/EtOAc = 5/1). White solid. Mp = 124-125 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.32 (s, 3H), 7.10-7.17 (m, 2 H), 7.22 (t, J = 7.6 Hz, 1H), 7.34 (dd, J = 8.0, 4.0 Hz, 1H), 7.38-7.44 (m, 4H), 7.49 (t, J = 8.0 Hz, 3H), 7.74 (d, J = 8.0 Hz, 2H), 7.79 (dd, J = 8.0, 1.6 Hz, 1H), 8.04 (dd, J = 8.0, 1.6 Hz, 1H), 8.23 (d, J = 1.6 Hz, 1 H), 8.56 (dd, J = 4.0, 1.6 Hz, 1H), 8.83 (dd, J = 8.0, 1.6 Hz, 1H), 9.89 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 20.22, 116.15, 121.35, 121.43, 125.86, 127.08, 127.21, 127.58, 127.69, 127.87, 128.88, 128.91, 129.91, 129.90, 130.25, 131.67, 134.54 135.88, 136.88, 136.46, 138.34, 139.29, 13985, 140.41, 147.52, 167.00; IR (KBr) 3309 w. 3054 w, 1660 m, 1598 w, 1525 s, 1481 s, 1423 m, 1380 m, 1324 m, 1255 m, 1220 m, 908 w, 823 m, 790 m, 757 s; MS *m/z*

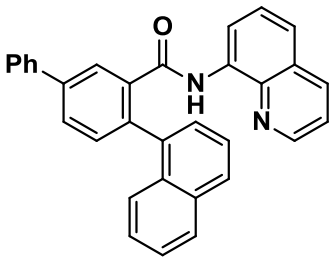
(relative intensity, %) 414 (M^+, 7), 272 (13), 271 (61), 228 (13), 166 (11), 145 (15), 144 (100). HRMS Calcd for $C_{29}H_{22}N_2O$: 414.1732; Found: 414.1735.

2-Methoxy-*N*-(quinolin-8-yl)-[1,1':4',1''-terphenyl]-2'-carboxamide (17b).



R_f 0.11 (hexane/EtOAc = 5/1). White solid. Mp = 162 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.56 (s, 3H), 6.66 (d, J = 8.0 Hz, 1H), 7.03 (t, J = 7.6 Hz, 1H), 7.17 (t, J = 7.6 Hz, 1H), 7.34-7.7.40 (m, 2H), 7.44-7.54 (m, 6H), 7.72 (d, J = 8.0 Hz, 2H), 7.81 (dd, J = 8.0, 1.6 Hz, 1H), 8.08 (d, J = 8.0 Hz, 1H), 8.18 (d, J = 1.6 Hz, 1H), 8.52 (d, J = 4.0 Hz, 1H), 8.86 (d, J = 7.6 Hz, 1H), 10.01 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 55.22, 120.90, 121.17, 121.35, 127.14, 127.21, 127.29, 127.60, 127.66, 128.55, 128.85, 129.15, 129.39, 131.01, 131.85, 134.76, 135.36, 135.92, 137.23, 138.66, 140.07, 140.45, 147.73, 156.38, 167.65; IR (KBr) 3315 w, 3052 w, 3302 w, 2993 w, 2832 w, 1664 m, 1598 w, 1523 s, 1481 s, 1425 m, 1380 m, 1324 m, 1245 m, 1124 w, 1105 w, 1024 m, 823 w, 790 w, 752 s, 694 m; MS *m/z* (relative intensity, %) 430 (M^+, 3), 400 (25), 399 (97), 398 (79), 397 (16), 288 (22), 287 (100), 273 (11), 272 (55), 244 (22), 215 (25),156 (14). HRMS Calcd for $C_{29}H_{22}N_2O_2$: 430.1681; Found: 430.1683.

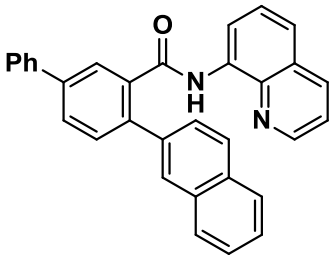
4-(Naphthalen-1-yl)-*N*-(quinolin-8-yl)-[1,1'-biphenyl]-3-carboxamide (18).



R_f 0.26 (hexane/EtOAc = 5/1). White solid. Mp = 232-234 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.20 (dd, J = 8.0, 4.0 Hz, 1H), 7.31 (d, J = 8.0 Hz, 1H), 7.36-7.61 (m, 10H), 7.1-7.86 (m, 5H), 7.93 (t, J = 8.0 Hz, 2H), 8.10 (d, J = 4.0 Hz, 1H), 8.40 (s, 1H), 8.69 (d, J = 8.0 Hz, 1H),9.78 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 115.98, 121.10, 121.28, 125.27, 125.84, 126.39, 127.00, 127.12 (two overlapping peaks), 127.36, 127.57, 127.76, 128.20, 128.25, 128.80, 128.92 (two overlapping peaks), 132.20, 132.55, 133.74, 135.66, 137.10, 137.28, 137.37, 138.00, 139.83, 140.82, 147.30, 166.85; IR (KBr) 3432 w, 3311 w, 3056 w, 3033 w, 1662 s, 1598 w, 1527 s, 1481 m, 1423 m, 1386 m, 1326 m, 1257 w, 1222 w, 906 w, 784 m, 757 m, 692 m; MS *m/z* (relative intensity, %) 451 (14),

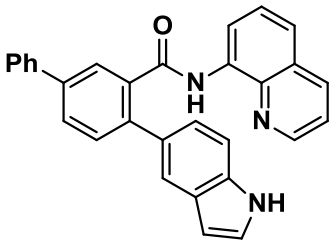
450 (M^+, 41), 308 (25), 307 (100), 276 (10), 144 (14). HRMS Calcd for $C_{32}H_{22}N_2O$: 450.1732; Found: 450.1730.

4-(Naphthalen-2-yl)-*N*-(quinolin-8-yl)-[1,1'-biphenyl]-3-carboxamide. (19)



R_f 0.26 (hexane/EtOAc = 3/1). White solid. Mp = 191-192 °C. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 7.10 (dd, J = 8.0, 4.0 Hz, 1H), 7.39-7.44 (m, 3H), 7.47-7.53 (m, 4H), 7.56-7.69 (m, 4H), 7.73-7.76 (m, 3H), 7.85 (dd, J = 8.0, 2.0 Hz, 1H), 7.94 (t, J = 7.2 Hz, 2H), 8.14 (s, 1H), 8.28 (d, J = 1.6 Hz, 1H), 8.80 (d, J = 8.0, 1H), 9.84 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 116.27, 121.15, 121.50, 125.99, 126.13, 127.07, 127.12, 127.18, 127.45, 127.58, 127.77, 128.01, 128.11, 128.17, 128.33, 128.93, 129.19, 131.52, 132.82, 133.62, 134.37, 135.62, 136.21, 137.22, 138.27, 139.03, 139.80, 140.63, 147.40, 167.40; IR (KBr) 3305 m, 3050 w, 1662 s, 1598 w, 1527 s, 1481 m, 1421 m, 1386 m, 1326 m, 1259 m, 1222 m, 898 w, 823 m, 759 m, 700m; MS *m/z* (relative intensity, %) 451 (14), 450 (M^+, 39), 308 (24), 307 (100), 278 (19), 277 (12), 276 (13), 226 (14), 144 (29). HRMS Calcd for $C_{32}H_{22}N_2O$: 450.1732; Found: 450.1737.

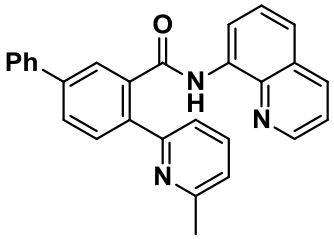
4-(1H-Indol-5-yl)-*N*-(quinolin-8-yl)-[1,1'-biphenyl]-3-carboxamide (20).



R_f 0.31 (CH_2Cl_2). White solid. Mp = 207-208 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.60 (s, 1H), 7.13-7.18 (m, 3H), 7.28 (dd, J = 8.4, 1.2 Hz, 1H), 7.37-7.40 (m, 2H), 7.46-7.50 (m, 3H), 7.62 (d, J = 8.4 Hz, 1H), 7.73 (d, J = 8.4 Hz, 2H), 7.79 (dd, J = 8.0, 1.6 Hz, 1H), 7.93 (s, 1H), 7.96 (dd, J = 8.4, 1.2 Hz, 1H), 8.02 (dd, J = 4.0, 1.6 Hz, 1H), 8.12 (brs, 1H), 8.23 (d, J = 2.0 Hz, 1H), 8.83 (dd, J = 8.0, 1.2 Hz, 1H), 9.88 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 103.05, 11.05, 116.25, 121.12, 121.30, 121.37, 123.62, 124.51, 127.10, 127.15, 127.51, 127.56, 128.16, 128.32, 128.87, 128.96, 131.39, 13 1.75, 134.64, 135.50, 135.61, 136.17, 138.35, 139.78, 140.04, 140.40, 147.50, 168.03; IR (KBr) 3305 m, 3029 w, 1644 s, 1531 s, 1482 m, 1423 m, 1324 m, 1095 w, 889 w, 757 m, 700 m; MS *m/z*

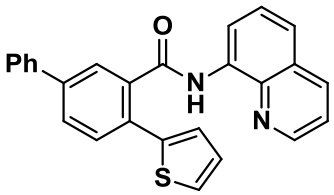
(relative intensity, %) 440 (32), 406 (M^+, 32), 297 (22), 296 (100), 295 (30), 241 (11), 220 (13), 144 (27). HRMS Calcd for $C_{30}H_{21}N_3O$: 439.1685; Found: 439.1685.

4-(6-Methylpyridin-2-yl)-*N*-(quinolin-8-yl)-[1,1'-biphenyl]-3-carboxamide. (21)



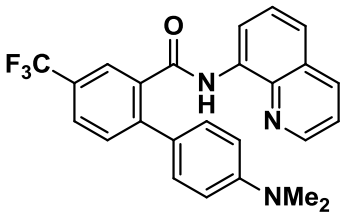
R_f 0.11 (hexane/EtOAc = 5/1). Pale Blue Oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.36 (s, 3H), 6.89 (dd, J = 7.2, 1.6 Hz, 1H), 7.33-7.49 (m, 7H), 7.69 (d, J = 7.2 Hz, 2H), 7.80 (d, J – 0.8 Hz, 1H), 8.06-8.09 (m, 2H), 8.58 (dd, J = 4.0, 1.6 Hz, 1 H), 8.84 (d, J = 8.0 Hz, 1H), 9.96 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 24.35, 116.31, , 120.14, 121.38, 121.43, 121.66, 127.11, 127.20, 127.28, 127.67, 127.77, 128.81, 128.86, 130.38, 134.70, 135.95, 136.45, 137.22, 137.89, 138.34, 139.79, 141.35, 14 7.87, 156.43, 158.01, 168.39; IR (neat) 3342 m, 3058 w, 3010 w, 1733 w, 1675 s, 1575 m, 1523 s, 1482 s, 1452 m, 1425 m, 1384 m, 1326 m, 1245 m, 916 w, 827 m, 796 m, 761 s: MS *m/z* (relative intensity, %) 417 (31), 416 (M^+, 100), 273 (16), 272 (75). HRMS Calcd for $C_{28}H_{21}N_3O$: 415.1685; Found: 416.1766.

***N*-(quinolin-8-yl)-4-(thiophen-2-yl)-[1,1'-biphenyl]-3-carboxamide. (22)**



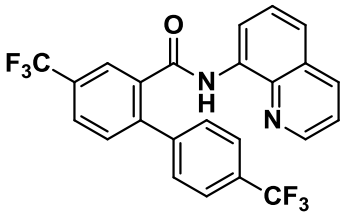
R_f 0.29 (hexane/EtOAc = 5/1). White solid. Mp = 68-69 °C. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 6.90-6.92 (m, 1H), 7.23-7.27 (m, 2H), 7.37-7.41 (m, 2H), 7.46-7.60 (m, 4H), 7.68 (t, J = 8.0 Hz, 3H), 7.76 (dt, J = 8.0, 2.0 Hz, 1H), 8.04 (s, 1H), 8.12 (dd, J = 8.0, 1.6 Hz, 1H), 8.62 (dd, J = 4.0, 2.0 Hz, 1H), 8.90 (d, J = 8.0 Hz, 1H), 10.5 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 166.52, 121.54, 121.78, 126.36, 127.05, 127.14, 127.31, 127.41, 127.70, 127.78, 127.87, 128.79, 128.94, 131.17, 131.28, 134.50, 136.10, 136.73, 138.40, 139.60, 140.71, 140.82, 147.98, 167.76; IR (KBr) 3434 w, 3326 w, 3052 w, 1668 m, 1596 w, 1523 s, 1481 s, 1423 m, 1382 m, 1324 m, 1257 m, 1222 w, 906 w, 825m, 790 w, 761 m, 696 m; MS *m/z* (relative intensity, %) 407 (13), 406 (M^+, 40), 264 (1119), 263 (100), 235 (15), 234 (24), 202 (11). HRMS Calcd for $C_{26}H_{18}N_2OS$: 406.1140; Found: 406.1141.

4'-(Dimethylamino)-*N*-(quinolin-8-yl)-4-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxamide. (25)



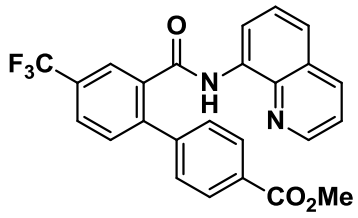
R_f 0.11 (hexane/EtOAc = 5/1). White solid. Mp = 169-170 °C. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 2.81 (s, 6H), 6.61 (d, J = 8.8 Hz, 2H), 7.30 (dd, J = 8.4, 4.0 Hz, 1H), 7.39 (d, J = 8.8 Hz, 2H), 7.46-7.60 (m, 3H), 7.75 (dd, J = 8.4, 1.2 Hz, 1H), 8.06 (dd, J = 8.4, 1.2 Hz, 1H), 8.16 (d, J = 0.8 Hz, 1H), 8.48 (dd, J = 4.0, 1.2 Hz, 1H), 8.83 (dd, J = 8.4, 1.2 Hz, 1H), 9.86 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 40.19, 112.29, 116.42, 121.30, 121.66, 124.00 (q, J = 270 Hz), 125.86, 126.56 (d, J = 3.8 Hz), 126.94 (d, J = 2.9 Hz), 127.20, 127.65, 128.65 (q, J = 32.4 Hz),129.77, 130.84, 134.38, 135.77, 135.91, 138.43, 143.85, 147.70, 150.53, 166.98; IR (KBr) 3305 w, 2985 w, 2815 w, 1664 m, 1608 m, 1527 s, 1486 m, 1357m, 1324 s, 1253 m, 1162 m, 1112 m, 919w, 815 w, 690m; MS *m/z* (relative intensity, %) 436 (20), 435 (M^+, 73), 306 (16), 293 (17), 292 (100). HRMS Calcd for $C_{25}H_{20}F_3N_3O$: 435.1558; Found: 435.1559.

_N_-(Quinolin-8-yl)-4,4'-bis(trifluoromethyl)-[1,1'-biphenyl]-2-carboxamide. (27)



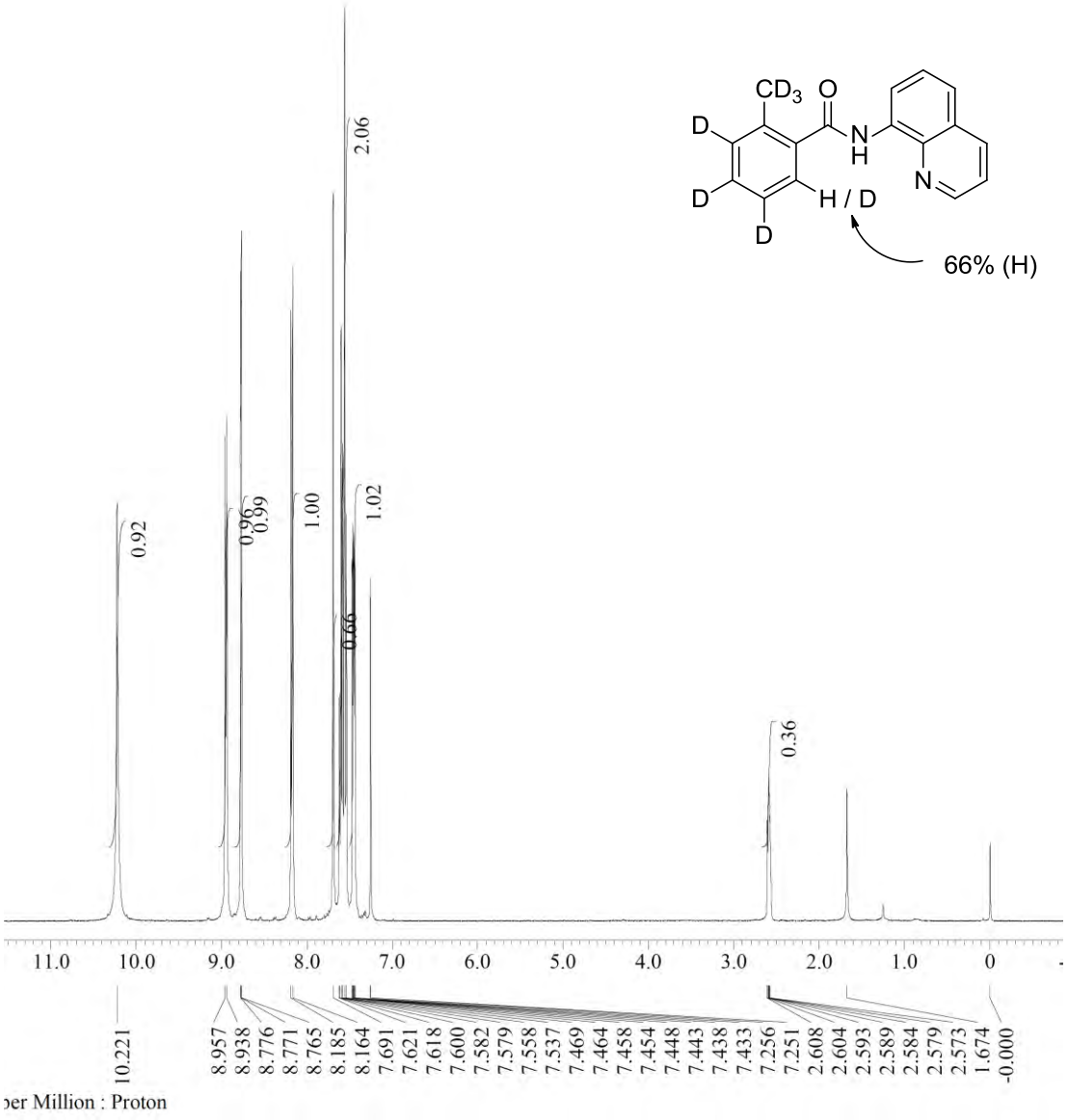
R_f 0.43 (hexane/EtOAc = 5/1). White solid. Mp = 137-138 °C. ^{1}H NMR ($CDCl_3$, 399.78 MHz) δ 7.37 (dd, J = 8.8, 4.8 Hz, 1H), 7.52-7.66 (m, 7H), 7.85 (dd, J = 8.0, 1.6 Hz, 1H), 8.10 (dd, J = 8.4, 1.6 Hz, 1H), 8.24 (dd, J = 0.8 Hz, 1H), 8.49 (dd, J = 4.0, 1.6 Hz, 1H), 8.76 (dd, J = 6.4, 1.6 Hz, 1H), 9.78 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100.53 MHz) δ 116.58, 121.59, 122.24, 123.62 (q, J = 271 Hz), 123.82 (q, J = 271 Hz), 125.58 (d, J = 3.8 Hz), 126.66 (d, J = 3.8 Hz), 127.18, 127.38 (d, J = 3.8 Hz), 127.71, 129.33 (two overlapping peaks), 130.81 (q, J = 32.4 Hz, two overlapping peaks), 131.16, 133.81, 136.18, 136.67, 138.21, 142.10, 142.18 (d, J = 15.3 Hz), 147.95, 165.60; IR 1670 m, 1618 w, 1525 s, 1485 m, 1425 w, 1386 w, 1322 s, 1258 m, 1168 m, 1124 s, 1069 m, 917 w, 826 m; MS *m/z* (relative intensity, %) 461 (19), 460 (M^+, 74), 459 (41), 319 (16), 317 (100), 269 (33), 220 (29), 171 (32), 144 (22). HRMS Calcd for $C_{27}H_{13}F_6N_2O$: 460.1010; Found: 460.1005.

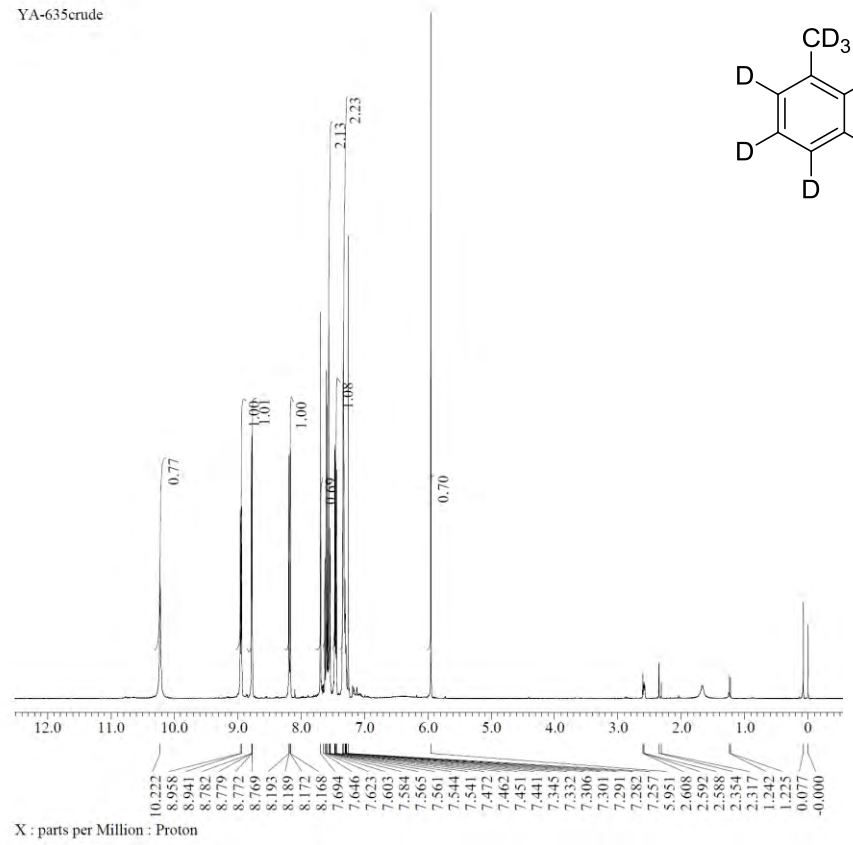
Methyl 2'-(quinolin-8-ylcarbamoyl)-4'-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate (29).

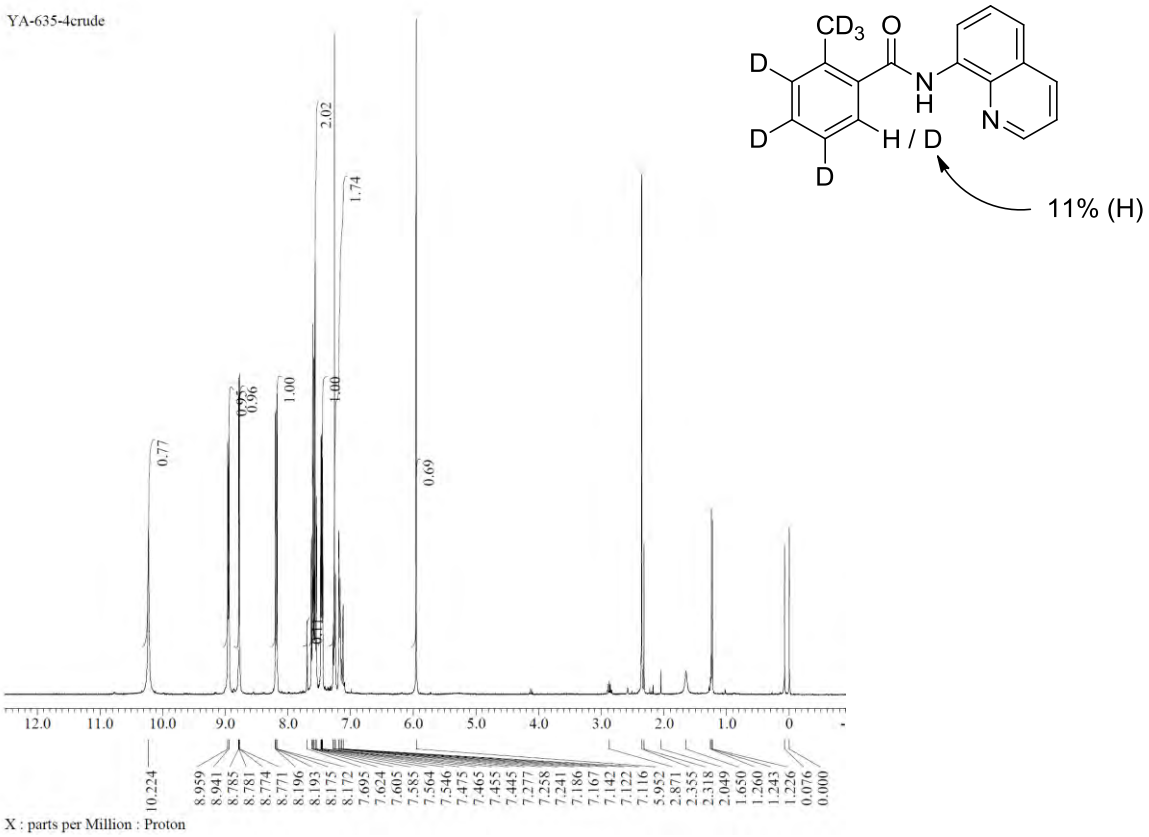


R_f 0.14 (hexane/EtOAc = 5/1). White solid. Mp = 171-172 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.84 (s, 3H), 7.36 (dd, J = 7.6, 4.0 Hz, 1H), 7.48-7.55 (m, 3H), 7.62 (t, J = 7.6 Hz, 3H), 7.84 (d, J = 8.0 Hz, 1H), 7.99 (d, J = 8.0 Hz, 1H), 8.09 (dd, J = 8.0, 1.2 Hz, 1H), 8.21 (s, 1H), 8.51 (dd, J = 4.4, 1.2 Hz, 1H), 8.76 (dd, J = 6.4, 2.0 Hz, 1H), 9.80 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 52.14, 116.55, 121.56, 122.16, 123.64 (q, J = 270 Hz), 126.45 (d, J = 2.8 Hz), 127.19, 127.42, 127.71, 128.92, 129.89, 129.96, 130.59 (q, J = 33.4 Hz), 131.09, 133.86, 136.14, 136.70, 138.22, 142.49, 143.21, 147.93, 165.79, 166.54; IR (KBr) 3343 m, 3050 w, 2954 w, 1724 s, 1681 s, 1610 w, 1529 s, 1484 m, 1428 m, 1388 m, 1334 s, 1286 s, 1224 w, 1172 m, 1120 s, 827 m, 788 w: MS *m/z* (relative intensity, %) 451 (27), 450 (M^+, 100), 449 (64), 264 (17), 636 (80), 248 (25), 219 (13), 1771 (42), 144 (44), 130. (10). HRMS Calcd for $C_{25}H_7F_3N_2O_3$: 450.1191; Found: 450.1187.

VI. Deuterium Labeling Experiments (eq. 4 and 5)



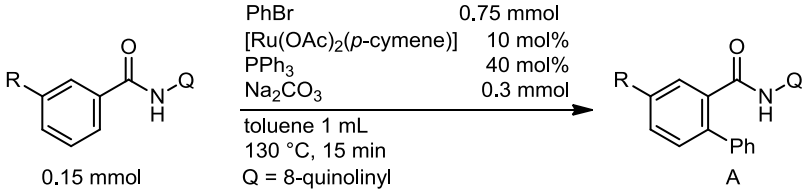

YA-635crude
CD3
O
N
H
D
D
D
H / D
N
70%(H)
X : parts per Million : Proton


YA-635-4crude
CD3
O
N
H
D
D
D
H / D
N
11% (H)
X : parts per Million : Proton

VII. Hammett plot of *m*-XC_6H_4CONHQ(Q = 8-quinolinyl) 7a-f with PhBr

To an oven-dried 5 mL screw-capped vial, 3-methyl-*N*-(8-quinolinyl)benzamide 7d (39mg, 0.15 mmol), bromobenzene (118 mg, 0.75 mmol), $[Ru(OAc)_2(p\text{-cymene})]_2$ (5 mg, 0.015 mmol), PPh_3 (16 mg, 0.06 mmol), Na_2CO_3 (32 mg, 0.3 mmol) and toluene (1 mL) were added under a gentle stream of nitrogen. The mixture was stirred for 15 min at 130 °C. After the reaction was finished, the screw-capped vial was cooled by ice bath. The mixture was filtered through a celite pad and concentrated *in vacuo*. The residue was analyzed by ^1H NMR spectroscopy. Conversions of starting materials were determined using tetrachloroethane as an internal standard.

Table S1.



	A	SM	conversion
R = NMe_2	3.6%	82.6%	17.4%
R = OMe	16.3%	69.5%	30.5%
R = Me	16.8%	70.4%	29.6%
R = Ph	22.2%	60.2%	39.8%
R = H	26.1%	57.9%	42.1%
R = CF_3	41.7%	45.1%	54.9%

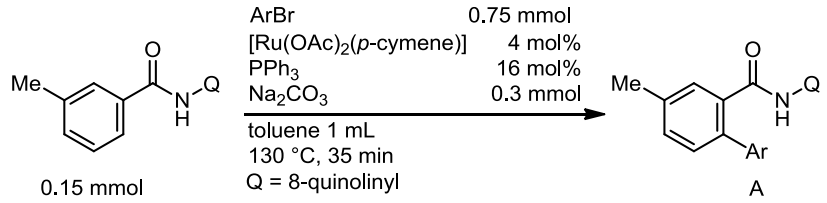
NMR yeild

	σ_p	log (conv. X / conv. H)
NMe_2	-0.83	-0.3837
OMe	-0.27	-0.1399
Me	-0.17	-0.1537
Ph	-0.01	0.02484
H	0	0
CF_3	0.54	0.1152

VIII. Hammett plot of 7d with *p*-X-C_6H_4Br

To an oven-dried 5 mL screw-capped vial, 3-methyl-*N*-(8-quinolinyl)benzamide 7d (39mg, 0.15 mmol), bromobenzene (118 mg, 0.75 mmol), $[Ru(OAc)_2(p\text{-cymene})]_2$ (2 mg, 0.06 mmol), PPh_3 (6 mg, 0.024 mmol), Na_2CO_3 (32 mg, 0.3 mmol) and toluene (1 mL) were added under a gentle stream of nitrogen. The mixture was stirred for 35 min at 130 °C. After completion of the reaction, the screw-capped vial was cooled in an ice bath. The mixture was filtered through a celite pad and concentrated *in vacuo*. The residue was analyzed by ^1H NMR spectroscopy. Conversions of starting materials were determined using tetrachloroethane as an internal standard.

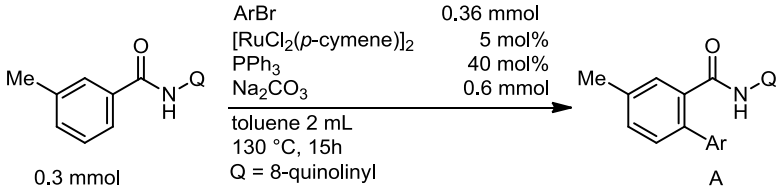
Table S2



	A	SM	conversion		σ⁻	log (con. X / conv. H)
R = OMe	28.3%	65.7%	34.3%	OMe	-0.26	0.07140
R = NMe_2	29.0%	71.4%	28.6%	NMe_2	-0.12	-0.007527
R = F	22.8%	75.7%	24.3%	F	-0.03	-0.07829
R = H	18.9%	70.9%	29.1%	H	0	0
R = Cl	18.6%	78.8%	21.2%	Cl	0.19	-0.1376
R = OTf	12.4%	86.8%	13.2%	OTf	0.49	-0.3433
R = CF_3	10.0%	87.1%	12.9%	CF_3	0.65	-0.3533
R = CO_2Me	25.8%	70.9%	29.1%	COOMe	0.75	0
R = COMe	29.8%	67.7%	32.3%	COMe	0.84	0.04531

NMR yeild

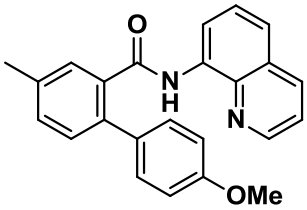
Spectroscopic Data for Arylated Products



	Isolated yeild
R = OMe	86%
R = NMe_2	76%
R = F	78%
R = H	74%
R = Cl [a]	80%
R = OTf [a]	70%
R = CF_3	76%
R = CO_2Me	78%
R = COMe	87%

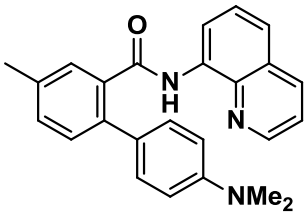
[a] Run at 130 °C for24h

4'-Methoxy-4-methyl-N-(quinolin-8-yl)-[1,1'-biphenyl]-2-carboxamide



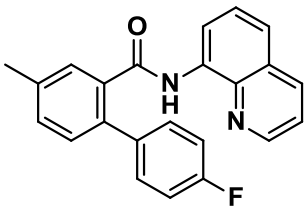
R_f 0.20 (hexane/EtOAc = 5/1). Colorless Oil ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.45 (s, 3H), 3.62 (s, 3H), 6.89 (d, J = 8.4 Hz, 2H), 7.24-7.36 (m, 3H), 7.43 (t, J = 8.4 Hz, 3H), 7.51 (t, J = 8.4 Hz, 1H), 7.71 (s, 1H), 8.50 (d, J = 1.6 Hz, 1H), 8.82 (d, J = 7.6 Hz, 1H), 9.78 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 20.97, 55.5, 113.82, 116.21, 121.29, 121.37, 127.20, 127.65, 129.73, 129.73, 130.06, 130.48, 131.21, 132.26, 134.56, 135.62, 135.91, 136.93, 137.03, 138.37, 147.62, 159.10, 168.16; IR (neat) 3325 m, 2837 w, 1709 m, 1666 s, 1610 w, 1523 S, 1484 s, 1425 m, 1382 w, 1247 m, 1178 w, 1037 w, 825 m, 755 s; MS *m/z* (relative intensity, %) 368 (M^+, 28), 226 (16), 225 (100). HRMS Calcd for $C_{24}H_{20}N_2O_2$: 368.1525; Found: 368.1525.

4'-(Dimethylamino)-4-methyl-N-(quinolin-8-yl)-[1,1'-biphenyl]-2-carboxamide



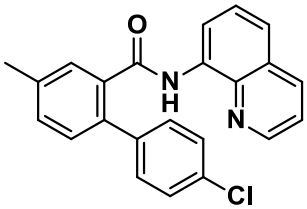
R_f 0.11 (hexane/EtOAc = 5/1). Pale yellow solid. Mp = 64-65 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.44 (s, 3H), 2.77 (s, 3H), 6.60 (d, J = 8.4 Hz, 2H), 7.29-7.37 (m, 5H), 7.43 (d, J = 8.4 Hz, 2H), 7.51 (t, J = 4.0 Hz, 1H), 7.69 (s, 1H), 8.04 (d, J = 8.4 Hz, 1H), 8.48 (d, J = 3.6 Hz, 1H), 8.84 (d, J = 7.2 Hz, 1H), 9.82 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 20.95, 40.38, 112.45, 116.19, 121.16, 121.19, 127.22, 127.64, 127.71, 129.69, 129.75, 130.37, 131.18, 134.80, 135.35, 135.82, 136.34, 137.54, 138.50, 147.58, 149.95, 168.58; IR (neat) 3428 w, 3010 w, 1664 s, 1612 s, 1525 s, 1484 s, 1425 m, 1382 m, 1335 m, 1326 m, 1120 w, 99 m, 1168 w, 944 w, 819 m, 755 s; MS *m/z* (relative intensity, %) 382 (18), 381 (M^+, 63), (239 (17), 238 (100), 223 (16). HRMS Calcd for $C_{25}H_{23}N_3O$: 381.1841; Found: 381.1843.

4'-Fluoro-4-methyl-N-(quinolin-8-yl)-[1,1'-biphenyl]-2-carboxamide



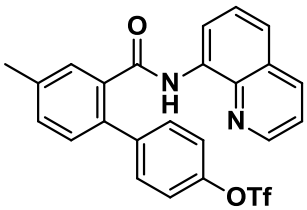
R_f 0.23 (hexane/EtOAc = 5/1). White solid. Mp = 153-154 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.46 (s, 3H), 6.52 (tt, J = 7.6, 3.2 Hz, 2H), 7.33-7.50 (m, 3H), 7.43-7.51 (m, 4H), 7.71 (s, 1H), 8.07 (dd, J = 4.0, 1.6 Hz, 1H), 8.52 (dd, J = 4.0, 1.2 Hz, 1H), 8.79 (dd, J = 8.0, 1.2 Hz, 1H), 9.75 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.02, 115.29 (d, J = 22 Hz), 116.26, 121.47, 121.58, 127.24, 127.71, 129.78, 130.53, 130.62, 131.31, 134.40, 135.98 (d, J = 3.8 Hz), 136.04, 136.24, 137.71, 138.34, 147.74, 162.45 (d, J = 245 Hz), 167.78; IR (neat) 3461 w, 3436 w, 1668 m, 1600 w, 1523 s, 1484 s, 1425 w, 1384 w, 1326 m, 1224 m, 1159 w, 823 m, 757 w; MS *m/z* (relative intensity, %) 357 (10), 356 (M^+, 39), 214 (15), 213 (100), 183 (12), 171 (16), 165 (10). HRMS Calcd for $C_{23}H_{17}FN_2O$:356.1352; Found: 356.1324.

4'-Chloro-4-methyl-N-(quinolin-8-yl)-[1,1'-biphenyl]-2-carboxamide



R_f 0.26 (hexane/EtOAc = 5/1). White solid. Mp = 161-162 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.47 (s, 3H), 7.23 (d, J = 8.0 Hz, 2H), 7.32-7.54 (m, 7H), 7.73 (s, 1H), 8.09 (d, J = 8.0 Hz, 1H), 8.54 (d, J = 4.0 Hz, 1H), 8.79 (d, J = 7.6 Hz, 1H), 9.77 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.04, 116.35, 121.47, 121.66, 127.22, 127.72, 128.53, 129.85, 130.29, 130.44, 131.39, 133.57, 134.37, 135.72, 136.04, 136.09, 137.95, 138.36, 138.44, 147.80, 167.63; IR (neat) 3328 m, 3014 m, 1664s, 1600 m, 1529 s, 1482 s, 1425 m, 1384 m, 1326 s, 1214 m, 1095 m, 1004 w, 900 w, 821 s, 759 s; MS *m/z* (relative intensity, %) 374 (14), 373 (12), 372 (M^+, 38), 231 (32), 230 (15), 229 (100), 166(30), 165 (27). HRMS Calcd for $C_{23}H_{17}ClN_2O$: 372.1029; Found: 372.1030.

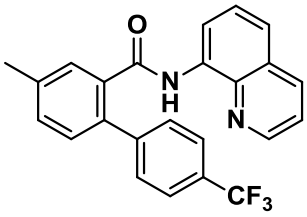
4'-Methyl-2'-(quinolin-8-ylcarbamoyl)-[1,1'-biphenyl]-4-yl trifluoromethanesulfonate



R_f 0.20 (hexane/EtOAc = 5/1). Colorless Oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.47 (s, 3H), 7.15 (d, J = 8.8, 2H), 7.33- 7.37 (m, 3H), 7.45-7.57 (m, 4H), 7.71 (s, 1H), 8.07 (dd, J = 8.0, 1.6 Hz, 1H), 8.52 (dd, J = 4.0, 1.2 Hz, 1H), 8.77 (dd, J = 8.0, 1.2 Hz, 1H), 9.74 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.06, 116.16, 120.62 (q, J = 319 Hz), 120.99, 121.16, 121.54, 121.76, 127.15, 127.71, 129.81, 130.40, 130.71, 131.46, 134.16, 135.29, 136.04, 138.20, 138.49, 140.50, 147.97, 148.99,

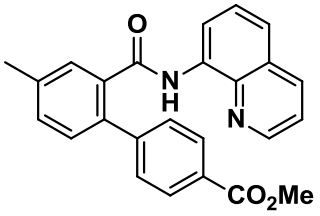
167.41; IR (neat) 3405 w, 3332 m, 1670 m, 1598 w, 1527 s, 1484 m, 1425 s, 1386 w, 1326 m, 1214 s, 1141 s, 889 s, 848 w, 825 m, 757 m; MS *m/z* (relative intensity, %) 486 (M^+, 17), 354 (26), 353 (100), 343 (25), 210 (14), 209 (23), 193 (13), 182 (16), 153 (13). HRMS Calcd for $C_{24}H_{17}F_3N_2O_4S$: 486.0861; Found: 486.0863.

4-Methyl-N-(quinolin-8-yl)-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxamide



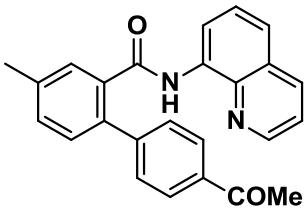
R_f 0.20 (hexane/EtOAc = 5/1). White solid. Mp = 126-127 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.49(s、3H), 7.33-7.43 (m, 3H), 7.46-7.54 (m, 4H), 7.60 (d, J = 8.4 Hz, 2H), 7.75 (s, 1H), 8.07 (dd, J = 8.0, 1.2 Hz, 1H), 8.48 (dd, J = 4.4, 1.2 Hz, 1H), 8.79 (d, J = 7.2 Hz, 1H), 9.75 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) 21.08, 116.32, 121.43, 121.76, 124.04 (q, J = 271 Hz), 125.23 (d, J = 3.8 Hz), 127.19, 127.69, 129.33, 129.41 (q, J = 32.5 Hz), 129.92, 130.49, 131.50, 134.24, 135.87, 136.07, 138.28, 138.49, 143.68, 147.80, 167.41; IR (neat) 3432 m, 33447 m, 1706 s, 1673 m, 1525 m, 1484 m, 1425 m, 1367 m, 1326 s, 1234 m, 1166 w, 1124 m, 1070 w, 825 w; MS *m/z* (relative intensity, %) 407 (11), 406 (M^+, 40), 405 (10), 264 (16), 263 (100), 215 (10), 166 (11), 165 (13). HRMS Calcd for $C_{24}H_{17}F_3N_2O$: 406.1293; Found: 406.1296.

Methyl 4'-methyl-2'-(quinolin-8-ylcarbamoyl)-[1,1'-biphenyl]-4-carboxylate



R_f 0.11 (hexane/EtOAc = 5/1).Pale yellow solid. Mp = 62-63 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.48 (s, 3H), 3.81 (s, 3H), 7.31-7.40 (m, 3H), 7.44-7.53 (m, 2H), 7.56 (d, J = 7.2 Hz, 2H), 7.72 (s, 1H), 7.94 (d, J = 7.2 Hz, 2H), 7.06 (d, J = 8.4 Hz, 1H), 8.50 (dd, J = 3.2, 1.6 Hz, 1H), 8.78 (d, J = 7.2 Hz, 1H), 9.77 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.06, 51.95, 116.30, 121.38, 121.65, 127.19, 127.68, 128.94, 129.60, 129.71, 130.41, 131.35, 134.28, 135.95, 136.02, 136.29, 138.28, 138.32, 144.74, 147.79, 1666.80, 167.56; IR (neat) 3018 m, 2950 w, 1772 s, 1668 s, 1610 m, 1525 s, 1482 s, 1428 m, 1384 m, 1326 m, 1280 s, 1182w, 1112 m, 827 m, 755 s; MS *m/z* (relative intensity, %) 397 (28), 396 (M^+, 100), 395 (28), 254 (11), 221 (18), 210 (18), 209 (89), 194 (31), 166 (28), 165 (47), 144 (16), 59 (12). HRMS Calcd for $C_{25}H_{20}N_2O_3$: 396.1474; Found: 396.1476.

4'-Acetyl-4-methyl-N-(quinolin-8-yl)-[1,1'-biphenyl]-2-carboxamide

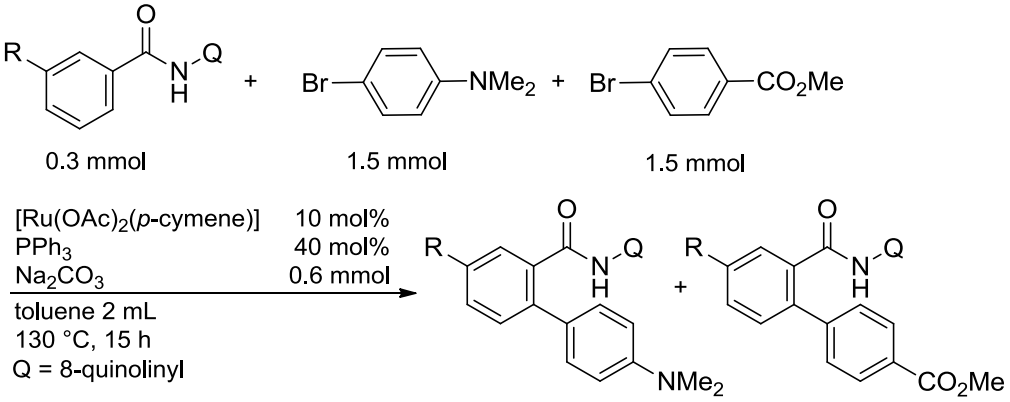


R_f 0.09 (hexane/EtOAc = 5/1). Pale yellow Oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.44 (s, 3H), 2.49 (s, 3H), 7.32-7.41 (m, 3H), 7.46-7.54 (m, 2H), 7.58 (d, J = 7.6 Hz, 2H), 7.73 (s, 1H), 7.85 (d, J = 7.6 Hz, 2H), 8.07 (d, J = 8.4 Hz, 1H), 8.51 (dd, J = 2.4, 1.2 Hz, 1H), 8.78 (d, J = 8.0 Hz, 1H), 9.79 (brs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.08, 26.51, 116.33, 121.41, 121.69, 127.23, 127.68, 128.37, 129.13, 129.68, 130.38, 131.39, 134.30, 135.79, 135.96, 136.06, 136.25, 138.28, 138.40, 144.93, 147.77, 167.57, 197.69; IR (neat) 3332 m, 3018 s, 1677 s, 1606 s, 1527 s, 1484 s, 1425 m, 1384 m, 1361 m, 1326 s, 1268 s, 1216 s, 1112 w, 958 w, 823 s, 669m; MS *m/z* (relative intensity, %) 381 (16), 380 (M^+, 56), 379(15), 237 (30), 196 ’15), 195 (100), 165 (16). HRMS Calcd for $C_{25}H_{20}N_2O_2$: 380.1525; Found: 380.1524.

IX. Competition Experiment (eq. 6).

To an oven-dried 5 mL screw-capped vial, 3-methyl-*N*-(8-quinolinyl)benzamide **7d** (79 mg, 0.3 mmol), 4-bromo-N,N-dimethylaniline (300 mg, 1.5 mmol), methyl 4-bromobenzoate (322 mg, 1.5 mmol), $[RuCl_2(p\text{-cymene})]_2$ (9 mg, 0.015 mmol), PPh_3 (31 mg, 0.12 mmol), Na_2CO_3 (64 mg, 0.6 mmol) and toluene (2 mL) were added under a gentle stream of nitrogen. The mixture was stirred for 15 h at 130 °C followed by cooling. The mixture was filtered through a celite pad and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel to afford the mixture product. The product ratio was determined by ^{1}H NMR spectroscopy.

Competition Experiment Using Electronically Diverse Aryl Bromides

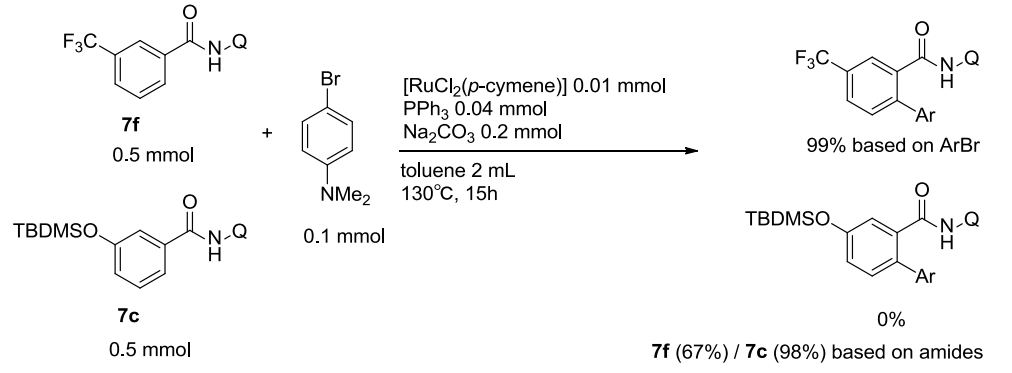


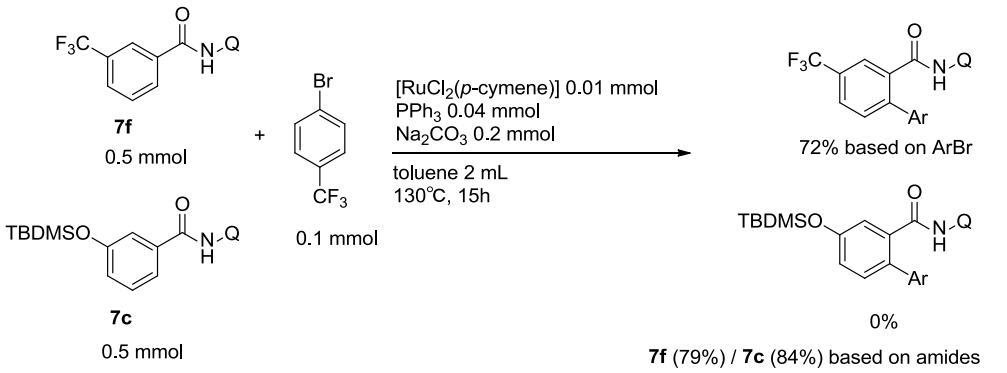
	product ratio	σ_p	log (selectivity)
R = CF_3	5.6 : 1	0.54	0.747
R = Me	2.6 : 1	-0.17	0.466
R = TBDMSO	2.3 : 1	-0.27[a]	0.356
R = NMe_2	1.6 : 1	-0.83	0.214

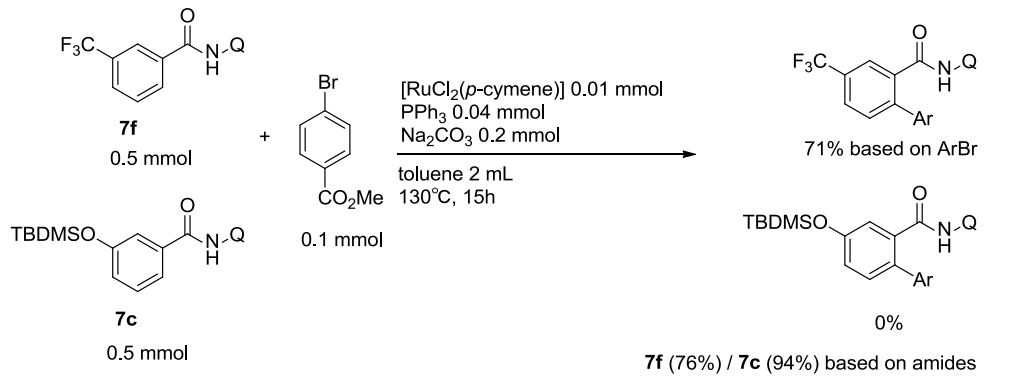
[a] the σ_p value of TMSO is used in place of TBDMSO

X. Competition Experiment (eq. 7).

To an oven-dried 5 mL screw-capped vial, *N*-(8-Quinolinyl)-3-(trifluoromethyl)benzamide 7f (158mg, 0.5 mmol), 3-(*tert*-Butyldimethylsilyloxy)-*N*-(8-quinolinyl)benzamide 7c (189 mg, 0.5 mmol), methyl 4-bromobenzoate (2.15 mg, 0.1 mmol), $[Ru(OAc)_2(p\text{-cymene})]_2$,(3.5 mg, 0.01 mmol), PPh_3 (10 mg, 0.04 mmol), Na_2CO_3 (21 mg, 0.2 mmol) and toluene (2 mL) were added under a gentle stream of nitrogen. The mixture was stirred for 15 h at 130 °C followed by cooling. The mixture was filtered through a celite pad and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (eluant: hexane/EtOAc= 20/1) to afford the desired arylated product **29** (32 mg, 71% based on ArBr) as a white solid. *N*-(8-Quinolinyl)-3-(trifluoromethyl)benzamide 7f and 3-(*tert*-Butyldimethylsilyloxy)-*N*-(8-quinolinyl)benzamide 7c was recovered 71% and 94%



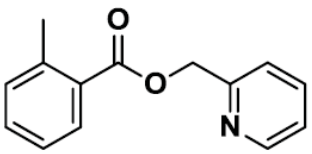




XI. Removal of 8-Aminoquinolinyl Directing Group. (eq. 8)

To an oven-dried 5 mL screw-capped vial, arylated amide **8d** (68 mg, 0.15 mmol) and 3 mL of 12 M HCl were added under a gentle stream of nitrogen. The mixture was stirred for 24 h at 110 °C followed by cooling. EtOAc (15 mL) and saturated aq. $NaHCO_3$ (10 mL) were added. The aqueous layer was extracted with EtOAc (2 × 5 mL). The combined organic layers were washed with brine (10 mL), dried over $MgSO_4$, filtered and concentrated in *in vacuo* to afford the 8-aminoquinoline (yellow solid, 23 mg, 99%). Then 1 M HCl was added in aqueous layer until pH 4. The aqueous layer was extracted with EtOAc (2 × 5 mL). The combined organic layers were washed with brine (10 mL), dried over $MgSO_4$, filtered and concentrated in *in vacuo*. The residue was purified by column chromatography on silica gel to afford the desired carboxylic acid (white solid, 31 mg, 98%)

^{1}H NMR of 4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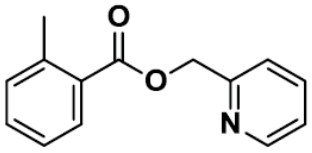
^{13}C NMR of 4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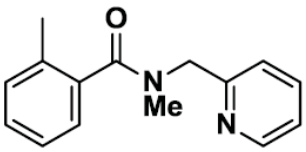
^{1}H NMR of 5

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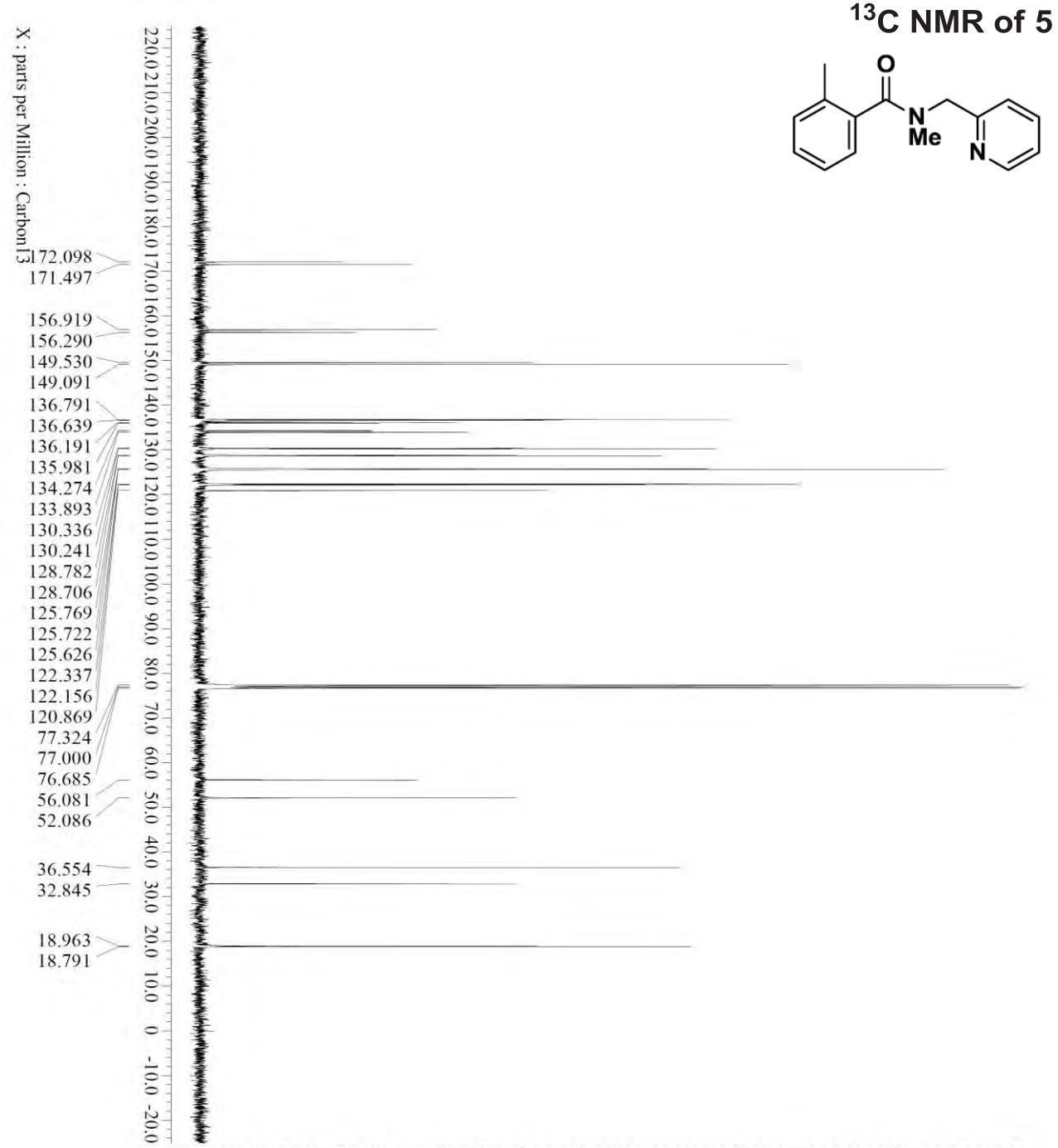
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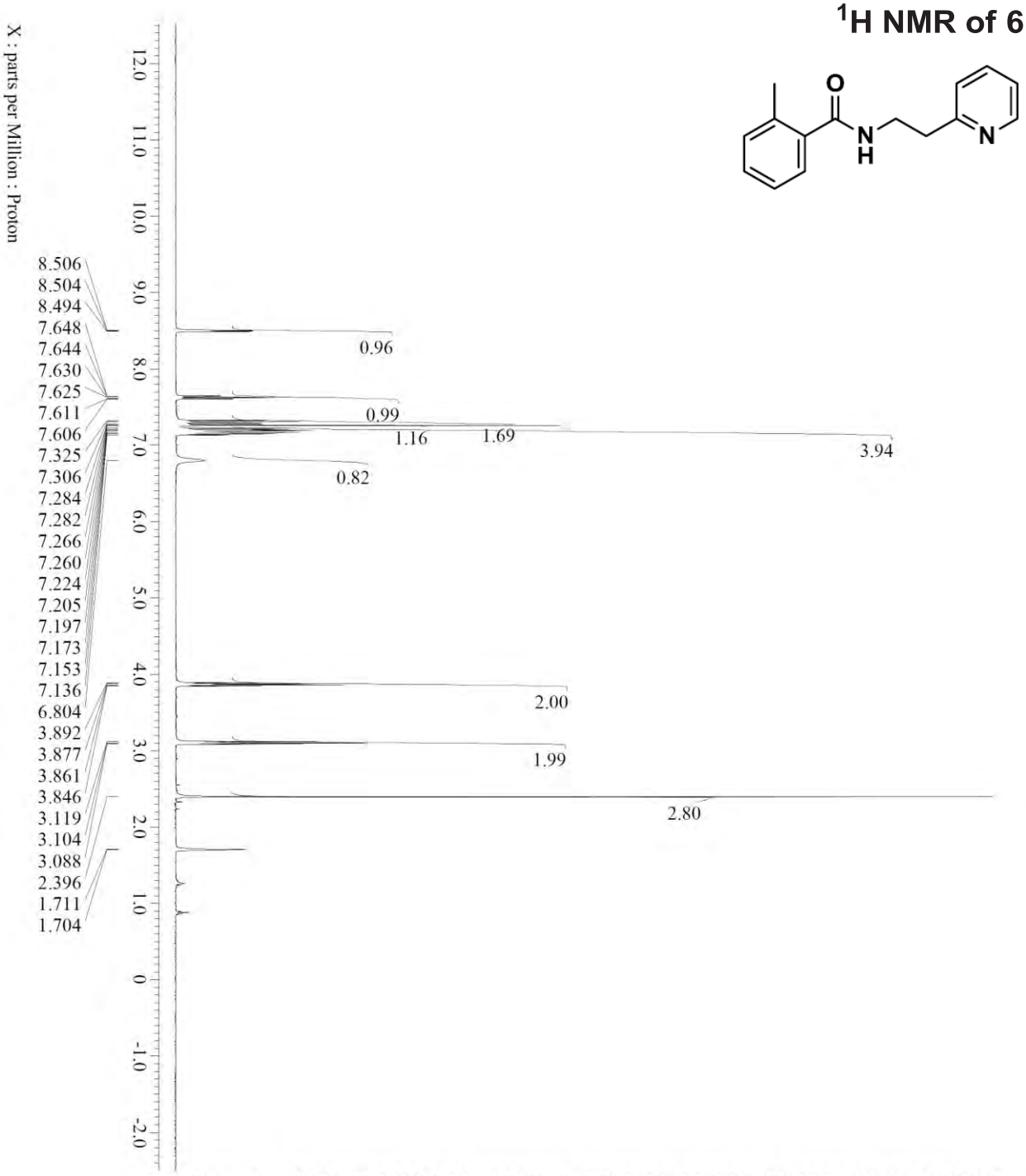
^{1}H NMR of 6

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Spectrometer            = DELTA2_NMR

Field_Strength          = 9.38976[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.50300l2[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 46
Temp_Get                = 19.5[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 538
Sawtooth_Range          = 4
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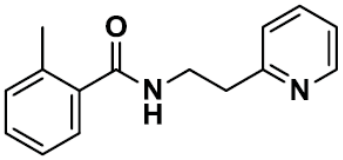
^{13}C NMR of 6

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Filename                = E:¥NMRデータ¥原料合成¥YAG-133sei
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YAG-133seisei
Solvent                 = CHLOROFORM-D
Creation_Time           = 23-NOV-2011 15:47:11
Revision_Time           = 23-NOV-2011 16:59:02
Current_Time            = 28-JUN-2012 16:37:09

Comment                 = YAG-133seisei
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 19.7[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 530
Sawtooth_Range          = 4
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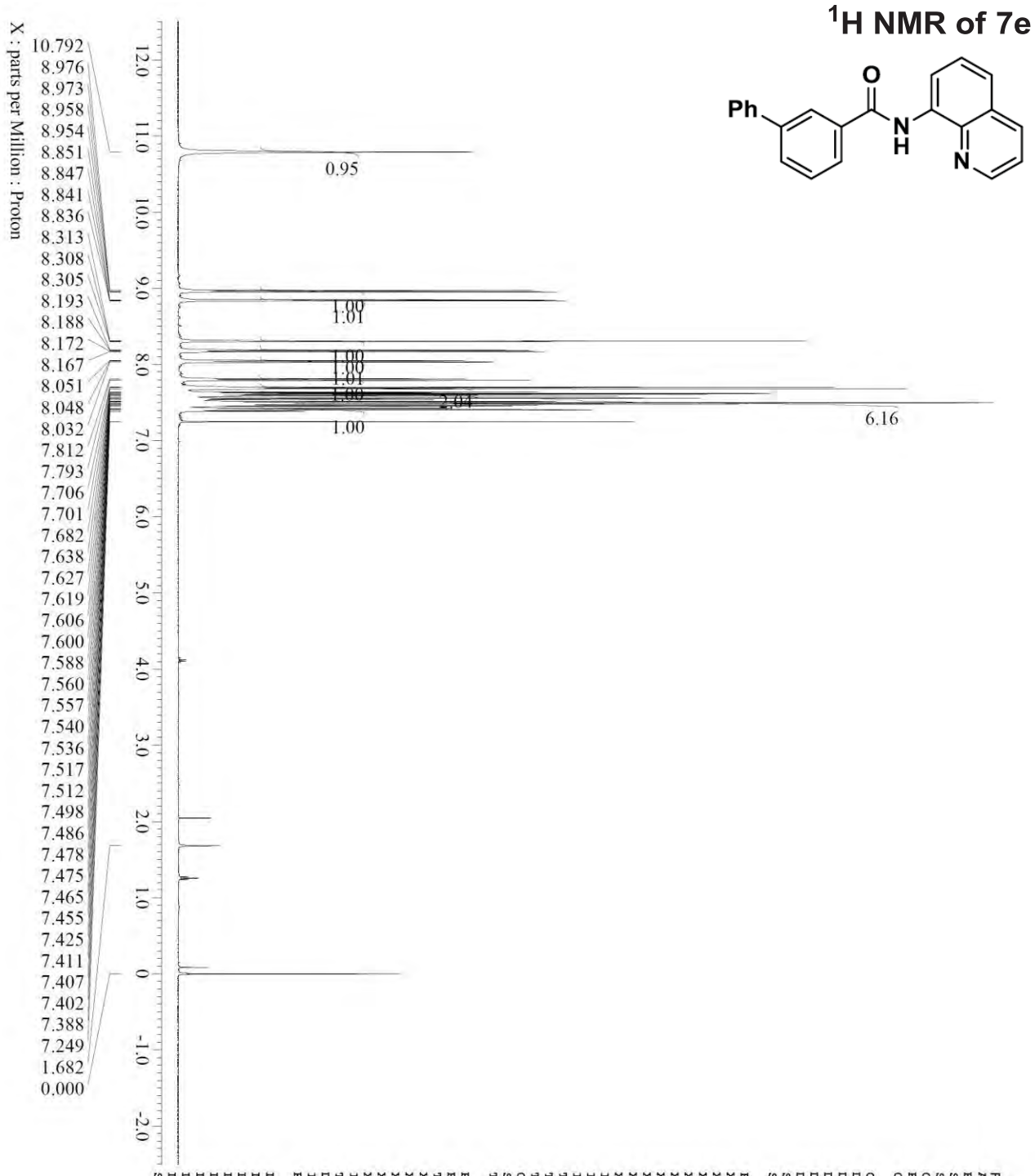
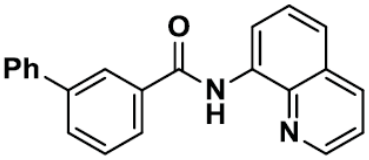

^{1}H NMR of 7e
O
Ph
N
H
N
X : parts per Million : Proton
10.792
8.976
8.973
8.958
8.954
8.851
8.847
8.841
8.836
8.313
8.308
8.305
8.193
8.188
8.172
8.167
8.051
8.048
8.032
7.812
7.793
7.706
7.701
7.682
7.638
7.627
7.619
7.606
7.600
7.588
7.560
7.557
7.540
7.536
7.517
7.512
7.498
7.486
7.478
7.475
7.465
7.455
7.425
7.411
7.407
7.402
7.388
7.249
1.682
0.000
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
0.95
1.00
1.01
1.00
1.01
1.00
2.04
1.00
6.16
Filename = E:¥NMRデータ¥原料合成¥m-Ph,Q-ami
Author = delta
Experiment = proton.jxp
Sample_Id = m-Ph,Q-amide
Solvent = CHLOROFORM-D
Creation_Time = 13-FEB-2012 18:16:51
Revision_Time = 28-JUN-2012 16:40:14
Current_Time = 28-JUN-2012 16:40:23
Comment = m-Ph,Q-amide
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 15.5[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 826
Sawtooth_Range = 4

^{13}C NMR of 7e

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Filename                = E:¥NMRデータ¥原料合成¥m-Ph,Q-ami
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = m-Ph,Q-amide
Solvent                 = CHLOROFORM-D
Creation_Time           = 13-FEB-2012 18:18:34
Revision_Time           = 28-JUN-2012 16:42:36
Current_Time            = 28-JUN-2012 16:42:44

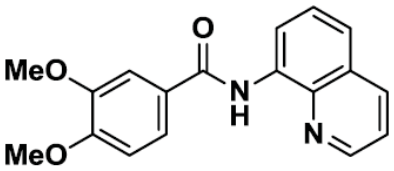
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
X_Domain                = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 957
Total_Scans             = 957

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 15.9[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe_Time                = TRUE
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 819
Sawtooth_Range          = 4
```

^{1}H NMR of SM for 10




```
Filename                = E:¥NMRデータ¥スペクトル¥アリール化¥3,4
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = 3,4-dimethoxy,Q-amide
Solvent                 = CHLOROFORM-D
Creation_Time           = 16-FEB-2012 00:21:44
Revision_Time           = 28-JUN-2012 16:44:10
Current_Time            = 28-JUN-2012 16:44:17

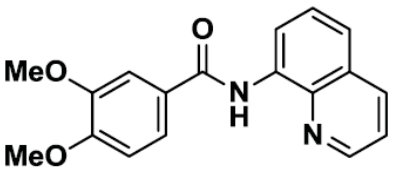
Comment                 = 3,4-dimethoxy,Q-amide
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.183659521s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.503012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 40
Temp_Get                = 15.8[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.183659521s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.183659521s]

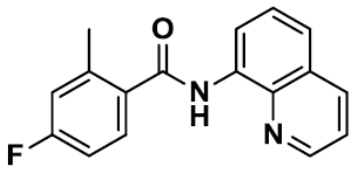
Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 862.0
Sawtooth_Range          = 4
```

^{13}C NMR of SM for 10



File name	= E:¥NMRデータ¥スペクトル¥アリール化¥3,
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= 3,4-dimethoxy,Q-amide
Solvent	= CHLOROFORM-D
Creation_Time	= 16-FEB-2012 00:23:27
Revision_Time	= 28-JUN-2012 16:44:55
Current_Time	= 28-JUN-2012 16:45:01
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 16.1[dC]
X_90_Width	= 9.2[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 6[dB]
X_Pulse	= 3.06666667[us]
Irr_Atn_Dec	= 22[dB]
Irr_Atn_Noe	= 22[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]
Lock_Gain	= 22
Lock_Level	= 180
Lock_Osc_Offset	= 7.26[ppm]
Lock_Osc_State	= 2H OSC ON
Lock_Phase	= 154.6875[deg]
Lock_State	= AUTOLOCK
Lock_Status	= LOCK IDLE
Lock_Strength	= 857
Sawtooth_Range	= 4

^{1}H NMR of SM for 12

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Filename                = E:¥NMRデータ¥原料合成¥YAG-155sei
Author                  = delta
Experiment              = proton.jxp
Sample_id               = YAG-155seiseigo
Solvent                 = CHLOROFORM-D
Creation_Time           = 20-FEB-2012 14:13:38
Revision_Time           = 28-JUN-2012 16:46:10
Current_Time            = 28-JUN-2012 16:46:16

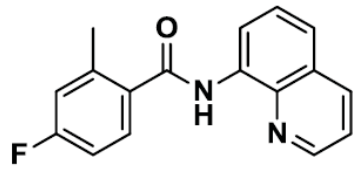
Comment                 = YAG-155seiseigo 1H
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.50300012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 42
Temp_Get                = 15.5[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 875
Sawtooth_Range          = 4
```

^{13}C NMR of SM for 12

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File name                = E:¥NMRデータ¥原料合成¥YAG-155sei
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = YAG-155seiseigo
Solvent                  = CHLOROFORM-D
Creation_Time            = 20-FEB-2012 14:15:15
Revision_Time            = 28-JUN-2012 16:46:35
Current_Time             = 28-JUN-2012 16:46:52

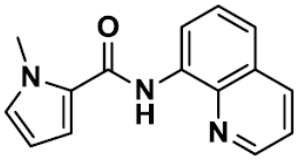
Comment                  = YAG-155seiseigo 13C
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Site                     = JNM-ECS400
Spectrometer             = DELTA2_NMR

Field_Strength           = 9.389766[T] (400[MHz])
X_Acq_Duration           = 1.04333312[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MHz]
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.95846665[Hz]
X_Sweep                  = 31.40703518[kHz]
X_Sweep_Clipped          = 25.12562814[kHz]
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MHz]
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 725
Total_Scans              = 725

Relaxation_Delay         = 2[s]
Recvr_Gain               = 60
Temp_Get                 = 15.6[dC]
X_90_Width               = 9.2[us]
X_Acq_Time               = 1.04333312[s]
X_Angle                  = 30[deg]
X_Atn                    = 6[dB]
X_Pulse                  = 3.06666667[us]
Irr_Atn_Dec              = 22[dB]
Irr_Noise                = WALTZ
Irr_Pwidth               = 0.115[ms]
Decoupling               = TRUE
Initial_Wait             = 1[s]
Noe                      = FALSE
Repetition_Time          = 3.04333312[s]

Lock_Gain                = 22
Lock_Level               = 180
Lock_Osc_Offset          = 7.26[ppm]
Lock_Osc_State           = 2H OSC ON
Lock_Phase               = 154.6875[deg]
Lock_State               = AUTOLOCK
Lock_Status              = LOCK IDLE
Lock_Strength            = 876
Sawtooth_Range           = 4
```

^{1}H NMR of SM for 13



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Author = delta
Experiment = proton.jxp
Sample_Id = YA-690GPC1
Solvent = CHLOROFORM-D
Creation_Time = 13-MAR-2012 21:39:45
Revision_Time = 28-JUN-2012 17:37:35
Current_Time = 28-JUN-2012 17:37:39

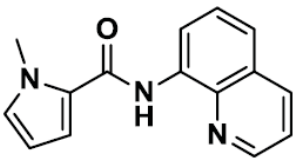
Comment = YA-690GPC1
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.50300l2[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 17.4[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]

Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 687
Sawtooth_Range = 4

^{13}C NMR of SM for 13



Filename = E:¥NMRデータ¥反応系(500-699)¥YA-
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-690GPC2
Solvent = CHLOROFORM-D
Creation_Time = 13-MAR-2012 22:22:12
Revision_Time = 13-MAR-2012 22:54:07
Current_Time = 28-JUN-2012 16:48:39

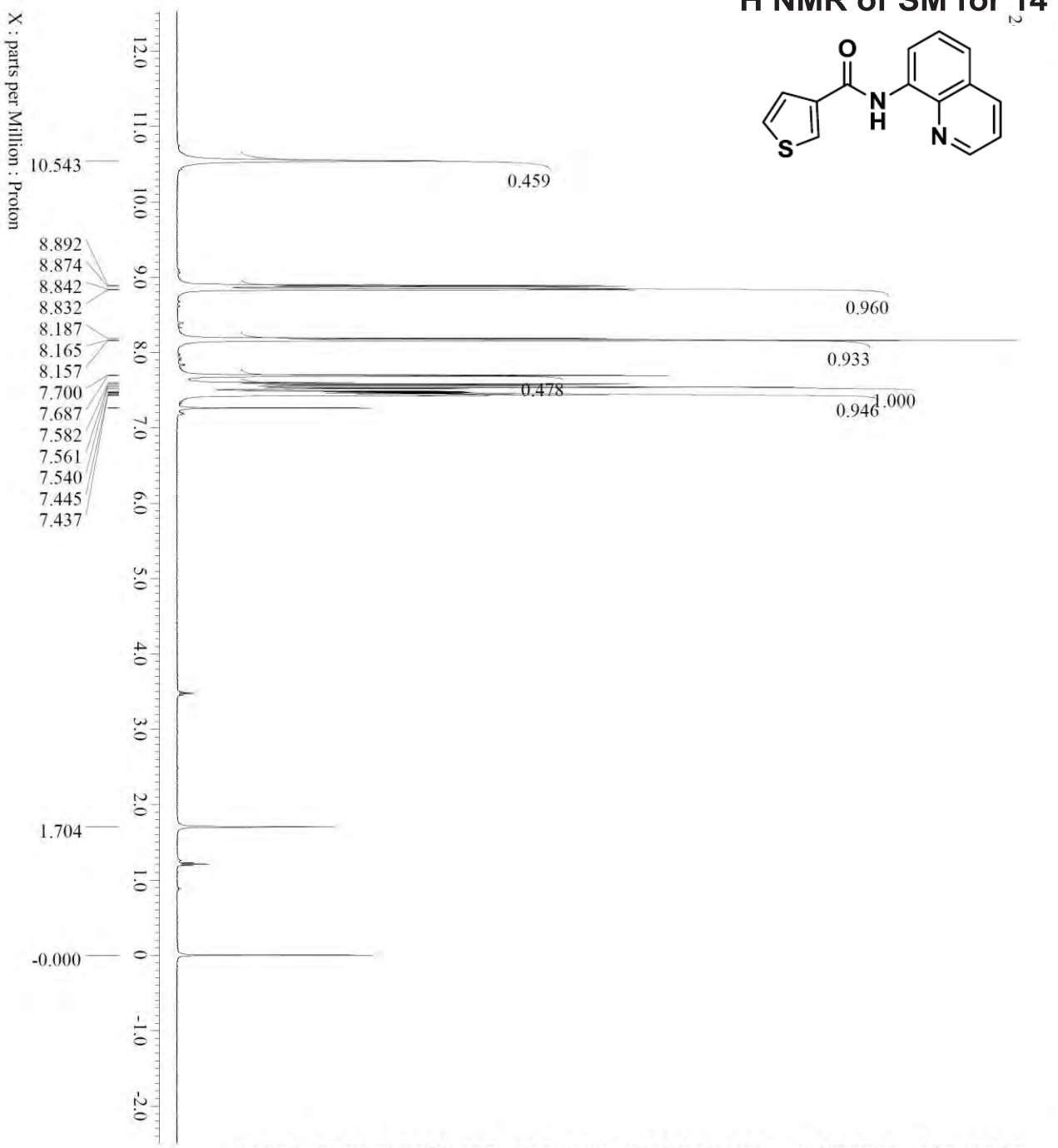
Comment = YA-690GPC2_Carbon
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 512
Total_Scans = 512

Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 16.8[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Atn = 30[deg]
X_Pulse = 6[dB]
Irr_Atn_Dec = 3.06666667[us]
Irr_Atn_Noe = 22[dB]
Irr_Noise = 22[dB]
Irr_Pwidth = WALTZ
Decoupling = 0.115[ms]
Initial_Wait = TRUE
Noe = 1[s]
Noe_Time = TRUE
Repetition_Time = 2[s]
= 3.04333312[s]

Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 790
Sawtooth_Range = 4

^{1}H NMR of SM for 14




```
Filename                = C:\Users\delta\Documents\J
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = 2-thio,Q-amide
Solvent                 = CHLOROFORM-D
Creation_Time           = 18-JUN-2012 13:37:18
Revision_Time           = 28-JUN-2012 20:19:27
Current_Time            = 28-JUN-2012 20:19:37

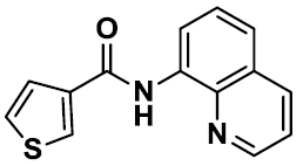
Comment                 = 2-thio,Q-amide
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.503012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 40
Temp_Get                = 19.7[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Status             = LOCK IDLE
Lock_Strength           = 477.0
```

^{13}C NMR of SM for 14



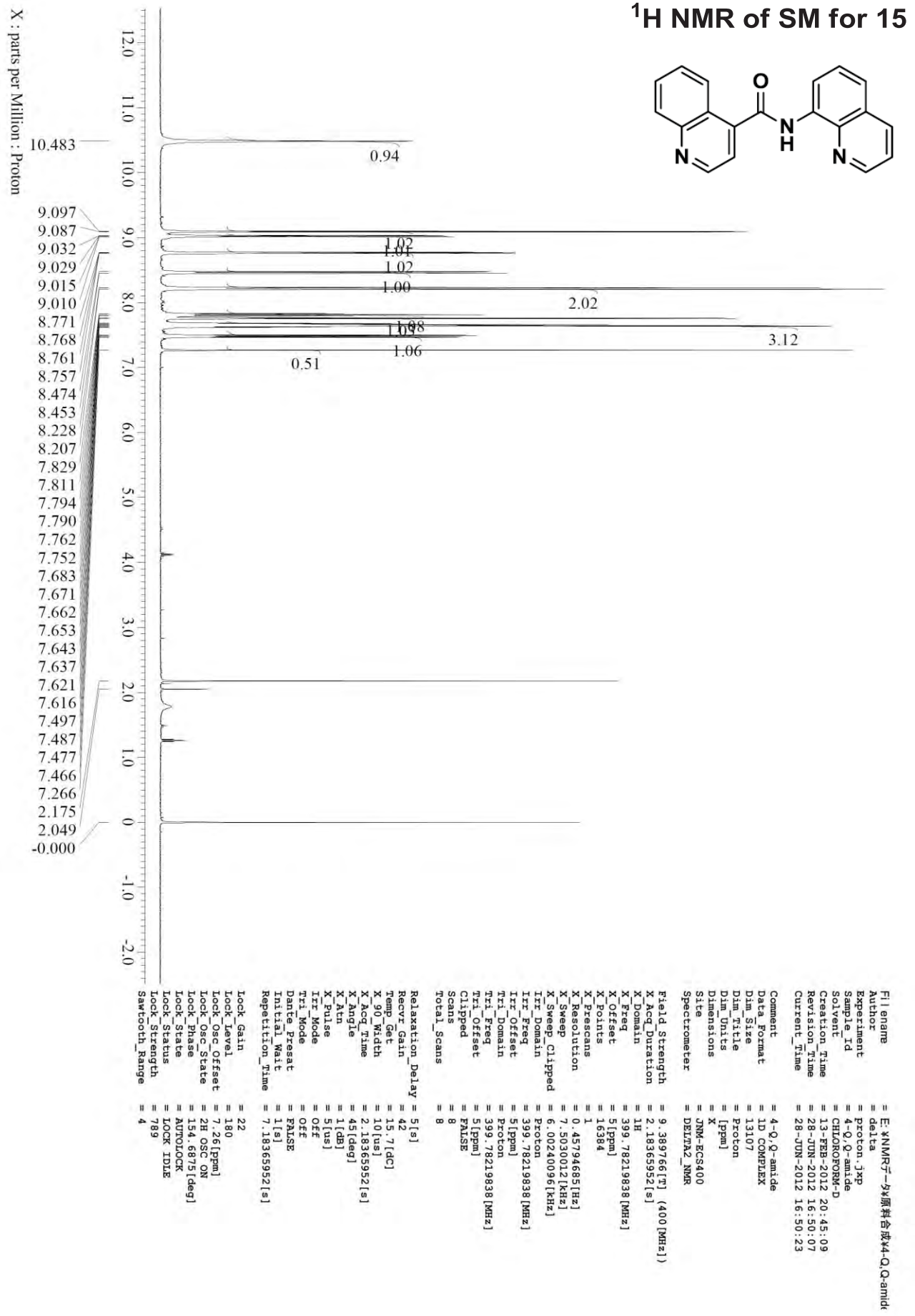

```
Filename                = C:\Users\delta\Documents\J
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = 2-thio,Q-amide
Solvent                 = CHLOROFORM-D
Creation_Time           = 18-JUN-2012 13:39:54
Revision_Time           = 18-JUN-2012 14:07:05
Current_Time            = 28-JUN-2012 20:19:01

Comment                 = 2-thio,Q-amide_Carbon
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

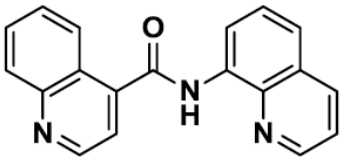
Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 20.3[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe_Time                = TRUE
Repetition_Time         = 2[s]
                        = 3.04333312[s]

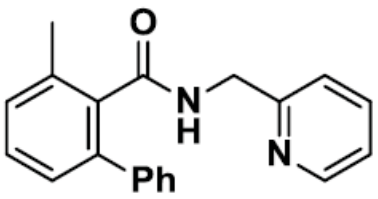
Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Status             = LOCK IDLE
Lock_Strength           = 485.0
```


^{1}H NMR of SM for 15
O
N
H
N
N
X : parts per Million : Proton
10.483
9.097
9.087
9.032
9.029
9.015
9.010
8.771
8.768
8.761
8.757
8.474
8.453
8.228
8.207
7.829
7.811
7.794
7.790
7.762
7.752
7.683
7.671
7.662
7.653
7.643
7.637
7.621
7.616
7.497
7.487
7.477
7.466
7.266
2.175
2.049
-0.000
0.94
1.02
1.01
1.02
1.00
2.02
1.08
1.09
3.12
1.06
0.51
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
Filename = E:¥NMRデータ¥原料合成¥4-Q,Q-amide
Author = delta
Experiment = proton.jxp
Sample_Id = 4-Q,Q-amide
Solvent = CHLOROFORM-D
Creation_Time = 13-FEB-2012 20:45:09
Revision_Time = 28-JUN-2012 16:50:07
Current_Time = 28-JUN-2012 16:50:23
Comment = 4-Q,Q-amide
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 15.7[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 789
Sawtooth_Range = 4

^{13}C NMR of SM for 15



^{1}H NMR of 2a




```
Filename                = E:¥NMRデータ¥スペクトル¥アリール化¥o-M
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = o-Me,Ph-amide
Solvent                 = CHLOROFORM-D
Creation_Time           = 17-NOV-2011 20:52:54
Revision_Time           = 17-NOV-2011 20:55:57
Current_Time            = 28-JUN-2012 16:53:13

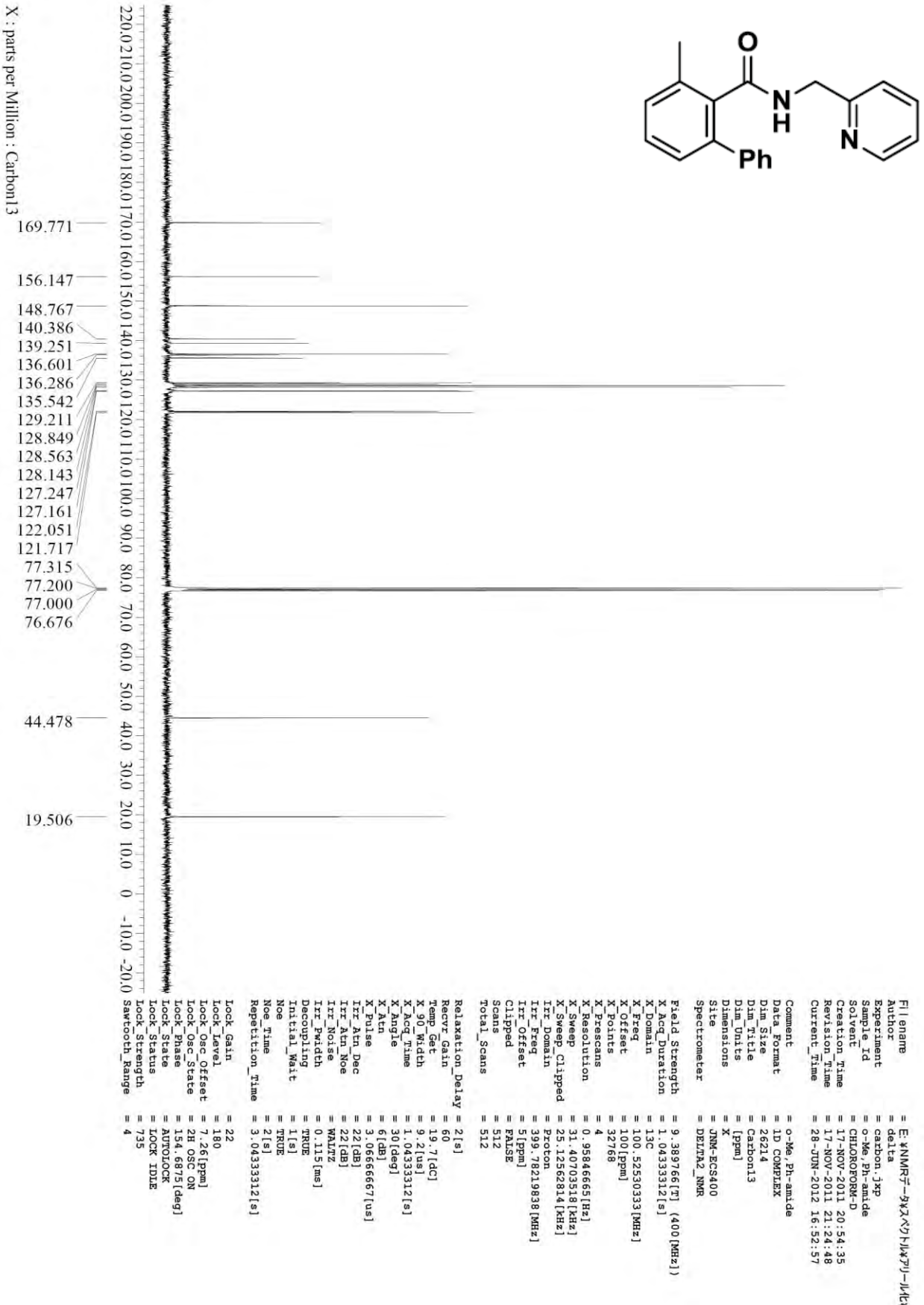
Comment                 = o-Me,Ph-amide
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.5030012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

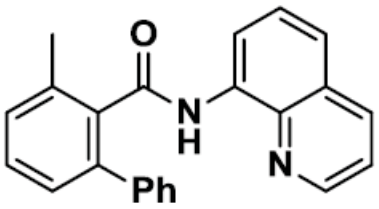
Relaxation_Delay        = 5[s]
Recvr_Gain              = 34
Temp_Get                = 19.5[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 740
Sawtooth_Range          = 4
```

^{13}C NMR of 2a


O
N
H
N
Ph
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
169.771
156.147
148.767
140.386
139.251
136.601
136.286
135.542
129.211
128.849
128.563
128.143
127.247
127.161
122.051
121.717
77.315
77.200
77.000
76.676
44.478
19.506
Filename = E:¥NMRデータ¥スペクトル¥アリール化¥o-
Author = delta
Experiment = carbon.jxp
Sample_Id = o-Me,Ph-amide
Solvent = CHLOROFORM-D
Creation_Time = 17-NOV-2011 20:54:35
Revision_Time = 17-NOV-2011 21:24:48
Current_Time = 28-JUN-2012 16:52:57
Comment = o-Me,Ph-amide
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-EC400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.7[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 735
Sawtooth_Range = 4

^{1}H NMR of 8a




```
Filename                = E:¥NMRデータ¥スペクトル¥アリール化¥o-1
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = o-Me,Ph,Quinoline-amide
Solvent                 = CHLOROFORM-D
Creation_Time           = 28-NOV-2011 17:54:25
Revision_Time           = 28-NOV-2011 18:05:37
Current_Time            = 28-JUN-2012 16:53:49

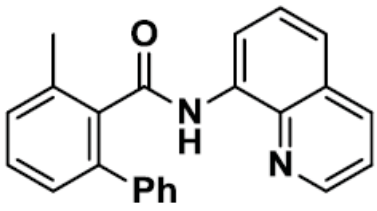
Comment                 = o-Me,Ph,Quinoline-amide
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.50300012[kHz]
X_Sweep_clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 44
Temp_Get                = 20[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 531
Sawtooth_Range          = 4
```

^{13}C NMR of 8a




```
Filename                = E:¥NMRデータ¥スペクトル¥アリール化¥o-M
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = o-Me,Ph,Quinoline-amide
Solvent                 = CHLOROFORM-D
Creation_Time           = 28-NOV-2011 17:56:08
Revision_Time           = 28-NOV-2011 20:41:40
Current_Time            = 28-JUN-2012 16:54:15

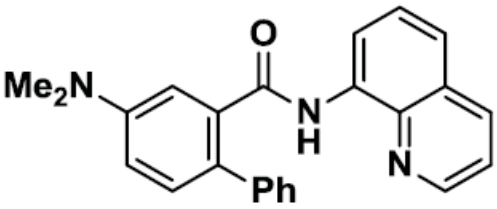
Comment                 = o-Me,Ph,Quinoline-amide 13
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 20[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = FALSE
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 530
Sawtooth_Range          = 4
```

^{1}H NMR of 8b




```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-557GPC1
Solvent                 = CHLOROFORM-D
Creation_Time           = 16-JAN-2012 22:16:19
Revision_Time           = 28-JUN-2012 17:07:25
Current_Time            = 28-JUN-2012 17:07:29

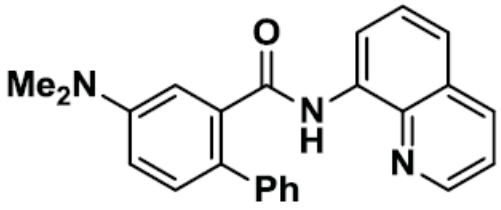
Comment                 = YA-557GPC1
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.5030012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 32
Temp_Get                = 15.8[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 845.0
Sawtooth_Range          = 4
```

^{13}C NMR of 8b




```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-557GPC1
Solvent                 = CHLOROFORM-D
Creation_Time           = 16-JAN-2012 22:20:47
Revision_Time           = 28-JUN-2012 17:01:33
Current_Time            = 28-JUN-2012 17:01:42

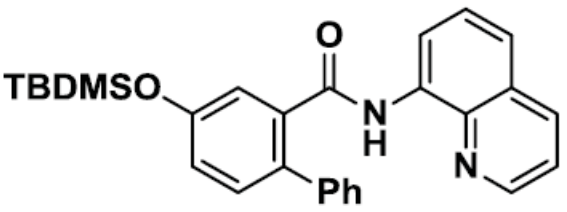
Comment                 = YA-557GPC1
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 15.9[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 845.0
Sawtooth_Range          = 4
```

^{1}H NMR of 8c

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Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-603f5-9
Solvent                 = CHLOROFORM-D
Creation_Time           =  6-FEB-2012 19:25:02
Revision_Time           = 29-JUN-2012 15:26:16
Current_Time            = 29-JUN-2012 15:26:29

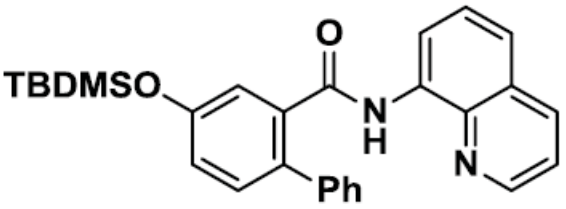
Comment                 = YA-603f5-9
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.503012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 34
Temp_Get                = 15.9[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

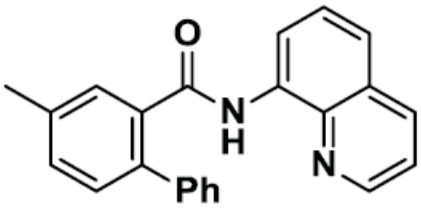
Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 610
Sawtooth_Range          = 4
```

^{13}C NMR of 8c


TBDMSO
O
N
H
N
Ph

X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
167.416
155.184
147.680
139.728
138.317
136.944
135.924
134.446
133.283
131.919
128.992
128.248
127.619
127.209
127.161
122.261
121.450
121.355
120.535
116.139
77.324
77.210
77.000
76.685
25.637
18.191
-4.101
-4.378
Filename = E:¥NMRデータ¥反応系(500-699)¥YA-
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-557GPC1
Solvent = CHLOROFORM-D
Creation_Time = 17-JAN-2012 15:07:03
Revision_Time = 17-JAN-2012 15:48:41
Current_Time = 28-JUN-2012 17:09:05
Comment = YA-557GPC1
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 16.2[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 836
Sawtooth_Range = 4

^{1}H NMR of 8d




```
Filename                = E:¥NMRデータ¥反応系(300-499)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-497GPC1
Solvent                 = CHLOROFORM-D
Creation_Time           = 9-DEC-2011 19:51:20
Revision_Time           = 28-JUN-2012 16:55:53
Current_Time            = 28-JUN-2012 16:55:57

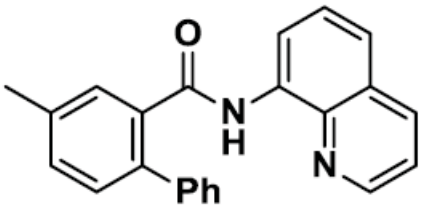
Comment                 = YA-497GPC1
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.5030012[kHz]
X_Sweep_clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 30
Temp_Get                = 17.9[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 545
Sawtooth_Range          = 4
```

^{13}C NMR of 8d




```
Filename                = E:¥NMRデータ¥反応系(300-499)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-497GPC1
Solvent                 = CHLOROFORM-D
Creation_Time           =  9-DEC-2011 21:20:59
Revision_Time           =  9-DEC-2011 21:42:34
Current_Time            = 28-JUN-2012 16:55:33

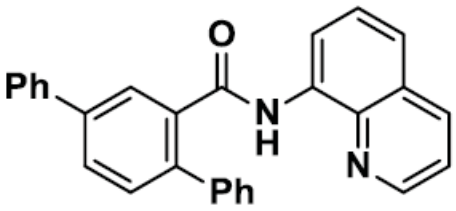
Comment                 = YA-497GPC1
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 256
Total_Scans             = 256

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 18.1[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 536
Sawtooth_Range          = 4
```

^{1}H NMR of 8e




```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-555f4-9
Solvent                 = CHLOROFORM-D
Creation_Time           = 17-JAN-2012 19:33:28
Revision_Time           = 28-JUN-2012 16:59:58
Current_Time            = 28-JUN-2012 17:00:36

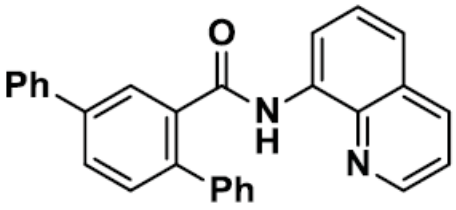
Comment                 = YA-555f4-9
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.5030012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 30
Temp_Get                = 16.2[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 766
Sawtooth_Range          = 4
```

^{13}C NMR of 8e



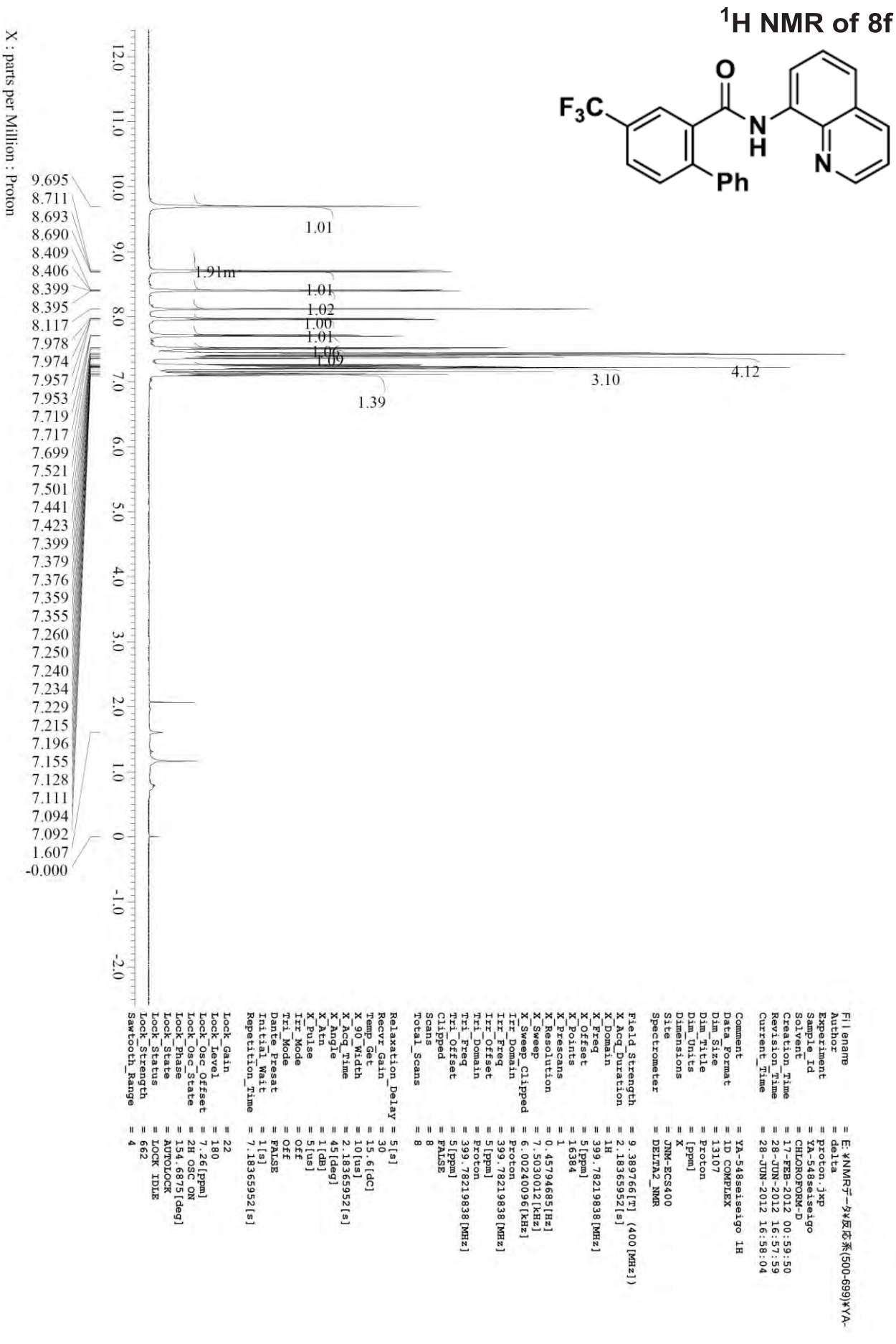

```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-555f4-9
Solvent                 = CHLOROFORM-D
Creation_Time           = 17-JAN-2012 19:35:12
Revision_Time           = 17-JAN-2012 20:33:00
Current_Time            = 28-JUN-2012 16:59:24

Comment                 = YA-555f4-9
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.043333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.1256214[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 16.2[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.043333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.066666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.043333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 769
Sawtooth_Range          = 4
```

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Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-548seiseigo
Solvent                 = CHLOROFORM-D
Creation_Time           = 17-FEB-2012 00:59:50
Revision_Time           = 28-JUN-2012 16:57:59
Current_Time            = 28-JUN-2012 16:58:04

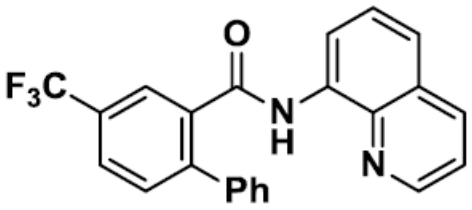
Comment                 = YA-548seiseigo 1H
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.50300121[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 30
Temp_Get                = 15.6[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 662
Sawtooth_Range          = 4
```

^{13}C NMR of 8f

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Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-548seiseigo
Solvent                 = CHLOROFORM-D
Creation_Time           = 17-FEB-2012 01:01:28
Revision_Time           = 28-JUN-2012 16:58:27
Current_Time            = 28-JUN-2012 16:58:33

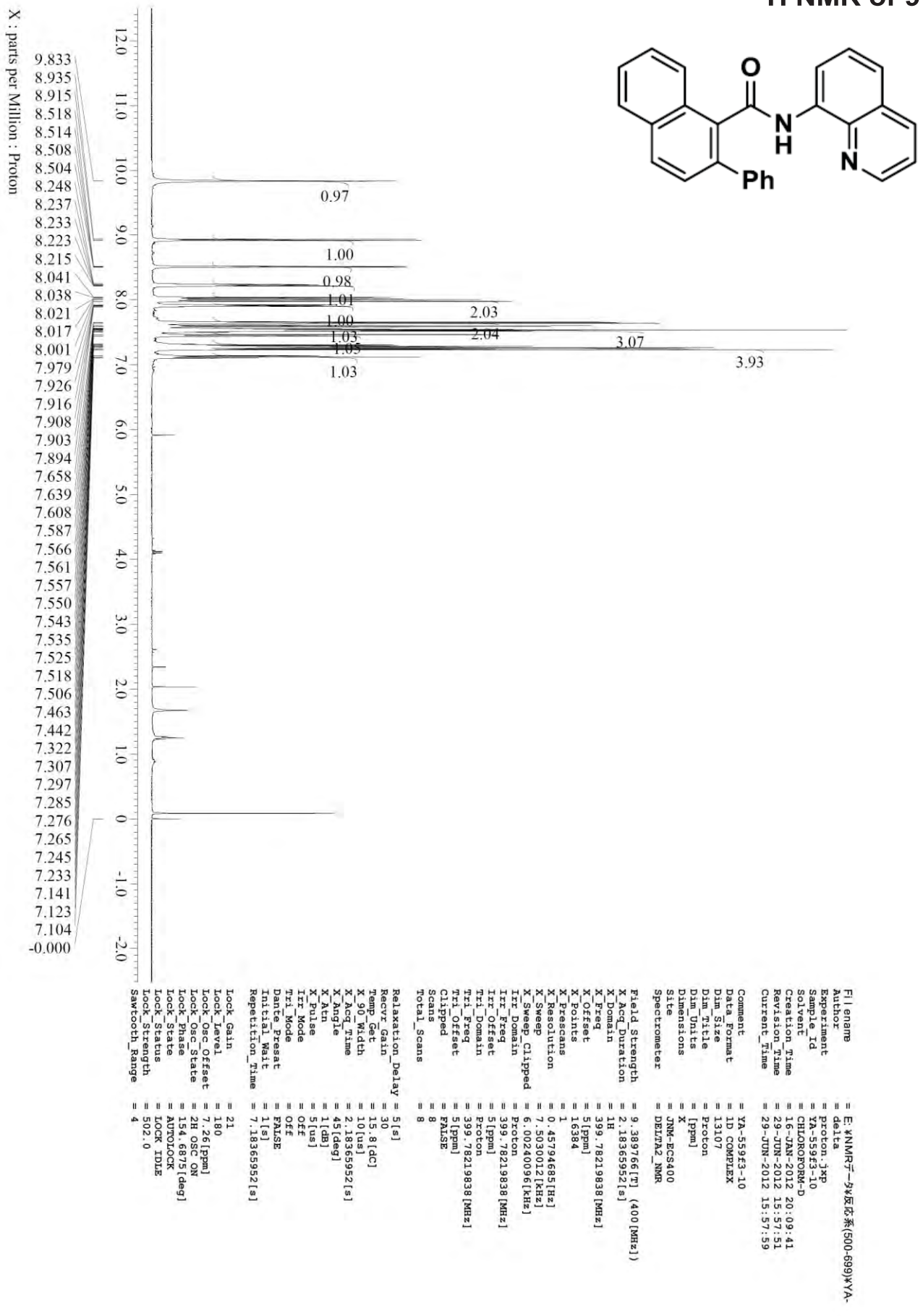
Comment                 = YA-548seiseigo 13C
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 7680
Total_Scans             = 7680

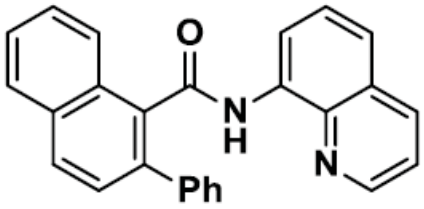
Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 15.9[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = FALSE
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 429
Sawtooth_Range          = 4
```

^{1}H NMR of 9


O
N
H
N
Ph
X : parts per Million : Proton
0.97
1.00
0.98
1.01
2.03
1.00
2.04
1.03
3.07
1.05
3.93
1.03

^{13}C NMR of 9




```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-559f3-10
Solvent                 = CHLOROFORM-D
Creation_Time           = 16-JAN-2012 20:12:31
Revision_Time           = 28-JUN-2012 17:11:51
Current_Time            = 28-JUN-2012 17:11:56

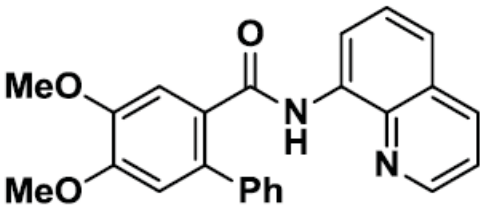
Comment                 = YA-559f3-10
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = TRUE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 16[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 503
Lock_Tooth_Range        = 4
```

^{1}H NMR of 10

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Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_id               = YA-593f18-23
Solvent                 = CHLOROFORM-D
Creation_Time           =  2-FEB-2012 23:13:37
Revision_Time           = 28-JUN-2012 17:25:48
Current_Time            = 28-JUN-2012 17:25:56

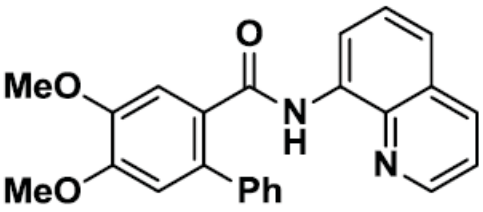
Comment                 = YA-593f18-23
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

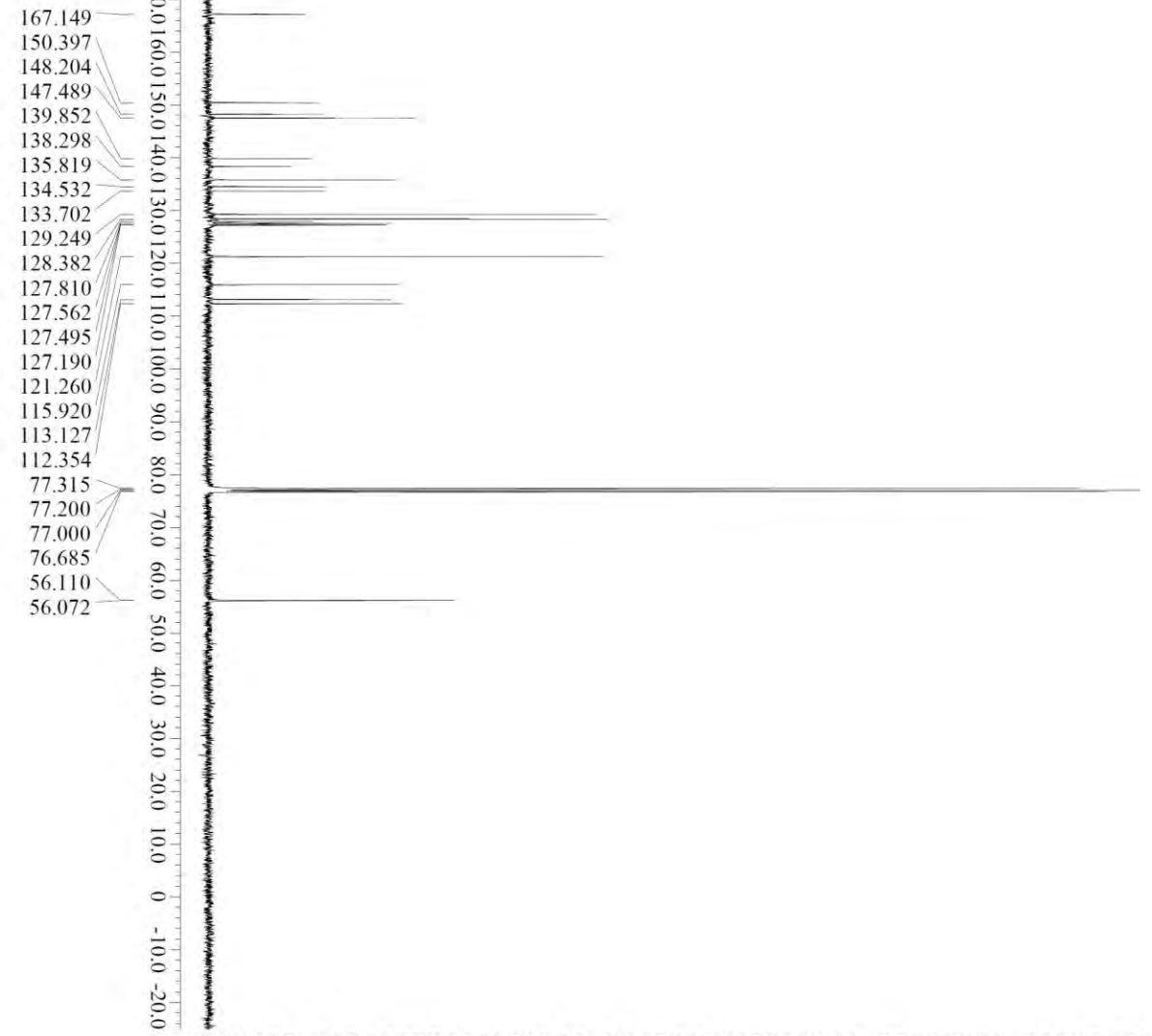
Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.5030012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 46
Temp_Get                = 15[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = off
Tri_Mode                = off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 627
Sawtooth_Range          = 4
```

^{13}C NMR of 10



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Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-593f24-30
Solvent                 = CHLOROFORM-D
Creation_Time           =  2-FEB-2012 23:21:38
Revision_Time           =  3-FEB-2012 09:42:06
Current_Time            =  28-JUN-2012 17:24:41

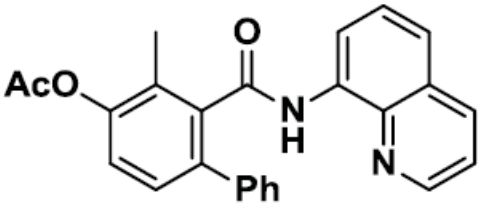
Comment                 = YA-593f24-30
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.043333312[s]
X_Domain                = 13C
X_Freq                  = 100.525303333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.958466665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = TRUE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 15.1[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.043333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.066666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.043333312[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 602
Sawtooth_Range          = 4
```

^{1}H NMR of 11

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Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-5889f11-13
Solvent                 = CHLOROFORM-D
Creation_Time           =  2-FEB-2012 00:24:46
Revision_Time           = 28-JUN-2012 17:33:16
Current_Time            = 28-JUN-2012 17:33:19

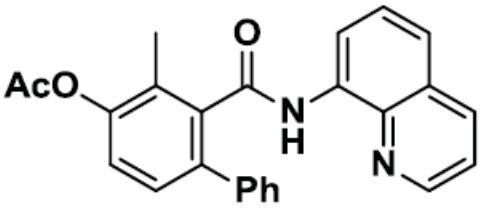
Comment                 = YA-5889f11-13
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Site                    = X
Dimensions              = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.503012[kHz]
X_Sweep_Clipped         = 6.002400961[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 30
Temp_Get                = 15.7[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 759
Sawtooth_Range          = 4
```

^{13}C NMR of 11


AcO
O
N
H
N
Ph

X : parts per Million : Carbon13
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169.438
167.159
148.652
147.994
139.604
138.317
138.202
137.506
135.971
134.103
128.620
128.553
128.143
128.086
127.619
127.343
127.066
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121.689
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77.324
77.210
77.000
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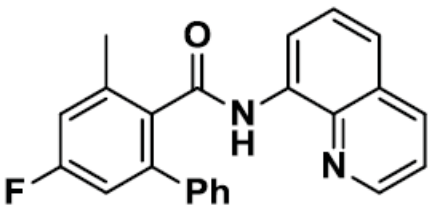
13.309
Filename = E:¥NMRデータ¥反応系(500-699)¥YA-
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-5889f11-13
Solvent = CHLOROFORM-D
Creation_Time = 2-FEB-2012 00:26:29
Revision_Time = 2-FEB-2012 00:56:35
Current_Time = 28-JUN-2012 17:33:38
Comment = YA-5889f11-13
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 15.9[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 769
Sawtooth_Range = 4

^{1}H NMR of 12



Filename = E:¥NMRデータ¥反応系(500-699)¥YA-
Author = delta
Experiment = proton.jxp
Sample_Id = YA-595f70-10
Solvent = CHLOROFORM-D
Creation_Time = 2-FEB-2012 22:46:39
Revision_Time = 28-JUN-2012 17:34:33
Current_Time = 28-JUN-2012 17:34:40

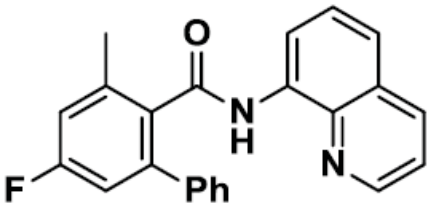
Comment = YA-595f70-10
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 15.1[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]

Lock_Gain = 21
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 632
Sawtooth_Range = 4

^{13}C NMR of 12

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Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-595f70-10
Solvent                 = CHLOROFORM-D
Creation_Time           =  2-FEB-2012 22:48:22
Revision_Time           =  2-FEB-2012 23:12:09
Current_Time            =  28-JUN-2012 17:34:08

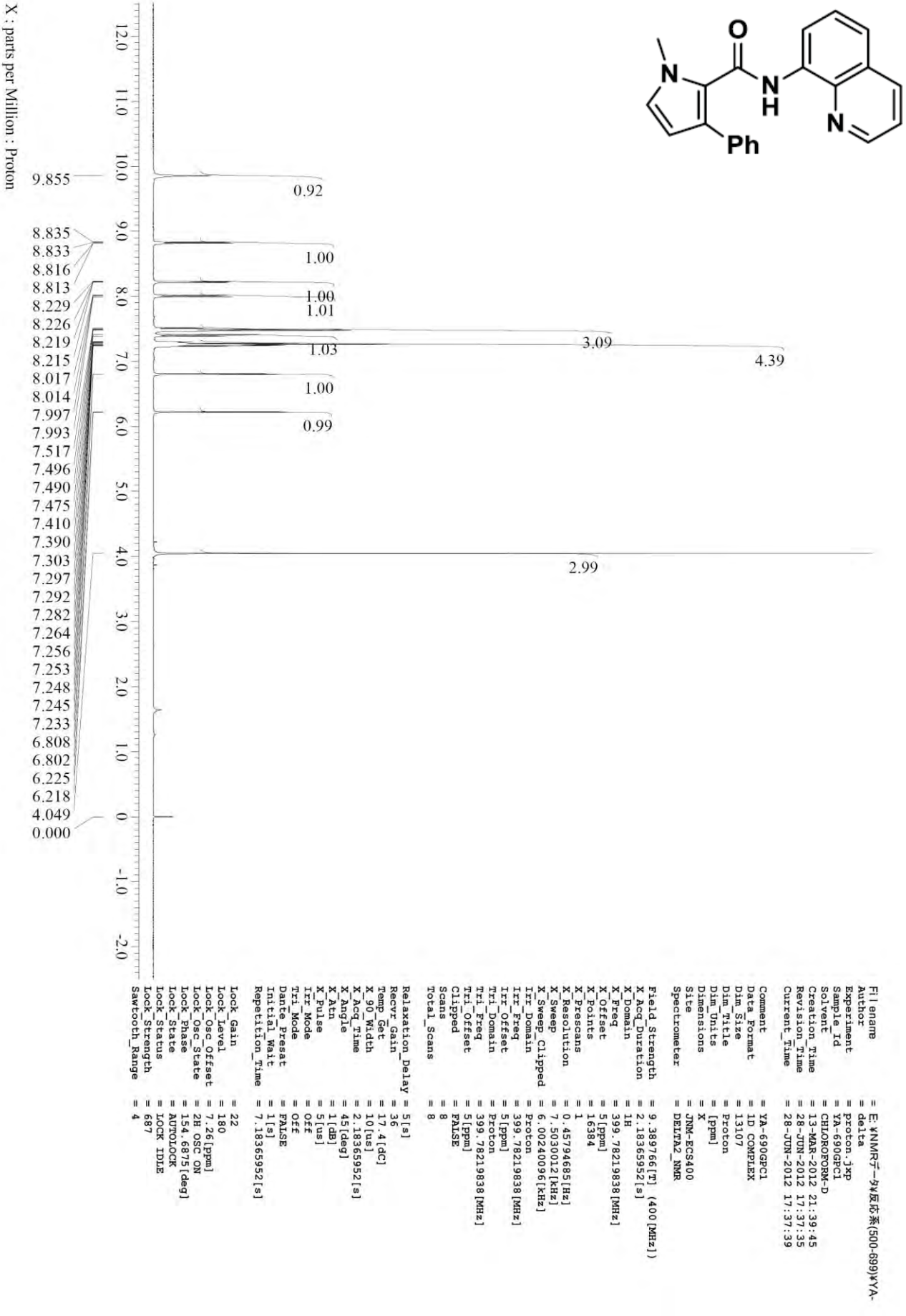
Comment                 = YA-595f70-10
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = TRUE
Scans                   = 296
Total_Scans             = 296

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 15.5[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 633
Sawtooth_Range          = 4
```

^{1}H NMR of 13


X : parts per Million : Proton
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8.813
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8.219
8.215
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7.993
7.517
7.496
7.490
7.475
7.410
7.390
7.303
7.297
7.292
7.282
7.264
7.256
7.253
7.248
7.245
7.233
6.808
6.802
6.225
6.218
4.049
0.000
0.92
1.00
1.00
1.01
1.03
3.09
4.39
1.00
0.99
2.99
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
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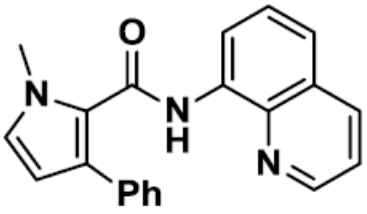
-2.0
Filename = E:¥NMRデータ¥反応系(500-699)¥YA-
Author = delta
Experiment = proton.jxp
Sample_Id = YA-690GPC1
Solvent = CHLOROFORM-D
Creation_Time = 13-MAR-2012 21:39:45
Revision_Time = 28-JUN-2012 17:37:35
Current_Time = 28-JUN-2012 17:37:39
Comment = YA-690GPC1
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 17.4[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 687
Sawtooth_Range = 4

^{13}C NMR of 13



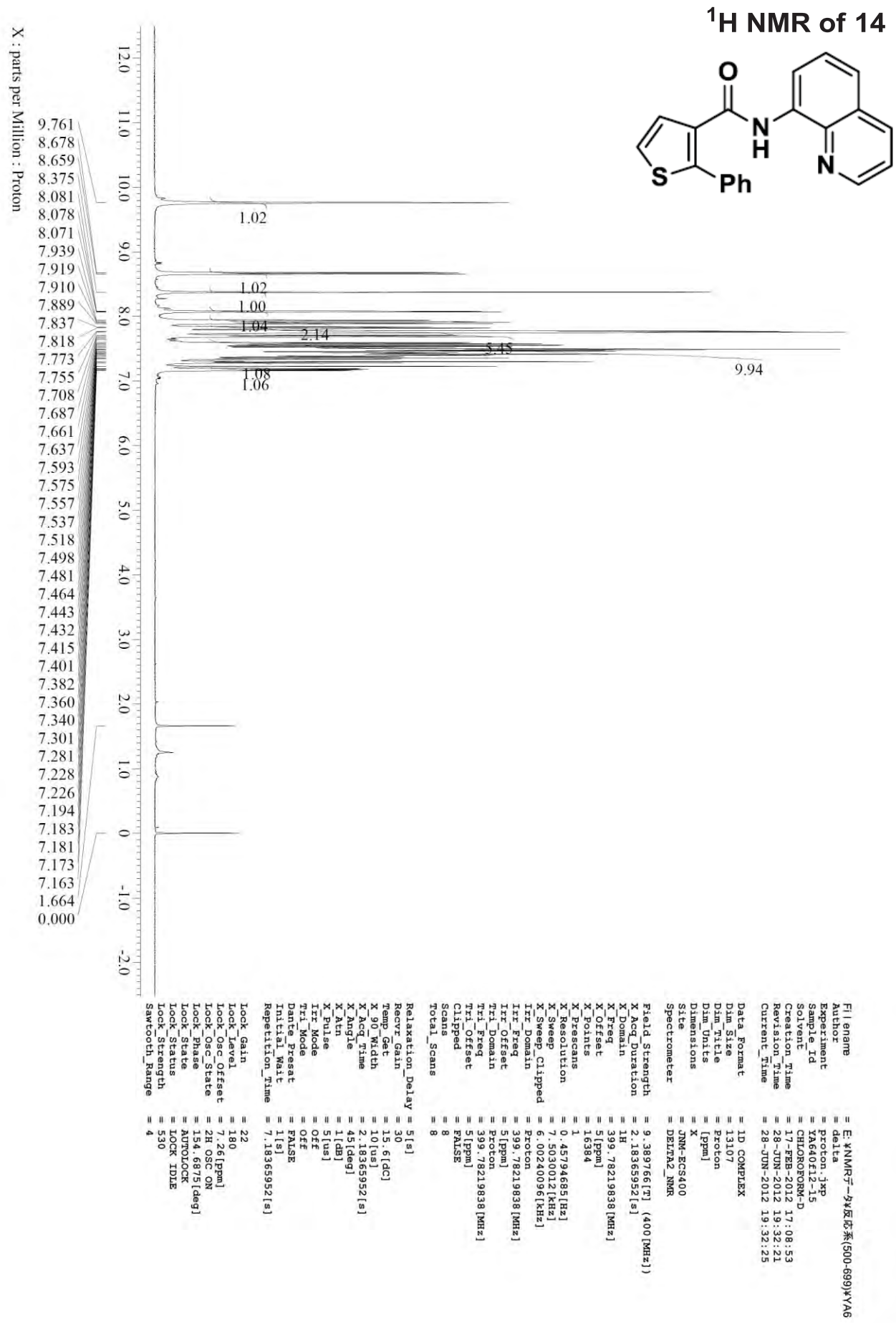
Filename = E:¥NMRデータ¥反応系(500-699)¥YA-
Author = delta
Experiment = carbon.jxp
Sample_id = YA-690GPC1
Solvent = CHLOROFORM-D
Creation_Time = 13-MAR-2012 21:41:26
Revision_Time = 13-MAR-2012 22:18:04
Current_Time = 28-JUN-2012 17:37:22

Comment = YA-690GPC1_Carbon
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR

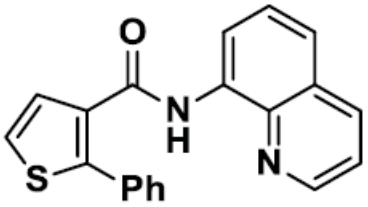
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 512
Total_Scans = 512

Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 17.4[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 667
Sawtooth_Range = 4


^{1}H NMR of 14
O
N
H
S
Ph
N
X : parts per Million : Proton
9.761
8.678
8.659
8.375
8.081
8.078
8.071
7.939
7.919
7.910
7.889
7.837
7.818
7.773
7.755
7.708
7.687
7.661
7.637
7.593
7.575
7.557
7.537
7.518
7.498
7.481
7.464
7.443
7.432
7.415
7.401
7.382
7.360
7.340
7.301
7.281
7.228
7.226
7.194
7.183
7.181
7.173
7.163
1.664
0.000
1.02
1.02
1.00
1.04
2.14
5.45
9.94
1.08
1.06
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
Filename = E:¥NMRデータ¥反応系(500-699)¥YA6
Author = delta
Experiment = proton.jxp
Sample_Id = YA640f12-15
Solvent = CHLOROFORM-D
Creation_Time = 17-FEB-2012 17:08:53
Revision_Time = 28-JUN-2012 19:32:21
Current_Time = 28-JUN-2012 19:32:25
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 30
Temp_Get = 15.6[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 530
Sawtooth_Range = 4

^{13}C NMR of 14

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Filename                = E:¥NMR子一タ¥反応系(500-699)¥YA6
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA640f12-15
Solvent                 = CHLOROFORM-D
Creation_Time           = 17-FEB-2012 17:10:36
Revision_Time           = 17-FEB-2012 18:34:43
Current_Time            = 28-JUN-2012 19:32:43

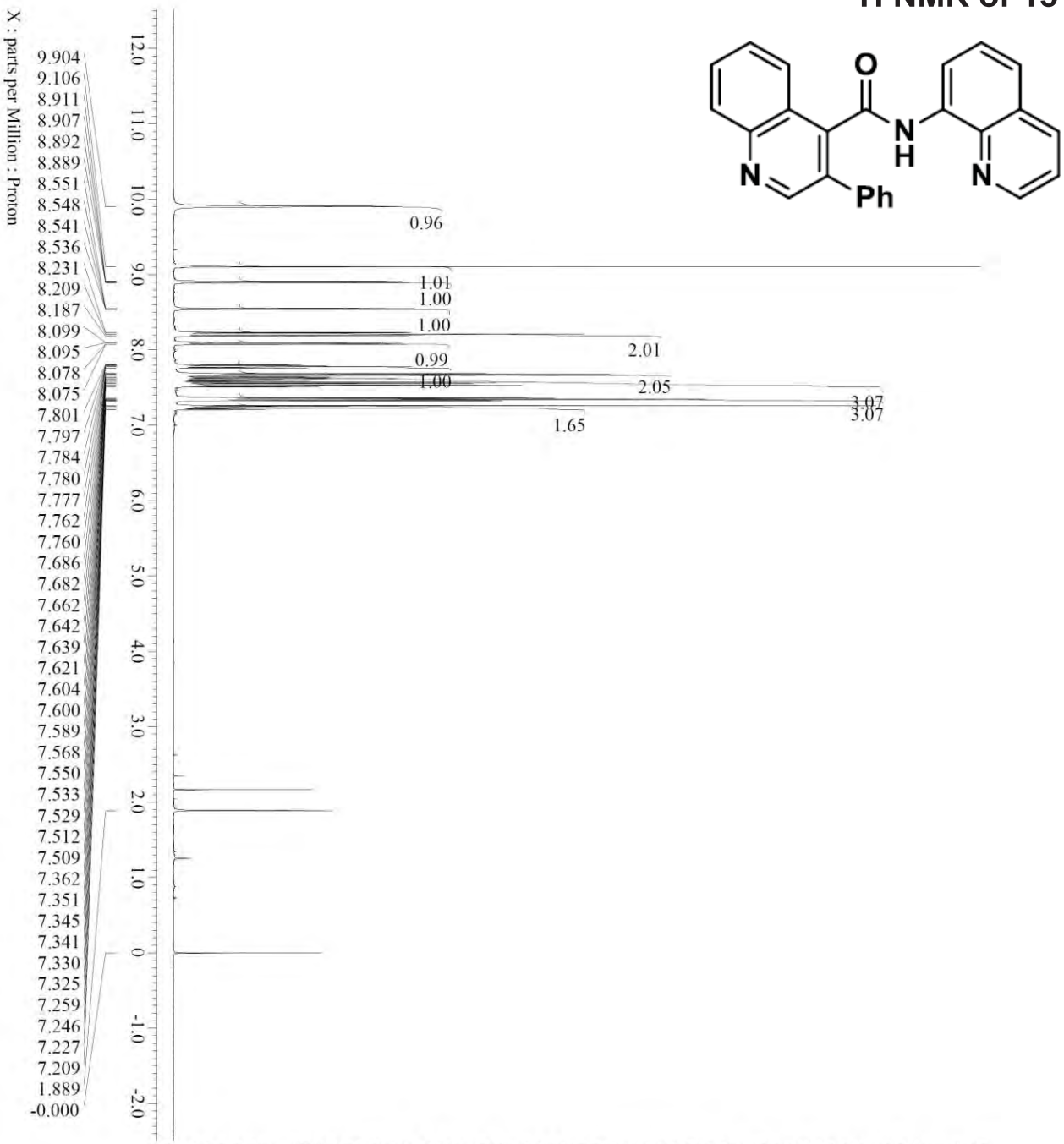
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
ClipPed                 = FALSE
Scans                   = 1536
Total_Scans             = 1536

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 15.6[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Atn                   = 30[deg]
X_Pulse                 = 6[dB]
Irr_Atn_Dec             = 3.06666667[us]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ2
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 537
Sawtooth_Range          = 4
```

^{1}H NMR of 15

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Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-604GPC1
Solvent                 = CHLOROFORM-D
Creation_Time           =  6-FEB-2012 23:44:28
Revision_Time           = 28-JUN-2012 17:39:05
Current_Time            = 28-JUN-2012 17:39:12

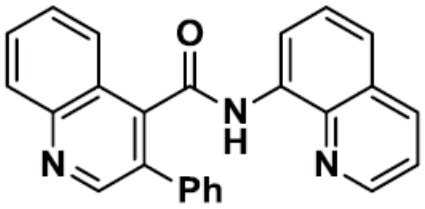
Comment                 = YA-604GPC1
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.5030012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 34
Temp_Get                = 16.4[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 564
Sawtooth_Range          = 4
```

^{13}C NMR of 15

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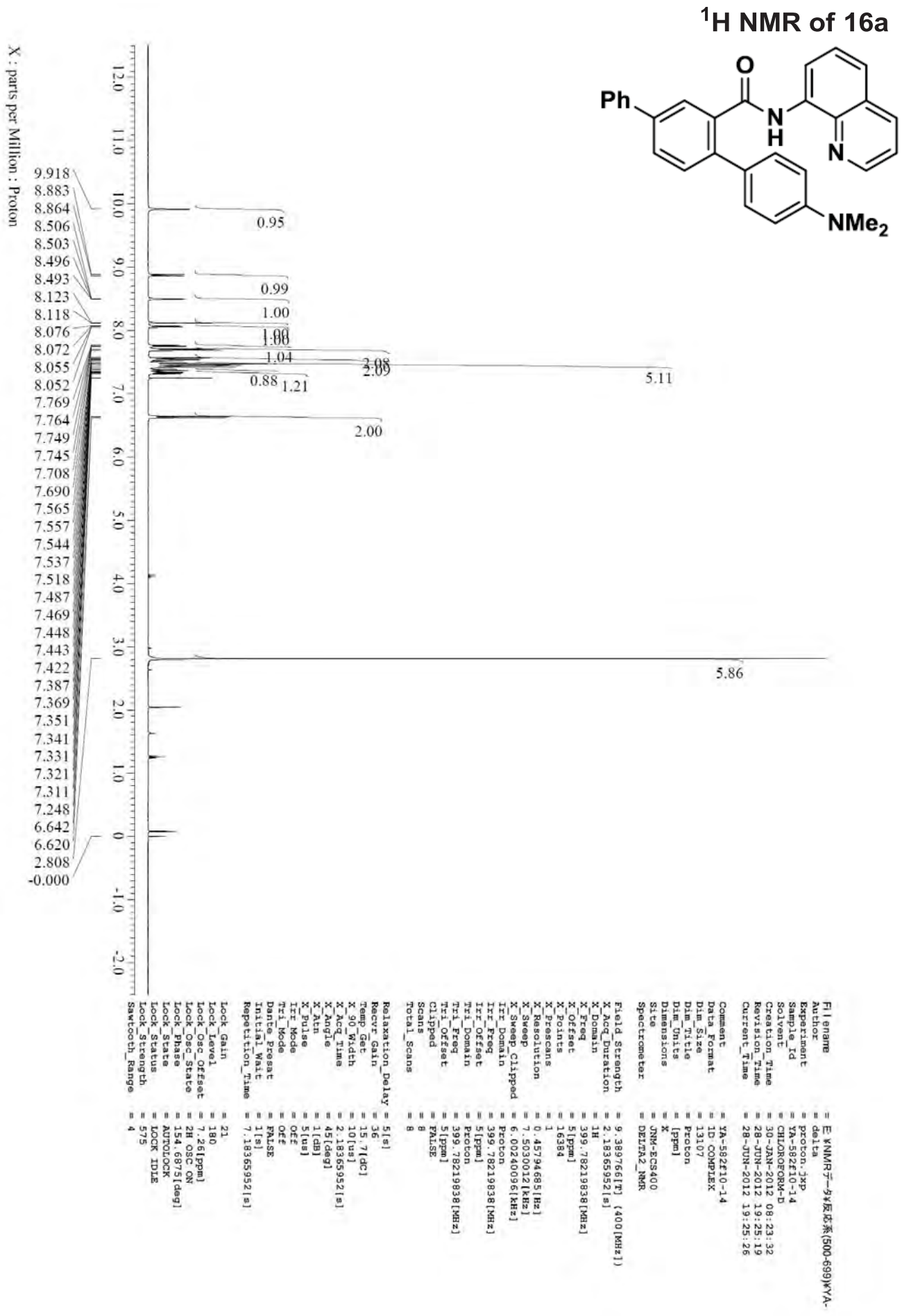
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-604GPC1
Solvent                 = CHLOROFORM-D
Creation_Time           = 6-FEB-2012 23:46:09
Revision_Time           = 7-FEB-2012 00:13:27
Current_Time            = 28-JUN-2012 17:39:52

Comment                 = YA-604GPC1_Carbon
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

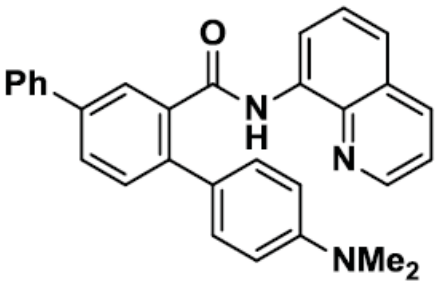
Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 16.5[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 565
Sawtooth_Range          = 4
```


^{1}H NMR of 16a
Ph
O
N
H
N
NMe$_2$
X : parts per Million : Proton
9.918
8.883
8.864
8.506
8.503
8.496
8.493
8.123
8.118
8.076
8.072
8.055
8.052
7.769
7.764
7.749
7.745
7.708
7.690
7.565
7.557
7.544
7.537
7.518
7.487
7.469
7.448
7.443
7.422
7.387
7.369
7.351
7.341
7.331
7.321
7.311
7.248
6.642
6.620
2.808
-0.000
0.95
0.99
1.00
1.00
1.00
1.04
2.08
2.05
0.88
1.21
5.11
2.00
5.86
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
Filename = E:¥NMRデータ¥反応系(500-699)¥YA-
Author = delta
Experiment = proton.jxp
Sample_Id = YA-582f10-14
Solvent = CHLOROFORM-D
Creation_Time = 30-JAN-2012 08:23:32
Revision_Time = 28-JUN-2012 19:25:19
Current_Time = 28-JUN-2012 19:25:26
Comment = YA-582f10-14
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.183659521[s]
X_Domain = 1H
X_Freq = 399.7821983[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.457946851[Hz]
X_Sweep = 7.503012[kHz]
X_Sweep_Clipped = 6.002409[kHz]
Irr_Domain = Proton
Irr_Freq = 399.7821983[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.7821983[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 15.7[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.183659521[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.183659521[s]
Lock_Gain = 21
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 575
Sawtooth_Range = 4

^{13}C NMR of 16a




```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-582f10-14
Solvent                 = CHLOROFORM-D
Creation_Time           = 30-JAN-2012 08:25:20
Revision_Time           = 28-JUN-2012 19:24:54
Current_Time            = 28-JUN-2012 19:25:00

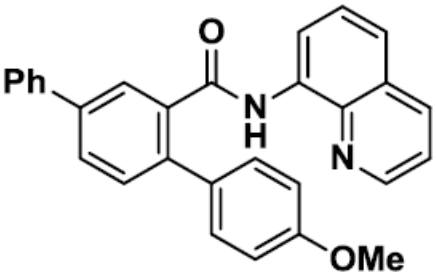
Comment                 = YA-582f10-14
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 15.7[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 561
Sawtooth_Range          = 4
```

^{1}H NMR of 16b

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Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-575f11-14
Solvent                 = CHLOROFORM-D
Creation_Time           = 27-JAN-2012 00:50:40
Revision_Time           = 28-JUN-2012 17:42:17
Current_Time            = 28-JUN-2012 17:42:21

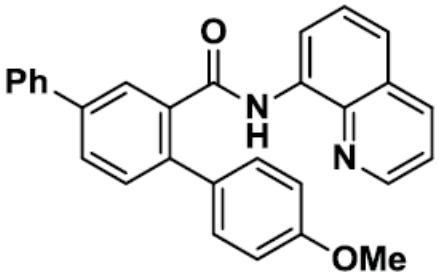
Comment                 = YA-575f11-14
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.50300212[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 30
Temp_Get                = 16.3[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 682
Sawtooth_Range          = 4
```

^{13}C NMR of 16b

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Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-575f11-14
Solvent                 = CHLOROFORM-D
Creation_Time           = 27-JAN-2012 01:19:11
Revision_Time           = 27-JAN-2012 09:10:10
Current_Time            = 28-JUN-2012 17:42:35

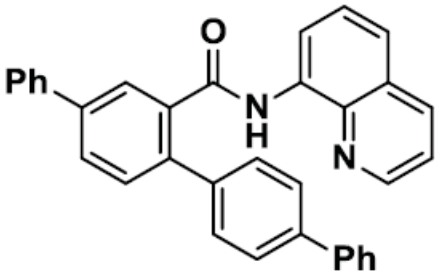
Comment                 = YA-575f11-14 13C
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 16.2[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 683
Sawtooth_Range          = 4
```

^{1}H NMR of 16c

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Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-583 seiseigo
Solvent                 = CHLOROFORM-D
Creation_Time           = 1-MAR-2012 01:06:57
Revision_Time           = 29-JUN-2012 16:32:27
Current_Time            = 29-JUN-2012 16:32:31

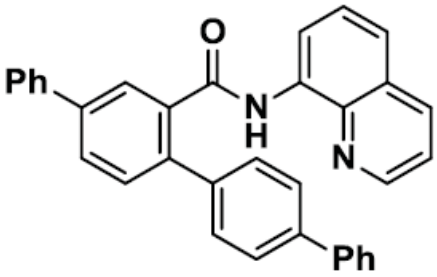
Comment                 = YA-583 seiseigo
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.50300l2[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 38
Temp_Get                = 17.1[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 707
Sawtooth_Range          = 4
```

^{13}C NMR of 16c



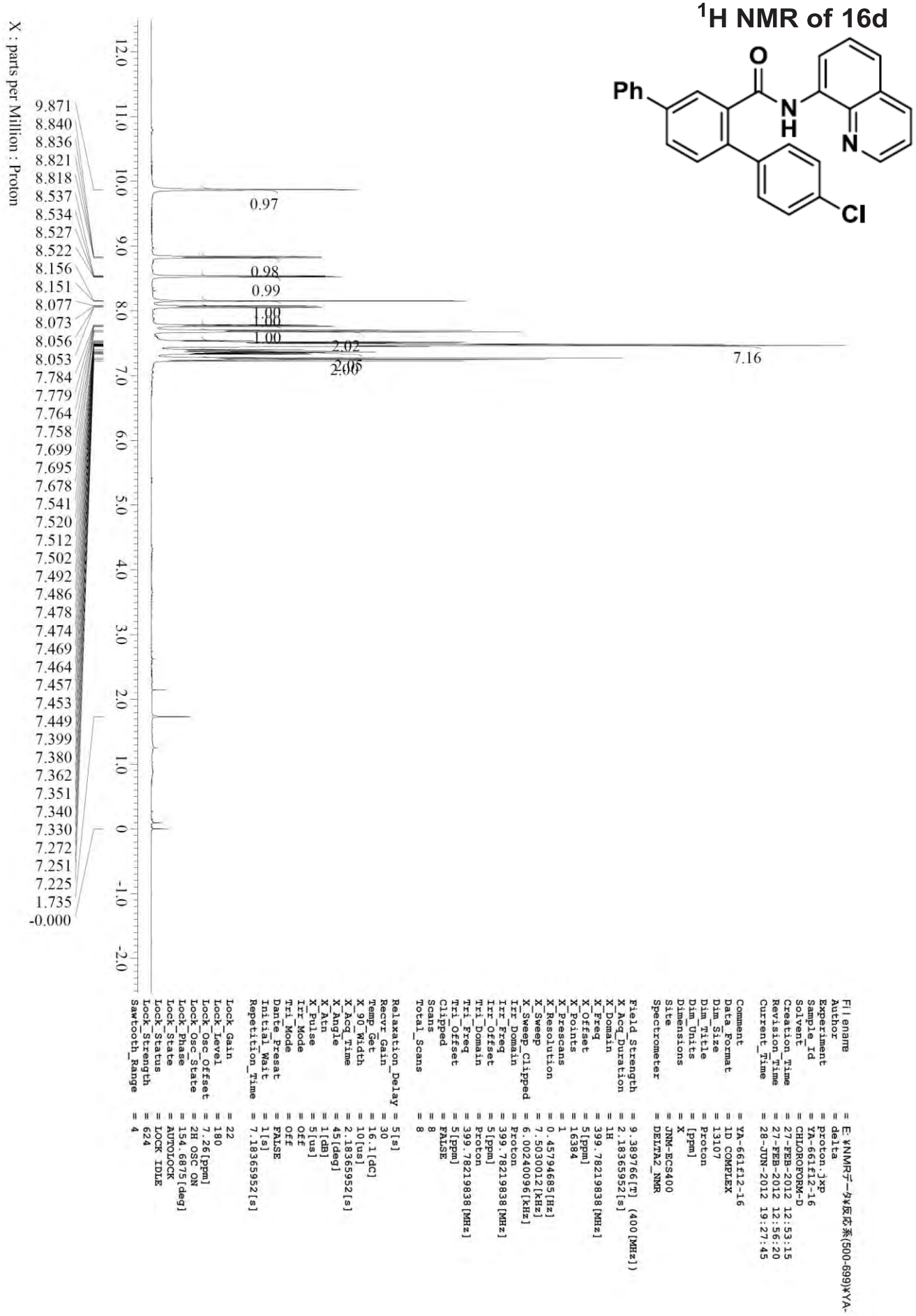

```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-583f3-6
Solvent                 = CHLOROFORM-D
Creation_Time           = 30-JAN-2012 15:19:20
Revision_Time           = 30-JAN-2012 17:02:36
Current_Time            = 28-JUN-2012 19:26:16

Comment                 = YA-583f3-6
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = TRUE
Scans                   = 1024
Total_Scans             = 1024

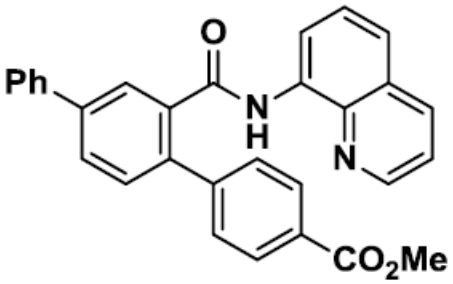
Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 15.3[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 740
Sawtooth_Range          = 4
```


^{1}H NMR of 16d
Ph
O
N
H
N
Cl
X : parts per Million : Proton
9.871
8.840
8.836
8.821
8.818
8.537
8.534
8.527
8.522
8.156
8.151
8.077
8.073
8.056
8.053
7.784
7.779
7.764
7.758
7.699
7.695
7.678
7.541
7.520
7.512
7.502
7.492
7.486
7.478
7.474
7.469
7.464
7.457
7.453
7.449
7.399
7.380
7.362
7.351
7.340
7.330
7.272
7.251
7.225
1.735
-0.000
0.97
0.98
0.99
1.00
1.00
1.00
2.02
2.05
7.16
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
Filename = E:¥NMRデータ¥反応系(500-699)¥YA-
Author = delta
Experiment = proton.jxp
Sample_Id = YA-661f12-16
Solvent = CHLOROFORM-D
Creation_Time = 27-FEB-2012 12:53:15
Revision_Time = 27-FEB-2012 12:56:20
Current_Time = 28-JUN-2012 19:27:45
Comment = YA-661f12-16
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 30
Temp_Get = 16.1[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 624
Sawtooth_Range = 4

13C NMR of 16d
Ph
O
N
H
N
Cl
X : parts per Million : Carbon13
167.340
147.823
140.786
139.537
138.269
138.021
137.669
136.286
136.019
134.236
133.826
131.023
130.222
129.078
128.906
128.601
127.867
127.829
127.667
127.161
127.037
121.755
121.479
116.349
77.315
77.200
77.000
76.676
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
Filename = E:¥NMRデータ¥反応系(500-699)¥YA-
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-661f12-16
Solvent = CHLOROFORM-D
Creation_Time = 27-FEB-2012 12:54:58
Revision_Time = 27-FEB-2012 13:40:08
Current_Time = 28-JUN-2012 19:27:29
Comment = YA-661f12-16 13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.043333l2[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 858
Total_Scans = 858
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 15.7[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.043333l2[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.043333l2[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 639
Sawtooth_Range = 4

^{1}H NMR of 16e




```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-579f12-16
Solvent                 = CHLOROFORM-D
Creation_Time           = 30-JAN-2012 08:57:09
Revision_Time           = 29-JUN-2012 16:22:05
Current_Time            = 29-JUN-2012 16:22:13

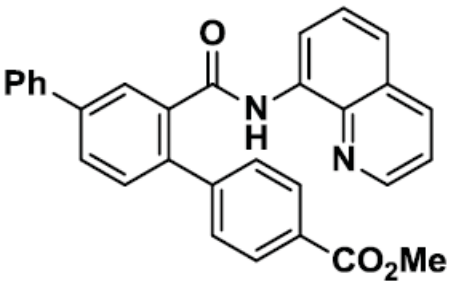
Comment                 = YA-579f12-16
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.5030012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr Gain_             = 38
Temp_Get                = 15.3[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 666
Sawtooth_Range          = 4
```

^{13}C NMR of 16e




```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-579f12-16
Solvent                 = CHLOROFORM-D
Creation_Time           = 30-JAN-2012 08:58:51
Revision_Time           = 30-JAN-2012 09:27:30
Current_Time            = 28-JUN-2012 19:23:36

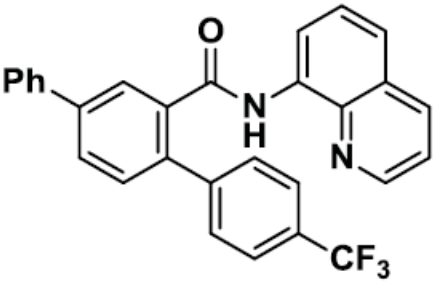
Comment                 = YA-579f12-16
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.043333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 15.6[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.043333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.043333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 631
Sawtooth_Range          = 4
```

^{1}H NMR of 16f



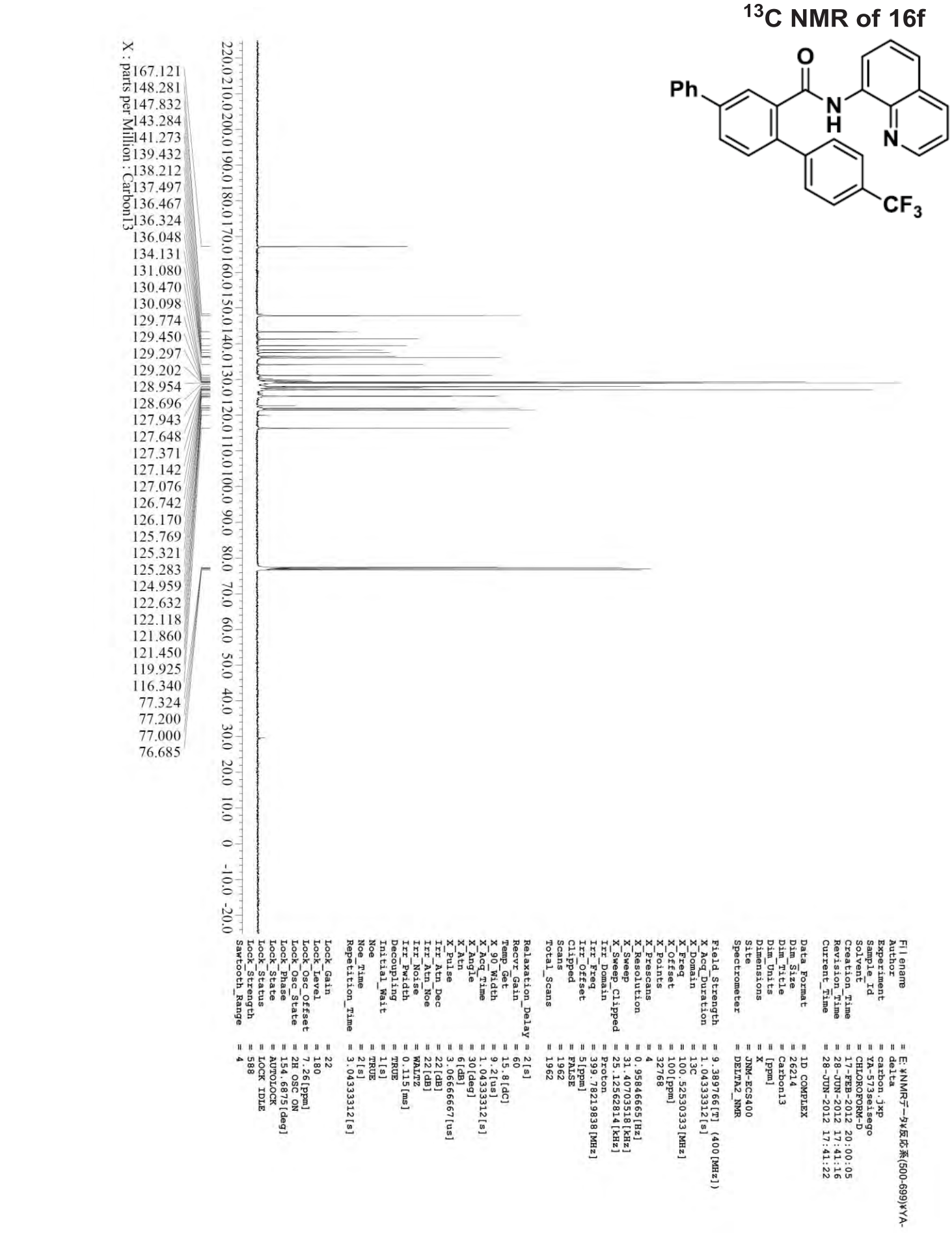

```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-573f-9-13
Solvent                 = CHLOROFORM-D
Creation_Time           = 27-JAN-2012 00:18:09
Revision_Time           = 28-JUN-2012 17:40:58
Current_Time            = 28-JUN-2012 17:41:02

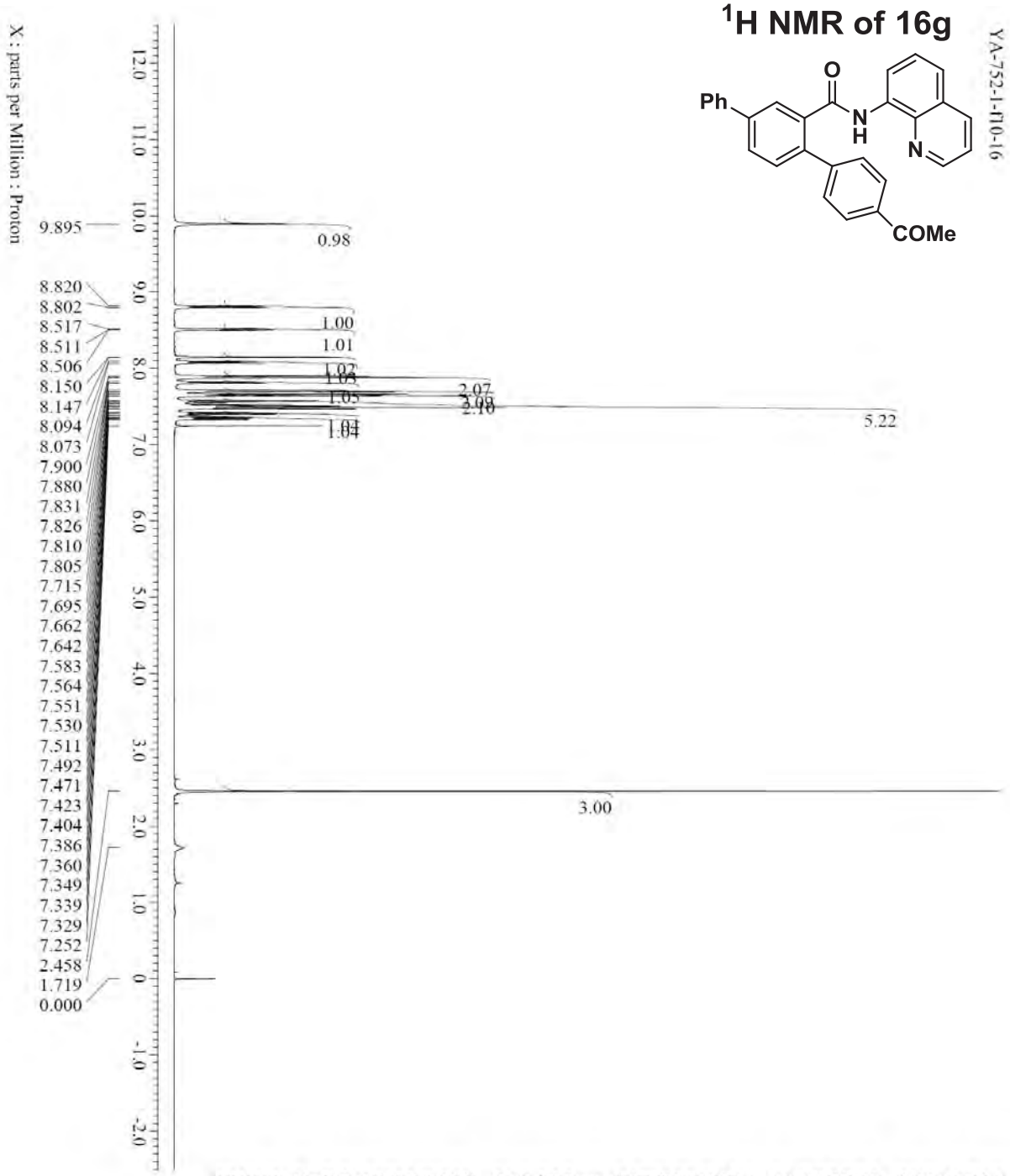
Comment                 = YA-573f-9-13
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.50300012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 30
Temp_Get                = 16.1[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 613
Sawtooth_Range          = 4
```


13C NMR of 16f
Ph
O
N
H
N
CF3
X : parts per Million : Carbon13
167.121
148.281
147.832
143.284
141.273
139.432
138.212
137.497
136.467
136.324
136.048
134.131
131.080
130.470
130.098
129.774
129.450
129.297
129.202
128.954
128.696
127.943
127.648
127.371
127.142
127.076
126.742
126.170
125.769
125.321
125.283
124.959
122.632
122.118
121.860
121.450
119.925
116.340
77.324
77.200
77.000
76.685
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
Filename = E:¥NMRデータ¥反応系(500-699)¥YA-
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-573seisego
Solvent = CHLOROFORM-D
Creation_Time = 17-FEB-2012 20:00:05
Revision_Time = 28-JUN-2012 17:41:16
Current_Time = 28-JUN-2012 17:41:22
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1962
Total_Scans = 1962
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 15.8[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 588
Sawtooth_Range = 4

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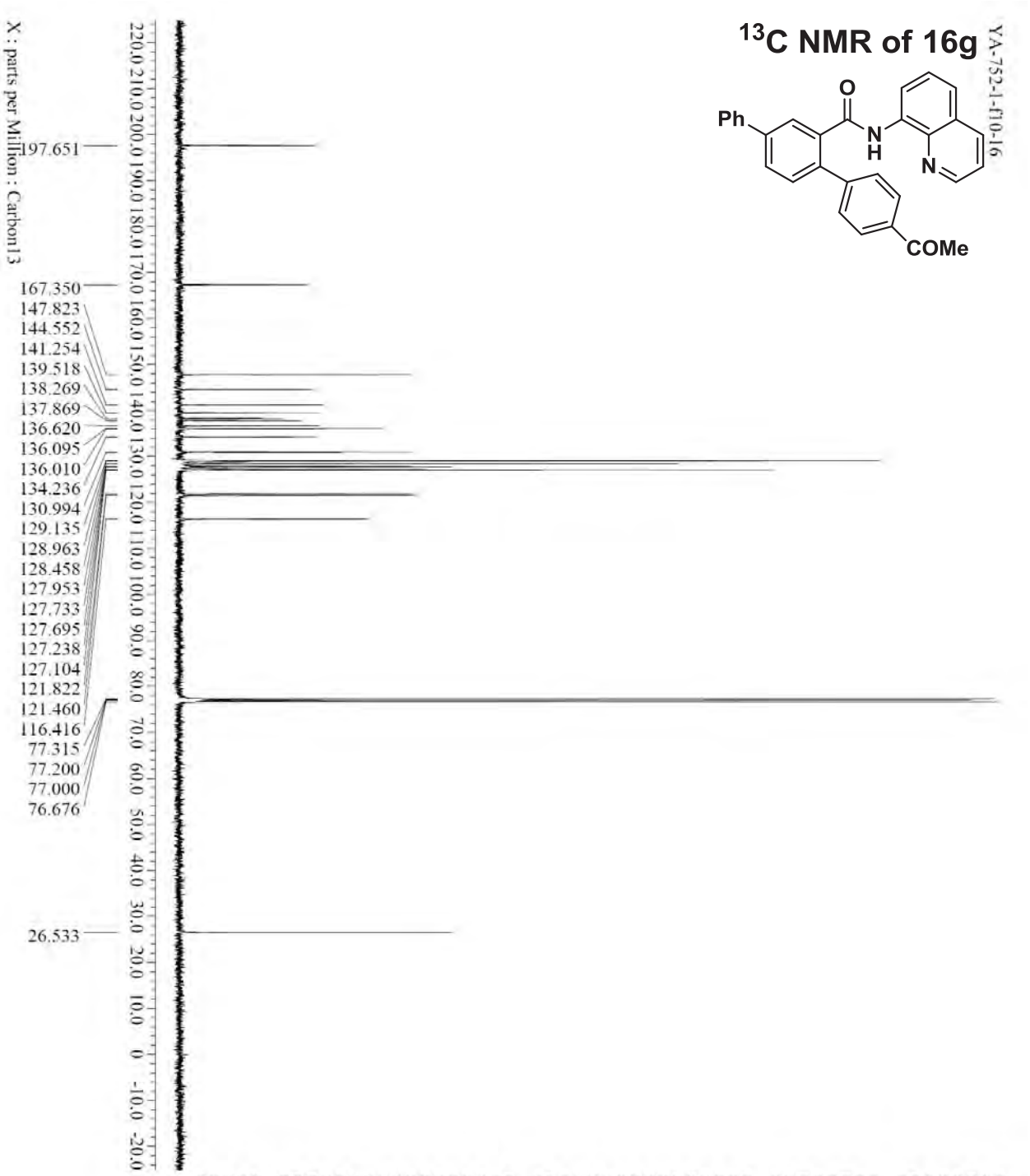
Filename                = E:\aihara NMR\YA-752-1-f10
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-752-1-f10-16
Solvent                 = CHLOROFORM-D
Creation_Time           = 30-MAY-2012 11:55:37
Revision_Time           = 18-AUG-2012 10:50:17
Current_Time            = 18-AUG-2012 10:52:58

Comment                 = YA-752-1-f10-16
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.5030012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 34
Temp_Get                = 18.7[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Status             = LOCK IDLE
Lock_Strength           = 663
```

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Filename                = E:\aihara NMR\YA-752-1-f10
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-752-1-f10-16
Solvent                 = CHLOROFORM-D
Creation_Time           = 30-MAY-2012 11:57:20
Revision_Time           = 18-AUG-2012 10:50:27
Current_Time            = 18-AUG-2012 10:53:13

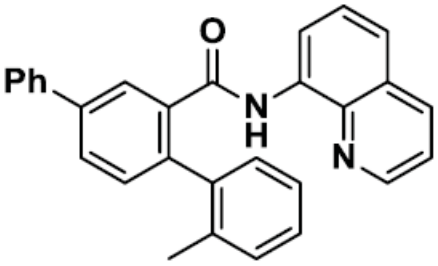
Comment                 = YA-752-1-f10-16
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.043333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.4070351[kHz]
X_Sweep_Clipped         = 25.1256281[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 711
Total_Scans             = 711

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 19[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.043333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Status             = LOCK IDLE
Lock_Strength           = 676
```

^{1}H NMR of 17a

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Filename                = E:¥NMRデータ反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-601f6-13
Solvent                 = CHLOROFORM-D
Creation_Time           =  6-FEB-2012 10:29:18
Revision_Time           = 28-JUN-2012 19:28:37
Current_Time            = 28-JUN-2012 19:28:43

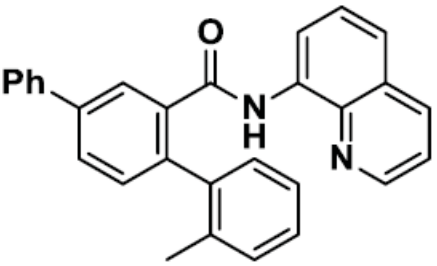
Comment                 = YA-601f6-13
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.50300012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 30
Temp_Get                = 15.8[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 747
Sawtooth_Range          = 4
```

^{13}C NMR of 17a



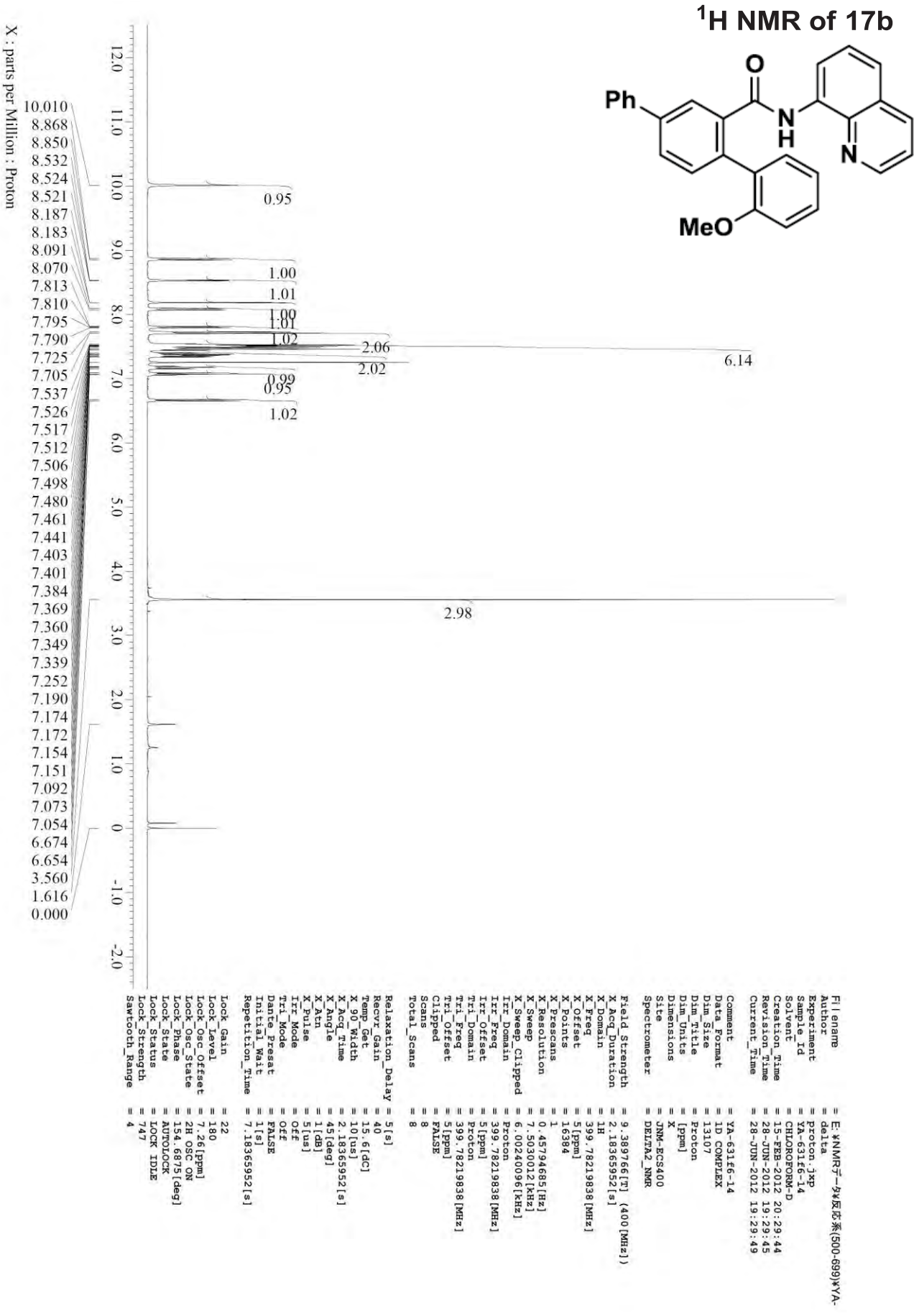

```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-601f6-13
Solvent                 = CHLOROFORM-D
Creation_Time           =  6-FEB-2012 10:33:41
Revision_Time           =  6-FEB-2012 11:01:38
Current_Time            = 28-JUN-2012 19:28:54

Comment                 = YA-601f6-13_Carbon
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

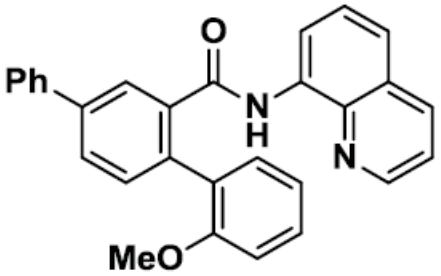
Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.043333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.7821938[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 15.7[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.043333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.043333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 751
Sawtooth_Range          = 4
```


^{1}H NMR of 17b
Ph
O
N
H
N
MeO
X : parts per Million : Proton
10.010
8.868
8.850
8.532
8.524
8.521
8.187
8.183
8.091
8.070
7.813
7.810
7.795
7.790
7.725
7.705
7.537
7.526
7.517
7.512
7.506
7.498
7.480
7.461
7.441
7.403
7.401
7.384
7.369
7.360
7.349
7.339
7.252
7.190
7.174
7.172
7.154
7.151
7.092
7.073
7.054
6.674
6.654
3.560
1.616
0.000
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
0.95
1.00
1.01
1.00
1.01
1.02
2.06
2.02
0.99
0.95
1.02
6.14
2.98
Filename = E:¥NMRデータ¥反応系(500-699)¥YA-
Author = delta
Experiment = proton.jxp
Sample_Id = YA-631f6-14
Solvent = CHLOROFORM-D
Creation_Time = 15-FEB-2012 20:29:44
Revision_Time = 28-JUN-2012 19:29:45
Current_Time = 28-JUN-2012 19:29:49
Comment = YA-631f6-14
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 15.6[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 747
Sawtooth_Range = 4

^{13}C NMR of 17b

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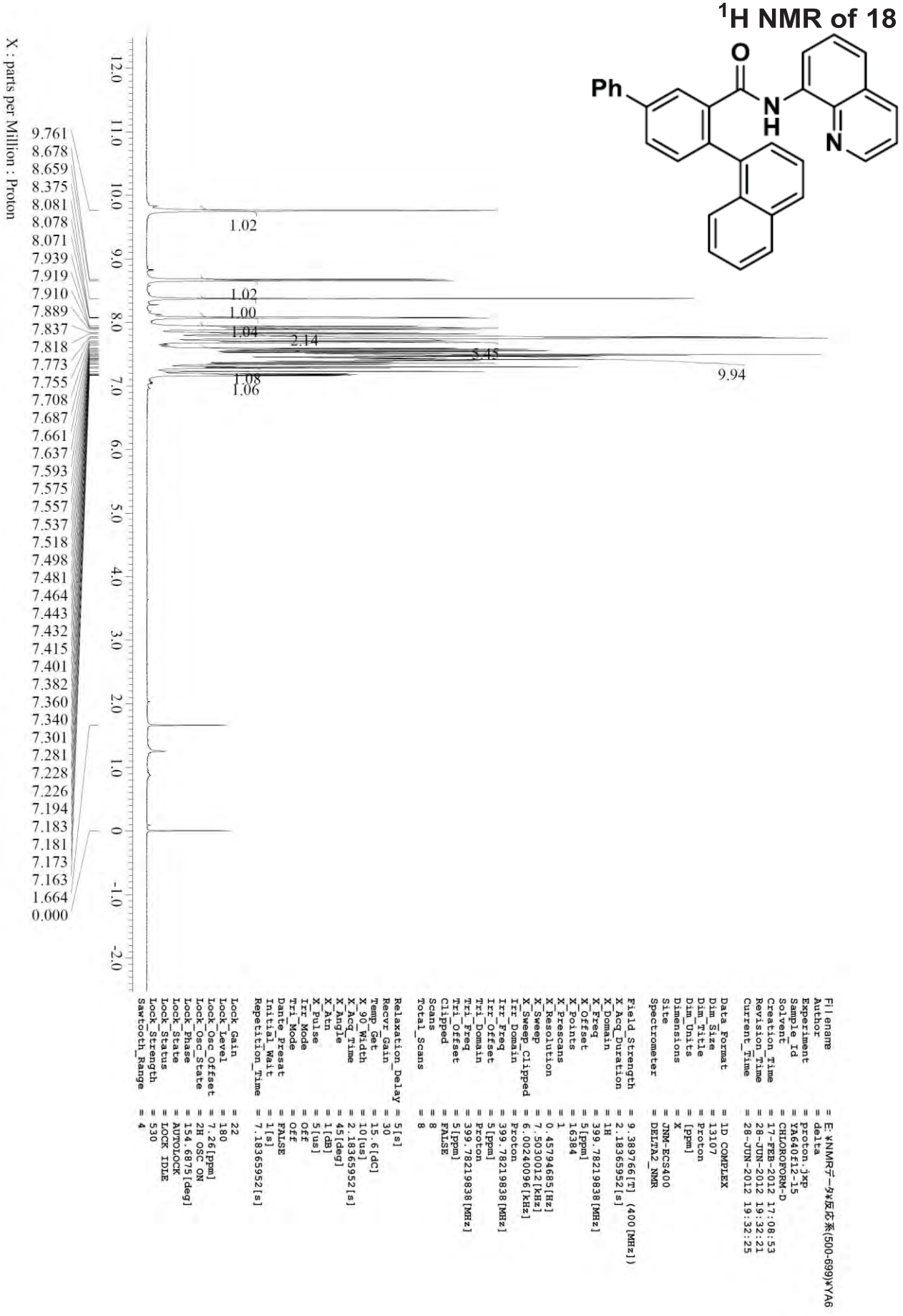
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-631f6-14
Solvent                 = CHLOROFORM-D
Creation_Time           = 15-FEB-2012 20:31:26
Revision_Time           = 15-FEB-2012 21:22:18
Current_Time            = 28-JUN-2012 19:30:01

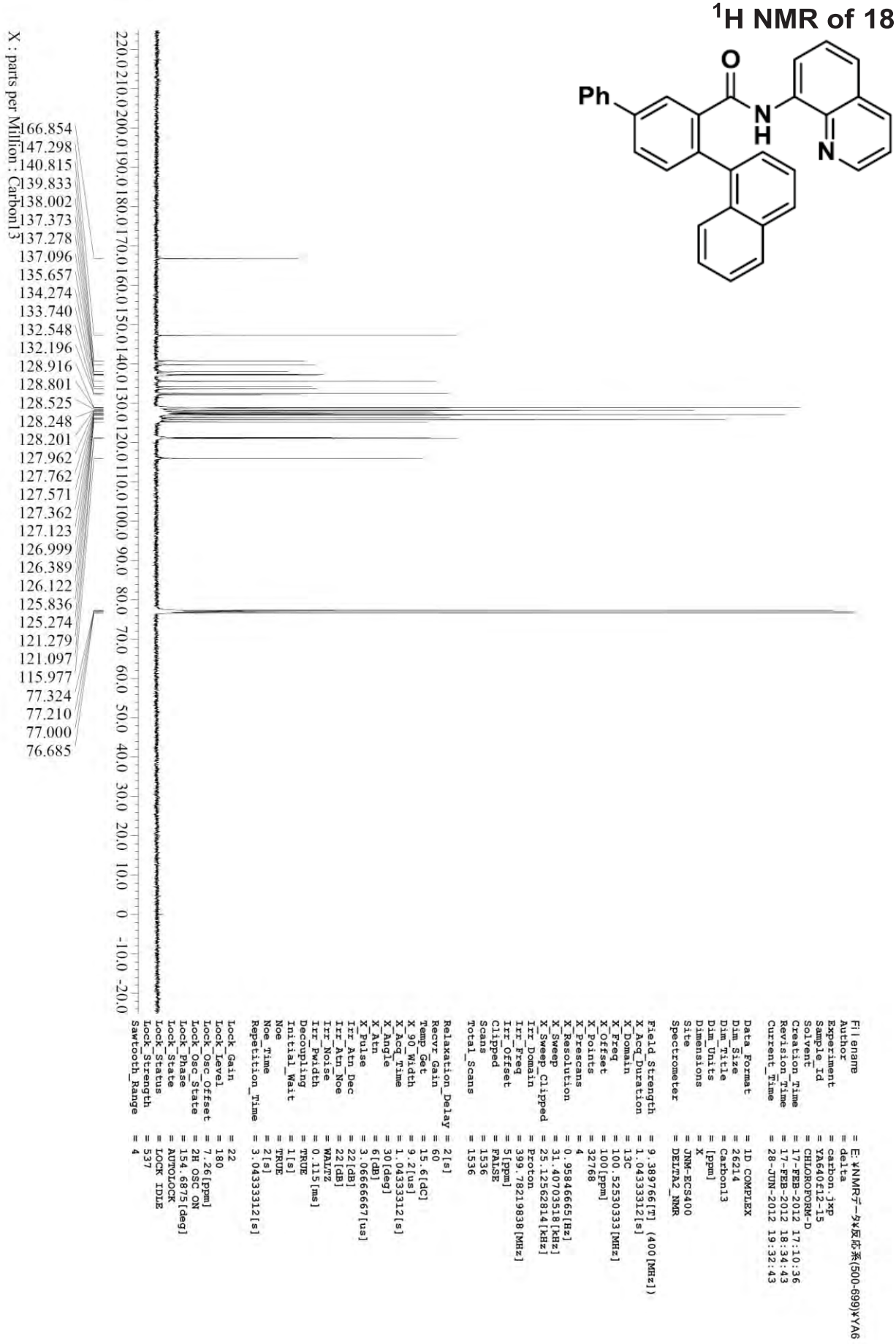
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 972
Total_Scans             = 972

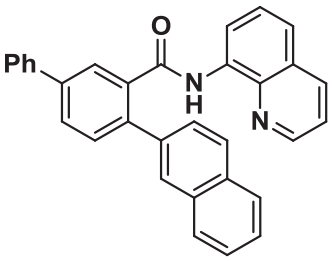
Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 15.7[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 746
Sawtooth_Range          = 4
```


^{1}H NMR of 18
Ph
O
N
H
N
X : parts per Million : Proton
9.761
8.678
8.659
8.375
8.081
8.078
8.071
7.939
7.919
7.910
7.889
7.837
7.818
7.773
7.755
7.708
7.687
7.661
7.637
7.593
7.575
7.557
7.537
7.518
7.498
7.481
7.464
7.443
7.432
7.415
7.401
7.382
7.360
7.340
7.301
7.281
7.228
7.226
7.194
7.183
7.181
7.173
7.163
1.664
0.000
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
1.02
1.02
1.00
1.04
2.14
3.45
1.08
1.06
9.94
Filename = E:¥NMR¥一分¥反応系(500-699)¥YA6
Author = delta
Experiment = proton.jxp
Sample_Id = YA640f12-15
Solvent = CHLOROFORM-D
Creation_Time = 17-FEB-2012 17:08:53
Revision_Time = 28-JUN-2012 19:32:21
Current_Time = 28-JUN-2012 19:32:25
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.503012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 30
Temp_Get = 15.6[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 530
Sawtooth_Range = 4


^{1}H NMR of 18
Ph
O
N
H
N
X : parts per Million : Carbon13
166.854
147.298
140.815
139.833
138.002
137.373
137.278
137.096
135.657
134.274
133.740
132.548
132.196
128.916
128.801
128.525
128.248
128.201
127.962
127.762
127.571
127.362
127.123
126.999
126.389
126.122
125.836
125.274
121.279
121.097
115.977
77.324
77.210
77.000
76.685
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
Filename = E:¥NMR データ¥反応系(500-699)¥YA6
Author = delta
Experiment = carbon.jxp
Sample_Id = YA640f12-15
Solvent = CHLOROFORM-D
Creation_Time = 17-FEB-2012 17:10:36
Revision_Time = 17-FEB-2012 18:34:43
Current_Time = 28-JUN-2012 19:32:43
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.043333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.958466665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1536
Total_Scans = 1536
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 15.6[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.043333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.066666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.043333312[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 537
Sawtooth_Range = 4

^{1}H NMR of 19

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Filename                = E:\aihara NMR\YA-641f7-10-
Author                  = delta
Experiment              = proton.jxp
Sample_id               = YA-641f7-10
Solvent                 = CHLOROFORM-D
Creation_Time           = 17-FEB-2012 19:52:46
Revision_Time           = 18-AUG-2012 10:44:03
Current_Time            = 18-AUG-2012 10:52:44

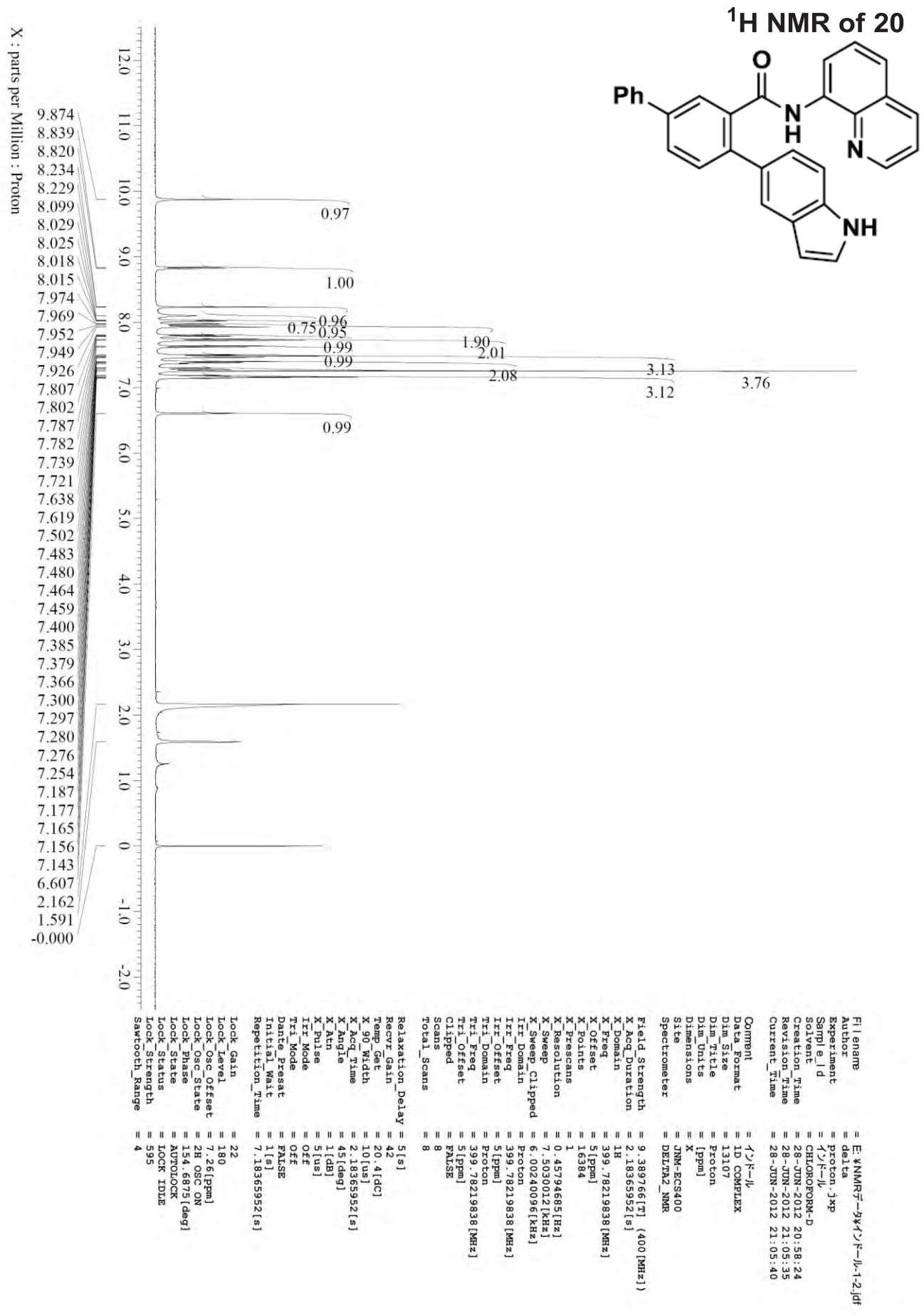
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.50300120[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

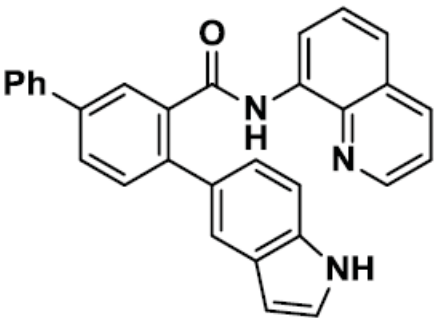
Relaxation_Delay        = 5[s]
Recvr_Gain              = 46
Temp_Get                = 15.8[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_offset         = 7.26[ppm]
Lock_Status             = LOCK IDLE
Lock_Strength           = 604
```


13C NMR of 19
Ph
O
N
H
N
X : parts per Million : Carbon13
167.397
147.394
140.634
139.795
139.032
138.269
137.220
136.210
135.619
134.370
133.616
132.815
131.519
129.192
128.925
128.334
128.172
128.105
128.010
127.772
127.581
127.447
127.180
127.123
127.066
126.132
125.989
121.498
121.145
116.273
77.315
77.200
77.000
76.676
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
Filename = E:\saihara NMR\YA641f7-10_C
Author = delta
Experiment = carbon.jxp
Sample_Id = YA641f7-10
Solvent = CHLOROFORM-D
Creation_Time = 17-FEB-2012 15:55:20
Revision_Time = 18-AUG-2012 10:44:32
Current_Time = 18-AUG-2012 10:50:33
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1366
Total_Scans = 1366
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 15.9[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Status = LOCK IDLE
Lock_Strength = 474



^{13}C NMR of 20




```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-651f8-9
Solvent                 = CHLOROFORM-D
Creation_Time           =  7-MAR-2012 18:57:22
Revision_Time           =  7-MAR-2012 20:56:04
Current_Time            = 28-JUN-2012 19:35:48

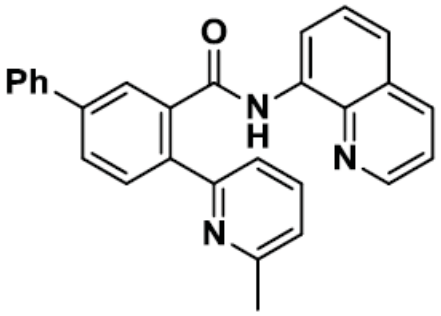
Comment                 = YA-651f8-9
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 2048
Total_Scans             = 2048

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 17.4[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 857
Sawtooth_Range          = 4
```

^{1}H NMR of 21



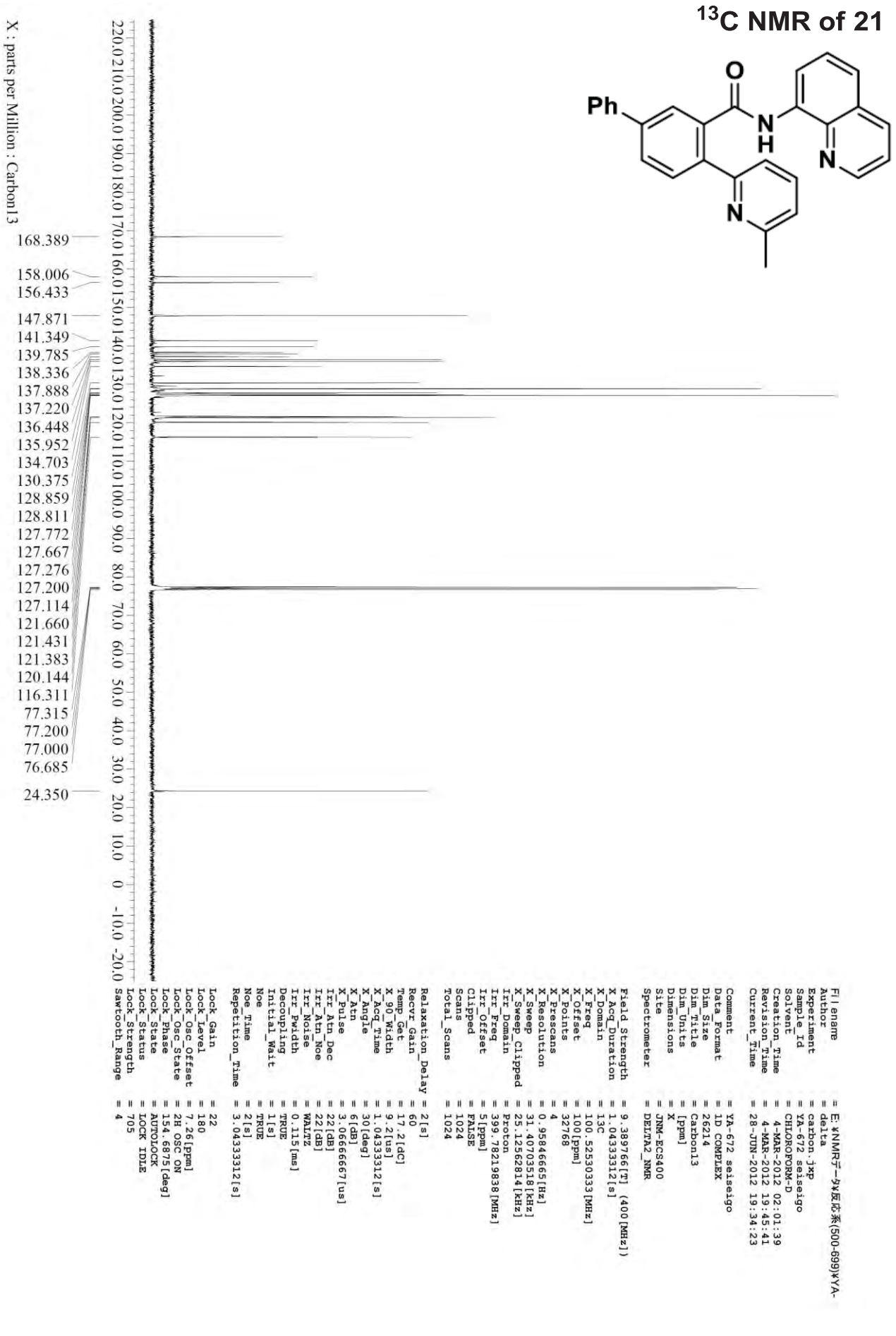

```
Filename                = E:¥NMRデータ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-672seiseigo
Solvent                 = CHLOROFORM-D
Creation_Time           = 3-MAR-2012 20:09:25
Revision_Time           = 29-JUN-2012 16:52:15
Current_Time            = 29-JUN-2012 16:52:20

Comment                 = YA-672seiseigo
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.5030012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr Gain              = 30
Temp_Get                = 17.1[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 21
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 510.0
Sawtooth_Range          = 4
```



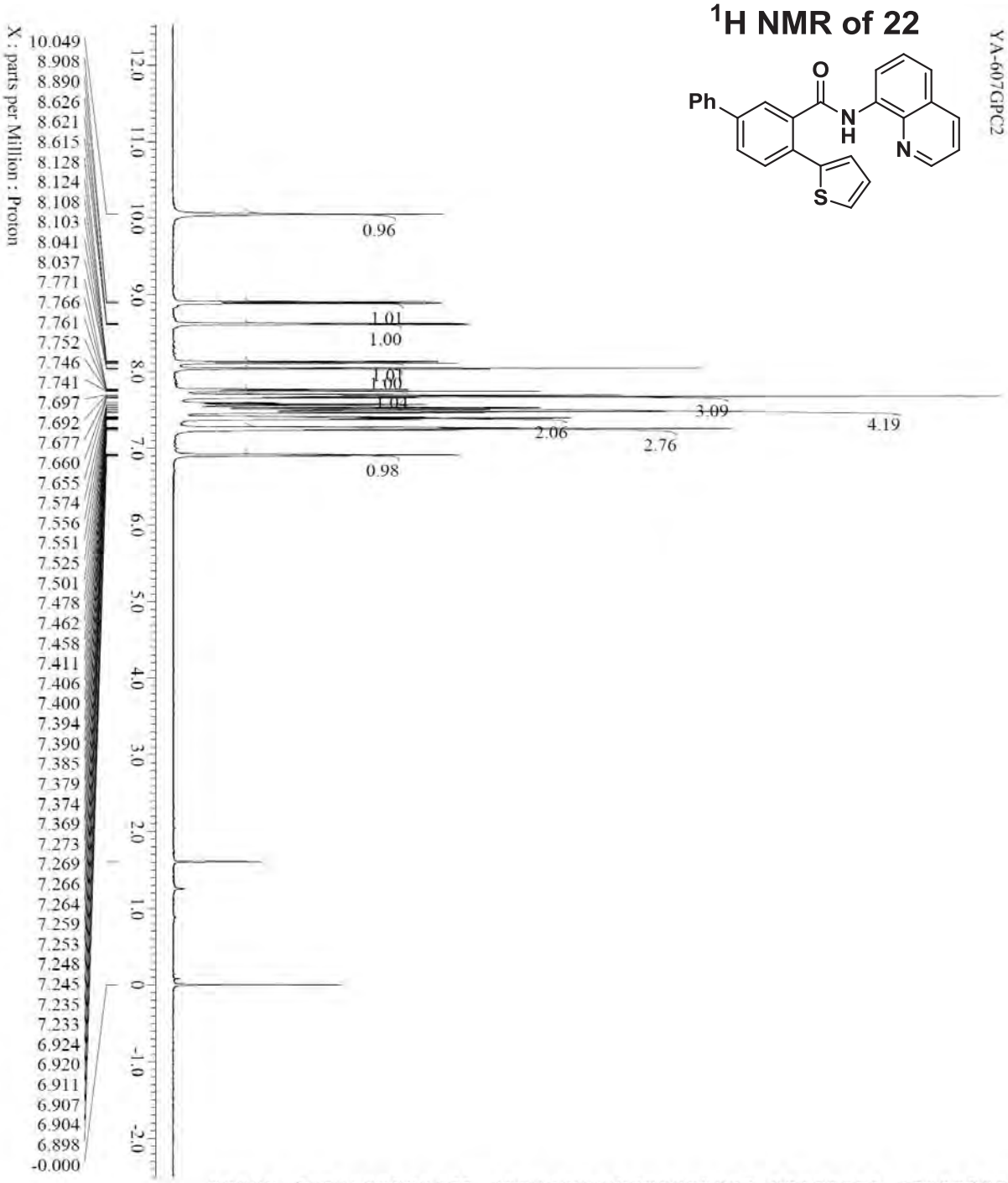

```
Filename                = E:¥NMR データ¥反応系(500-699)¥YA-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-672 seisei go
Solvent                 = CHLOROFORM-D
Creation_Time           = 4-MAR-2012 02:01:39
Revision_Time           = 4-MAR-2012 19:45:41
Current_Time            = 28-JUN-2012 19:34:23

Comment                 = YA-672 seisei go
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 1024
Total_Scans             = 1024

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 17.2[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 705
Sawtooth_Range          = 4
```



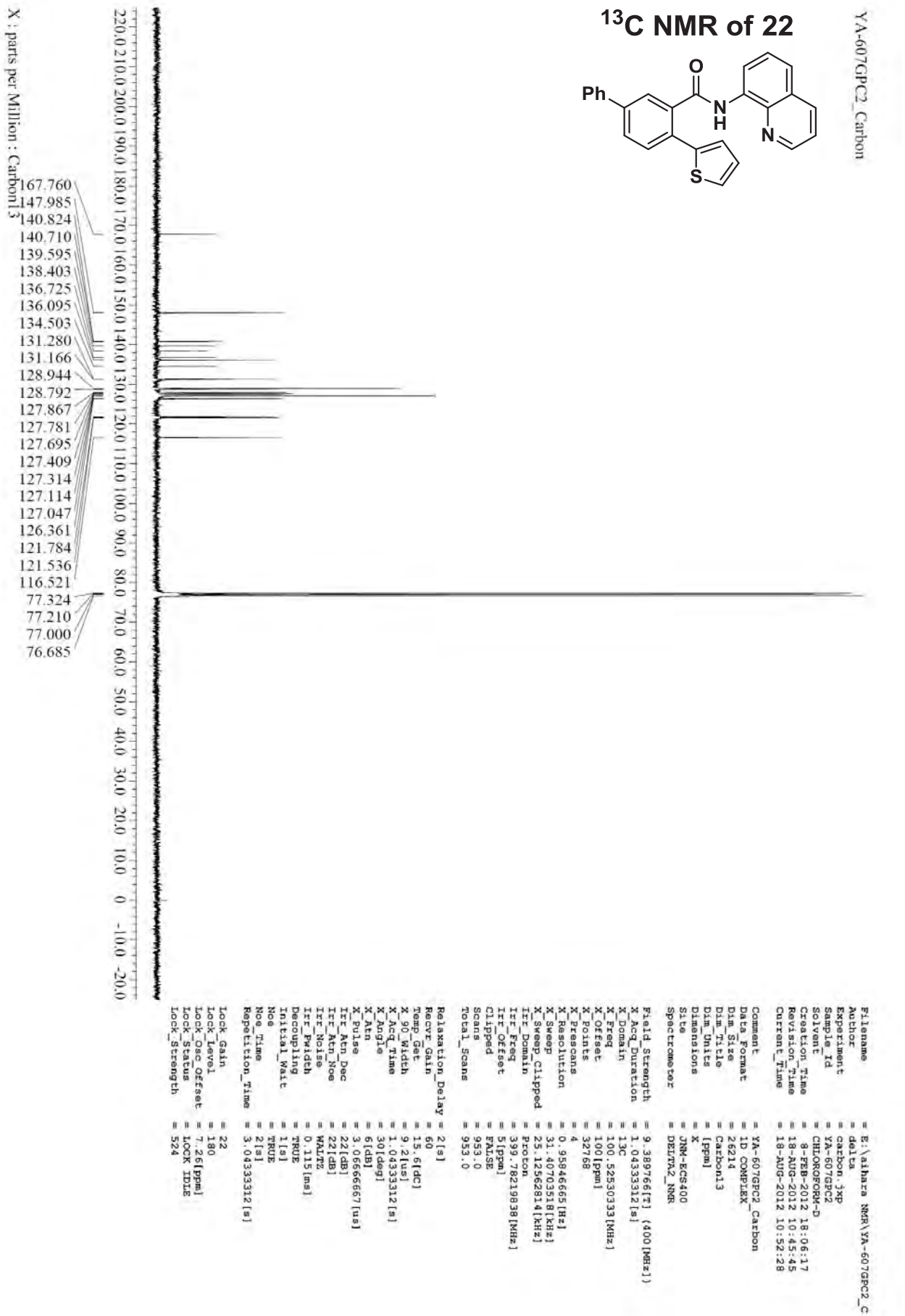

```
Filename                = E:\aihara NMR\YA-607GPC2-1
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-607GPC2
Solvent                 = CHLOROFORM-D
Creation_Time           =  8-FEB-2012 18:04:27
Revision_Time           = 18-AUG-2012 10:45:30
Current_Time            = 18-AUG-2012 10:52:02

Comment                 = YA-607GPC2
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

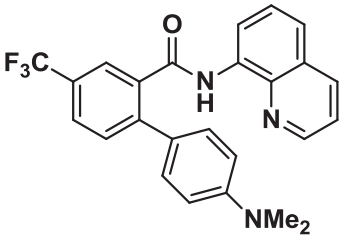
Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.50300121[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 40
Temp_Get                = 15.8[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Status             = LOCK IDLE
Lock_Strength           = 529
```


^{13}C NMR of 22
Ph
O
N
H
N
S
YA-607GPC2_Carbon
X : parts per Million : Carbon13
167.760
147.985
140.824
140.710
139.595
138.403
136.725
136.095
134.503
131.280
131.166
128.944
128.792
127.867
127.781
127.695
127.409
127.314
127.114
127.047
126.361
121.784
121.536
116.521
77.324
77.210
77.000
76.685
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
Filename = E:\ashara NMR\YA-607GPC2_C
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-607GPC2
Solvent = CHLOROFORM-D
Creation_Time = 8-FEB-2012 18:06:17
Revision_Time = 18-AUG-2012 10:45:45
Current_Time = 18-AUG-2012 10:52:28
Comment = YA-607GPC2_Carbon
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 953.0
Total_Scans = 953.0
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 15.6[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Status = LOCK IDLE
Lock_Strength = 524

^{1}H NMR of 25




```
Filename                = E:\aihara NMR\YA674pure_pr
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA674pure
Solvent                 = CHLOROFORM-D
Creation_Time           = 29-MAR-2012 18:59:52
Revision_Time           = 18-AUG-2012 10:46:48
Current_Time            = 18-AUG-2012 10:51:46

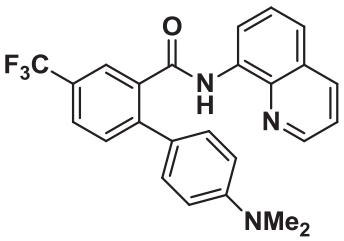
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.50300121[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 32
Temp_Get                = 18.2[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Preset            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Status             = LOCK IDLE
Lock_Strength           = 759
```

^{13}C NMR of 25



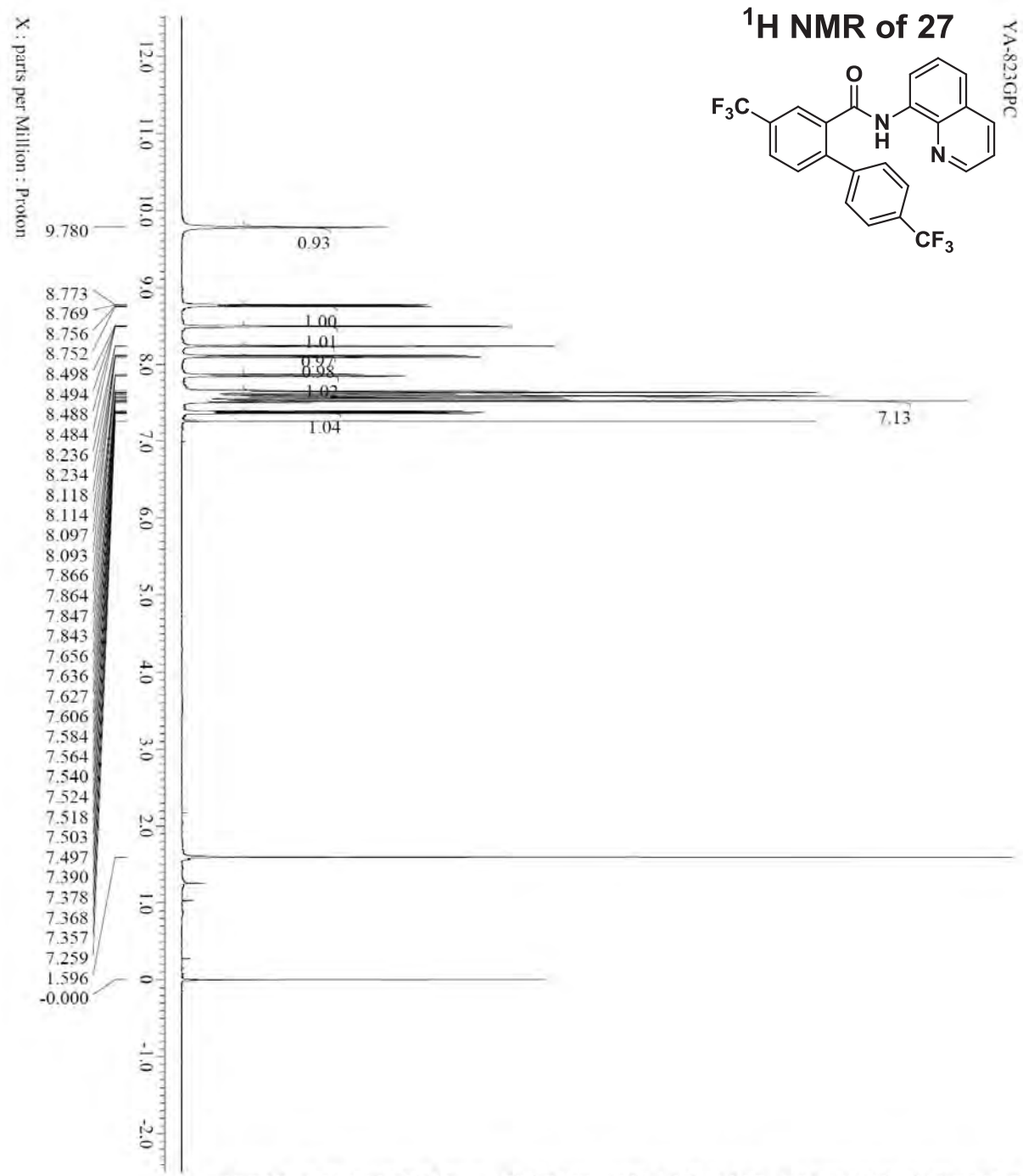

```
Filename                = E:\ashara NMR\YA674pure_Ca
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA674pure
Solvent                 = CHLOROFORM-D
Creation_Time           = 29-MAR-2012 19:01:40
Revision_Time           = 18-AUG-2012 10:47:02
Current_Time            = 18-AUG-2012 10:51:22

Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.043333312[s]
X_Domain                = 13C
X_Freq                  = 100.525303333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.958466665[Hz]
X_Sweep                 = 31.407035181[kHz]
X_Sweep_Clipped         = 25.125628141[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.782199838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 1287
Total_Scans             = 1287

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 18.5[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.043333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.066666671[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.043333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Status             = LOCK IDLE
Lock_Strength           = 756
```




```
Filename                = E:\aihara NMR\YA-823GPC-1-
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-823GPC
Solvent                 = CHLOROFORM-D
Creation_Time           = 16-AUG-2012 16:46:07
Revision_Time           = 18-AUG-2012 10:48:02
Current_Time            = 18-AUG-2012 10:53:26

Comment                 = YA-823GPC
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.7821938[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.503012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.7821938[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.7821938[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 42
Temp_Get                = 22[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Status             = LOCK IDLE
Lock_Strength           = 741
```

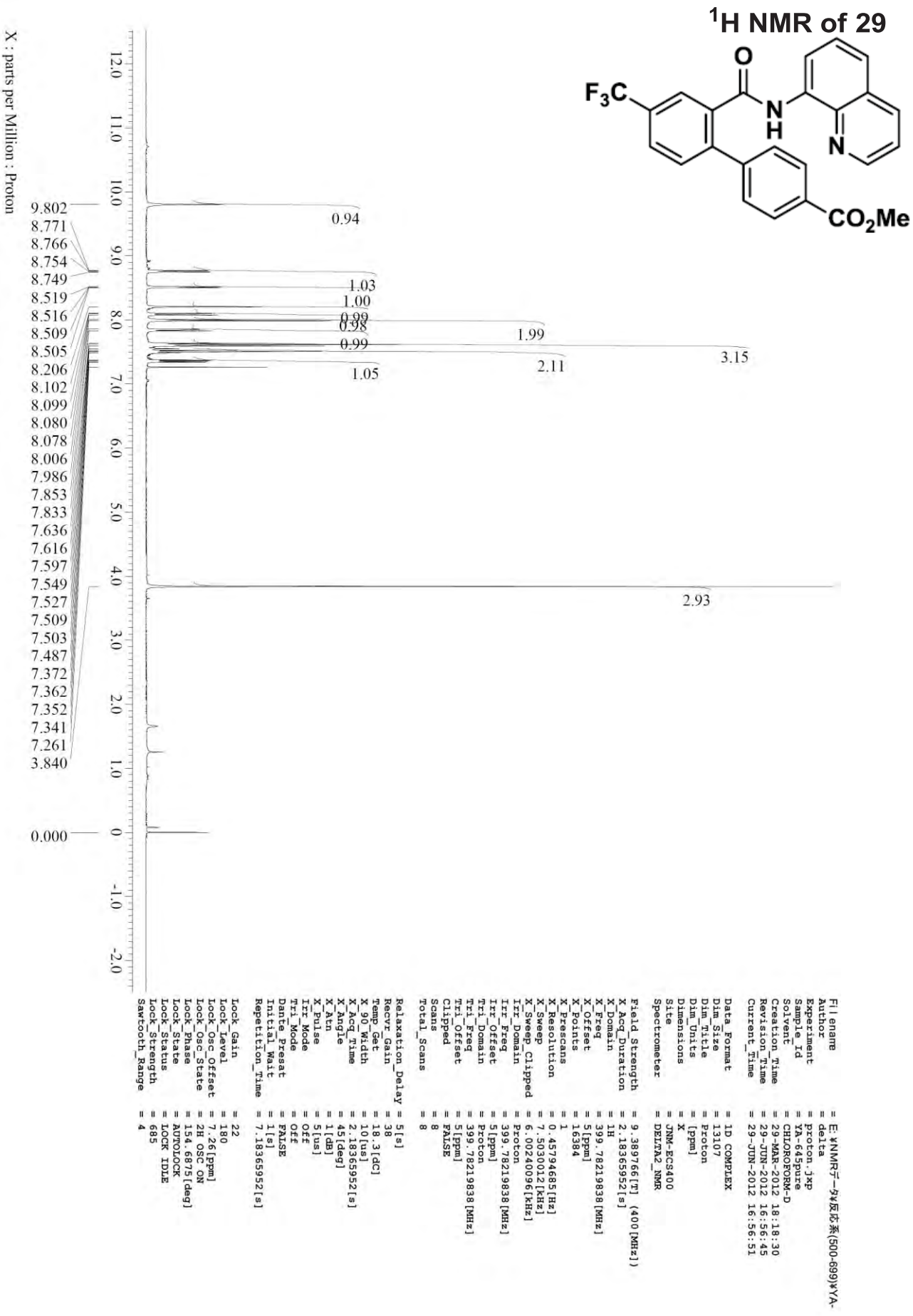

```
Filename                = E:\aihara NMR\YA-823GPC_Ca
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-823GPC
Solvent                 = CHLOROFORM-D
Creation_Time           = 16-AUG-2012 22:03:06
Revision_Time           = 18-AUG-2012 10:47:51
Current_Time            = 18-AUG-2012 10:53:42

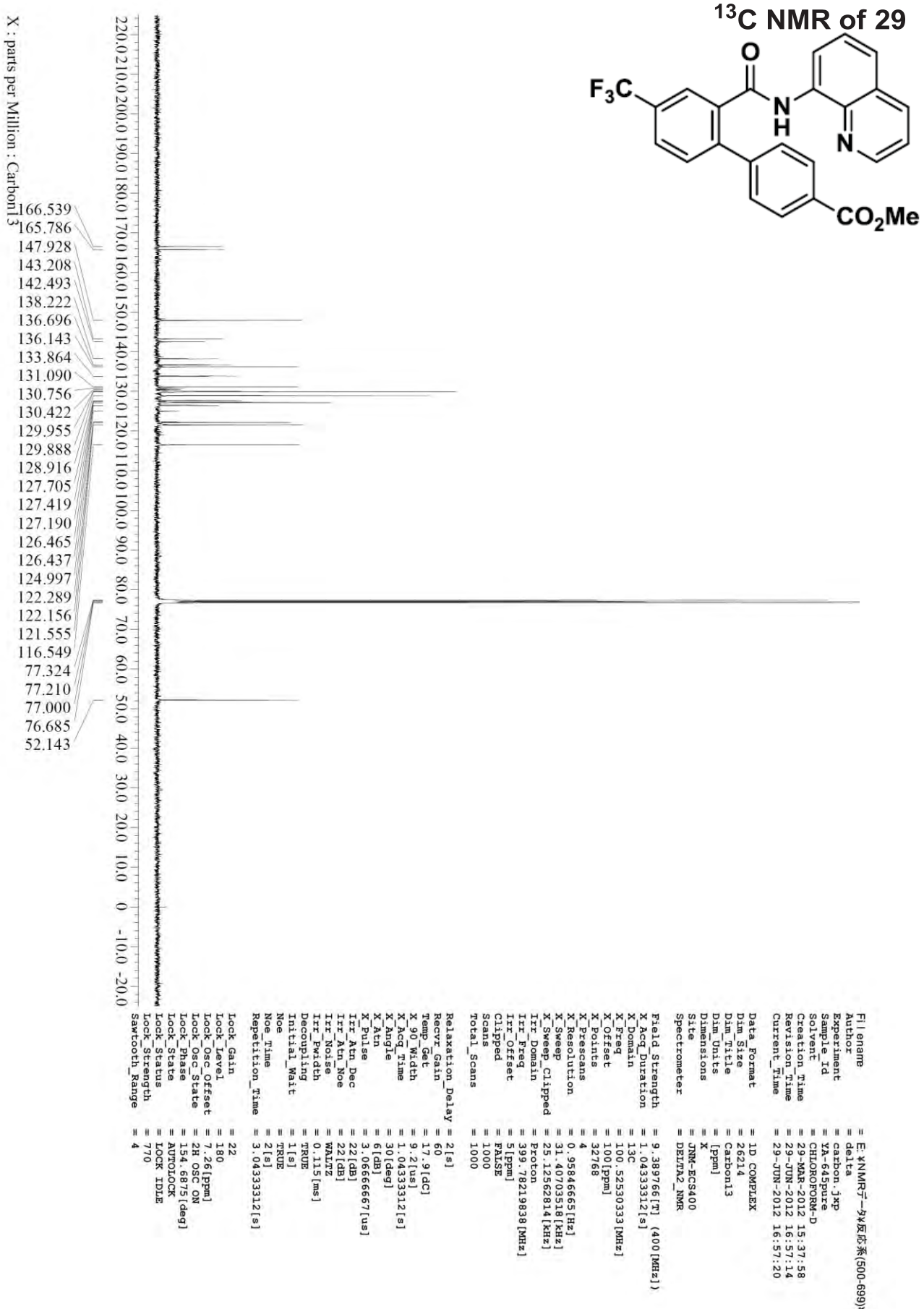
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

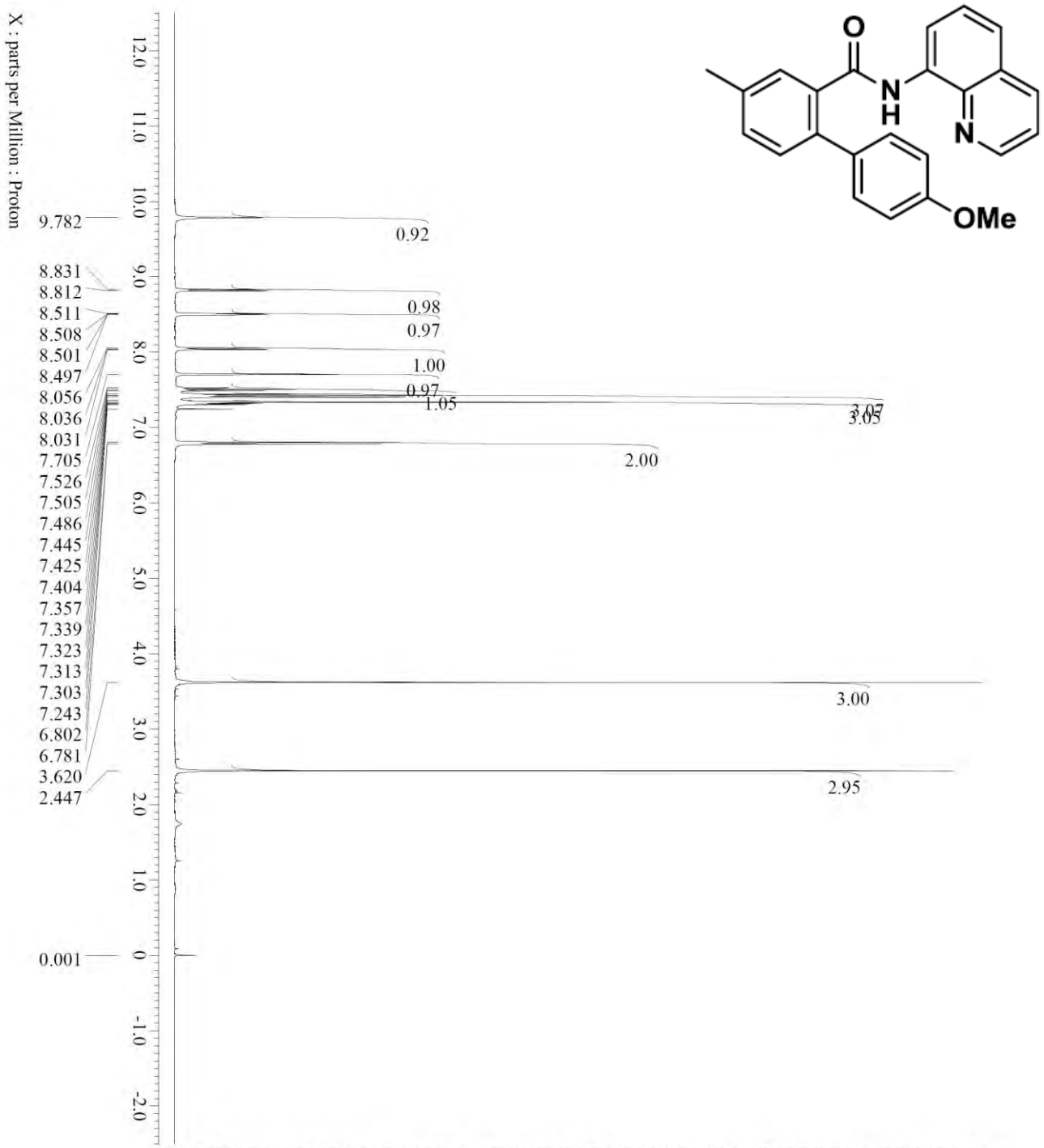
Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 13650
Total_Scans             = 13650

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 20.8[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Status             = LOCK IDLE
Lock_Strength           = 782
```


^{1}H NMR of 29
F3C
O
N
H
N
CO2Me
X : parts per Million : Proton
9.802
8.771
8.766
8.754
8.749
8.519
8.516
8.509
8.505
8.206
8.102
8.099
8.080
8.078
8.006
7.986
7.853
7.833
7.636
7.616
7.597
7.549
7.527
7.509
7.503
7.487
7.372
7.362
7.352
7.341
7.261
3.840
0.000
0.94
1.03
1.00
0.99
0.98
1.99
0.99
2.11
1.05
3.15
2.93
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
Filename = E:¥NMRデータ¥反応系(500-699)¥YA-
Author = delta
Experiment = proton.jxp
Sample_Id = YA-645pure
Solvent = CHLOROFORM-D
Creation_Time = 29-MAR-2012 18:18:30
Revision_Time = 29-JUN-2012 16:56:45
Current_Time = 29-JUN-2012 16:56:51
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.50300012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 18.3[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 685
Sawtooth_Range = 4


^{13}C NMR of 29
O
F_3C
N
H
N
CO_2Me
X : parts per Million : Carbon13
166.539
165.786
147.928
143.208
142.493
138.222
136.696
136.143
133.864
131.090
130.756
130.422
129.955
129.888
128.916
127.705
127.419
127.190
126.465
126.437
124.997
122.289
122.156
121.555
116.549
77.324
77.210
77.000
76.685
52.143
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
Filename = E:¥NMR¥データ¥反応系(500-699)¥YA-
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-645pure
Solvent = CHLOROFORM-D
Creation_Time = 29-MAR-2012 15:37:58
Revision_Time = 29-JUN-2012 16:57:14
Current_Time = 29-JUN-2012 16:57:20
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.043333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1000
Total_Scans = 1000
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 17.9[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.043333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.066666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.043333312[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 770
Sawtooth_Range = 4



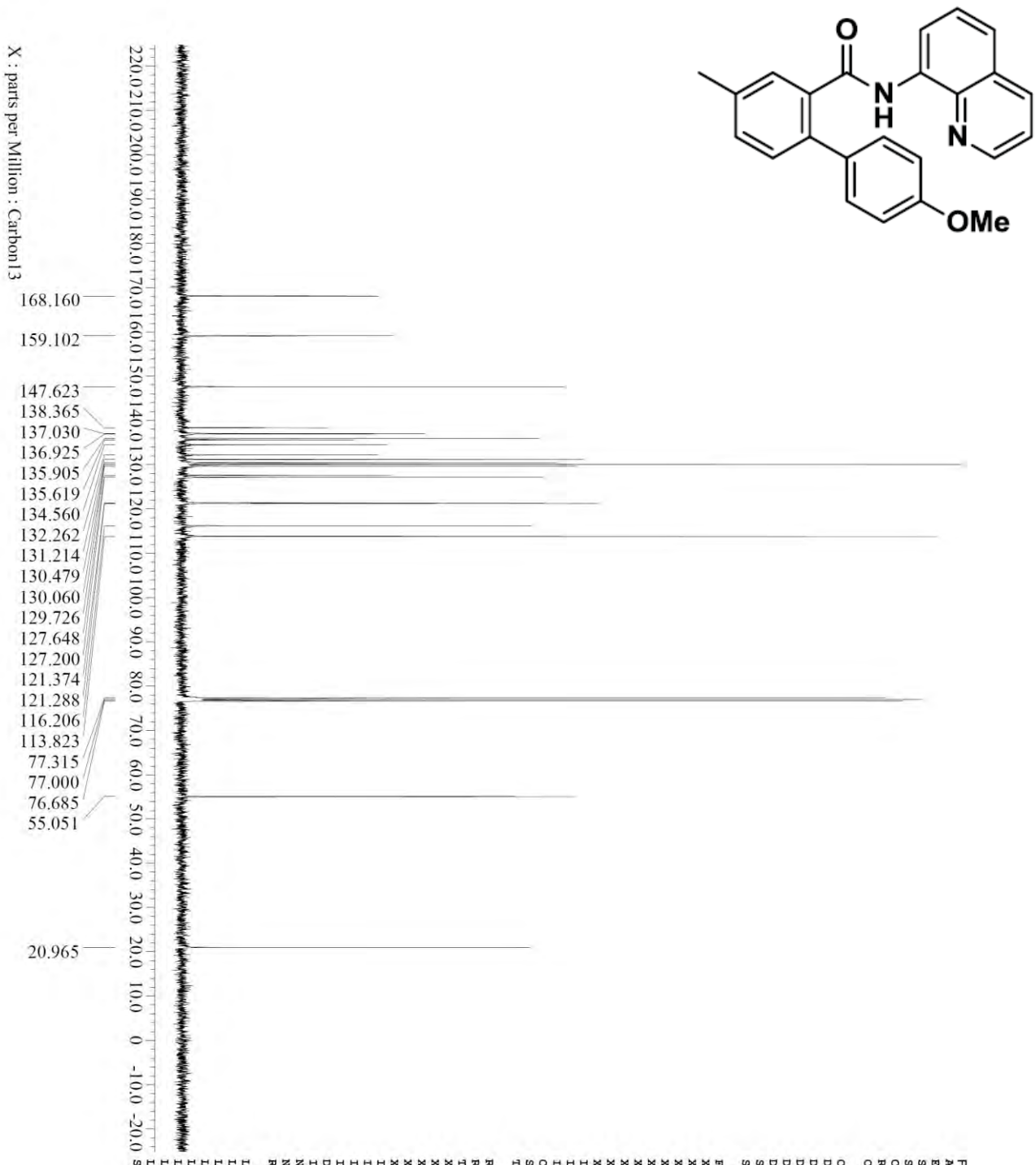

```
Filename                = E:¥NMRデータ¥反応系(700-900)2¥YA
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-764-1f8-10
Solvent                 = CHLOROFORM-D
Creation_Time           = 11-JUN-2012 20:22:41
Revision_Time           = 28-JUN-2012 20:00:35
Current_Time            = 28-JUN-2012 20:00:40

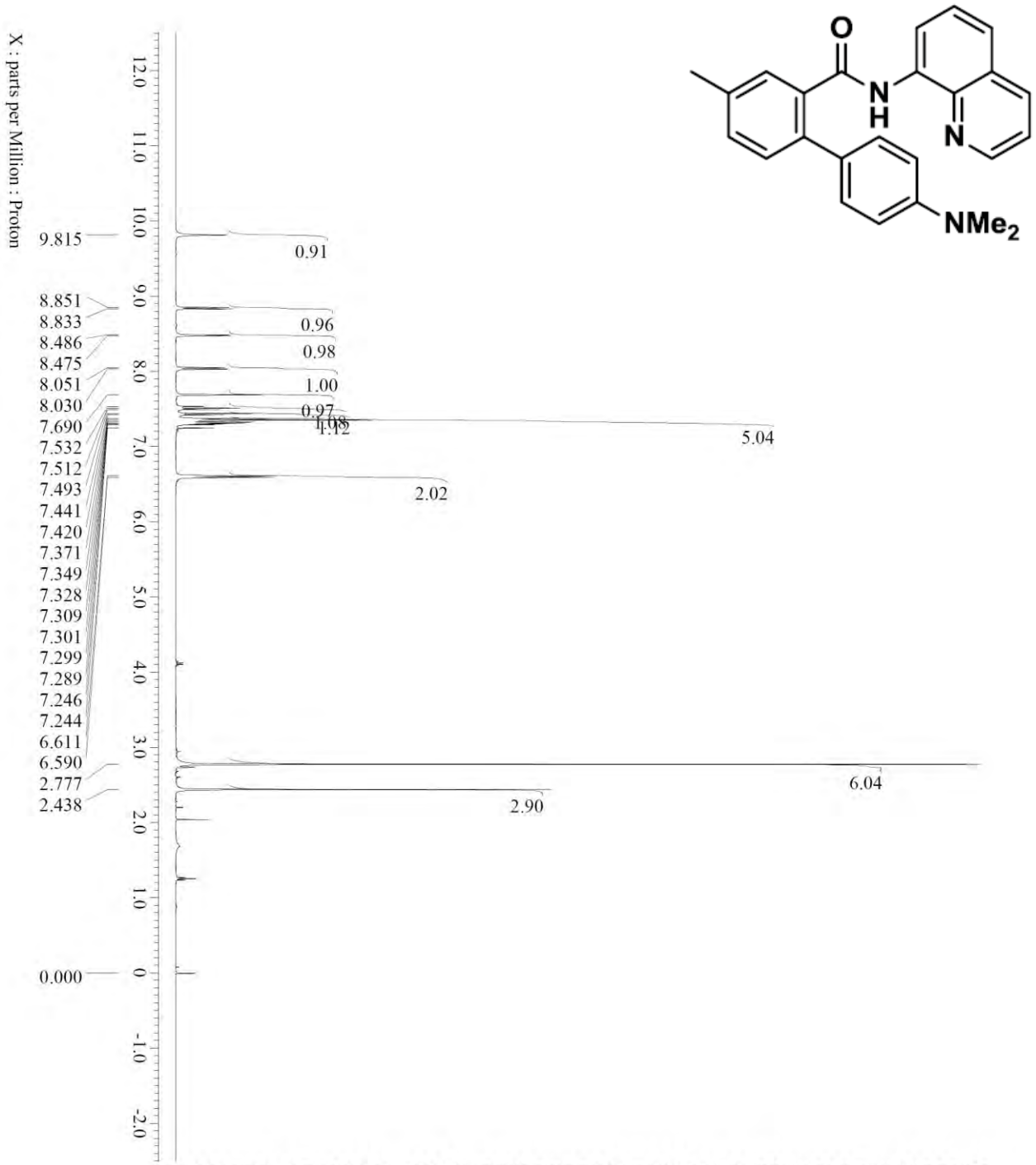
Comment                 = YA-764-1f8-10
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.5030012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 30
Temp_Get                = 19.8[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = off
Tri_Mode                = off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 613
Sawtooth_Range          = 4
```


O
NH
N
OMe
X : parts per Million : Carbon13
168.160
159.102
147.623
138.365
137.030
136.925
135.905
135.619
134.560
132.262
131.214
130.479
130.060
129.726
127.648
127.200
121.374
121.288
116.206
113.823
77.315
77.000
76.685
55.051
20.965
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
Filename = E:¥NMRデータ¥反応系(700-900)2¥YA
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-764-1f8-10
Solvent = CHLOROFORM-D
Creation_Time = 11-JUN-2012 20:24:24
Revision_Time = 11-JUN-2012 20:39:26
Current_Time = 28-JUN-2012 20:00:02
Comment = YA-764-1f8-10
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 273
Total_Scans = 273
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.8[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 612
Sawtooth_Range = 4



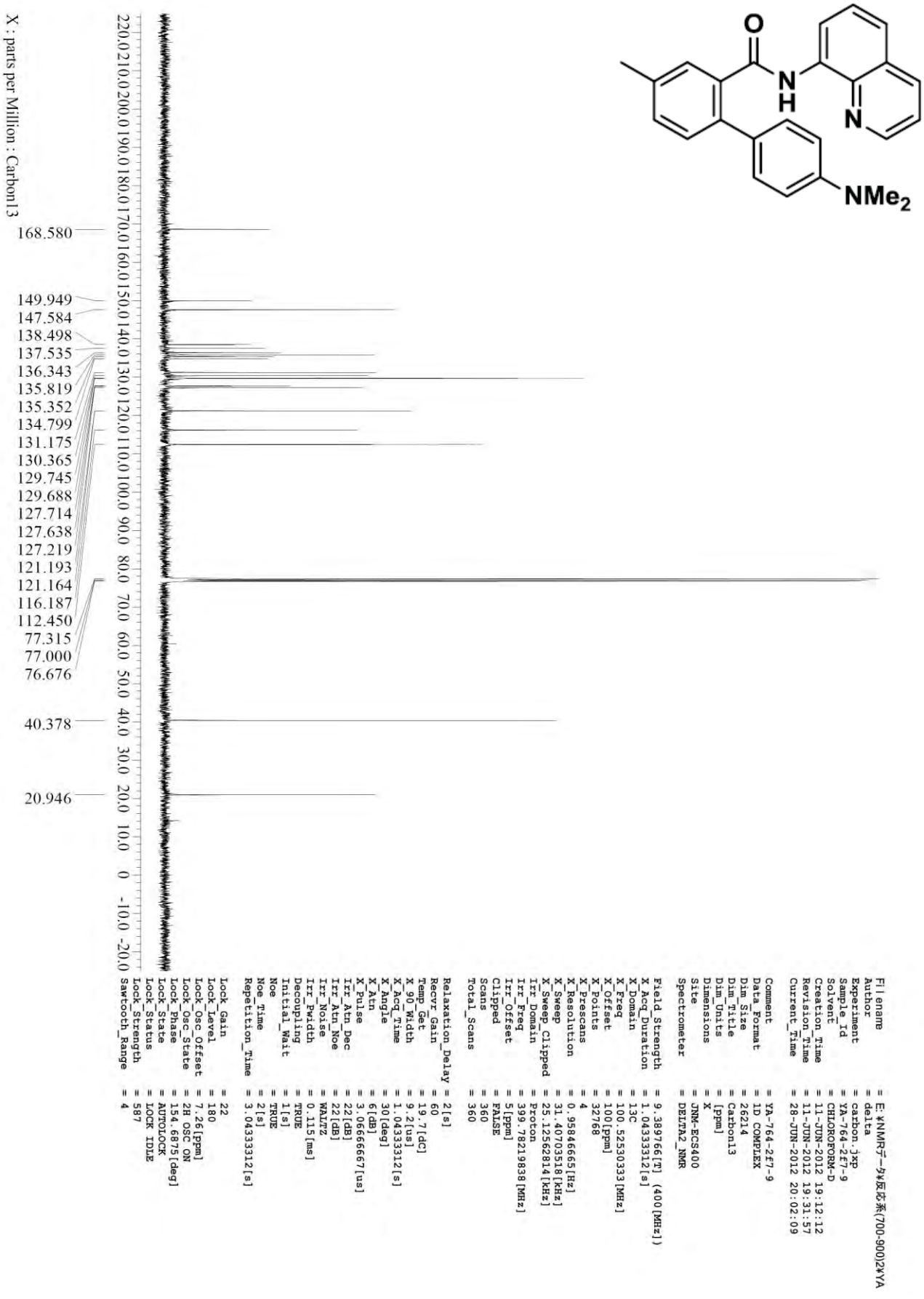

```
Filename                = E:¥NMRデータ¥反応系(700-900)2¥YA
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-764-2f7-9
Solvent                 = CHLOROFORM-D
Creation_Time           = 11-JUN-2012 19:10:30
Revision_Time           = 29-JUN-2012 19:39:46
Current_Time            = 29-JUN-2012 19:39:53

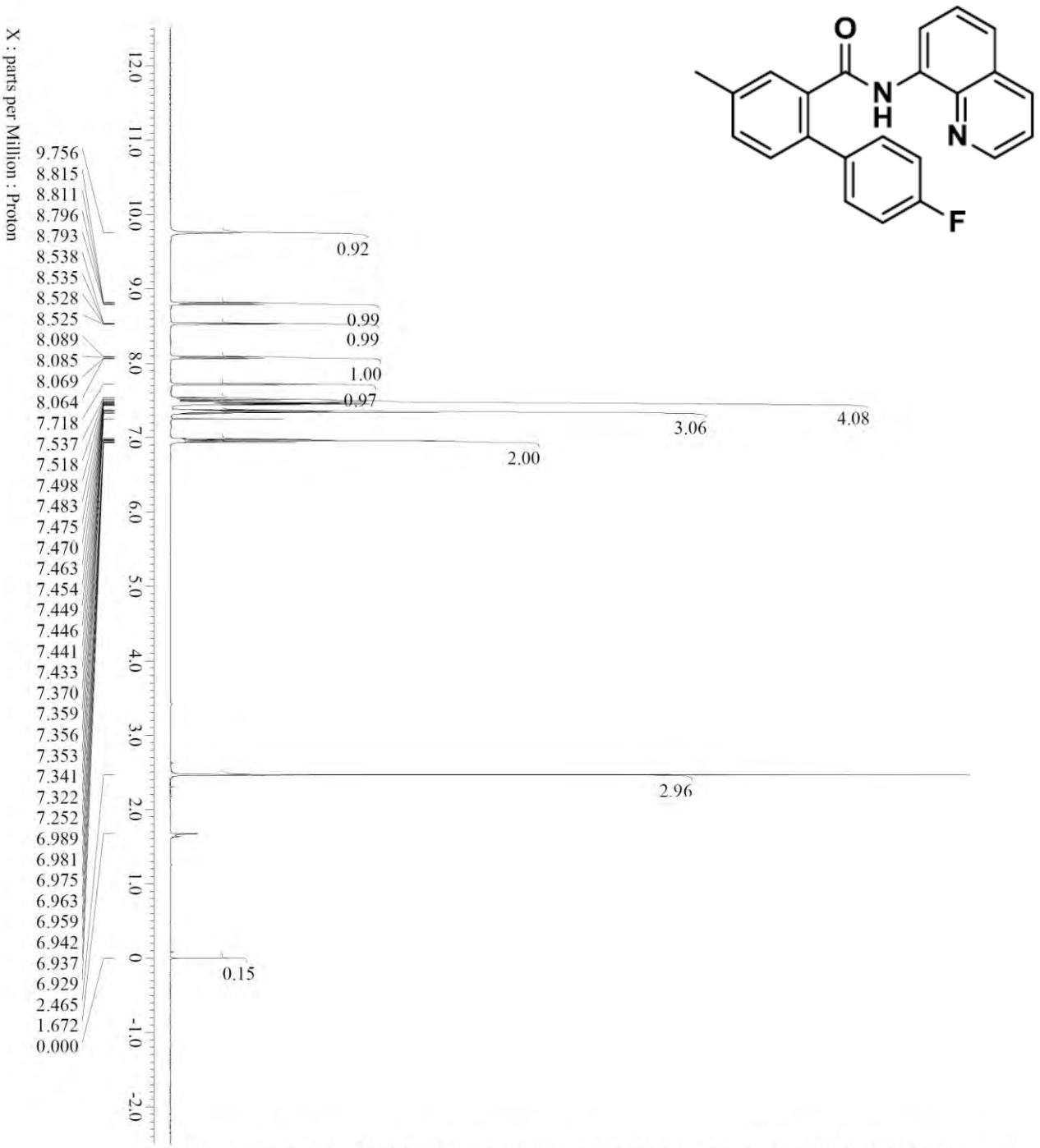
Comment                 = YA-764-2f7-9
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.5030012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 34
Temp_Get                = 19.8[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 590
Sawtooth_Range          = 4
```


O
N
H
N
NMe2
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
168.580
149.949
147.584
138.498
137.535
136.343
135.819
135.352
134.799
131.175
130.365
129.745
129.688
127.714
127.638
127.219
121.193
121.164
116.187
112.450
77.315
77.000
76.676
40.378
20.946
Filename = E:¥NMR¥データ¥反応系(700-900)2¥YA
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-764-2f7-9
Solvent = CHLOROFORM-D
Creation_Time = 11-JUN-2012 19:12:12
Revision_Time = 11-JUN-2012 19:31:57
Current_Time = 28-JUN-2012 20:02:09
Comment = YA-764-2f7-9
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 360
Total_Scans = 360
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.7[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 587
Sawtooth_Range = 4



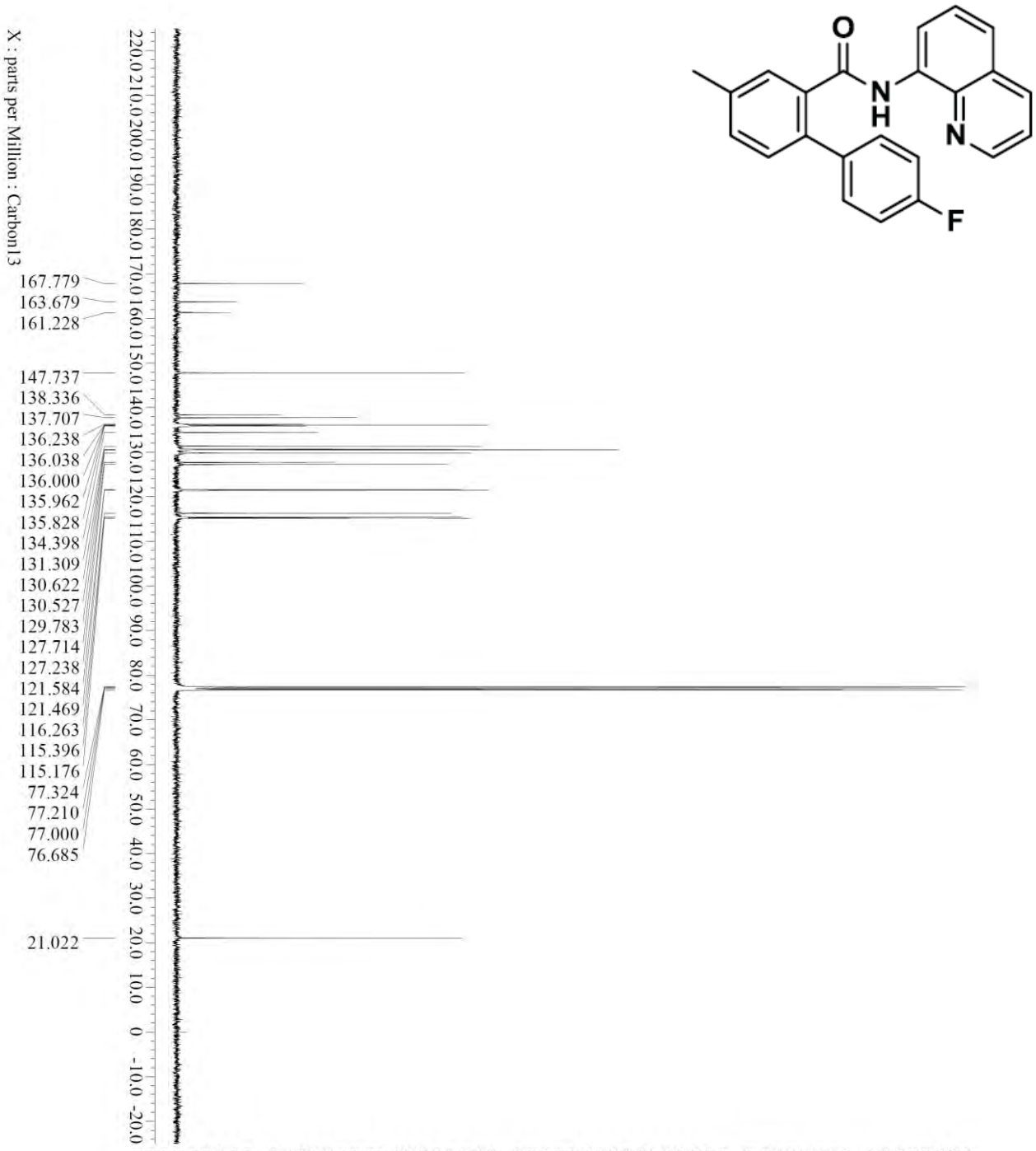

```
File_name                = E:¥NMR¥データ¥反応系(700-900)2¥YA
Author                   = delta
Experiment               = proton.jxp
Sample_Id                = YA-766-1GPC1
Solvent                  = CHLOROFORM-D
Creation_Time            = 12-JUN-2012 15:46:32
Revision_Time            = 28-JUN-2012 20:03:12
Current_Time             = 28-JUN-2012 20:03:17

Comment                  = YA-766-1GPC1
Data_Format              = 1D COMPLEX
Dim_Size                 = 13107
Dim_Title                = Proton
Dim_Units                = [ppm]
Dimensions               = X
Site                     = JNM-ECS400
Spectrometer             = DELTA2_NMR

Field_Strength           = 9.389766[T] (400[MHz])
X_Acq_Duration           = 2.18365952[s]
X_Domain                 = 1H
X_Freq                   = 399.78219838[MHz]
X_Offset                 = 5[ppm]
X_Points                 = 16384
X_Prescans               = 1
X_Resolution             = 0.45794685[Hz]
X_Sweep                  = 7.50300012[kHz]
X_Sweep_Clipped          = 6.00240096[kHz]
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MHz]
Irr_Offset               = 5[ppm]
Tri_Domain               = Proton
Tri_Freq                 = 399.78219838[MHz]
Tri_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 8
Total_Scans              = 8

Relaxation_Delay         = 5[s]
Recvr_Gain               = 36
Temp_Get                 = 19.4[dC]
X_90_Width               = 10[us]
X_Acq_Time               = 2.18365952[s]
X_Angle                  = 45[deg]
X_Atn                    = 1[dB]
X_Pulse                  = 5[us]
Irr_Mode                 = Off
Tri_Mode                 = Off
Dante_Presat             = FALSE
Initial_Wait             = 1[s]
Repetition_Time          = 7.18365952[s]

Lock_Gain                = 22
Lock_Level               = 180
Lock_Osc_Offset          = 7.26[ppm]
Lock_Osc_State           = 2H OSC ON
Lock_Phase               = 154.6875[deg]
Lock_State               = AUTOLOCK
Lock_Status              = LOCK IDLE
Lock_Strength            = 764
Sawtooth_Range           = 4
```



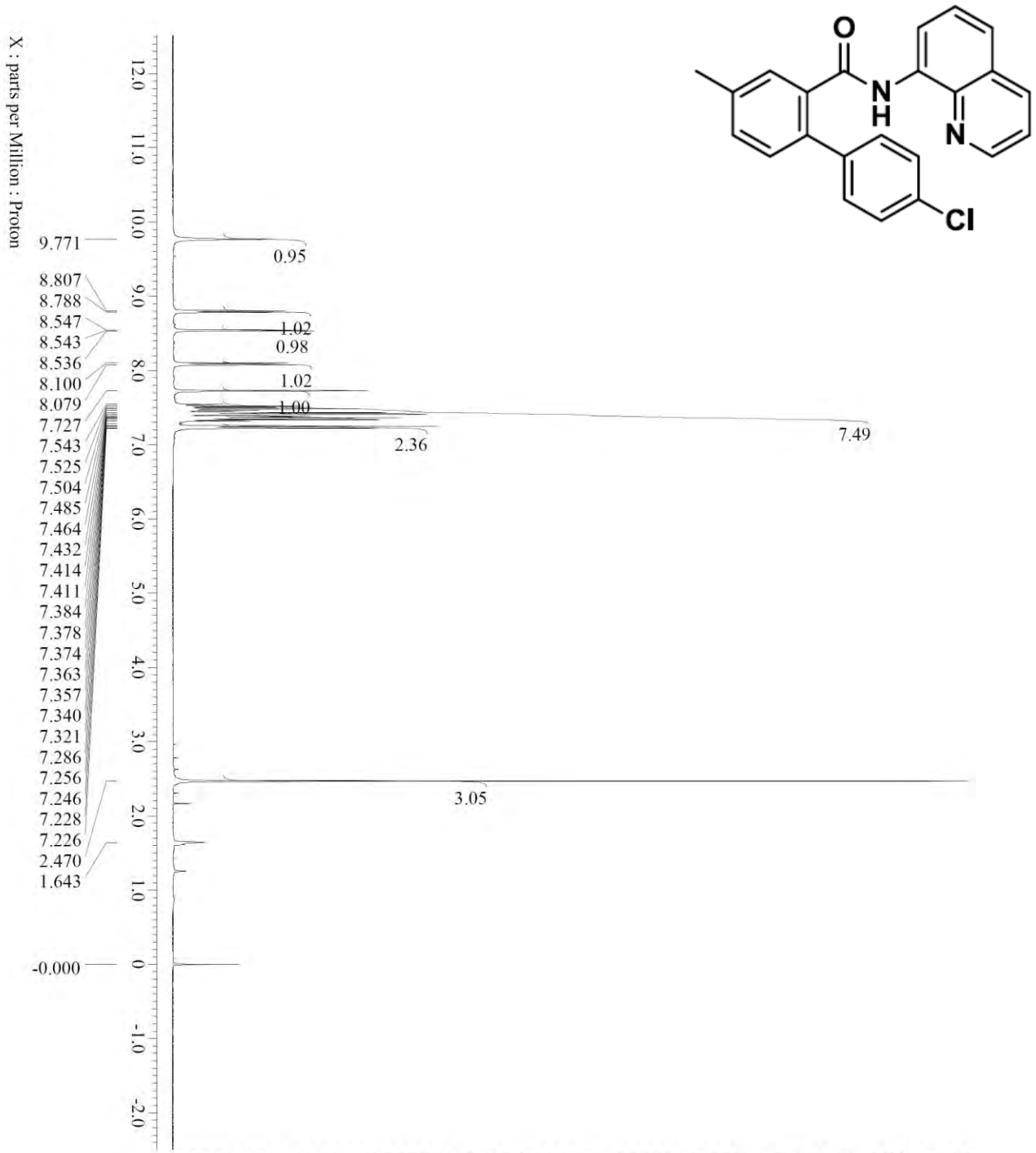

```
Filename                = E:¥NMRデータ¥反応系(700-900)2¥YA
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-766-1GPC1
Solvent                 = CHLOROFORM-D
Creation_Time           = 12-JUN-2012 15:48:15
Revision_Time           = 28-JUN-2012 20:03:32
Current_Time            = 28-JUN-2012 20:03:34

Comment                 = YA-766-1GPC1
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.043333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333 [MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838 [MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 1024
Total_Scans             = 1024

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 19.4[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.043333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.066666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.043333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 752
Sawtooth_Range          = 4
```



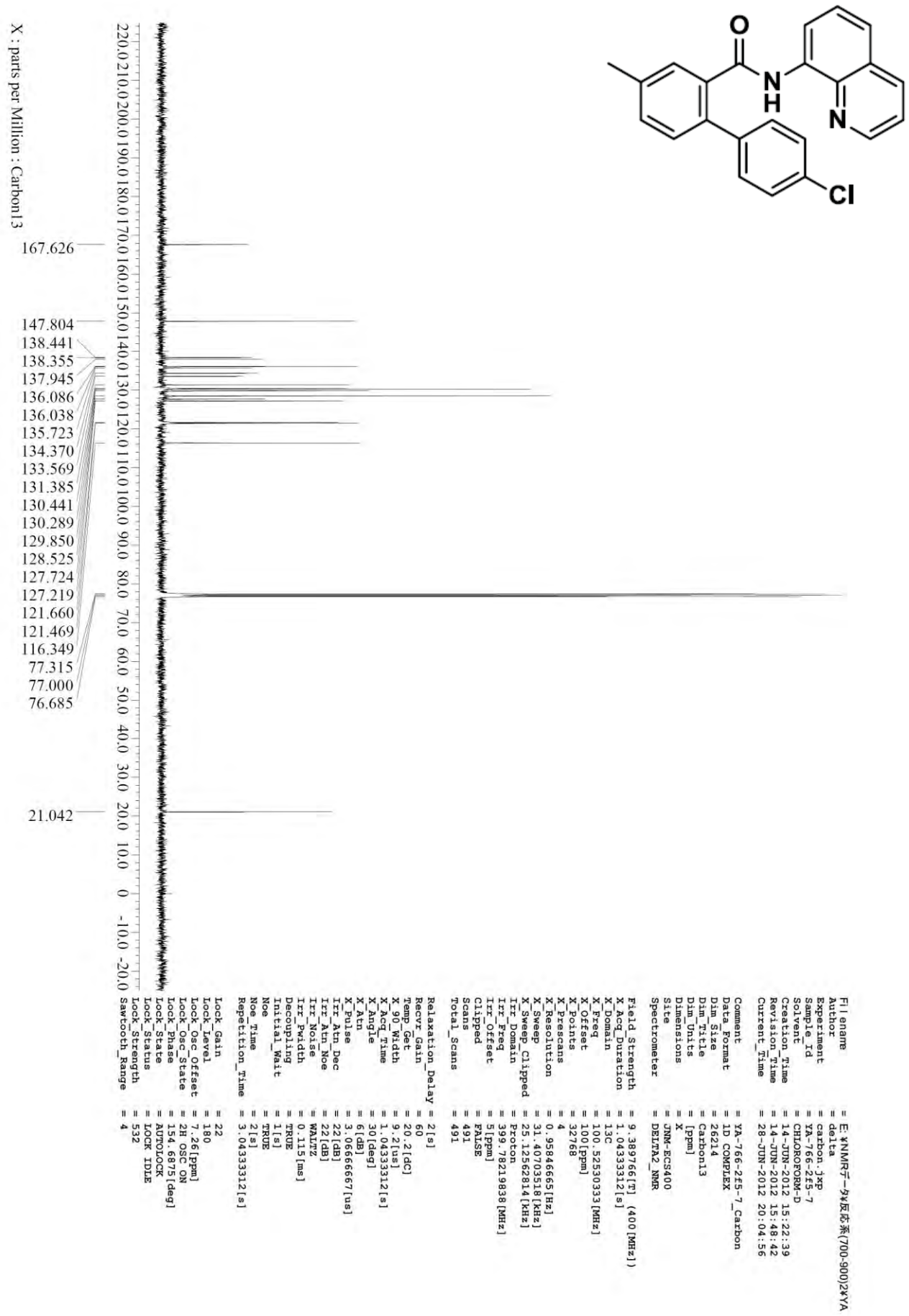

```
Filename                = E:¥NMRデータ¥反応系(700-900)2¥YA
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = YA-766-2f5-7
Solvent                 = CHLOROFORM-D
Creation_Time           = 14-JUN-2012 15:20:02
Revision_Time           = 28-JUN-2012 20:04:39
Current_Time            = 28-JUN-2012 20:04:45

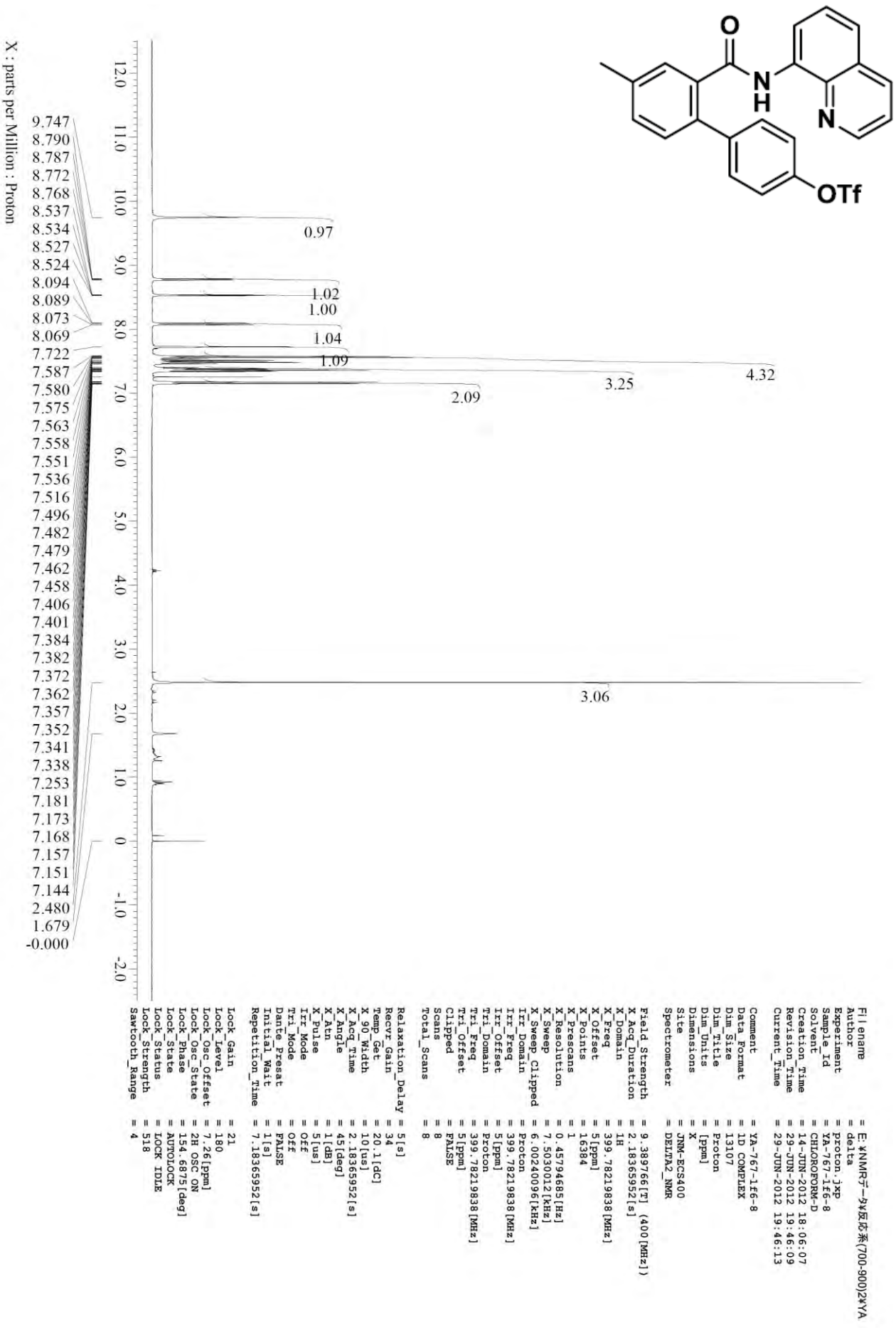
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

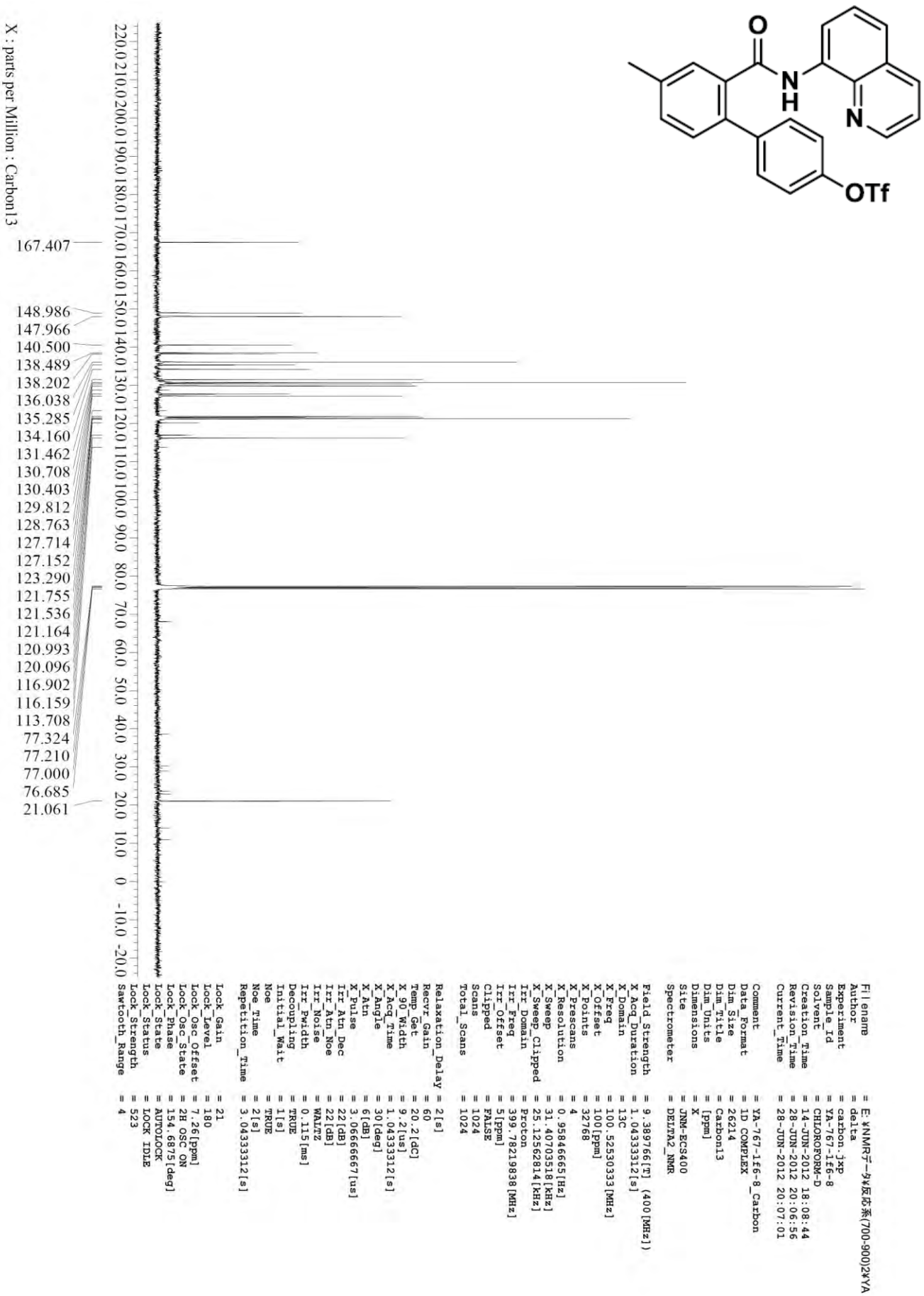
Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18365952[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45794685[Hz]
X_Sweep                 = 7.5030012[kHz]
X_Sweep_Clipped         = 6.00240096[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

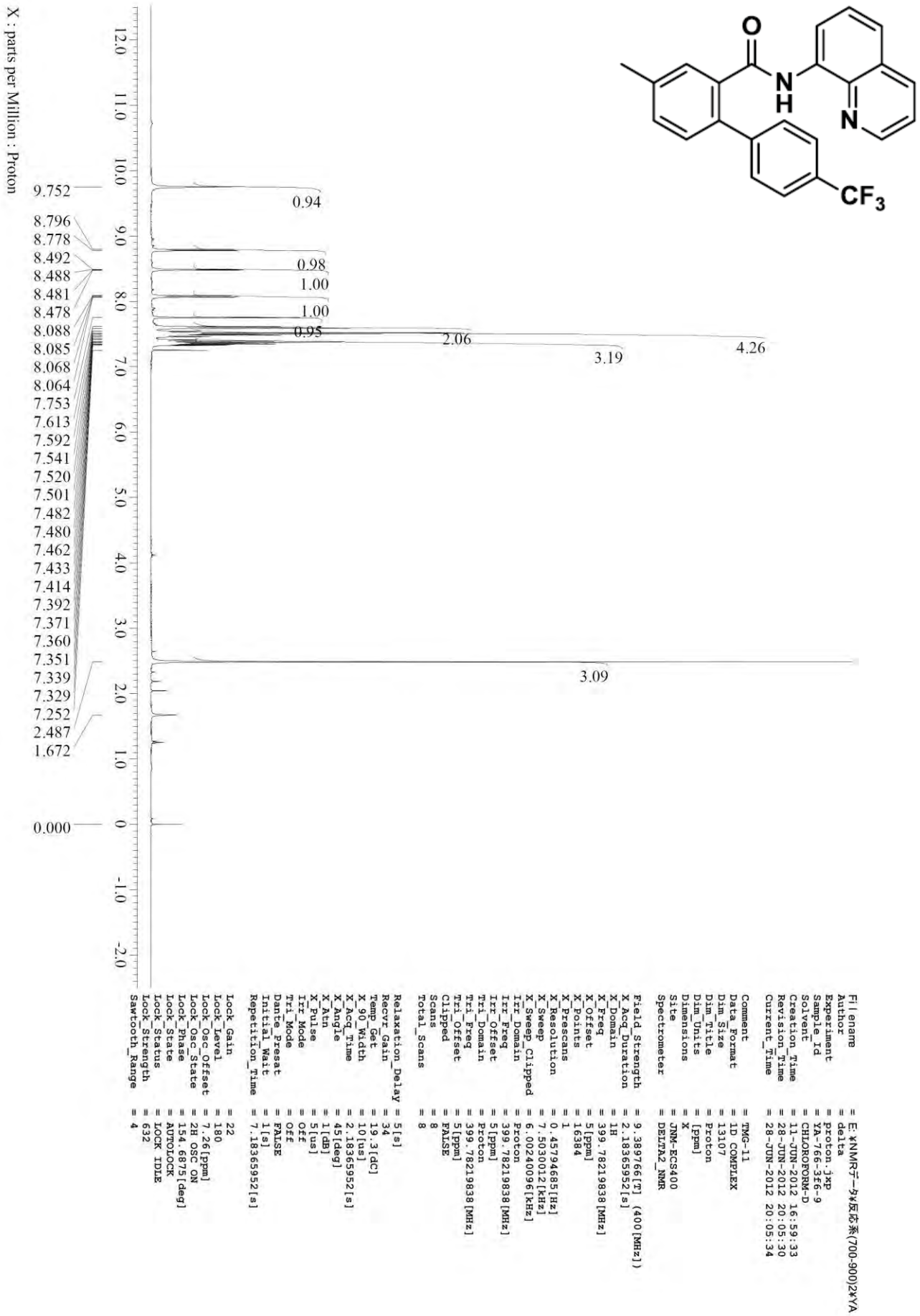
Relaxation_Delay        = 5[s]
Recvr_Gain              = 38
Temp_Get                = 19.9[dC]
X_90_Width              = 10[us]
X_Acq_Time              = 2.18365952[s]
X_Angle                 = 45[deg]
X_Atn                   = 1[dB]
X_Pulse                 = 5[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Presat            = FALSE
Initial_Wait            = 1[s]
Repetition_Time         = 7.18365952[s]

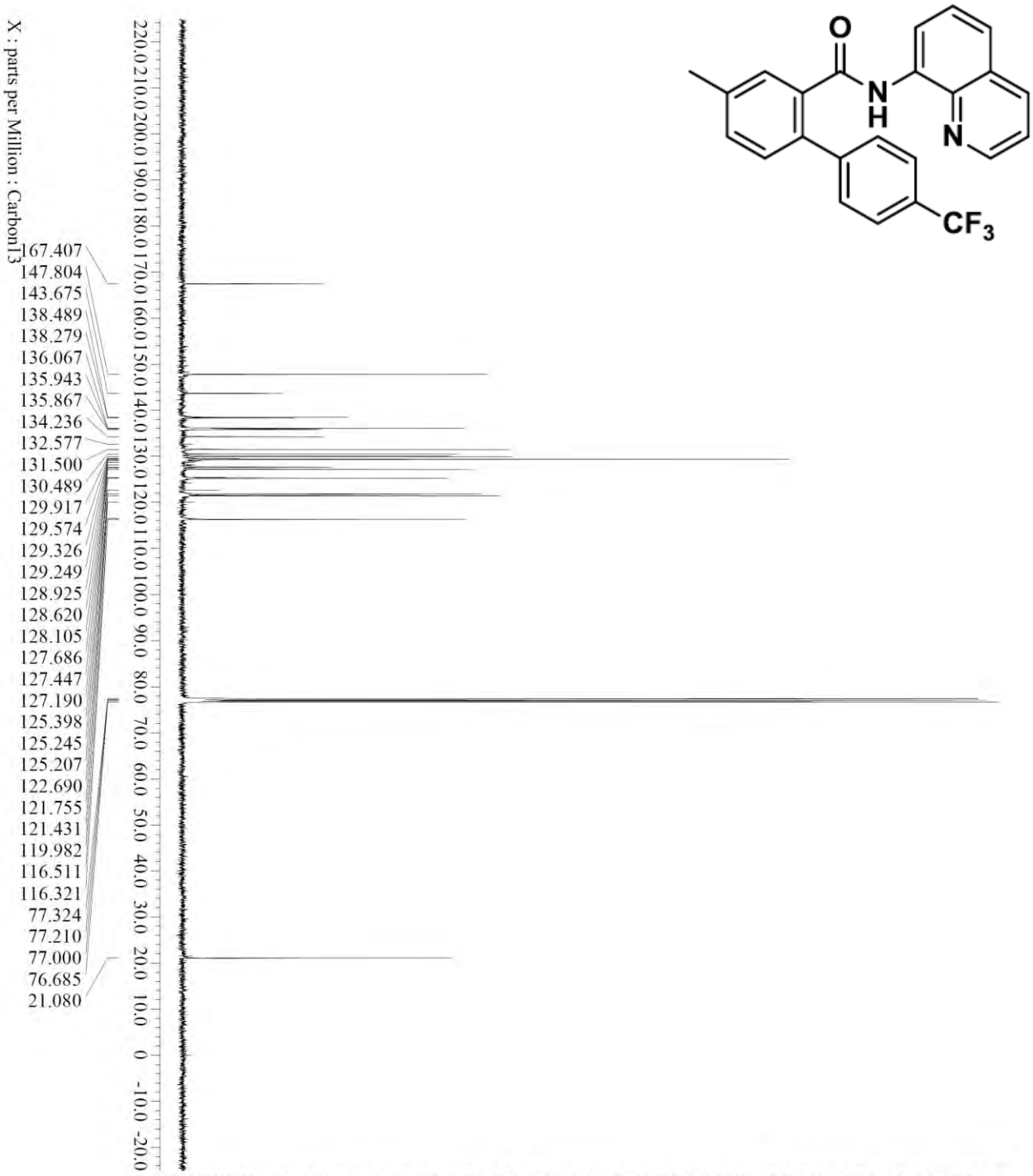
Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 528
Sawtooth_Range          = 4
```

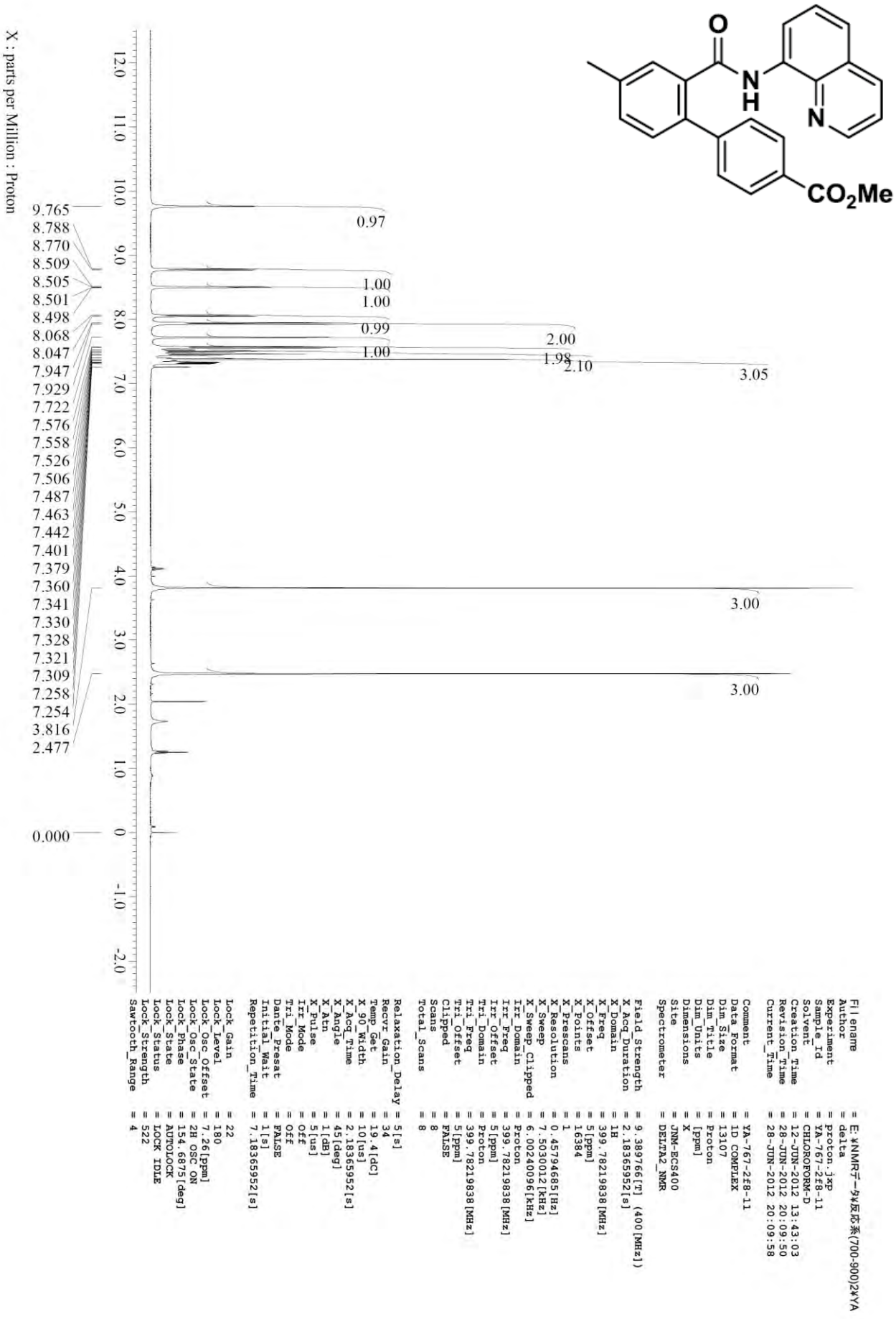

O
N
H
N
Cl
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
167.626
147.804
138.441
138.355
137.945
136.086
136.038
135.723
134.370
133.569
131.385
130.441
130.289
129.850
128.525
127.724
127.219
121.660
121.469
116.349
77.315
77.000
76.685
21.042
Filename = E:¥NMR¥データ¥反応系(700-900)2¥YA
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-766-2f5-7
Solvent = CHLOROFORM-D
Creation_Time = 14-JUN-2012 15:22:39
Revision_Time = 14-JUN-2012 15:48:42
Current_Time = 28-JUN-2012 20:04:56
Comment = YA-766-2f5-7_Carbon
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 491
Total_Scans = 491
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.2[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 532
Sawtooth_Range = 4

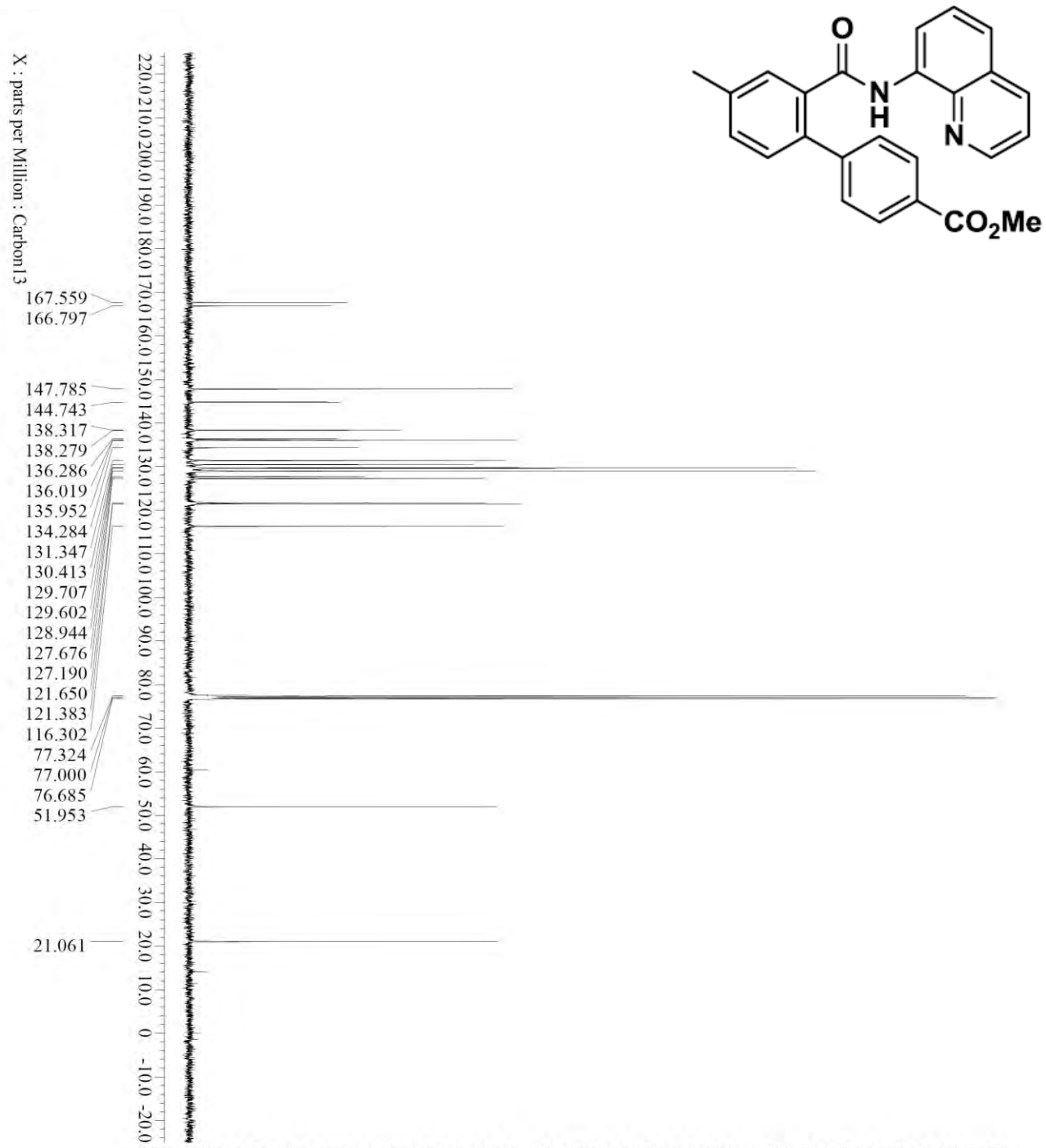

O
N
H
N
OTf
X : parts per Million : Proton
9.747
8.790
8.787
8.772
8.768
8.537
8.534
8.527
8.524
8.094
8.089
8.073
8.069
7.722
7.587
7.580
7.575
7.563
7.558
7.551
7.536
7.516
7.496
7.482
7.479
7.462
7.458
7.406
7.401
7.384
7.382
7.372
7.362
7.357
7.352
7.341
7.338
7.253
7.181
7.173
7.168
7.157
7.151
7.144
2.480
1.679
-0.000
0.97
1.02
1.00
1.04
1.09
2.09
3.25
4.32
3.06
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
Filename = E:¥NMRデータ¥反応系(700-900)2¥YA
Author = delta
Experiment = proton.jxp
Sample_Id = YA-767-1f6-8
Solvent = CHLOROFORM-D
Creation_Time = 14-JUN-2012 18:06:07
Revision_Time = 29-JUN-2012 19:46:09
Current_Time = 29-JUN-2012 19:46:13
Comment = YA-767-1f6-8
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 34
Temp_Get = 20.1[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]
Lock_Gain = 21
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.68875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 518
Sawtooth_Range = 4


O
N
H
N
OTf
X : parts per Million : Carbon13
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
167.407
148.986
147.966
140.500
138.489
138.202
136.038
135.285
134.160
131.462
130.708
130.403
129.812
128.763
127.714
127.152
123.290
121.755
121.536
121.164
120.993
120.096
116.902
116.159
113.708
77.324
77.210
77.000
76.685
21.061
Filename = E:¥NMRデータ¥反応系(700-900)2¥YA
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-767-1f6-8
Solvent = CHLOROFORM-D
Creation_Time = 14-JUN-2012 18:08:44
Revision_Time = 28-JUN-2012 20:06:56
Current_Time = 28-JUN-2012 20:07:01
Comment = YA-767-1f6-8_Carbon
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.2[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Atn = 30[deg]
X_Pulse = 6[dB]
Irr_Atn_Dec = 3.06666667[us]
Irr_Atn_Noe = 22[dB]
Irr_Noise = 22[dB]
Irr_Pwidth = WALTZ
Decoupling = 0.115[ms]
Initial_Wait = TRUE
Noe = 1[s]
Noe_Time = TRUE
Repetition_Time = 2[s]
= 3.04333312[s]
Lock_Gain = 21
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 523
Sawtooth_Range = 4


X : parts per Million : Proton
9.752
8.796
8.778
8.492
8.488
8.481
8.478
8.088
8.085
8.068
8.064
7.753
7.613
7.592
7.541
7.520
7.501
7.482
7.480
7.462
7.433
7.414
7.392
7.371
7.360
7.351
7.339
7.329
7.252
2.487
1.672
0.000
0.94
0.98
1.00
1.00
0.95
2.06
3.19
4.26
3.09
O
N
H
N
CF3
Filename = E:¥NMRデータ¥反応系(700-900)2¥YA
Author = delta
Experiment = proton.jxp
Sample_Id = YA-766-3f6-9
Solvent = CHLOROFORM-D
Creation_Time = 11-JUN-2012 16:59:33
Revision_Time = 28-JUN-2012 20:05:30
Current_Time = 28-JUN-2012 20:05:34
Comment = TMG-11
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.50300l2[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 34
Temp_Get = 19.3[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 632
Sawtooth_Range = 4


O
N
H
N
CF3
X : parts per Million : Carbon13
167.407
147.804
143.675
138.489
138.279
136.067
135.943
135.867
134.236
132.577
131.500
130.489
129.917
129.574
129.326
129.249
128.925
128.620
128.105
127.686
127.447
127.190
125.398
125.245
125.207
122.690
121.755
121.431
119.982
116.511
116.321
77.324
77.210
77.000
76.685
21.080
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
Filename = E:¥NMRデータ¥反応系(700-900)2¥YA
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-766-3f6-9
Solvent = CHLOROFORM-D
Creation_Time = 11-JUN-2012 17:02:08
Revision_Time = 11-JUN-2012 17:56:45
Current_Time = 28-JUN-2012 20:05:59
Comment = YA-766-3f6-9
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[KHz]
X_Sweep_Clipped = 25.12562814[KHz]
Irr_Domain = proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.7[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 643
Sawtooth_Range = 4


O
N
H
N
CO2Me
X : parts per Million : Proton
9.765
8.788
8.770
8.509
8.505
8.501
8.498
8.068
8.047
7.947
7.929
7.722
7.576
7.558
7.526
7.506
7.487
7.463
7.442
7.401
7.379
7.360
7.341
7.330
7.328
7.321
7.309
7.258
7.254
3.816
2.477
0.000
0.97
1.00
1.00
0.99
1.00
2.00
1.98
2.10
3.05
3.00
3.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
File name = E:¥NMRデータ¥反応系(700-900)2¥YA
Author = delta
Experiment = proton.jxp
Sample_Id = YA-767-2f8-11
Solvent = CHLOROFORM-D
Creation_Time = 12-JUN-2012 13:43:03
Revision_Time = 28-JUN-2012 20:09:50
Current_Time = 28-JUN-2012 20:09:58
Comment = YA-767-2f8-11
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.50300120[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 34
Temp_Get = 19.4[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 522
Sawtooth_Range = 4



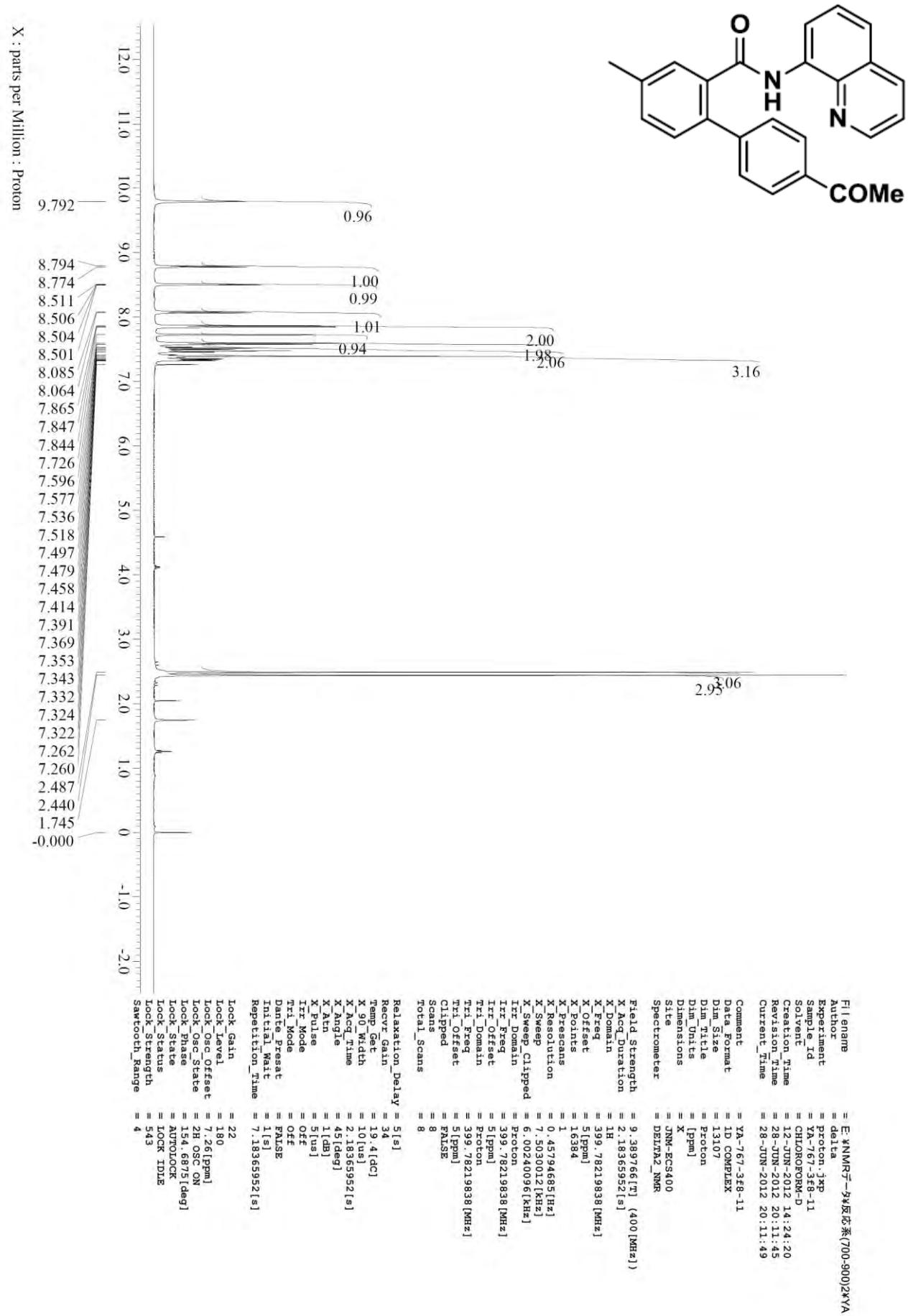

```
Filename                = E:¥NMRデータ¥反応系(700-900)2¥YA
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = YA-767-2f8-11
Solvent                 = CHLOROFORM-D
Creation_Time           = 12-JUN-2012 13:45:58
Revision_Time           = 12-JUN-2012 14:21:49
Current_Time            = 28-JUN-2012 20:08:18

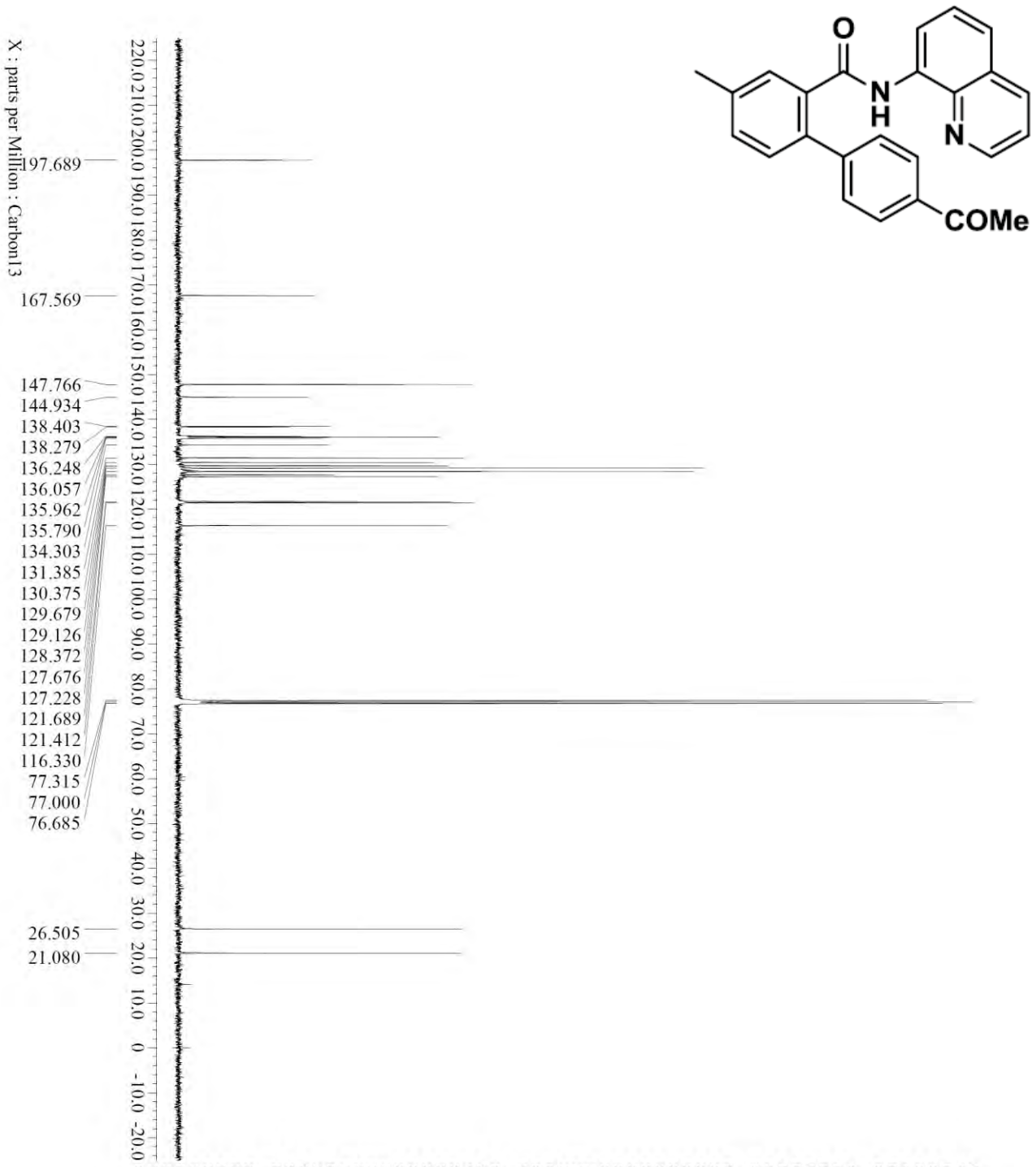
Comment                 = YA-767-2f8-11
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Site                    = JNM-ECS400
Spectrometer            = DELTA2_NMR

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 1.04333312[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.95846665[Hz]
X_Sweep                 = 31.40703518[kHz]
X_Sweep_Clipped         = 25.12562814[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 665
Total_Scans             = 665

Relaxation_Delay        = 2[s]
Recvr_Gain              = 60
Temp_Get                = 19.5[dC]
X_90_Width              = 9.2[us]
X_Acq_Time              = 1.04333312[s]
X_Angle                 = 30[deg]
X_Atn                   = 6[dB]
X_Pulse                 = 3.06666667[us]
Irr_Atn_Dec             = 22[dB]
Irr_Atn_Noe             = 22[dB]
Irr_Noise               = WALTZ
Irr_Pwidth              = 0.115[ms]
Decoupling              = TRUE
Initial_Wait            = 1[s]
Noe                     = TRUE
Noe_Time                = 2[s]
Repetition_Time         = 3.04333312[s]

Lock_Gain               = 22
Lock_Level              = 180
Lock_Osc_Offset         = 7.26[ppm]
Lock_Osc_State          = 2H OSC ON
Lock_Phase              = 154.6875[deg]
Lock_State              = AUTOLOCK
Lock_Status             = LOCK IDLE
Lock_Strength           = 525
Sawtooth_Range          = 4
```


O
N
H
N
COMe
X : parts per Million : Proton
9.792
8.794
8.774
8.511
8.506
8.504
8.501
8.085
8.064
7.865
7.847
7.844
7.726
7.596
7.577
7.536
7.518
7.497
7.479
7.458
7.414
7.391
7.369
7.353
7.343
7.332
7.324
7.322
7.262
7.260
2.487
2.440
1.745
-0.000
0.96
1.00
0.99
1.01
0.94
2.00
1.98
2.06
3.16
2.93
3.06
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
Filename = E:¥NMR¥データ¥反応系(700-900)2¥YA
Author = delta
Experiment = proton.jxp
Sample_Id = YA-767-3f8-11
Solvent = CHLOROFORM-D
Creation_Time = 12-JUN-2012 14:24:20
Revision_Time = 28-JUN-2012 20:11:45
Current_Time = 28-JUN-2012 20:11:49
Comment = YA-767-3f8-11
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.50300012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 34
Temp_Get = 19.4[dC]
X_90_Width = 10[us]
X_Acq_Time = 2.18365952[s]
X_Atn = 45[deg]
X_Angle = 1[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]
Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = ZH OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 543
Sawtooth_Range = 4



Filename = E:¥NMRデータ¥反応系(700-900)2¥YA
Author = delta
Experiment = carbon.jxp
Sample_Id = YA-767-3f8-11
Solvent = CHLOROFORM-D
Creation_Time = 12-JUN-2012 14:26:03
Revision_Time = 12-JUN-2012 15:37:10
Current_Time = 28-JUN-2012 20:10:47

Comment = YA-767-3f8-11
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024

Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.4[dC]
X_90_Width = 9.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3.06666667[us]
Irr_Atn_Dec = 22[dB]
Irr_Atn_Noe = 22[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

Lock_Gain = 22
Lock_Level = 180
Lock_Osc_Offset = 7.26[ppm]
Lock_Osc_State = 2H OSC ON
Lock_Phase = 154.6875[deg]
Lock_State = AUTOLOCK
Lock_Status = LOCK IDLE
Lock_Strength = 546
Sawtooth_Range = 4