Tetrabutylammonium Bromide-Mediated Ring Opening Reactions of *N*-Tosylaziridines with Carboxylic Acids in DMF

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Supporting Information

Table of Contents

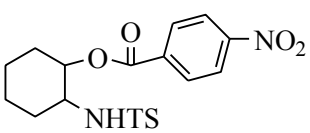
1. General Information

^{1}H NMR spectra were taken with a Bruker AVANCE III 600 MHz NMR spectrometers. The chemical shifts are reported in ppm downfield to the $CDCl_3$ resonance (δ = 7.27). Spectra are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration, and assignment. ^{13}C NMR data were collected at 150 MHz with complete proton decoupling. The chemical shifts are reported in ppm downfield to the central $CDCl_3$ resonance (δ = 77.0). High-resolution mass spectra were performed on a micrOTOF-Q II instrument with an ESI source. Melting points were measured with a RD-II melting point apparatus and are uncorrected. Unless otherwise noted, Reagents obtained from commercial sources were used without further purification. All solvents were purchased from commercial sources and used with further purification. Deuterated solvents were purchased from aladdin. Column chromatography was performed on silica gel (200-300 mesh). All yields were referred to isolated yields (average of two runs) of compounds. The corresponding preparation about *N*-tosylaziridines are listed in references.

2. General procedure for the ring opening of *N*-Tosylaziridines

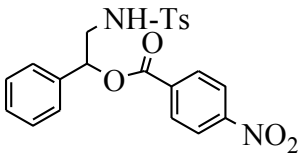
General Procedure: DMF (2.0 mL) was added to a mixture of *N*-tosylaziridine **1** (50 mg, 0.2 mmol), carboxylic acid **2** (40.1 mg, 0.24 mmol) and TBAB (6.4 mg, 0.02 mmol, 10 mol%). The reaction mixture was stirred at 65 ^{o}C under air atmosphere until the *N*-tosylaziridine disappeared indicated by TLC. The crude mixture was washed with 5% (m/m) K_2CO_3 solution (20 mL) to remove the remains of carboxylic acid. The water phase was extracted with CH_2Cl_2 (3 × 5 mL). The organic extracts were combined and dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuum. The resultant product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the corresponding product.

3. Characterization data of products



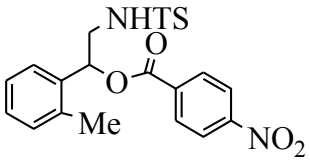
2-(4-methylphenylsulfonamido)cyclohexyl 4-nitrobenzoate (3a) White solid; mp 150-152 ^{o}C; 1H NMR (600 MHz, $CDCl_3$) : δ 1.27-1.52 (m, 4H), 1.71-1.78 (m, 2H), 2.03-2.09 (m, 2H), 2.23 (s, 3H), 3.37-3.42 (m, 1H), 4.82-4.86 (m, 1H), 4.88-4.89 (d, 1H), 7.01-7.02 (d, 2H), 7.61-7.62 (d, *J* =

8.4 Hz, 2H), 7.98-8.00 (d, *J* = 8.4 Hz , 2H), 8.19-8.21 (d, 2H**)** ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.4, 23.7, 24.3, 31.1, 33.6, 56.9, 75.8, 123.2, 126.6, 129.5, 130.9, 135.2, 138.5, 142.9, 150.5, 164.7 ppm; MS (ESI): Calcd for $C_{20}H_{22}N_2O_6S$+Na 441.1096, found 441.1093.



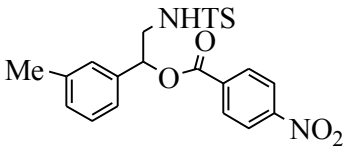
2-(4-methylphenylsulfonamido)-1-phenylethyl 4-nitrobenzoate (3b)

White solid; mp 143-145 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.29 (s, 3H), 2.39 (s, 3H), 3.43-3.54 (m, 2H), 4.44-4.47 (dd, *J* = 11.4, 5.4 Hz, 1H), 4.50-4.53 (dd, *J* = 11.4, 7.8 Hz, 1H), 4.77-4.80 (td, *J* = 7.8, 4.8 Hz, 1H), 5.57-5.60 (d, 1H), 6.00-6.02 (dd, *J* = 7.8, 3.6 Hz, 1H), 6.06-6.08 (d, *J* = 7.8 Hz, 1H), 7.04-7.06 (d, *J* = 7.8 Hz, 2H), 7.18-7.34 (m, 12H), 7.57-7.59 (d, *J* = 8.4 Hz, 2H), 7.70-7.71 (d, *J* = 8.4 Hz, 2H), 8.05-8.19 (m, 8H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): 21.5, 47.7, 56.8, 67.8, 75.9, 123.4, 127.0, 128.8, 128.9, 129.5, 129.8, 130.9, 134.8, 135.0, 136.5, 136.8, 136.9, 137.3, 143.4, 143.7, 150.6, 163.8, 164.4 ppm; MS (ESI): Calcd for $C_{22}H_{20}N_2O_6S$+Na 463.0940, found 463.0940.



2-(4-methylphenylsulfonamido)-1-o-tolylethyl 4-nitrobenzoate (3c)

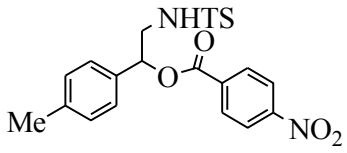
White solid; mp 164-166 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.17 (s, 3H), 2.39 (d, 3H), 3.39-3.50 (m, 1H), 4.41-4.44 (m, 1H), 5.27-5.30 (t, *J* = 7.2 Hz, 1H), 6.19-6.21 (q, 1H), 7.02-7.03 (d, 1H), 7.07-7.08 (d, 1H), 7.13-7.24 (m, 3H), 7.29-7.30 (d, 1H), 7.52-7.53 (m, 1H), 7.70-7.71 (d, 1H), 8.07-8.10 (dt, *J* = 9.0, 1.8 Hz, 1H), 8.15-8.17 (dt, *J* = 9.0, 1.8 Hz, 1H), 8.22-8.24 (d, *J* = 9.0 Hz, 2H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 19.1, 21.4, 46.9, 73.1, 123.5, 125.5, 126.6, 127.0, 128.2, 128.8, 129.4, 129.9, 130.9, 134.9, 135.0, 135.4, 143.7, 150.6, 164.5 ppm; MS (ESI): Calcd for $C_{23}H_{22}N_2O_6S$+Na 477.1096, found 477.1093.



2-(4-methylphenylsulfonamido)-1-m-tolylethyl 4-nitrobenzoate (3d)

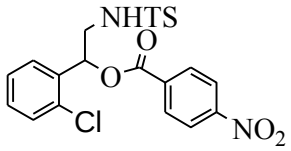
Mixture of **3d** and **4d.** Inseparable white solid (**3d:4d** = 1.2:1); white solid; mp 137-144 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.21 (s, 3H), 2.29 (s, 3H), 2.31 (s, 3H), 2.39 (s, 3H), 3.41-3.45 (m, 1H), 3.49-3.53 (m, 1H), 4.42-4.45 (dd, *J* = 11.4, 4.8 Hz, 1H), 4.49-4.52 (dd, *J* = 11.4 , 7.8 Hz, 1H), 4.71-4.75 (td, J=7.8, 4.8 Hz, 1H), 5.41-5.44 (t, 1H), 5.84-5.85 (d, *J* = 7.8 Hz, 1H), 5.95-5.97 (dd, *J* = 7.8, 4.2 Hz, 1H), 6.90 (s, 1H), 6.98-6.99 (d, *J* = 7.8 Hz, 1H), 7.02-7.06 (q, 3H), 7.10-7.13 (t, 4H), 7.21-7.7.23 (t, *J* = 8.4 Hz, 3H), 7.56-7.7.57 (d, *J* = 8.4 Hz, 2H), 7.69-7.70 (d, *J* = 8.4 Hz, 2H), 8.06-8.08 (dt, *J* = 9.0, 2.4 Hz, 2H), 8.14-8.16 (dt, *J* = 9.0, 2.4 Hz, 2H), 8.18-8.21 (m, 4H) ppm; ^{13}C NMR (150 MHz,

$CDCl_3$): δ 21.2, 21.4, 21.5, 47.7, 56.9, 67.7, 75.9, 123.4, 127.0, 127.1, 128.8, 129.4, 129.8, 130.9, 134.8, 135.0, 136.4, 136.6, 137.0, 137.4, 138.5, 138.7, 143.4, 143.6, 150.6, 163.8, 164.5 ppm; MS (ESI): Calcd for $C_{23}H_{22}N_2O_6S$+Na 477.1096, found 477.1091.



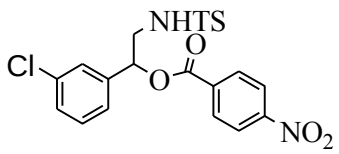
2-(4-methylphenylsulfonamido)-1-p-tolylethyl 4-nitrobenzoate (3e)

White solid; mp 140-142 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.33 (s, 3H), 2.40 (s, 3H), 3.44-3.53 (m, 1H), 4.43-4.54 (m ,1H), 5.19-5.21 (m, 1H), 5.96-5.98 (dd, *J* = 7.8, 4.2 Hz, 1H), 7.05-7.08 (m, 2H), 7.14-7.15 (d, *J* = 7.8 Hz, 2H), 7.20-7.24 (q, 2H), 7.57-7.58 (d, *J* = 8.4 Hz, 1H), 7.68-7.70 (d, *J* = 8.4 Hz, 1H), 8.06-8.07 (d, *J* = 9.0 Hz, 1H), 8.15-8.17 (d, *J* = 9.0 Hz, 1H), 8.20-8.22 (q, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.2, 21.5, 47.6, 75.7, 123.5, 126.4, 127.0, 129.6, 129.8, 130.9, 133.4, 135.1, 137.0, 139.0, 143.7, 150.6, 163.8 ppm; MS (ESI): Calcd for $C_{23}H_{22}N_2O_6S$+Na 477.1096, found 477.1093.



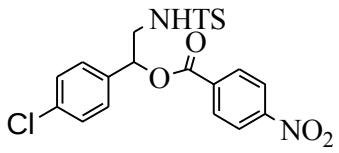
2-(4-methylphenylsulfonamido)-1-(2-chlorophenyl)ethyl 4-nitrobenzoate (3f)

White solid; mp 175-177 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.29 (s, 3H), 4.43-4.46 (dd, *J* = 11.4, 4.8 Hz, 1H), 4.57-4.60 (dd, *J* = 11.4, 7.8 Hz, 1H), 5.22-5.25 (m, 1H), 5.83-5.84 (d, *J* = 7.8 Hz, 1H), 7.05-7.07 (d, *J* = 7.8 Hz, 2H), 7.14-7.20 (m, 2H), 7.28-7.30 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.32-7.33 (q, 1H), 7.60-7.61 (d, *J* = 8.4 Hz, 2H), 8.04-8.07 (dt, *J* = 9.0, 2.4 Hz, 2H), 8.22-8.24 (dt, *J* = 8.4, 2.4 Hz, 2H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.4, 54.4, 66.3, 123.5, 127.0, 127.2, 128.7, 129.5, 129.9, 130.9, 132.5, 134.3, 134.6, 136.9, 143.5, 150.7, 164.5 ppm; MS (ESI): Calcd for $C_{22}H_{19}ClN_2O_6S$+Na 497.0550, found 497.0550.



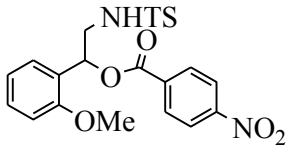
2-(4-methylphenylsulfonamido)-1-(3-chlorophenyl)ethyl 4-nitrobenzoate (3g)

White solid; mp 146-148 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.31 (s, 3H), 3.44-3.49 (m, 1H), 4.42-4.49 (m, 1H), 4.45-4.76 (td, *J* = 7.8, 1.8 Hz, 1H), 6.17-6.19 (d, *J* = 7.8 Hz, 1H), 7.06-7.07 (d, *J* = 7.8 Hz, 1H), 7.09-7.7.14 (m, 2H), 7.17-7.18 (m, 1H), 7.23-7.24 (d, *J* = 7.8 Hz, 1H), 7.27-7.28 (m, 1H), 7.56-7.57 (m, 1H), 7.69-7.70 (q, 1H), 8.04-8.20 (m, 4H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.4, 56.4, 674, 124.4, 125.0, 126.9, 127.2, 128.4, 129.5, 129.9, 130.1, 130.9, 134.6, 137.0, 138.8, 143.7, 150.6, 164.4 ppm.



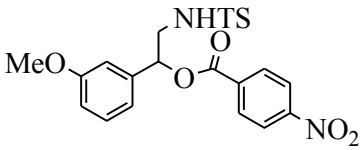
2-(4-methylphenylsulfonamido)-1-(4-chlorophenyl)ethyl 4-nitrobenzoate (3h)

Mixture of **3h** and **4h.** Inseparable white solid (**3h:4h** = 2:1); mp 134-137 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.31 (s, 3H), 2.40 (s, 3H), 3.41-3.51 (m, 2H), 4.40-4.43 (dd, *J* = 11.4, 4.8 Hz, 1 H), 4.46-4.49 (dd, *J* = 11.4, 7.2 Hz, 1H), 4.73-4.77 (td, *J* = 7.2, 4.8 Hz, 1H), 5.57-5.59 (t, 1H), 5.97-5.99 (q, 1H), 6.08-6.09 (d, *J* = 7.8 Hz, 1H), 7.06-7.07 (d, *J* = 7.8 Hz, 2H), 7.12-7.13 (d, *J* = 8.4 Hz, 2H), 7.17-7.19 (dt, *J* = 8.4, 1.8 Hz, 2H), 7.19-7.22 (m, 6H), 7.54-7.56 (d, *J* = 8.4 Hz, 2H), 7.66-7.68 (d, 2H), 8.03-8.05 (dt, *J* = 8.4, 2.4 Hz, 2H), 8.14-8.19 (m, 6H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.5, 29.6, 47.4, 56.3, 67.4, 75.2, 123.5, 126.9, 127.9, 128.2, 128.9, 129.1, 129.5, 129.8, 130.9, 134.3, 134.6, 134.9, 135.0, 135.4, 136.8, 137.1, 143.7, 143.8, 150.7, 163.7, 164.4 ppm; MS (ESI): Calcd for $C_{22}H_{19}ClN_2O_6S$+Na 497.0550, found 497.0556.



2-(4-methylphenylsulfonamido)-1-(2-methoxyphenyl)ethyl 4-nitrobenzoate (3i)

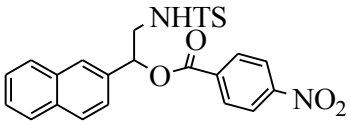
White solid; mp 149-151 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.38 (s, 3H), 3.44-3.49 (m, 1H), 3.53-3.57 (m, 1H), 3.82 (s, 3H), 4.95-4.97 (t, 1H), 6.36-6.38 (q, 1H), 6.85-6.87 (d, 1H), 6.91-6.94 (t, 1H), 7.19-7.21 (d, 2H), 7.28-7.30 (m, 2H), 7.67-7.69 (d, 2H), 8.12-8.28 (m, 4H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.5, 46.3, 55.8, 70.9, 110.8, 120.9, 123.5, 124.6, 126.5, 127.0, 129.2, 129.6, 130.9, 135.2, 137.3, 143.4, 150.7, 156.0, 163.7 ppm; MS (ESI): Calcd for $C_{23}H_{22}N_2O_7S$+Na 493.1045, found 493.1044.



2-(4-methylphenylsulfonamido)-1-(3-methoxyphenyl)ethyl 4-nitrobenzoate (3j)

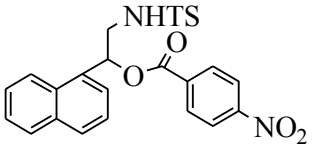
Mixture of **3j** and **4j.** Inseparable white solid (**3j:4j** = 1.4:1); white solid; mp 87-89 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.30 (s, 3H), 2.39 (s, 3H), 3.43-3.53 (m, 2H), 3.69 (s, 3H), 3.77 (s, 3H), 4.44-4.46 (dd, *J* = 12.0, 4.8 Hz, 1H), 4.51-4.54 (dd, *J* = 12.0, 7.8 Hz, 1H), 4.73-4.76 (td, *J* = 7.2, 4.8 Hz, 1H), 5.26-5.29 (m, 1H), 5.77-5.78 (d, *J* = 7.8 Hz, 1H), 5.96-5.98 (dd, *J* = 7.8, 4.2 Hz, 1H), 6.67 (t, 1H), 6.75-6.77 (m, 2H), 6.84-6.86 (m, 2H), 6.89-6.91 (d, 1H), 7.06-7.07 (d, *J* = 8.4 Hz, 2H), 7.14-7.16 (t, *J* = 8.4 Hz, 1H), 7.23-7.24 (m, 3H), 7.57-7.59 (d, *J* = 8.4 Hz, 2H), 7.69-7.70 (d, *J* = 8.4 Hz, 2H), 8.07-8.08 (q, 2H), 8.15-8.17 (dd, *J* = 7.2, 1.8 Hz, 2H), 8.19-8.22 (td, *J* = 7.8, 1.8 Hz, 4H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.4, 21.5, 47.6, 55.3, 67.7, 75.6, 112.4, 113.9, 118.5, 118.9, 123.5, 127.0, 129.5, 129.8, 130.1, 130.9, 134.8, 137.0, 137.3, 138.0, 138.3,

143.4, 143.7, 150.6, 159.9, 163.7, 164.5 ppm; MS (ESI): Calcd for $C_{23}H_{22}N_2O_7S$+Na 493.1045, found 493.1047.



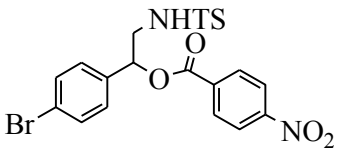
2-(4-methylphenylsulfonamido)-1-(naphthalen-7-yl)ethyl 4-nitrobenzoate (3k)

White solid; mp 183-186 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.35 (s, 3H), 3.53-3.63 (m, 2H), 5.36-5.38 (t, 1H), 6.16-6.18 (dd, *J* = 7.8, 4.8 Hz, 1H), 6.92-6.94 (d, *J* = 7.8 Hz, 1H), 7.16-7.17 (d, *J* = 8.4 Hz, 2H), 7.40-7.41 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.48-7.49 (m, 2H), 7.54-7.57 (d, *J* = 8.4 Hz, 1H), 7.65-7.67 (d, *J* = 8.4 Hz, 2H), 7.77-7.81 (m, 3H), 8.17-8.21 (m, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.5, 47.6, 75.9, 123.5, 126.1, 126.7, 126.7, 126.9. 127.7, 128.1, 128.9, 129.4, 129.8, 130.9, 133.0, 133.4, 133.7, 135.0, 136.9, 143.7, 150.6, 163.8 ppm; MS (ESI): Calcd for $C_{26}H_{22}N_2O_6S$+Na 513.1096, found 513.1095.



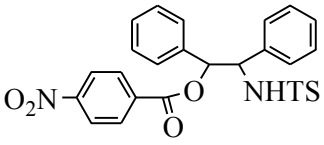
2-(4-methylphenylsulfonamido)-1-(naphthalen-5-yl)ethyl 4-nitrobenzoate (3l)

White solid; mp 189-191 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.37 (s, 3H), 3.63-3.66 (m, 2H), 5.18-5.21 (t, 1H), 6.80-6.82 (q, 1H), 7.19-7.21 (d, *J* = 8.4 Hz, 2H), 7.42-7.44 (t, 1H), 7.52-7.55 (m, 3H), 7.67-7.68 (d, *J* = 8.4 Hz, 2H), 7.82-7.83 (d, *J* = 8.4 Hz, 1H), 7.87-7.88 (d, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 8.22-8.27 (m, 4H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.5, 47.2, 73.3, 122.4, 123.6, 124.0, 125.2, 126.2, 127.0, 127.0, 129.2, 129.5, 129.8, 130.0, 131.0, 132.2, 133.8, 135.0, 137.0, 143.7, 150.7, 163.9 ppm; MS (ESI): Calcd for $C_{26}H_{22}N_2O_6S$+Na513.1096, found 513.1097.



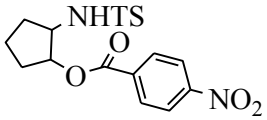
2-(4-methylphenylsulfonamido)-1-(4-bromophenyl)ethyl 4-nitrobenzoate (3m)

Mixture of **3m** and **4m.** Inseparable white solid (**3m:4m** = 2:1); white solid; mp 152-156 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.32 (s, 3H), 2.40 (s, 3H), 3.42-3.51(m, 2H), 4.40-4.43 (dd, *J* = 11.4, 4.2 Hz, 1H), 4.46-4.49 (dd, *J* = 11.4, 7.8 Hz, 1H), 4.72-4.4.75 (td, *J* = 7.8, 4.8 Hz, 1H), 5.41-5.44 (m, 1H), 5.95-5.97 (m, 2H), 7.06-7.08 (m, 4H), 7.19-7.20 (d, *J* = 8.4 Hz, 2H), 7.23-7.24 (d, 2H), 7.33-7.35 (d, *J* = 8.4 Hz, 2H), 7.44-7.45 (d, *J* = 8.4 Hz, 2H), 7.54-7.55 (d, *J* = 7.8 Hz, 2H), 7.66-7.67 (d, *J* = 8.4 Hz, 2H), 8.15-8.16 (d, *J* = 9.0 Hz, 2H), 8.19-8.22 (dd, *J* = 9.0, 7.2 Hz, 4H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 122.4, 123.1, 123.5, 126.9, 128.1, 128.5, 129.5, 129.8, 130.9, 131.9, 132.1, 134.5, 134.7, 135.5, 135.9, 136.8, 137.1, 143.7, 150.7, 163.6, 164.4 ppm; MS (ESI): Calcd for $C_{22}H_{19}BrN_2O_6$+Na 541.0045, found 541.0041.



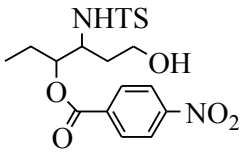
2-(4-methylphenylsulfonamido)-1,2-diphenylethyl 4-nitrobenzoate (3n)

White solid; mp 194-196 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 2.28 (s, 3H), 4.84-4.87 (t, *J* = 8.4 Hz, 1H), 5.72-5.74 (d, *J* = 8.4 Hz, 1H), 6.17-6.18 (d, 1H), 6.93-6.94 (d, *J* = 8.4 Hz, 2H), 6.97-6.99 (d, *J* = 8.4 Hz, 2H), 7.05-7.08 (t, *J* = 7.2 Hz, 2H), 7.10-7.12 (dt, *J* = 7.2, 2.4 Hz, 1H), 7.14-7.22 (m, 5H), 7.43-7.45 (d, *J* = 8.4 Hz, 2H), 8.19-8.21 (dt, *J* = 9.0, 1.8 Hz, 2H), 8.22-8.24 (dt, *J* = 8.4, 1.8 Hz, 2H) ppm; ^{13}CNMR (150 MHz, $CDCl_3$): δ 21.4, 62.4, 79.0, 123.6, 126.8, 127.1, 127.4, 128.0, 128.4, 128.4, 128.7, 129.3, 131.0, 134.9, 135.7, 136.6, 137.4, 143.1, 150.7, 164.0 ppm; MS (ESI): Calcd for $C_{28}H_{24}N_2O_6S$+Na 539.1253, found 539.1251.



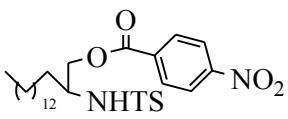
2-(4-methylphenylsulfonamido)cyclopentyl 4-nitrobenzoate (3o)

White solid; mp 142-144 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 1.55-1.58 (m, 1H), 1.71-1.78(m, 4H), 2.08-2.13 (td, *J* = 13.2, 7.2 Hz, 1H), 2.29 (s, 3H), 3.70-3.74 (ddd, *J* = 13.8, 7.2, 6.0 Hz, 1H), 5.13-5.16 (td, *J* = 7.8, 5.4 Hz, 1H), 5.38-5.39 (d, *J* = 6.0 Hz, 1H), 7.15-7.16 (d, *J* = 7.8 Hz, 2H), 7.72-7.74 (d, *J* = 8.4 Hz, 2H), 8.04-8.05 (dt, *J* = 9.0, 1.8 Hz, 2H), 8.24-8.26 (dt, *J* = 8.4, 2.4 Hz, 2H) ppm; ^{13}CNMR (150 MHz, $CDCl_3$): δ 20.7, 21.4, 29.5, 31.0, 59.6, 81.0, 123.4, 127.1, 129.6, 130.8, 135.2, 137.4, 143.4, 150.6, 164.4 ppm; MS (ESI): Calcd for $C_{19}H_{20}N_2O_6S$+Na 427.0940, found 427.0938.



2-(4-methylphenylsulfonamido)-6-hydroxyhexan-3-yl 4-nitrobenzoate (4p)

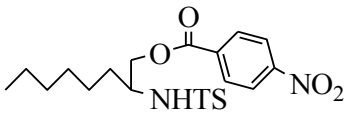
Colourless liquid; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 0.81-0.84 (t, 3H), 1.32-1.41 (m, 2H), 1.89-1.93 (m, 2H), 2.45 (s, 3H), 2.97-3.01 (m, 1H), 3.68-3.74 (m, 2H), 4.43-4.47 (m, 1H), 4.56-4.60 (m, 1H), 4.80-4.81 (d, 1H), 7.29-7.30 (d, 1H), 7.33-7.35 (d, 2H), 7.75-7.77 (dt, *J* = 8.4, 1.8 Hz, 1H), 7.82-7.84 (dt, *J* = 8.4, 1.8 Hz, 2H), 8.18-8.20 (dt, *J* = 9.0, 1.8 Hz, 1H), 8.28-8.30 (dt, *J* = 9.0, 1.8 Hz, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 11.5, 21.5, 29.1, 33.3, 46.9, 60.8, 68.9, 127.0, 128.1, 129.6, 130.7, 135.4, 150.6, 165.0 ppm; MS (ESI): Calcd for $C_{20}H_{24}N_2O_7S$+Na 459.1202, found 459.1202.



2-(4-methylphenylsulfonamido)pentyl 4-nitrobenzoate (4q)

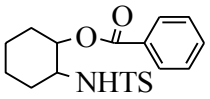
White solid; mp 106-108 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 0.87-0.89 (t, 3H), 1.13-1.26 (m, 24 H), 1.41-1.58 (m, 2H), 2.36 (s, 3H), 3.61-3.63 (m, 1H), 4.23-4.30 (m, 2H), 5.35-5.37 (d, *J* = 8.4 Hz, 1H), 7.20-7.21 (d, *J* = 8.4 Hz, 2H),

7.74-7.76 (d, 2H), 8.11-8.13 (dt, *J* = 8.4, 2.4 Hz, 2H), 8.20-8.21 (dt, *J* = 8.4, 2.4 Hz, 2H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 14.1, 21.5, 22.7, 25.4, 29.1, 29.4, 29.5, 29.7, 31.9, 32.3, 52.8, 67.3, 123.4, 126.9, 129.7, 130.9, 135.0, 138.0, 143.5, 150.6, 164.5 ppm; MS (ESI): Calcd for $C_{30}H_{44}N_2O_6S$+Na 583.2818, found 583.2821.



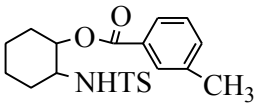
2-(4-methylphenylsulfonamido)octyl 4-nitrobenzoate (4r)

White solid; mp 116-118 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 0.82-0.85 (t, 3H), 1.10-1.22 (m, 8H), 1.46-1.53 (m, 2H), 2.40 (s, 3H), 3.60-3.63 (m, 1H), 4.23-4.30 (m, 2H), 5.33-5.34 (d, *J* = 8.4 Hz, 1H), 7.20-7.22 (d, 2H), 7.74-7.76 (d, *J* = 8.4 Hz, 2H), 8.11-8.13 (dt, *J* = 8.4, 2.4 Hz, 2H), 8.20-8.22 (dt, *J* = 8.4, 2.4 Hz, 2H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 13.9, 21.4, 22.4, 25.4, 28.8, 31.5, 32.3, 52.9, 67.3, 123.4, 126.9, 129.7, 130.8, 135.0, 138.5, 143.5, 150.6, 164.5 ppm; MS (ESI): Calcd for $C_{22}H_{28}N_2O_6S$+Na 471.1566, found 471.1562.



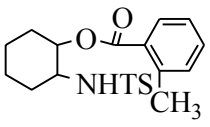
2-(4-methylphenylsulfonamido)cyclohexyl benzoate (3s)

White solid; mp 155-157 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 1.28-1.48 (m, 4H), 1.69-1.76 (m, 2H), 2.00-2.04 (m, 1H), 2.18 (s, 3H), 2.18-2.23 (m, 1H), 3.31-3.32 (m, 1H), 4.79-4.84 (m, 1H), 5.14-5.15 (d, 1H), 6.90-6.92 (d, *J* = 7.8, 2H), 7.35-7.37 (t, *J* = 7.8 Hz, 2H), 7.53-7.55 (t, *J* = 7.8 Hz, 1H), 7.58-7.59 (d, 2H), 7.77 (dd, *J* = 7.8, 1.2 Hz, 2H) ppm.



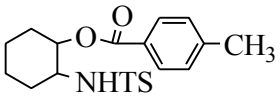
2-(4-methylphenylsulfonamido)cyclohexyl 3-methylbenzoate (3t)

White solid; mp 129-131 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 1.29-1.49 (m, 3H), 1.68-1.76 (m, 3H), 2.02 (m, 1H), 2.19 (s, 3H), 2.38-2.46 (s, 1H), 2.46 (s, 3H), 3.30-3.32 (m, 1H), 4.80-4.82 (m, 1H), 5.11-5.12 (m, 1H), 6.90-6.92 (d, 2H), 7.16-7.20 (m, 1H), 7.23-7.26 (t, *J* = 7.2 Hz, 1H), 7.37-7.40 (td, *J* = 7.2, 1.2 Hz, 1H), 7.57-7.59 (dt, *J* = 7.8, 2.4 Hz, 2H), 7.65-7.66 (dd, *J* = 7.8, 1.2 Hz, 1H) ppm.



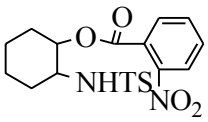
2-(4-methylphenylsulfonamido)cyclohexyl 2-methylbenzoate (3u)

White solid; mp 130-132 °C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 1.25-1.50 (m, 4H), 1.69-1.79 (m, 2H), 1.99-2.02 (m, 1H), 2.17 (s, 3H), 2.22-2.24 (m, 1H), 2.38 (s, 3H), 3.29-3.31(m, 1H), 4.79-4.83 (m, 1H), 5.07 (d, 1H), 6.89-6.92 (d, *J* = 7.8 Hz, 2H), 7.24-7.26 (t, *J* = 7.8 Hz, 1H), 7.35-7.36 (d, 1H), 7.55-7.60 (m, 4H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.4, 22.0, 23.8, 24.2, 31.3, 34.0, 57.3, 74.3, 125.5, 126.5, 128.8, 129.3, 131.0, 131.6, 132.2, 138.2, 140.6, 142.7, 167.6 ppm; MS (ESI): Calcd for $C_{21}H_{25}NO_4S$+Na 410.1402, found 410.1403.



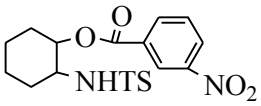
2-(4-methylphenylsulfonamido)cyclohexyl 4-methylbenzoate (3v)

White solid; mp 144-146 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 1.28-1.47 (m, 4H), 1.69-1.79 (m, 2H), 2.00-2.02 (m, 1H), 2.16 (s, 1H), 2.18 (s, 3H), 2.42 (s, 3H), 3.29-3.31 (m, 1H), 4.78-4.82 (m, 1H), 5.16-5.17 (d, 1H), 6.90-6.92 (d, *J* = 8.4 Hz, 2H), 7.15-7.16 (d, *J* = 8.4 Hz , 2H), 7.57-7.59 (dt, *J* = 8.4, 1.8 Hz, 2H), 7.64-7.65 (d, *J* = 8.4 Hz, 2H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.3, 21.6, 23.8, 24.2, 31.3, 34.1, 57.3, 74.4, 126.6, 127.0, 128.8, 129.3, 129.8, 138.1, 142.6, 143.6, 166.9 ppm; MS (ESI): Calcd for $C_{21}H_{25}NO_4S$ + Na 410.1402, found 410.1402.



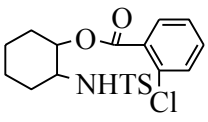
2-(4-methylphenylsulfonamido)cyclohexyl 2-nitrobenzoate (3w)

White solid; mp 135-137 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 1.21-1.41 (m, 4H), 1.59-1.71 (m, 2H), 1.87-1.89 (m, 1H), 2.01-2.04 (m, 1H), 2.28 (s, 3H), 3.23-3.29 (m, 1H), 4.81-4.85 (m, 1H), 5.47-5.48 (d, 1H), 7.05-7.06 (d, *J* = 7.8 Hz, 2H), 7.60-7.62 (m, 2H), 7.64-7.65 (d, *J* = 7.8 Hz, 2H), 7.71-7.72 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.83-7.85 (dd, J=7.2, 1.2 Hz, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.5, 23.4, 24.1, 30.2, 32.8, 56.3, 76.2, 123.6, 126.7, 127.4, 129.4, 130.2, 131.6, 132.9, 138.4, 142.8, 147.9, 165.2 ppm; MS (ESI): Calcd for $C_{20}H_{22}N_2O_6S$+Na 441.1096, found 441.1088.



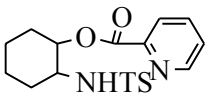
2-(4-methylphenylsulfonamido)cyclohexyl 3-nitrobenzoate (3x)

White solid; mp 138-140 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 1.29-1.39 (m, 3H), 1.51 (m, 1H), 1.70-1.75 (m, 2H), 2.04-2.07 (m, 2H), 2.17 (s, 3H), 3.35-3.41 (m, 1H), 4.86-4.90 (m, 1H), 5.17-5.18 (d, *J* = 7.8 Hz, 1H), 6.97-6.99 (d, *J* = 7.8 Hz, 2H), 7.57-7.59 (d, *J* = 7.8 Hz, 1H), 7.60-7.62 (m, 2H), 8.18-8.20 (dt, *J* = 7.8, 1.2 Hz, 1H), 8.36-8.38 (ddd, *J* = 7.8, 2.4, 1.2 Hz, 1H), 8.56 (t, *J* = 1.8 Hz, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.3, 23.7, 24.2, 31.1, 33.5, 56.9, 75.8, 124.6, 126.6, 127.2, 129.4, 131.7, 135.5, 138.4, 142.8, 148.1, 164.4 ppm; MS (ESI): Calcd for $C_{20}H_{22}N_2O_6S$+Na 441.1096, found 441.1096.



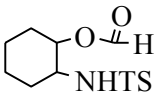
2-(4-methylphenylsulfonamido)cyclohexyl 2-chlorobenzoate (3y)

White solid; mp 137-139 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 1.27-1.50 (m, 4H), 1.66-1.74 (m, 2H), 2.07-2.10 (m, 2H), 2.23 (s, 3H), 3.34-3.36 (m, 1H), 4.83-4.87 (m, 1H), 5.13-5.14 (d, *J* = 7.8 Hz, 1H), 7.00-7.02 (d, *J* = 7.8 Hz, 2H), 7.24-7.27 (m, 1H), 7.41-7.42 (d, 2H), 7.65-7.69 (q, 3H) ppm.



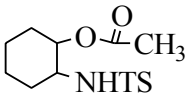
2-(4-methylphenylsulfonamido)cyclohexyl picolinate (3z)

White solid; mp 220-222 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 1.26-1.42 (m, 4H), 1.56-1.57 (m, 1H), 1.71-1.76 (m, 2H), 2.05-2.07 (m, 1H), 2.19 (s, 3H), 3.38-3.44 (m, 1H), 4.89-4.91 (m, 1H), 5.04-5.06 (d, 1H), 6.93-6.94 (d, *J* = 7.8 Hz, 2H), 7.44-7.47 (m, 1H), 7.60-7.62 (dt, *J* = 7.8, 2.4 Hz, 2H), 7.75-7.78 (td, *J* = 7.8, 1.8 Hz, 1H), 7.88-7.90 (dt, *J* = 7.8, 1.2 Hz, 1H), 8.71-8.72 (m, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.4, 23.8, 24.2, 31.1, 34.0, 57.1, 75.6, 125.3, 126.7, 129.3, 136.7, 138.3, 142.5, 147.6, 149.8, 165.1 ppm; MS (ESI): Calcd for $C_{19}H_{22}N_2O_4S$+Na 397.1198, found 397.1192.



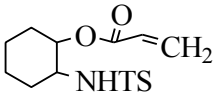
2-(4-methylphenylsulfonamido)cyclohexyl formate (3za)

White solid; mp 116-118 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 1.11-1.24 (m, 4H), 1.56-1.73 (m, 3H), 2.00-2.02 (m, 1H), 2.43 (s, 3H), 2.84-2.87 (m, 2H), 3.31-3.33 (m, 1H), 5.20-5.22 (d, 1H), 7.31-7.32 (d, 2H), 7.79-7.81 (d, 2H) ppm.



2-(4-methylphenylsulfonamido)cyclohexyl acetate (3zb)

White solid; mp 124-126 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 1.22-1.35 (m, 4H), 1.64-1.70 (m, 2H), 1.76 (s, 3H), 1.91-1.93 (m, 1H), 2.02-2.04 (m, 1H), 2.42 (s, 3H), 3.20 (m, 1H), 4.54-4.58 (m, 1H), 4.90-4.91 (d, *J* = 7.8 Hz, 1H), 7.29-7.30 (d, 2H), 7.74-7.75 (dt, *J* = 7.8, 1.8 Hz, 2H) ppm.



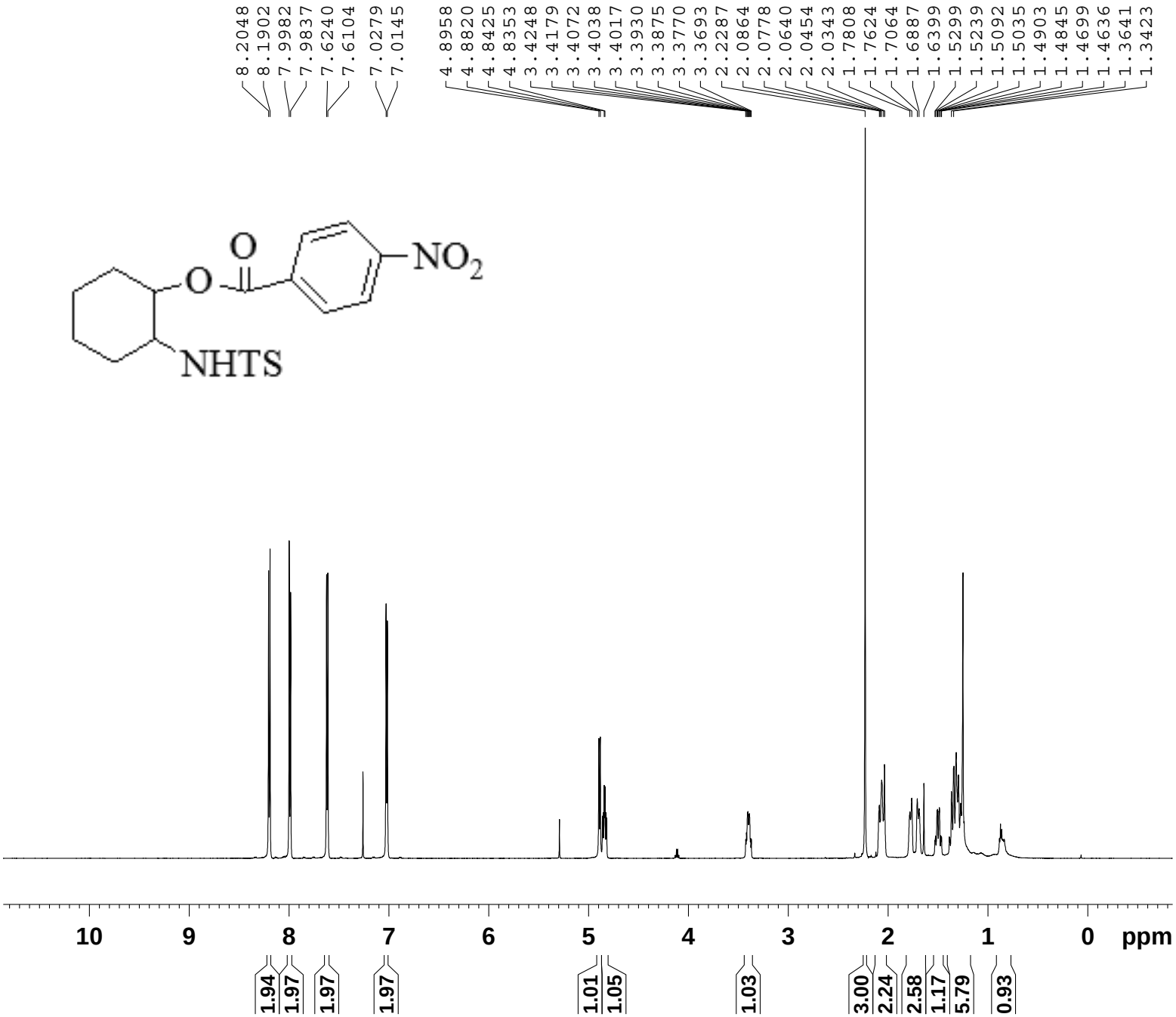
2-(4-methylphenylsulfonamido)cyclohexyl acrylate (3zc)

White solid; mp 105-107 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) : δ 1.23-1.38 (m, 4H), 1.67-1.73 (m, 2H), 1.95-2.12 (m, 2H), 2.41 (s, 3H), 3.23-3.24 (m, 1H), 4.61-4.65 (td, 10.2, 4.2 Hz, 1H), 4.82-4.84 (d, 1H), 5.70-5.72 (d, *J* = 10.2 Hz, 1H), 5.75-5.80 (dd, *J* = 16.8, 10.2 Hz, 1H), 6.21-6.24 (dd, *J* = 16.8, 1.2 Hz, 1H), 7.24-7.27 (d, 2H), 7.69-7.71 (d, 2H) ppm.

4. Reference

The corresponding preparation about *N*-tosylaziridines, see: (a) D. Kano, S. Minakata, M. Komatsu, J. Chem. Soc., Perkin Trans. 1 **2001**, 3186; (b) V. V. Thakur, A. Sudalai, *Tetrahedron Lett.* **2003**, *44*, 989.

5. ^{1}H, ^{13}C NMR, HRMS spectrum of products



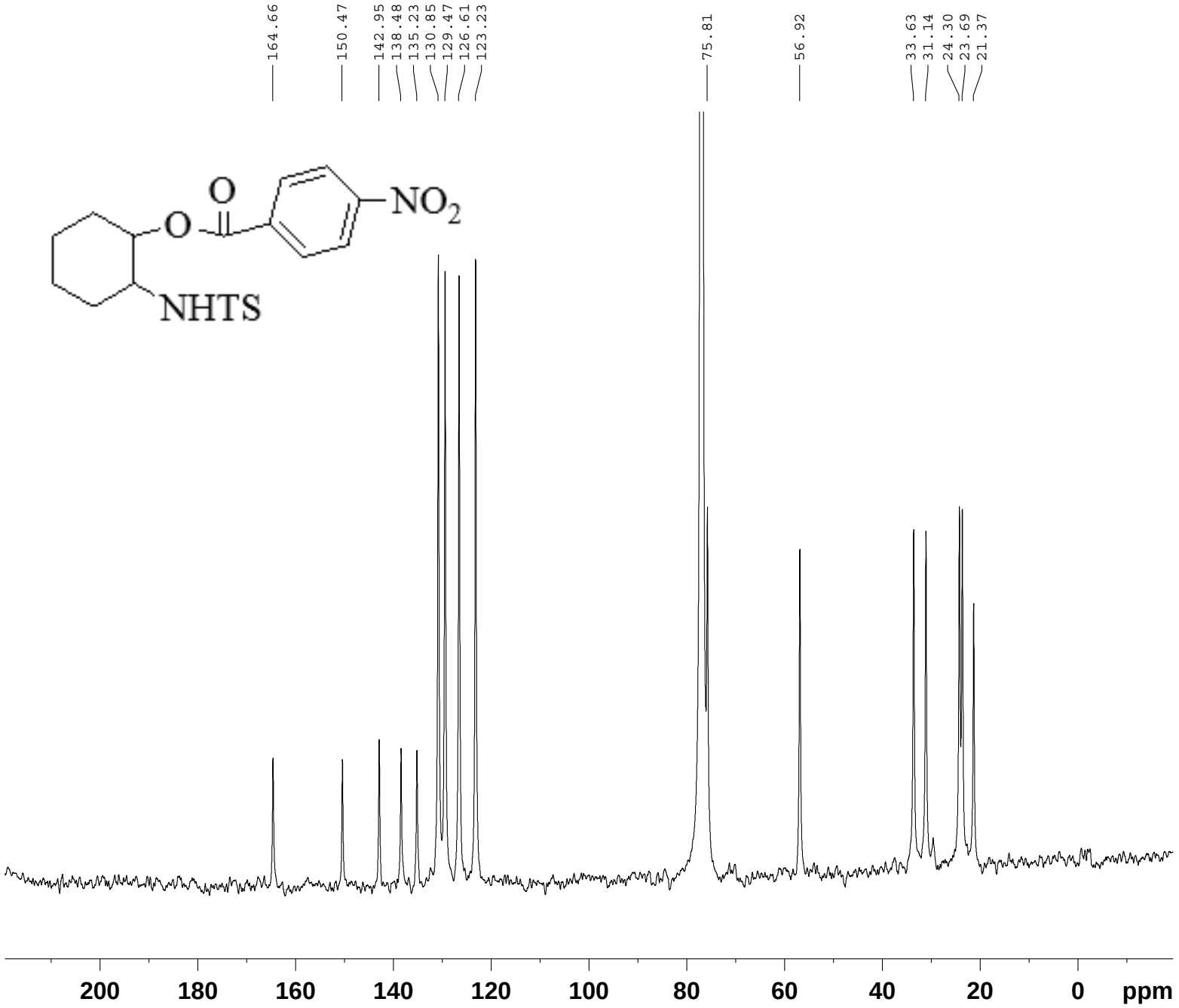
Current Data Parameters
NAME 201012311igong
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101231
Time 17.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 57
DW 40.533 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.74 usec
PL1 -1.00 dB
PL1W 15.52678299 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300171 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

suosuan

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Current Data Parameters
NAME      20110111ligong
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110112
Time                0.24
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1334
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9088159 sec
RG                  203
DW               13.867 usec
DE                6.50 usec
TE                300.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 11.16 usec
PL1                -1.00 dB
PL1W       103.40647888 W
SFO1        150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               14.96 dB
PL13               15.05 dB
PL2W       15.52678299 W
PL12W       0.39362392 W
PL13W       0.38555068 W
SFO2       600.1324005 MHz

F2 - Processing parameters
SI                 32768
SF          150.9028096 MHz
WDW                   EM
SSB       0
LB                 40.00 Hz
GB        0
PC                  1.40
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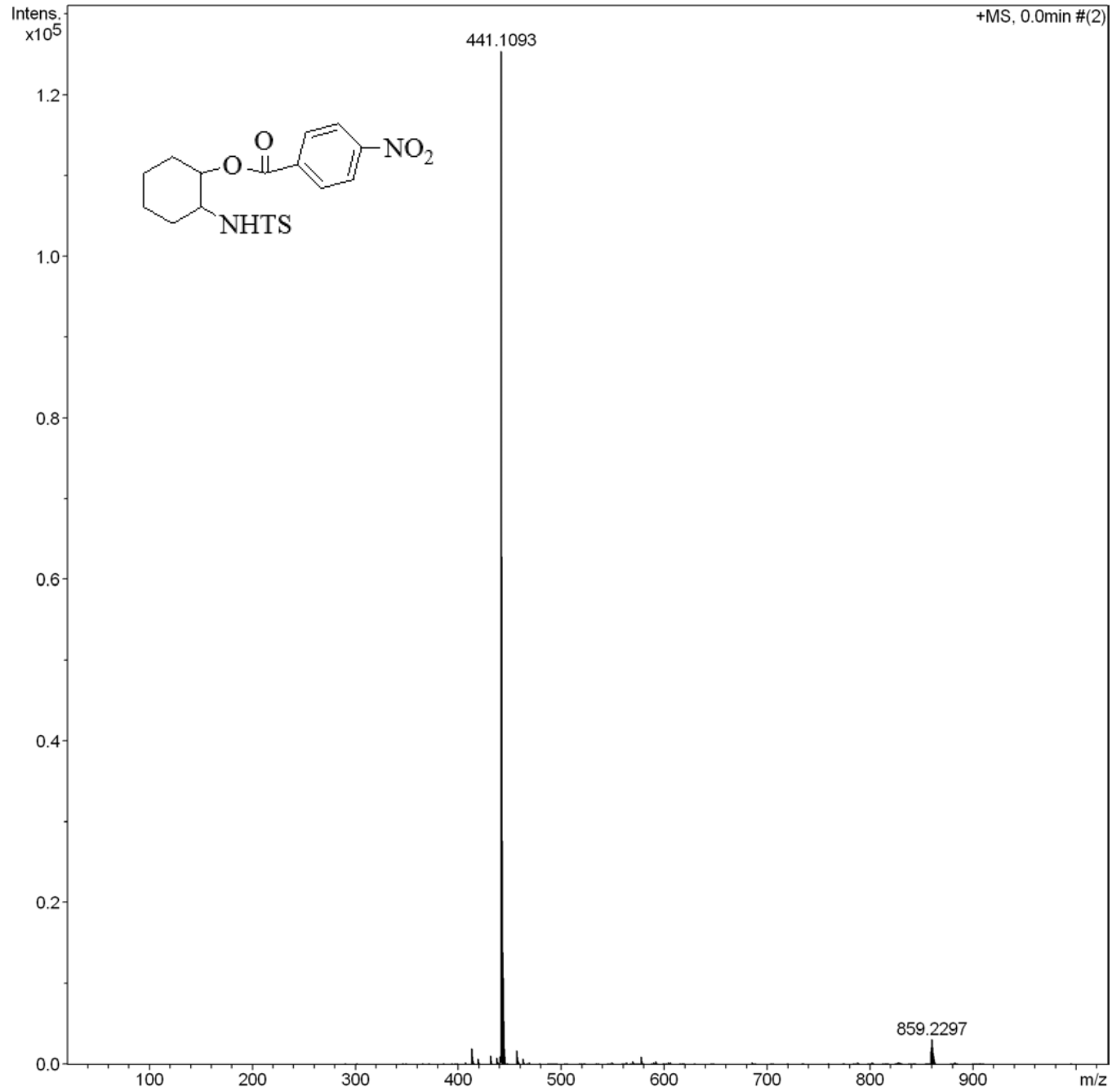
Display Report

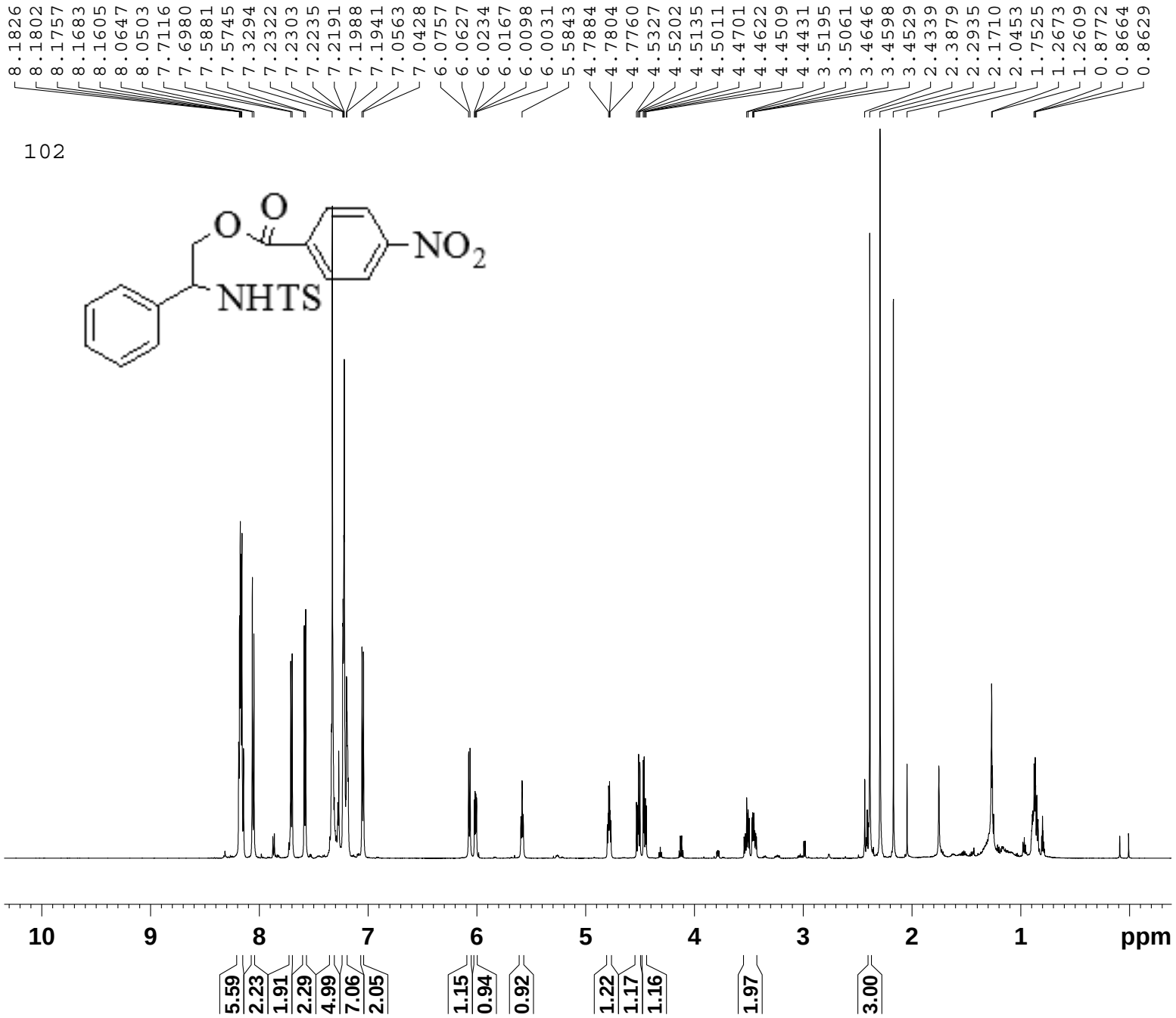
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-1.d	Acquisition Date	7/20/2011 8:46:33 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste





BRUKER

```
Current Data Parameters
NAME      20110629ligong
EXPNO                  8
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110629
Time               10.31
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ              2.6564426 sec
RG                  40.3
DW                40.533 usec
DE                 6.50 usec
TE                300.2 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.60 usec
PLW1         13.99600029 W
SFO1         600.1328806 MHz

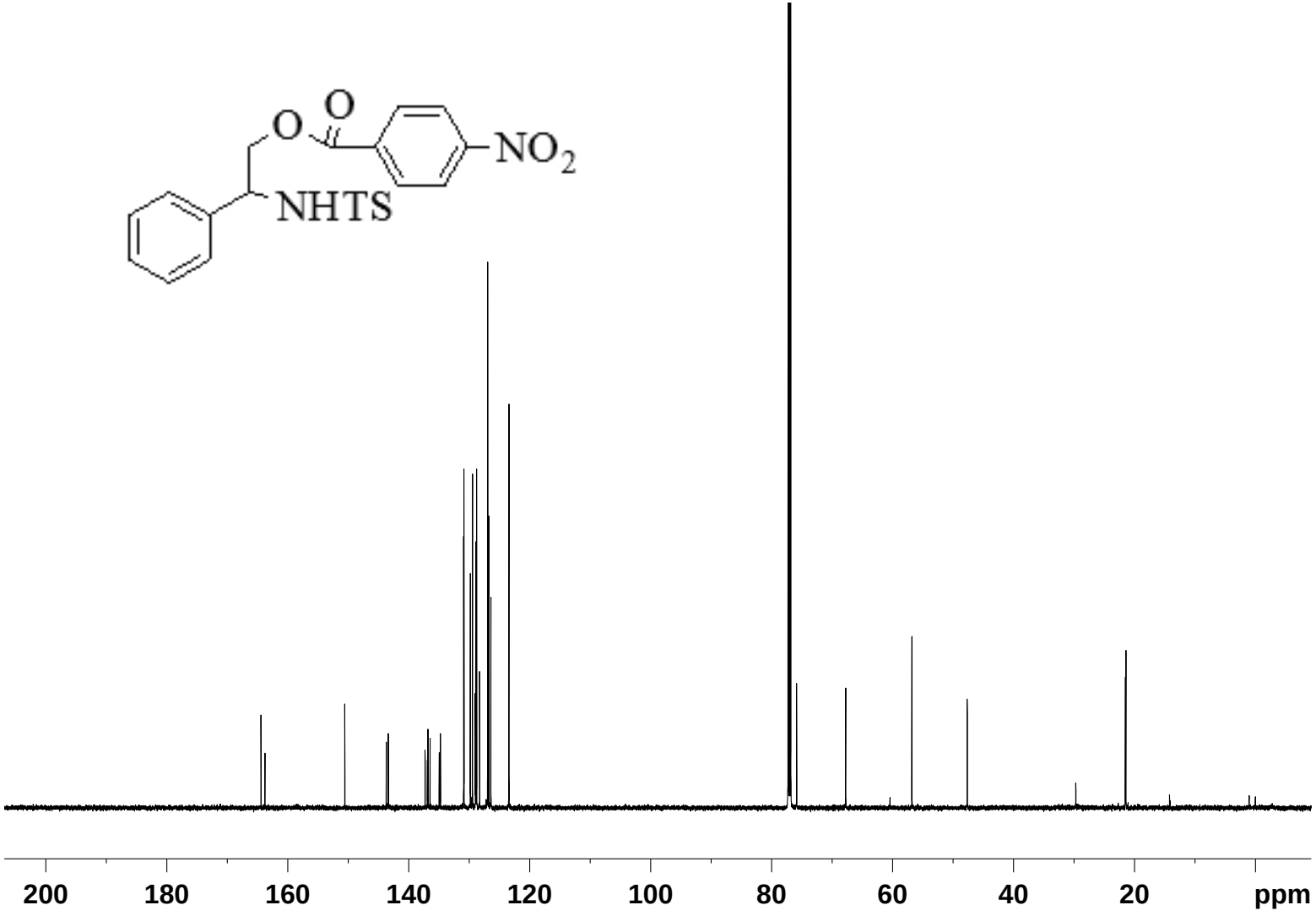
F2 - Processing parameters
SI                 32768
SF          600.1300098 MHz
WDW                   EM
SSB       0
LB                -0.10 Hz
GB        0
PC                 1.00
```

102

164.4292
163.7777
150.5795
143.7208
143.4010
137.3009
136.9232
136.8296
136.4779
134.9711
134.7733
130.9290
130.8719
129.8225
129.4641
128.9310
128.7859
126.9545
123.4344

75.8660
67.7552
56.8058
47.6589

21.5047
21.4167



Current Data Parameters
NAME 20110727ligong
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110727
Time 9.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1147
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
PLW1 92.68299866 W
SFO1 150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 13.99600029 W
PLW12 0.45346999 W
PLW13 0.22220001 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

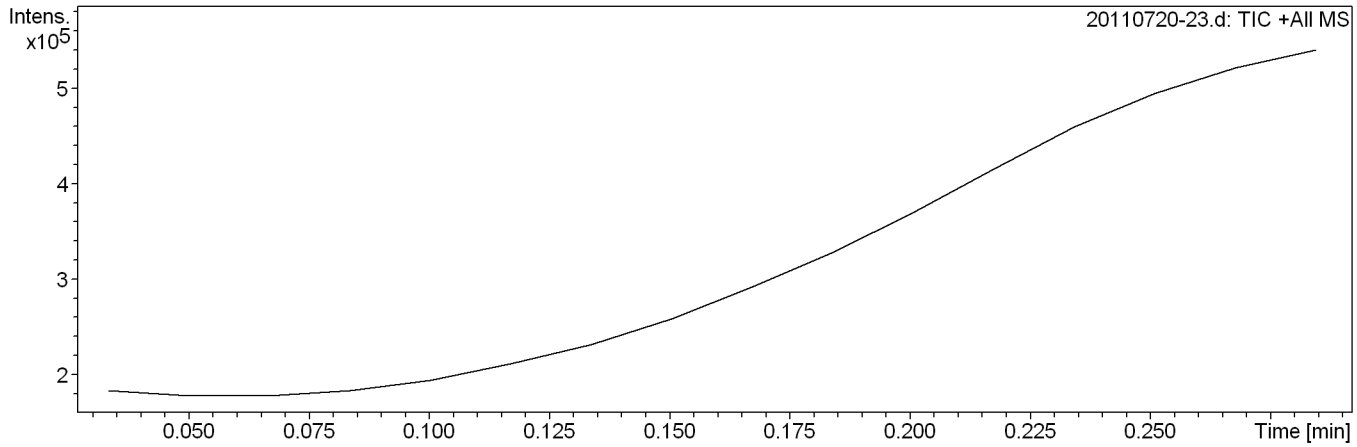
Display Report

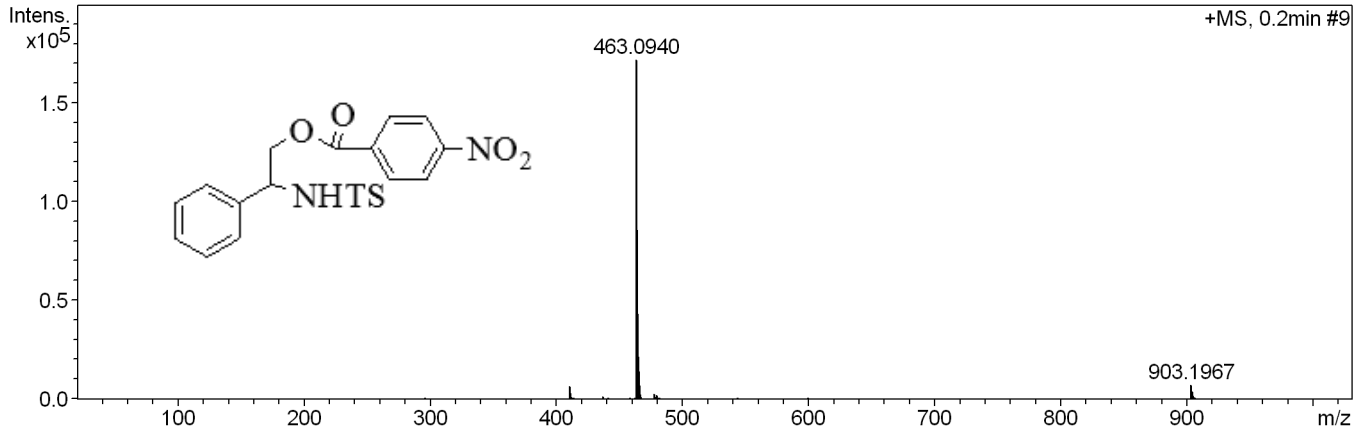
Analysis Info

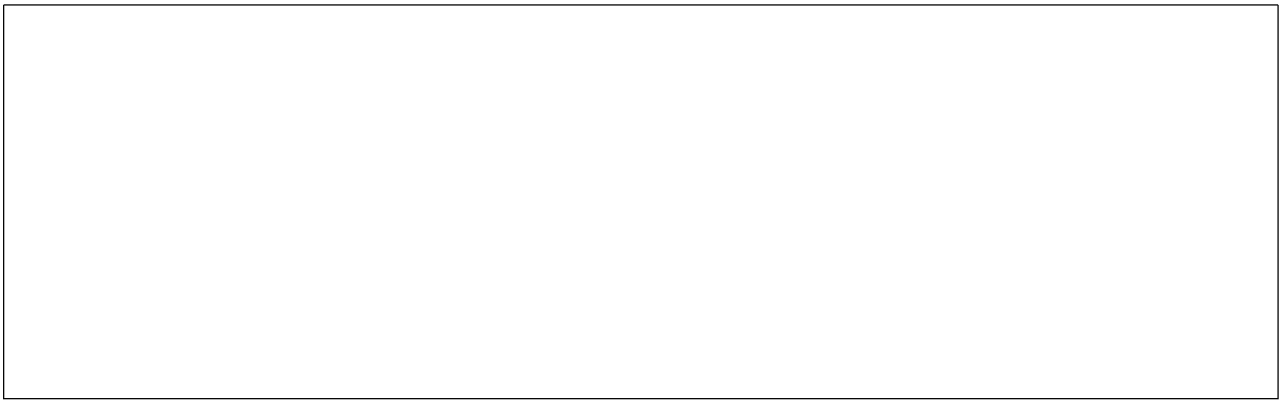
Analysis Name	D:\Data\Chang-HongHong\20110720-23.d	Acquisition Date	7/20/2011 9:06:51 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

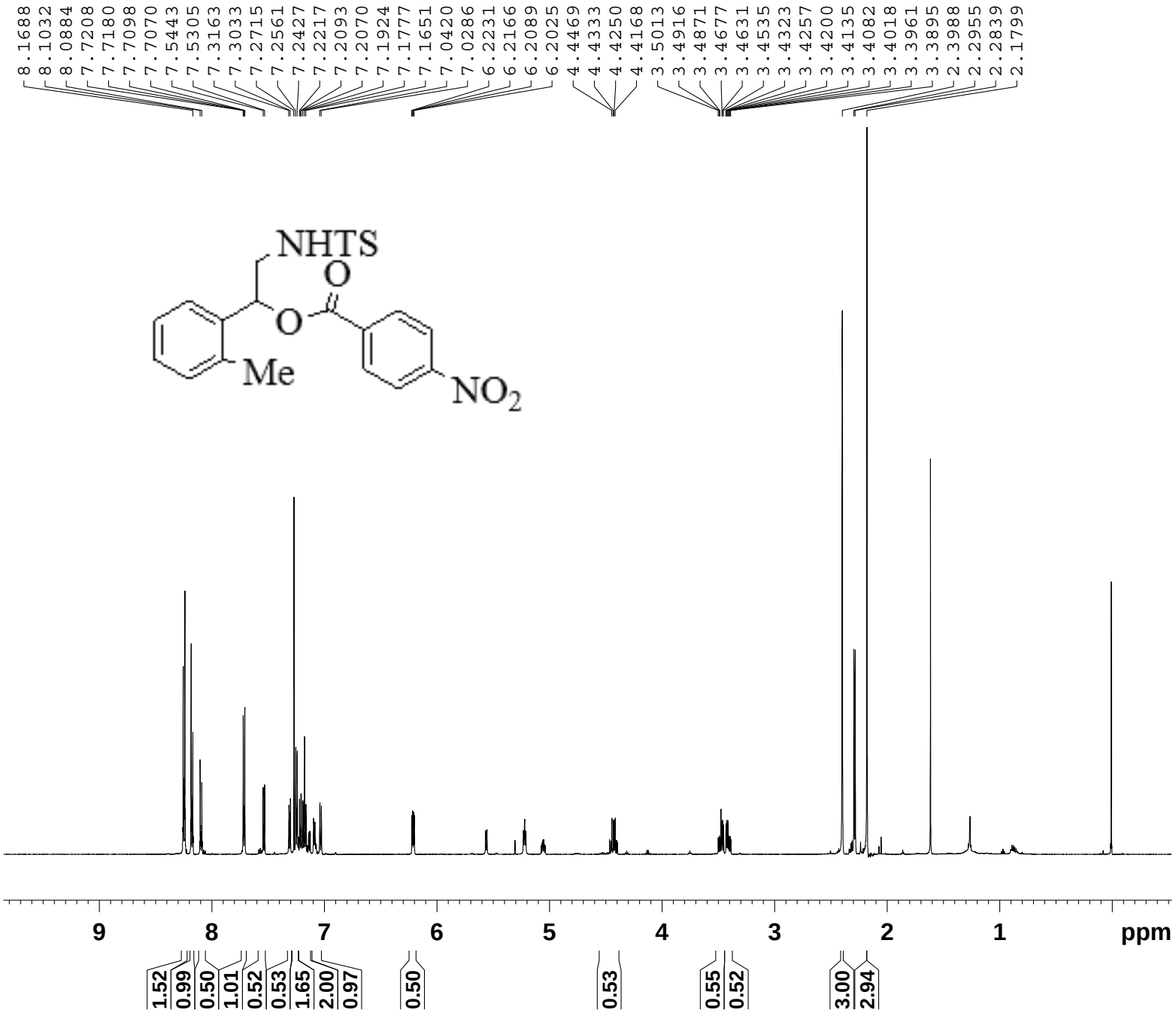
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste







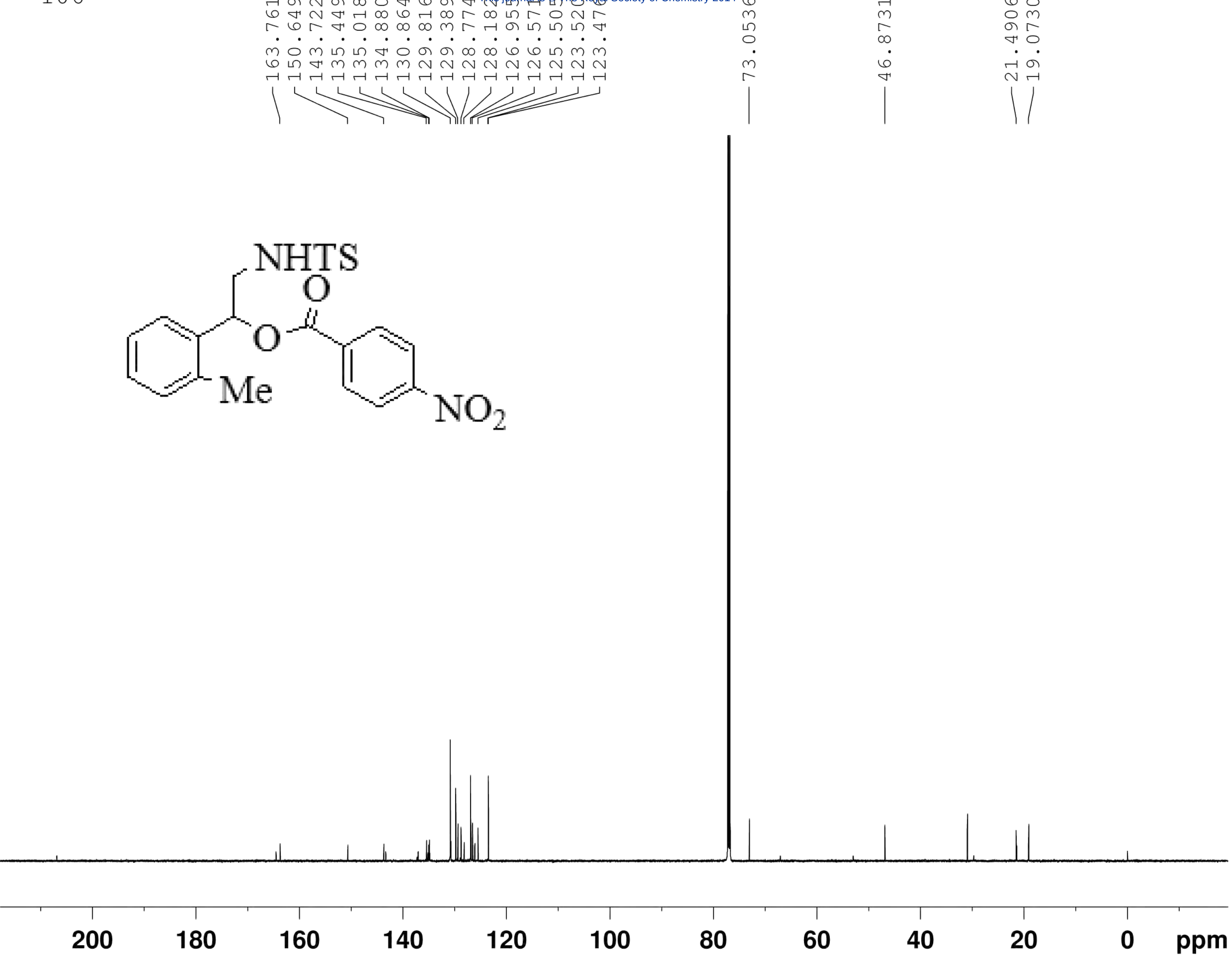



```
Current Data Parameters
NAME      20110711ligong
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110711
Time                9.50
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                   114
DW                40.533 usec
DE                 6.50 usec
TE                296.3 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                12.60 usec
PLW1        13.99600029 W
SFO1        600.1328806 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300096 MHz
WDW                   EM
SSB       0
LB                -0.10 Hz
GB        0
PC                 1.00
```



Current Data Parameters
NAME 20110718ligong
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110722
Time 10.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6652
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
PLW1 92.68299866 W
SFO1 150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 13.99600029 W
PLW12 0.45346999 W
PLW13 0.22220001 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

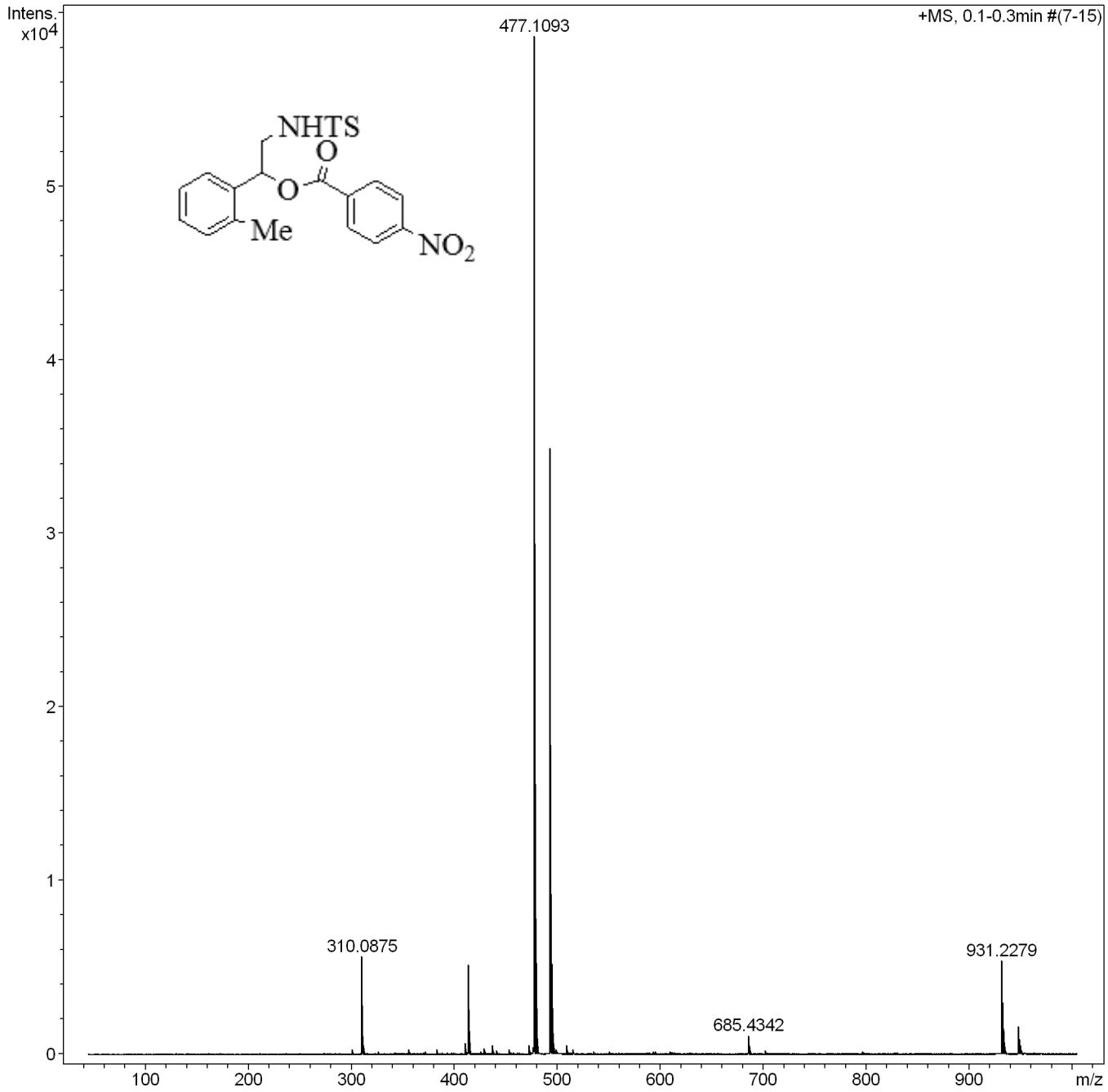
Display Report

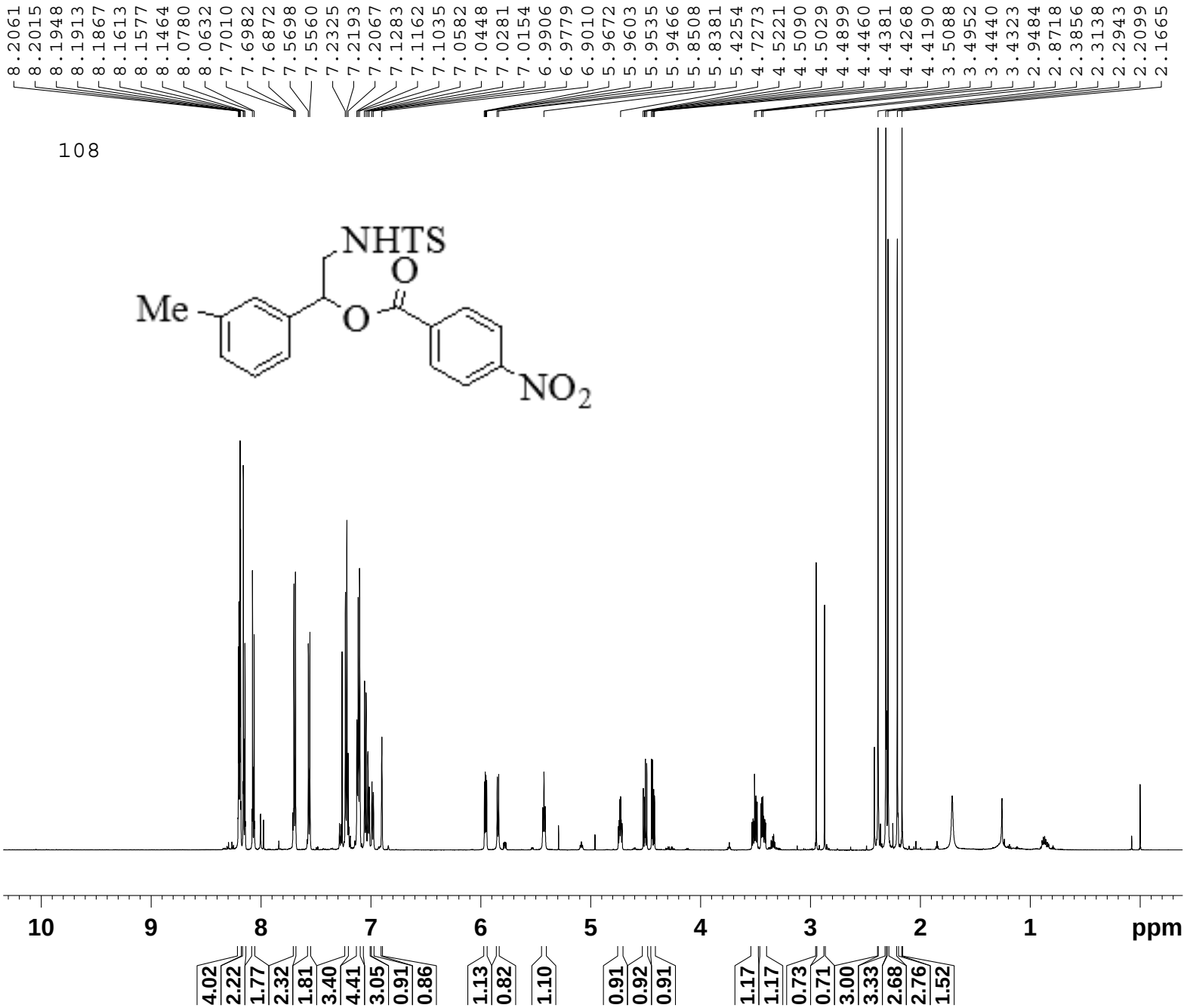
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-8.d	Acquisition Date	7/20/2011 9:19:16 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste





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```
Current Data Parameters
NAME      20110704ligong
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110704
Time               10.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                    64
DW               40.533 usec
DE                6.50 usec
TE               299.0 K
D1            1.00000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                12.60 usec
PLW1         13.99600029 W
SFO1         600.1328806 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300145 MHz
WDW                   EM
SSB       0
LB                -0.10 Hz
GB        0
PC                 1.00
```

108

164.4707
163.7883
150.5979
143.6691
143.3054
138.7373
138.4760
137.4112
137.0096
136.6182
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136.3749
135.0358
134.8475
130.9172
130.8765
129.7976
129.3848
128.8428
127.1050
126.9844
126.9553
123.4470
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123.4130

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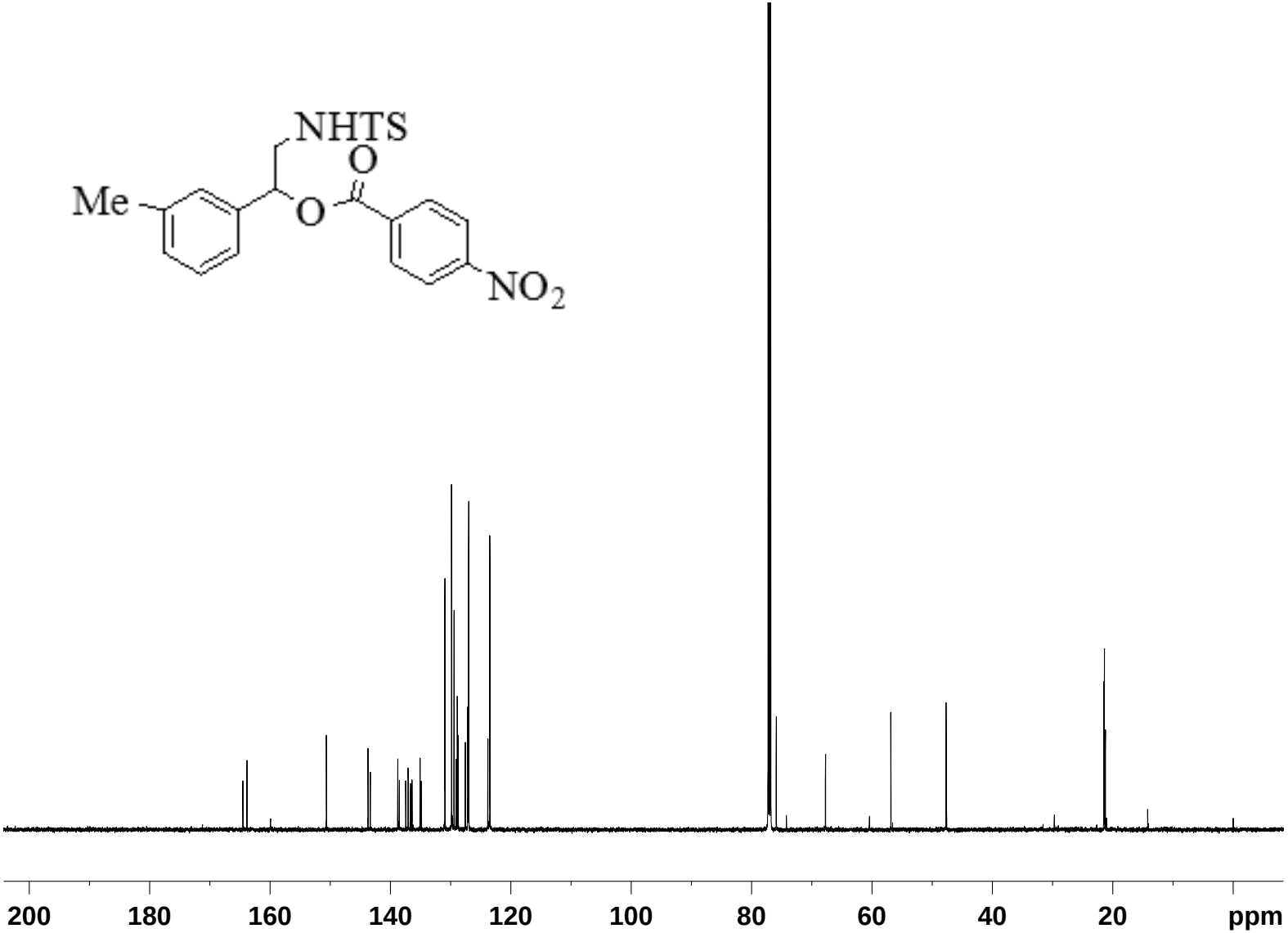


Current Data Parameters
NAME 20110727ligong
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110727
Time 13.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 300.3 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
PLW1 92.68299866 W
SFO1 150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 13.99600029 W
PLW12 0.45346999 W
PLW13 0.22220001 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

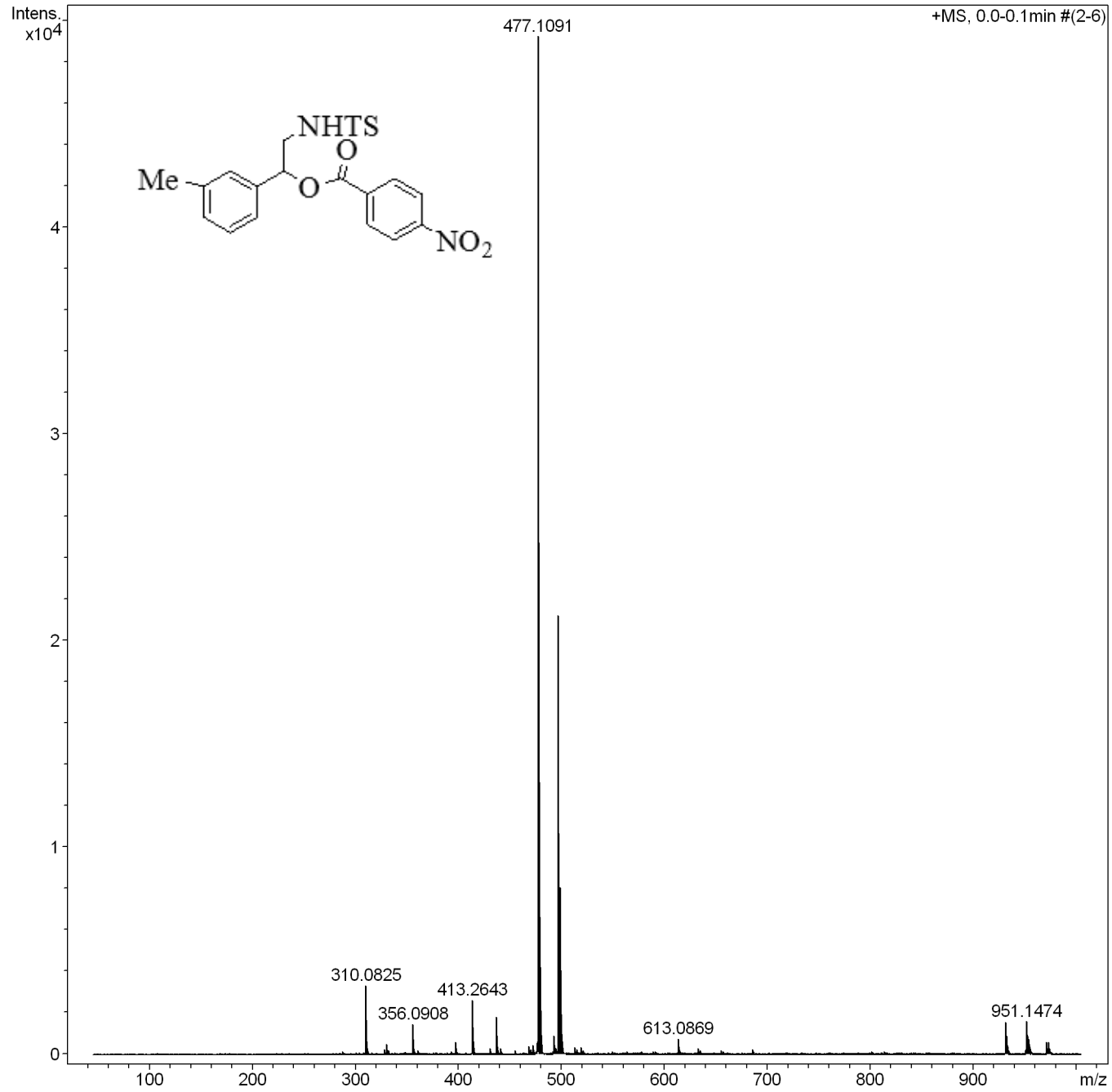
Display Report

Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-12.d	Acquisition Date	7/20/2011 8:29:54 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



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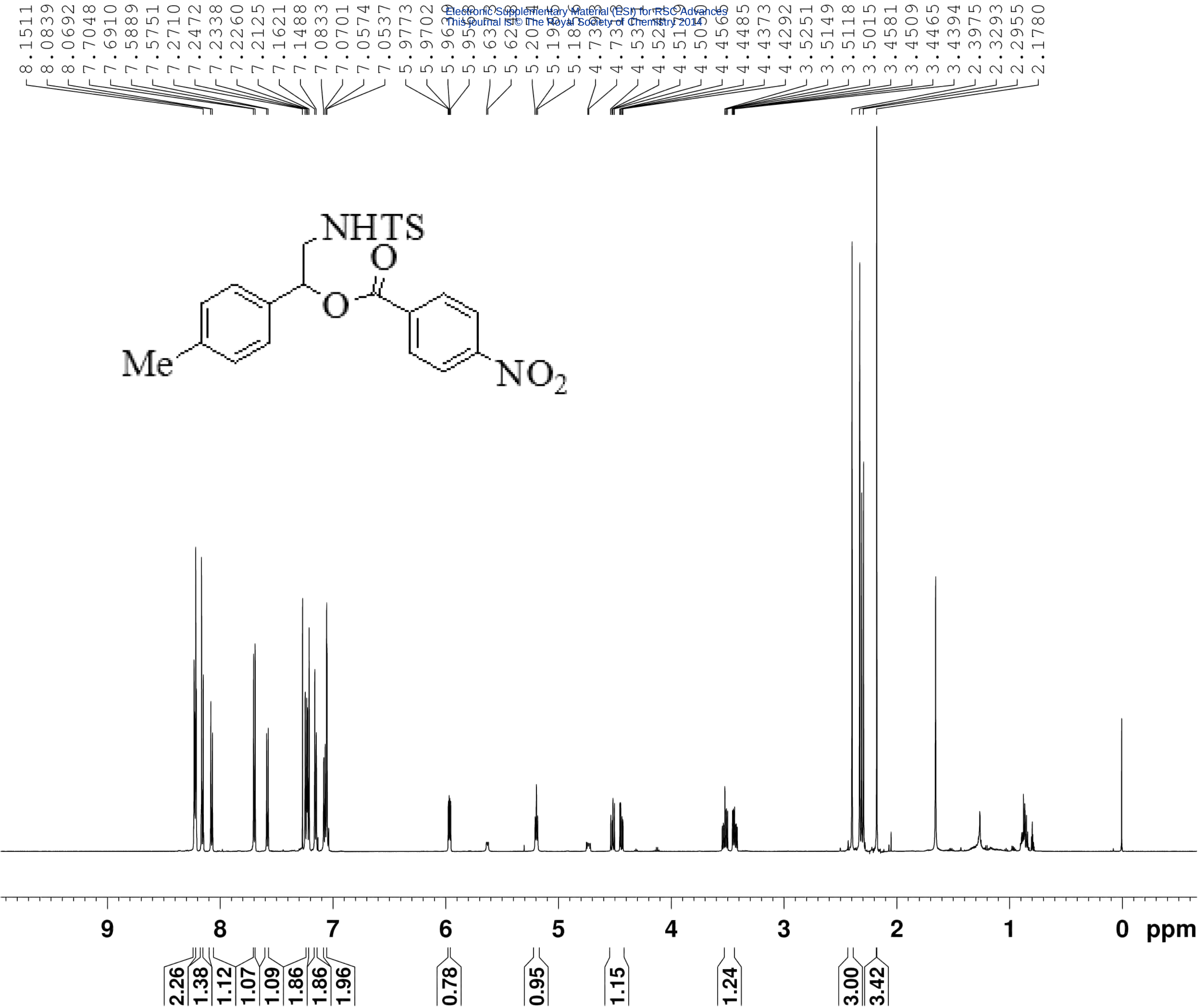

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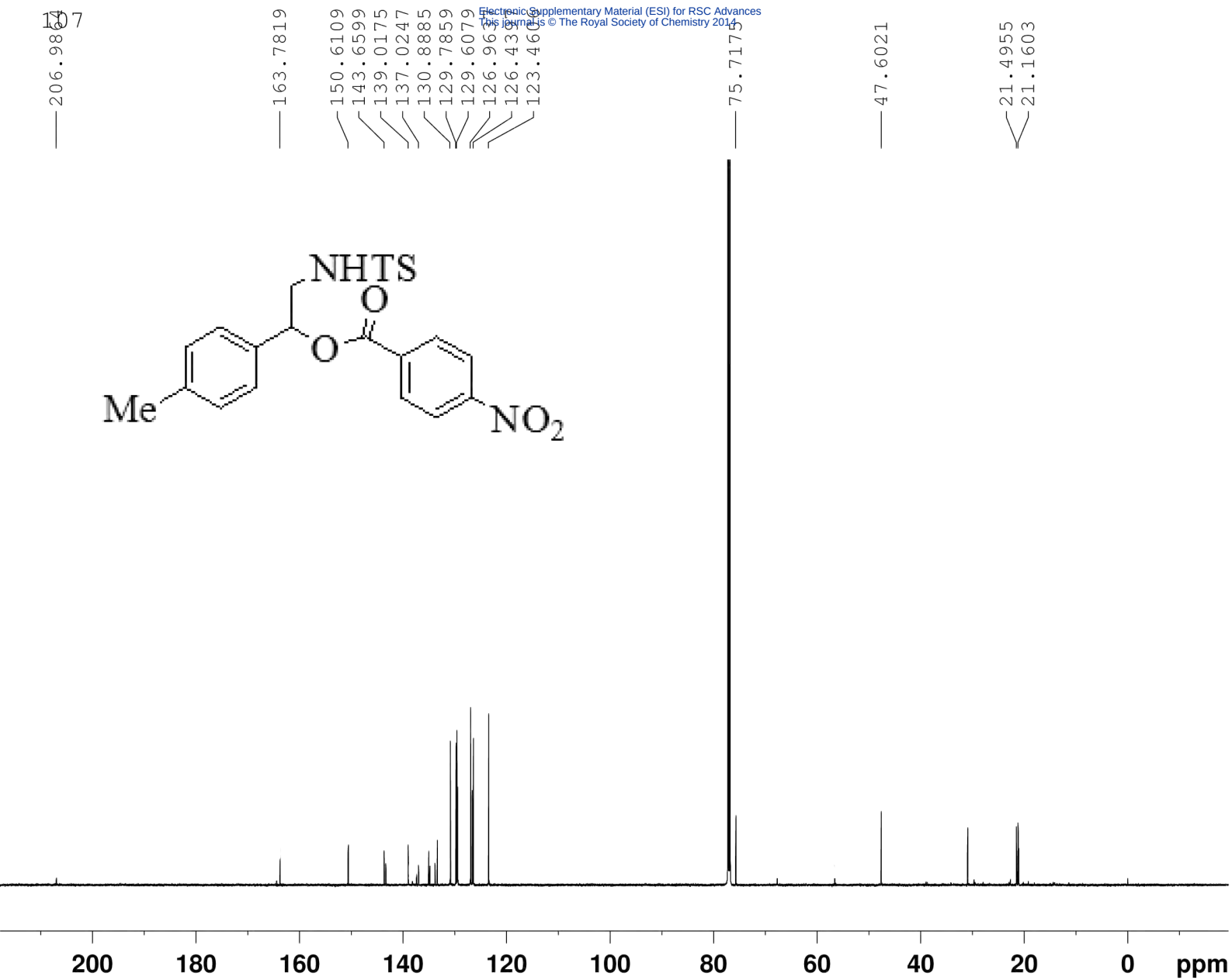
Current Data Parameters
NAME 20110711ligong
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110711
Time 9.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 114
DW 40.533 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300096 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20110718ligong
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110725
Time 9.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7899
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
PLW1 92.68299866 W
SFO1 150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 13.99600029 W
PLW12 0.45346999 W
PLW13 0.22220001 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

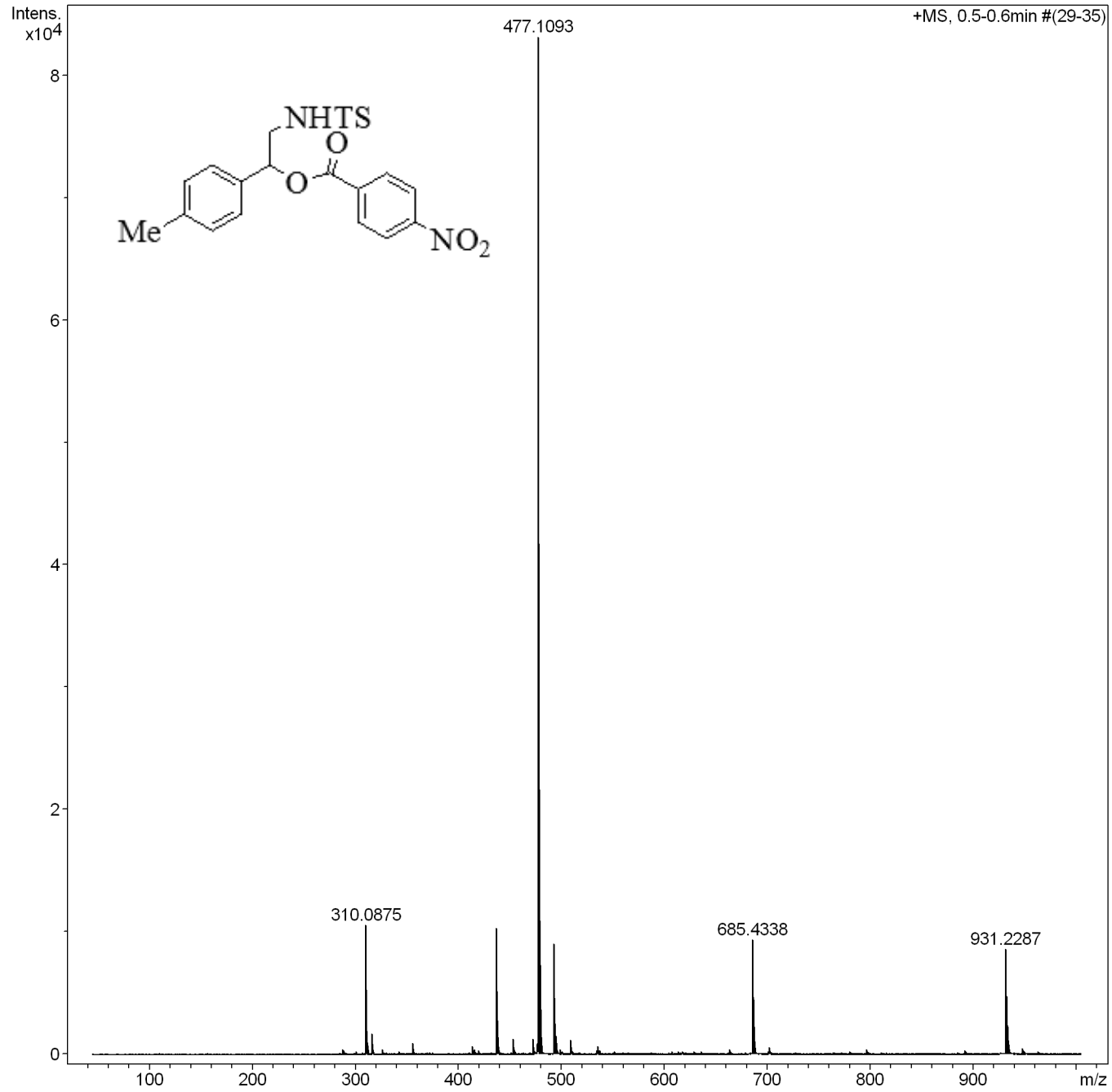
Display Report

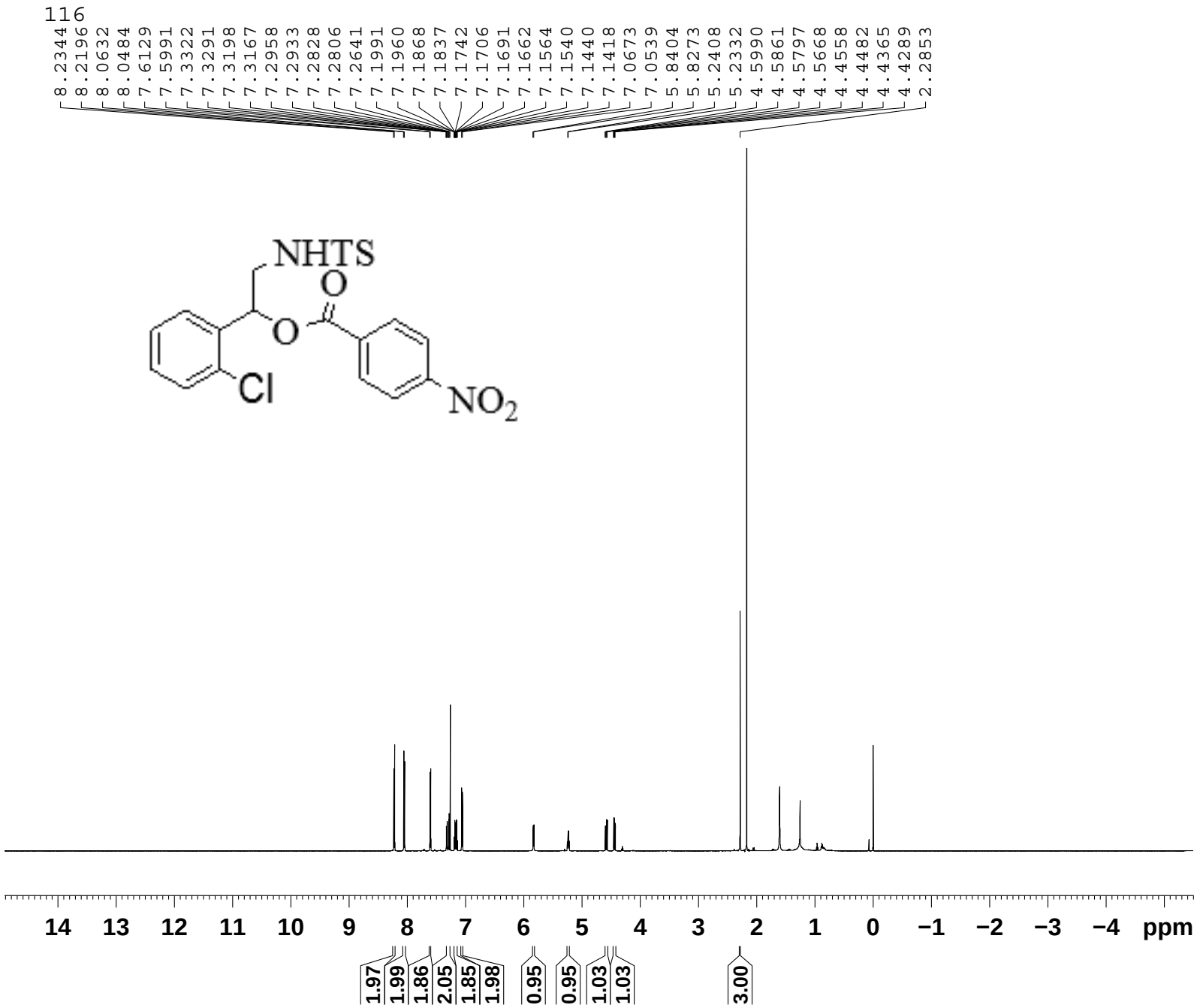
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-9.d	Acquisition Date	7/20/2011 9:28:13 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste





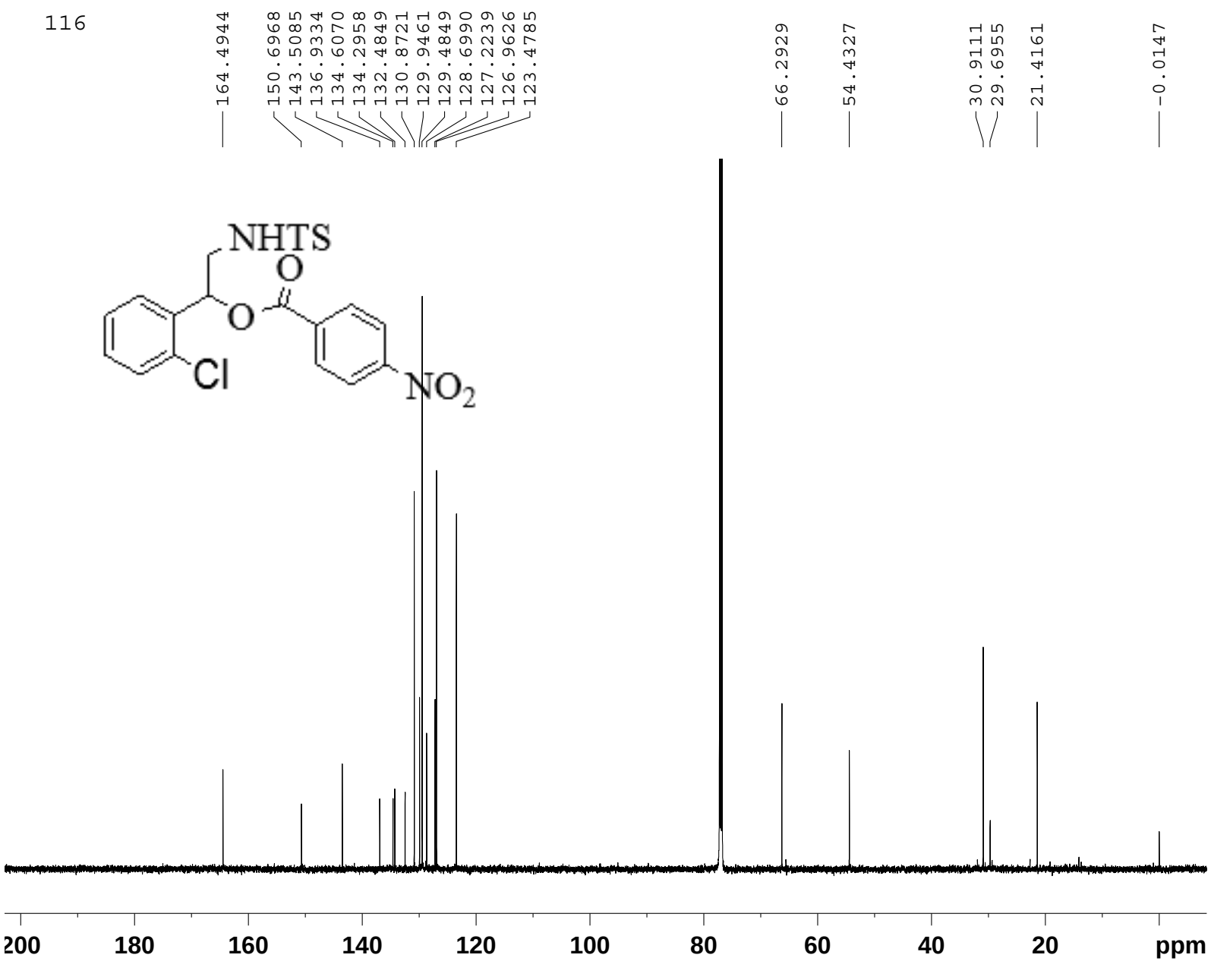
Current Data Parameters
NAME 20110711ligong
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110711
Time 10.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 144
DW 40.533 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300139 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

116



Current Data Parameters
NAME 20110712ligong
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110713
Time 15.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6080
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
PLW1 92.68299866 W
SFO1 150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 13.99600029 W
PLW12 0.45346999 W
PLW13 0.22220001 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

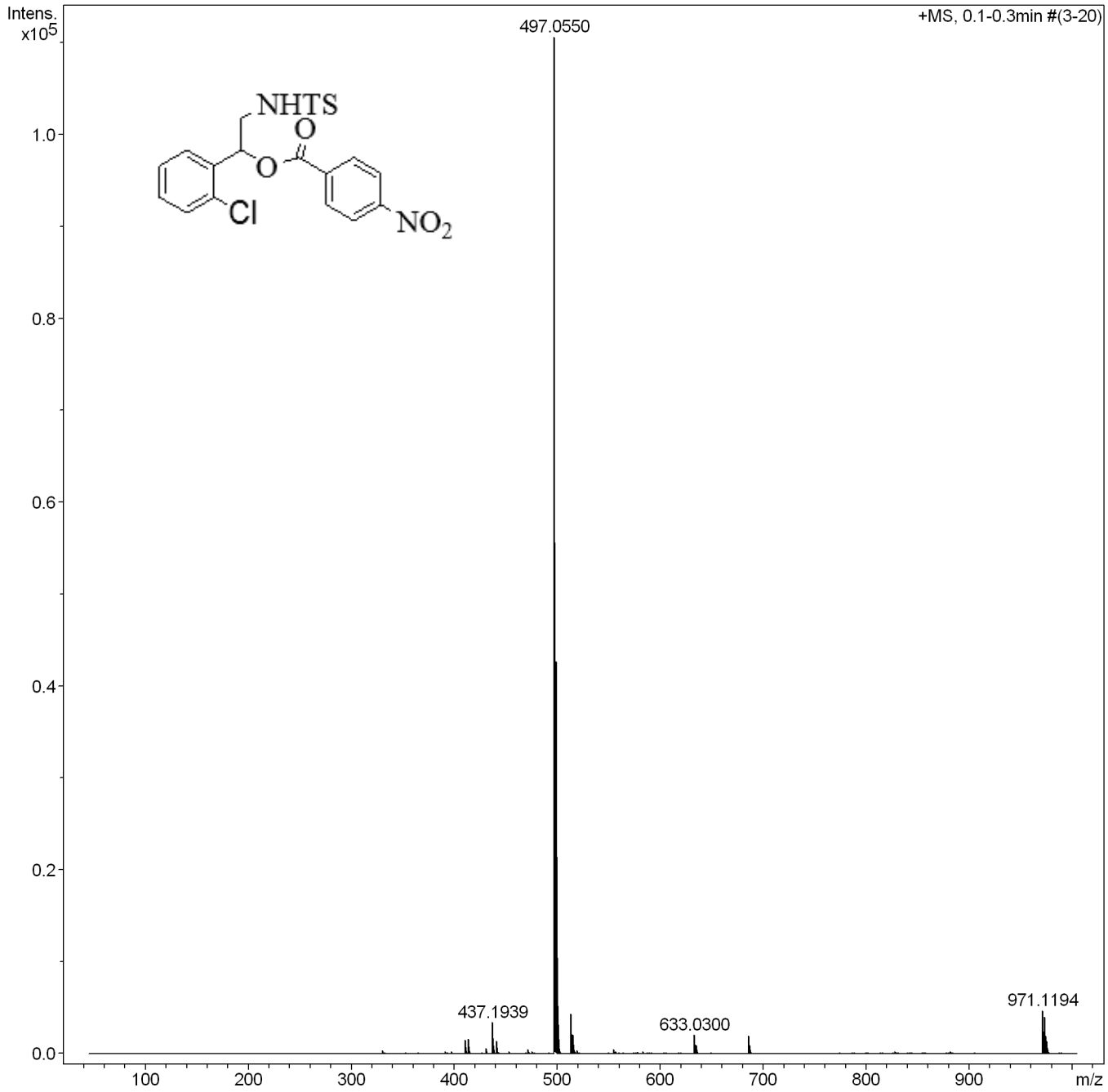
Display Report

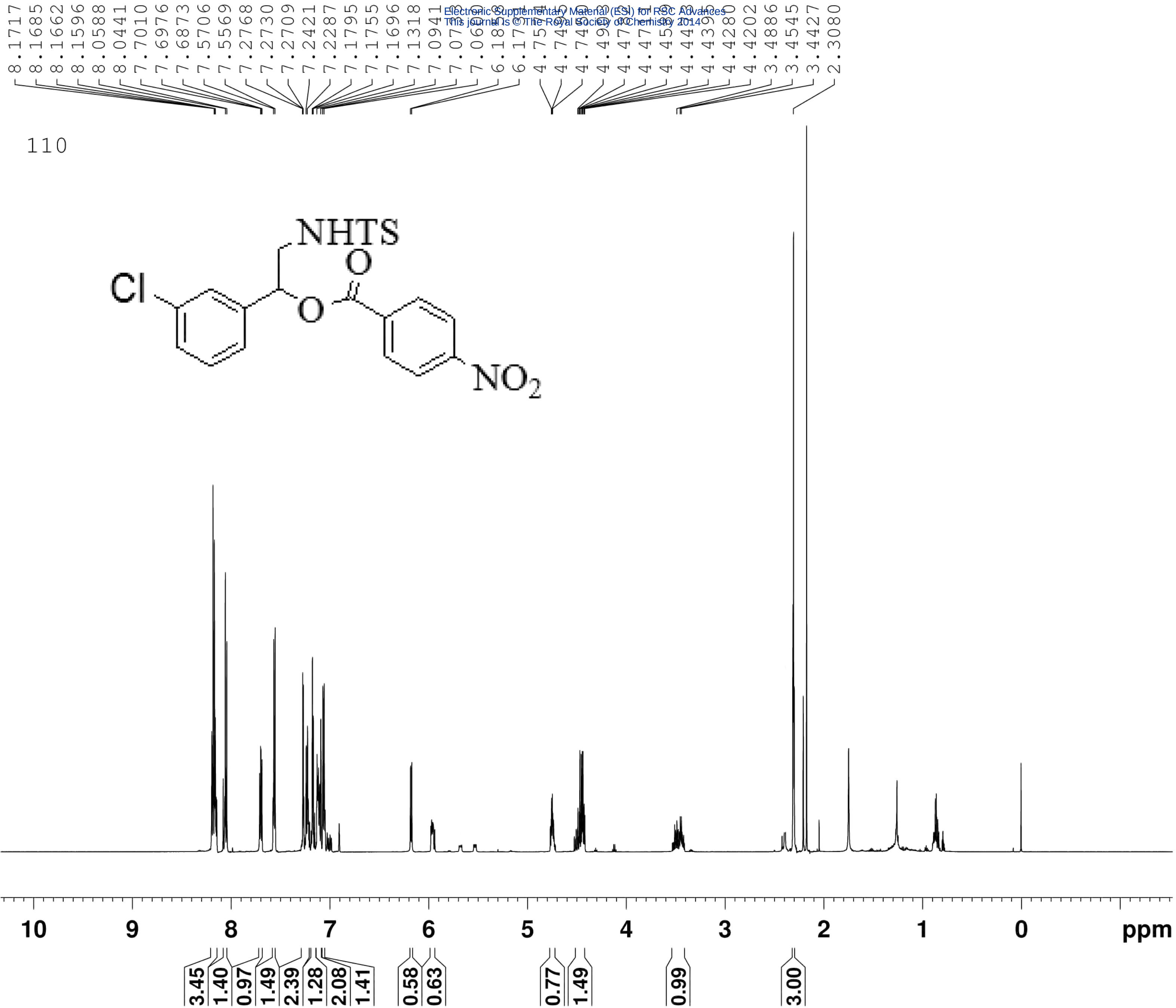
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-11---.d	Acquisition Date	7/20/2011 10:24:06 PM
Method	tune_wide.m	Operator	TJU
Sample Name		Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



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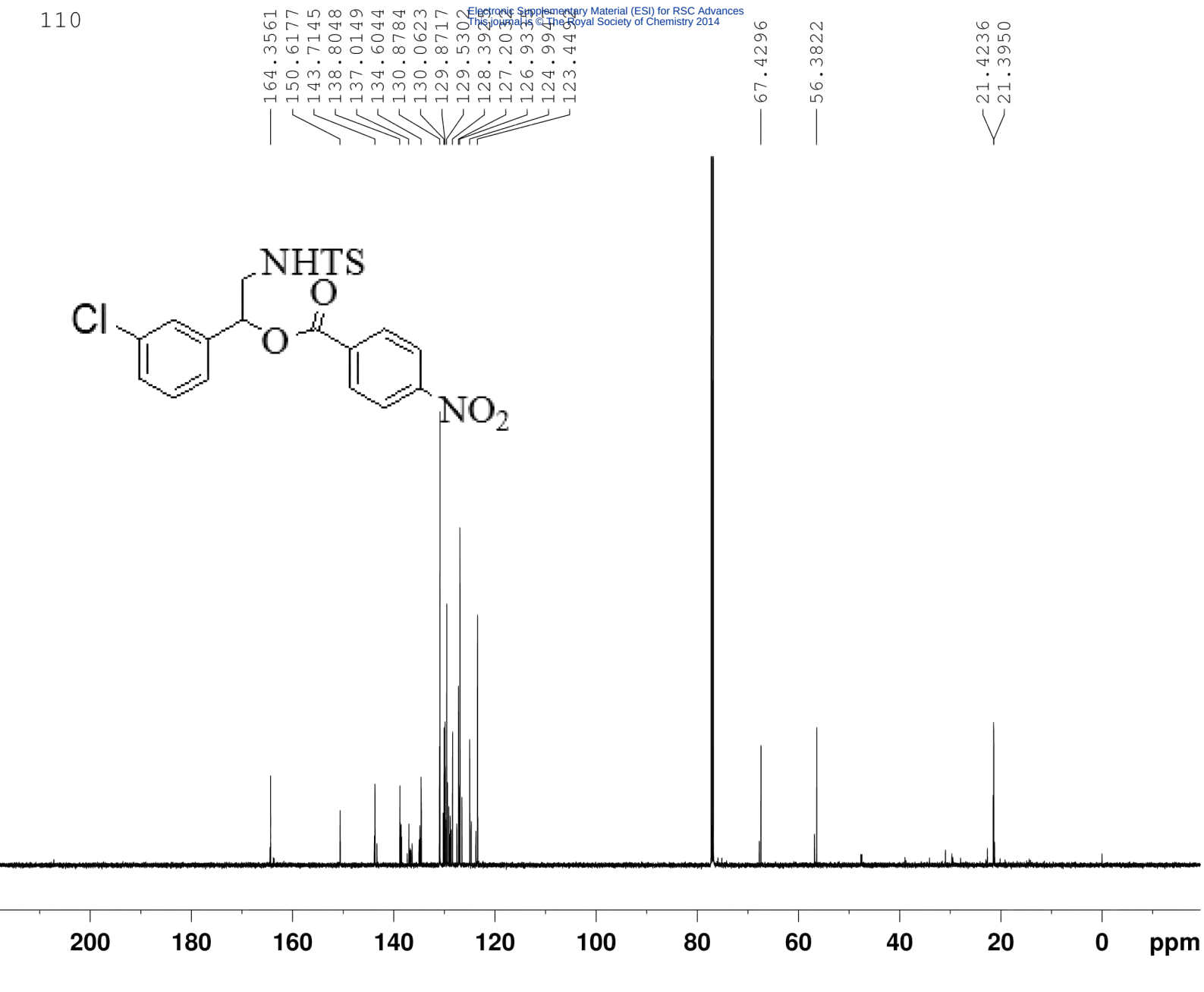
Current Data Parameters
NAME        20110711ligong
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_             20110711
Time                 10.04
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      32
DS                       2
SWH             12335.526 Hz
FIDRES           0.188225 Hz
AQ              2.6564426 sec
RG                      57
DW                  40.533 usec
DE                    6.50 usec
TE                   296.5 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.60 usec
PLW1           13.99600029 W
SFO1          600.1328806 MHz

F2 - Processing parameters
SI                   32768
SF            600.1300096 MHz
WDW                     EM
SSB      0
LB                   -0.10 Hz
GB       0
PC                    1.00
```



BRUKER

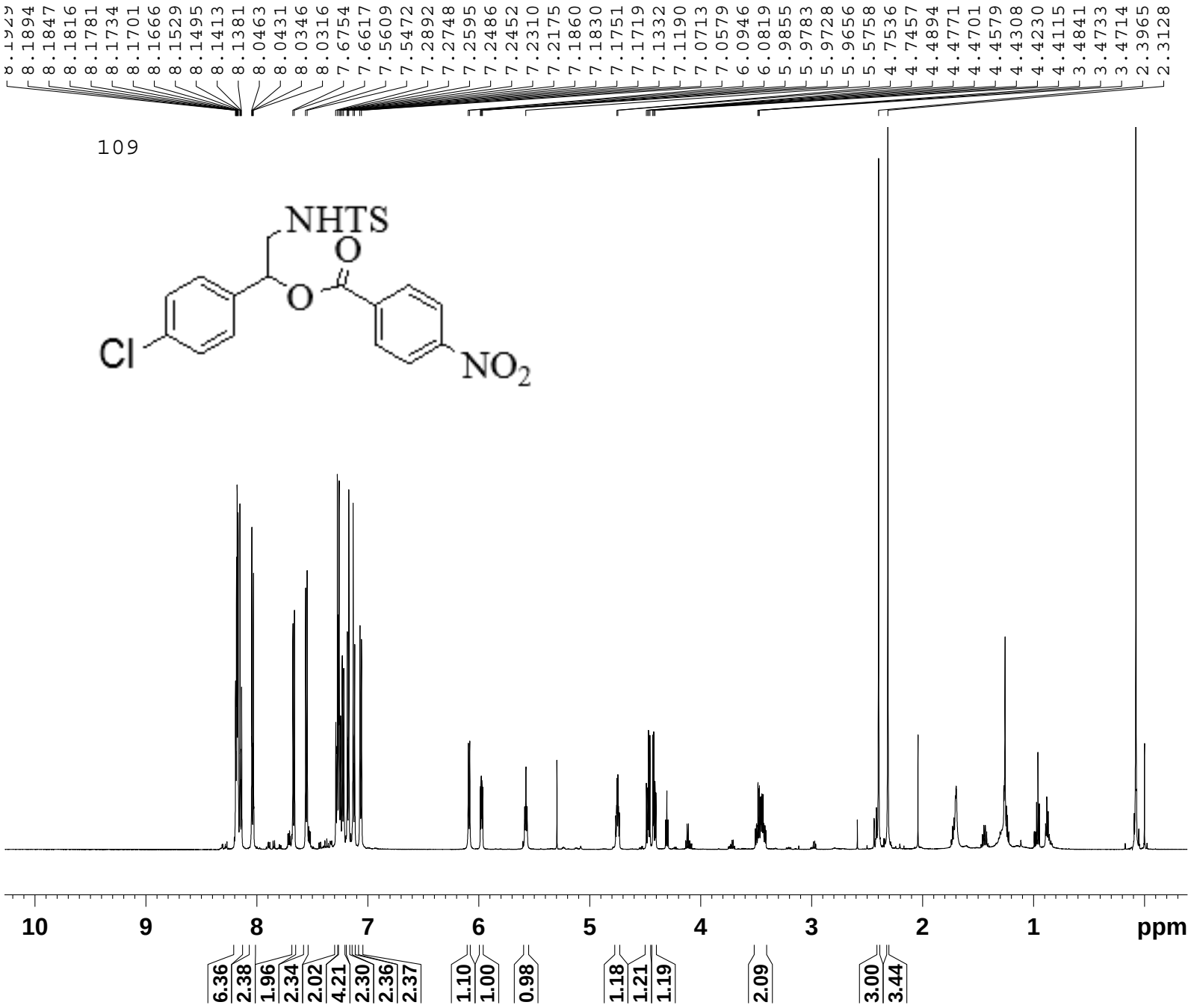
```
Current Data Parameters
NAME      20110718ligong
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110718
Time                9.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2205
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9088159 sec
RG                  203
DW               13.867 usec
DE                6.50 usec
TE               296.7 K
D1           2.00000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                11.30 usec
PLW1        92.68299866 W
SFO1       150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            70.00 usec
PLW2        13.99600029 W
PLW12        0.45346999 W
PLW13        0.22220001 W
SFO2       600.1324005 MHz

F2 - Processing parameters
SI                 32768
SF          150.9028096 MHz
WDW                   EM
SSB       0
LB                 0.10 Hz
GB        0
PC                 1.40
```



BRUKER

```
Current Data Parameters
NAME      20110704ligong
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110704
Time               10.39
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                    64
DW               40.533 usec
DE                6.50 usec
TE               299.1 K
D1            1.00000000 sec

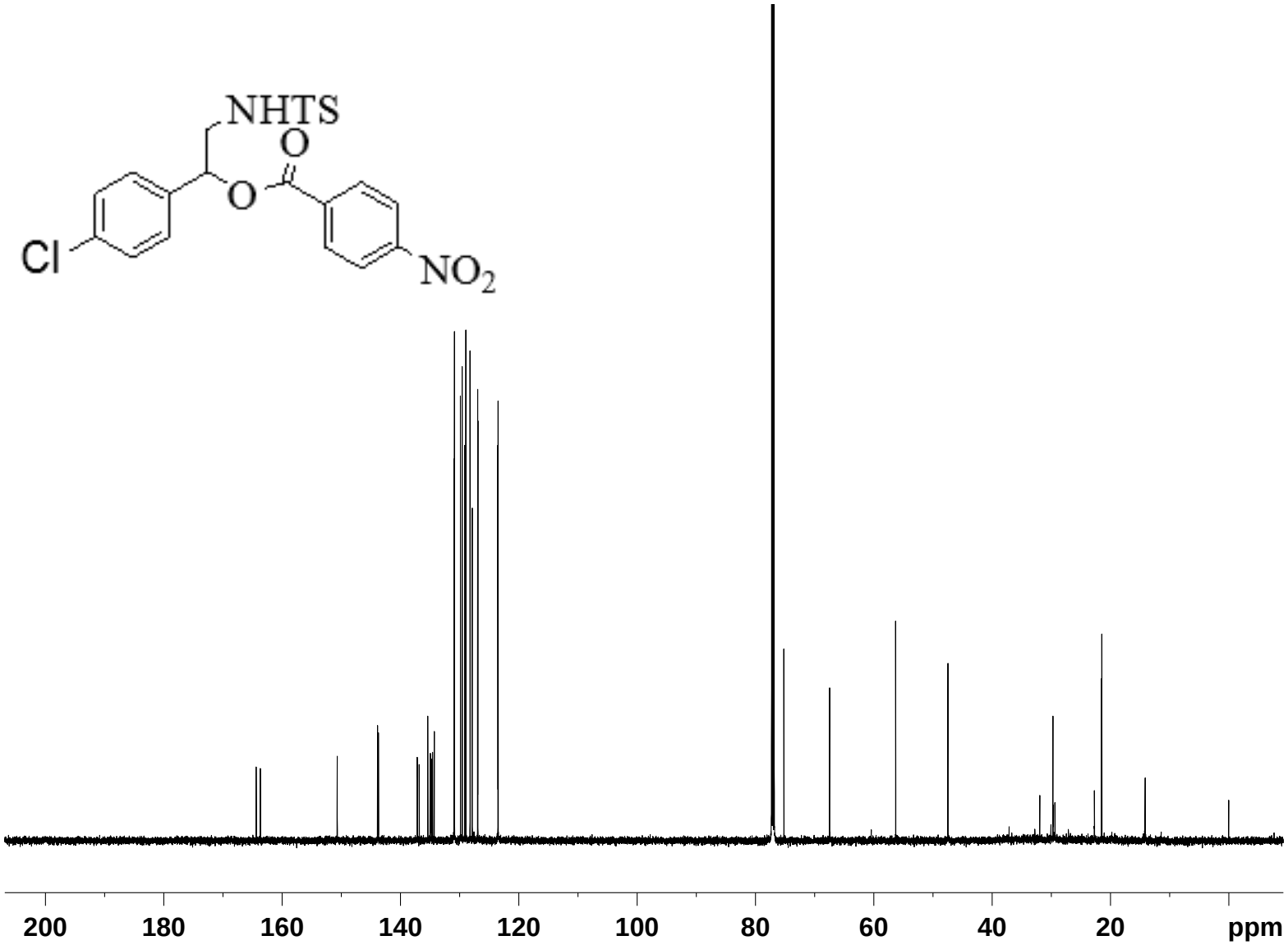
======== CHANNEL f1 ========
NUC1                  1H
P1                12.60 usec
PLW1         13.99600029 W
SFO1         600.1328806 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300135 MHz
WDW                   EM
SSB       0
LB                -0.10 Hz
GB        0
PC                 1.00
```

109

164.3688
163.6615
150.6819
150.6636
143.8511
143.6971
137.1332
136.8125
135.3626
134.9746
134.9339
134.7228
134.5476
134.2612
130.9287
130.8566
129.8355
129.5366
129.1130
128.9313
128.2094
127.8607
126.9408
126.9045
123.4981
123.4629

75.1676
67.4388
56.2665
47.4424
31.9184
29.6873
29.6491
29.3504
22.6795
21.5034
21.4166
14.1033



BRUKER

```
Current Data Parameters
NAME      20110727ligong
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20110727
Time              15.45
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2060
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9088159 sec
RG                  203
DW                13.867 usec
DE                 6.50 usec
TE                300.8 K
D1           2.00000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                11.30 usec
PLW1        92.68299866 W
SFO1       150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             70.00 usec
PLW2        13.99600029 W
PLW12        0.45346999 W
PLW13        0.22220001 W
SFO2       600.1324005 MHz

F2 - Processing parameters
SI                32768
SF          150.9028096 MHz
WDW                 EM
SSB       0
LB                 0.50 Hz
GB        0
PC                 1.40
```

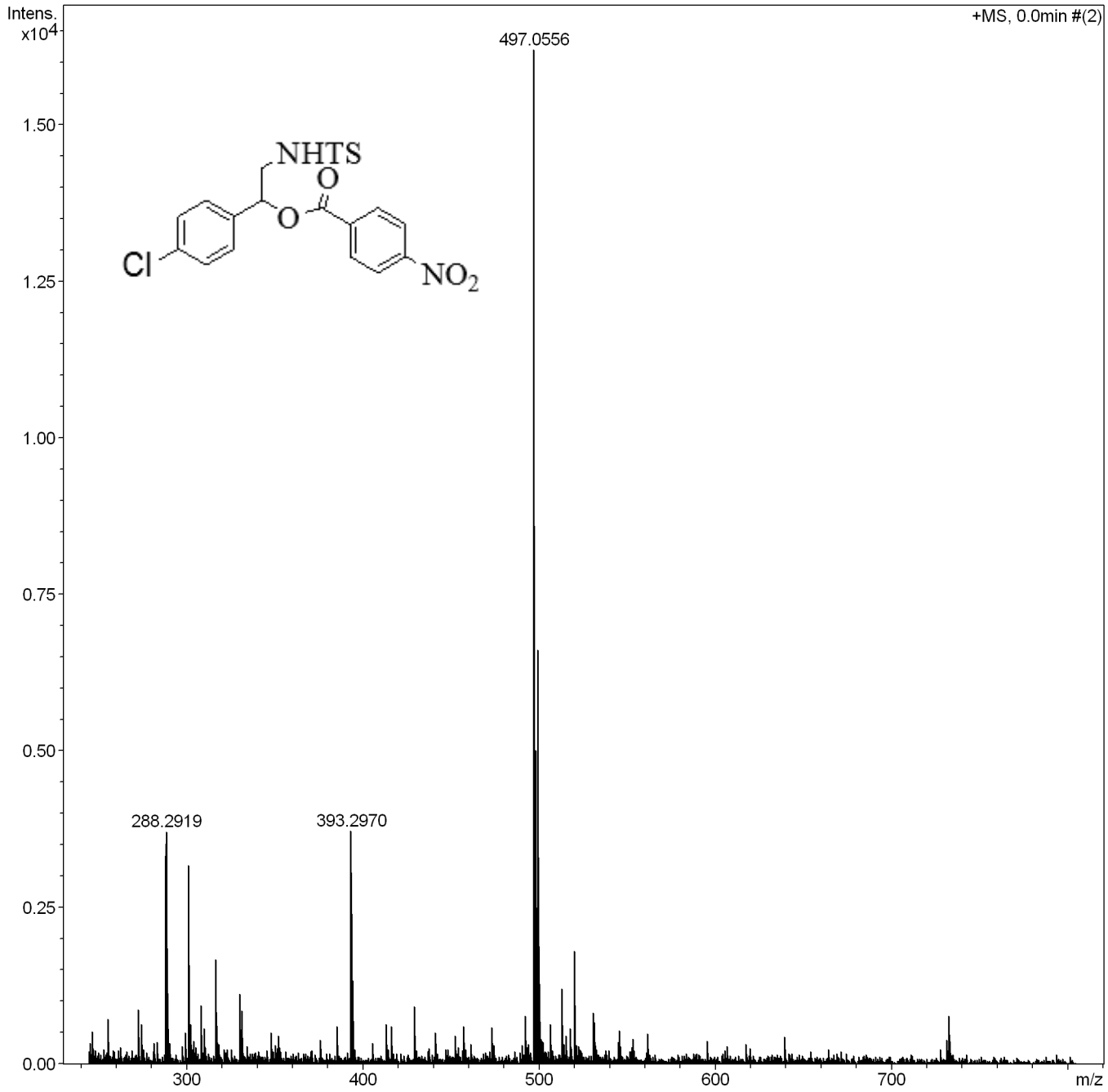
Display Report

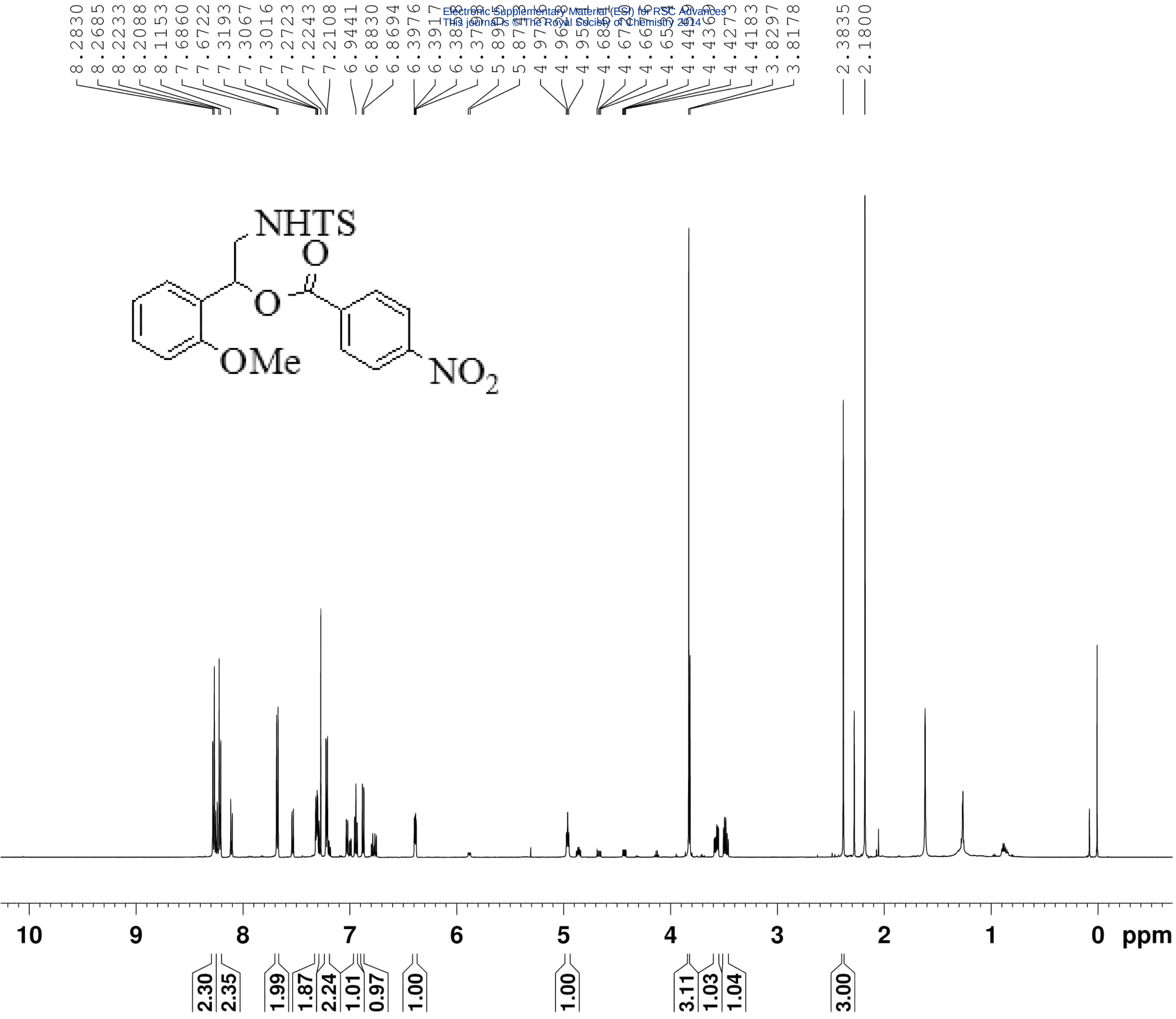
Analysis Info

Analysis Name	D:\Data\20110730_10-1.d	Acquisition Date	7/30/2011 11:38:04 AM
Method	Na FA_low.m	Operator	TJU
Sample Name	20110707_ZJT_1_3-3_M6	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	250 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	800 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source





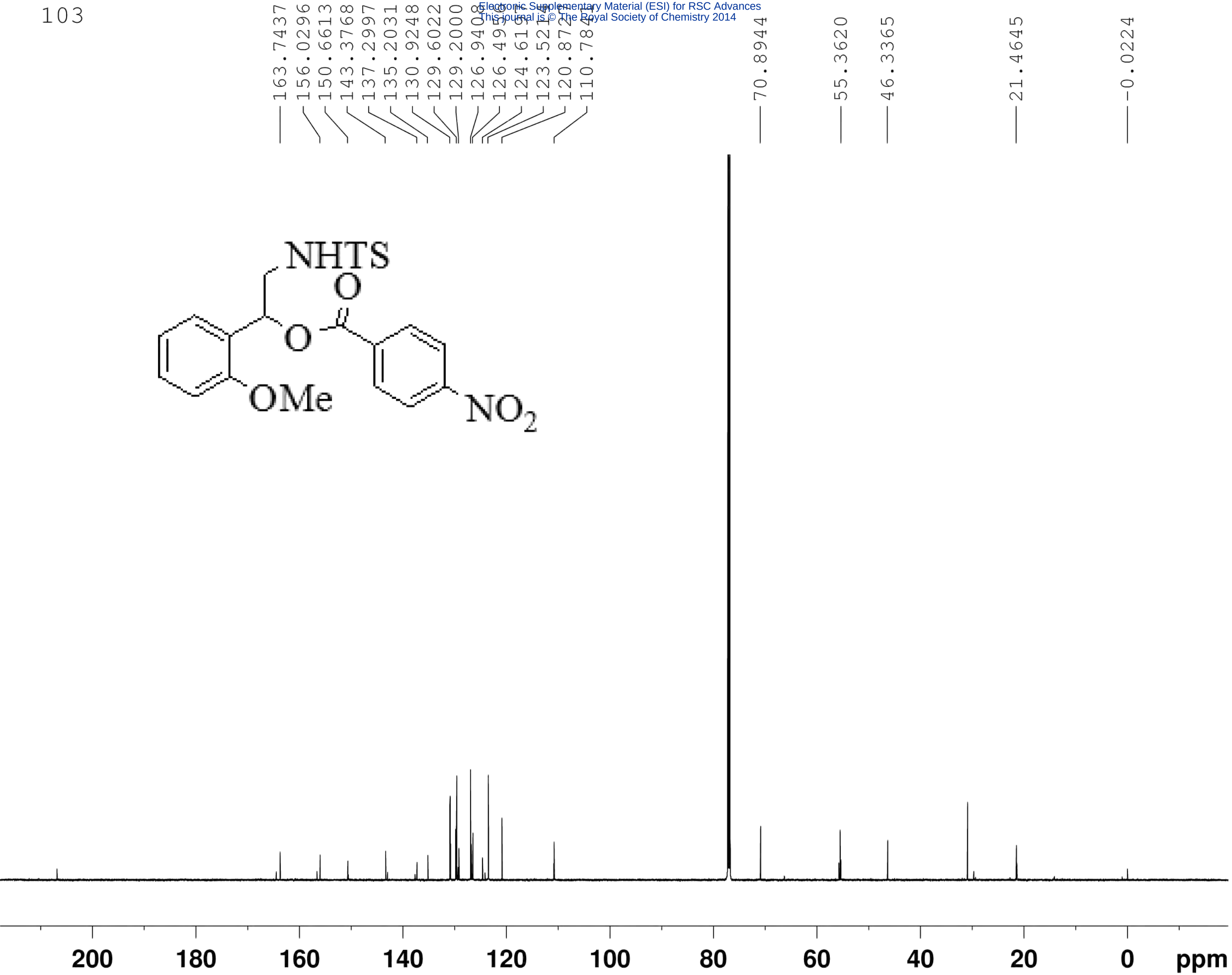

```
Current Data Parameters
NAME     20110711ligong
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20110711
Time               9.46
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH           12335.526 Hz
FIDRES         0.188225 Hz
AQ            2.6564426 sec
RG                  114
DW               40.533 usec
DE                 6.50 usec
TE                296.3 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                12.60 usec
PLW1        13.99600029 W
SFO1       600.1328806 MHz

F2 - Processing parameters
SI                32768
SF          600.1300096 MHz
WDW                  EM
SSB      0
LB                -0.10 Hz
GB       0
PC                 1.00
```

103



Current Data Parameters
NAME 20110718ligong
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110721
Time 8.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6144
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 300.5 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
PLW1 92.68299866 W
SFO1 150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 13.99600029 W
PLW12 0.45346999 W
PLW13 0.22220001 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

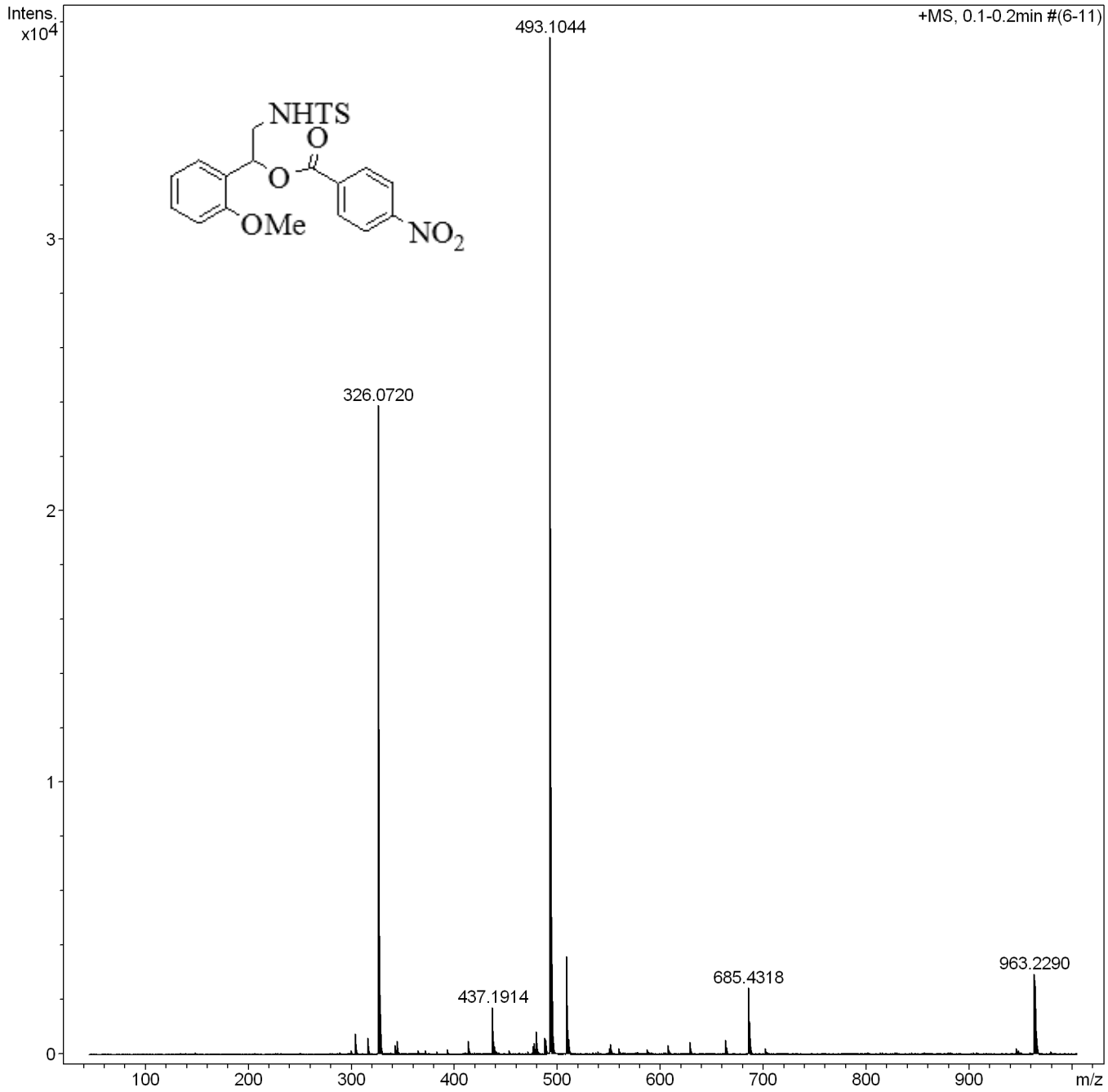
Display Report

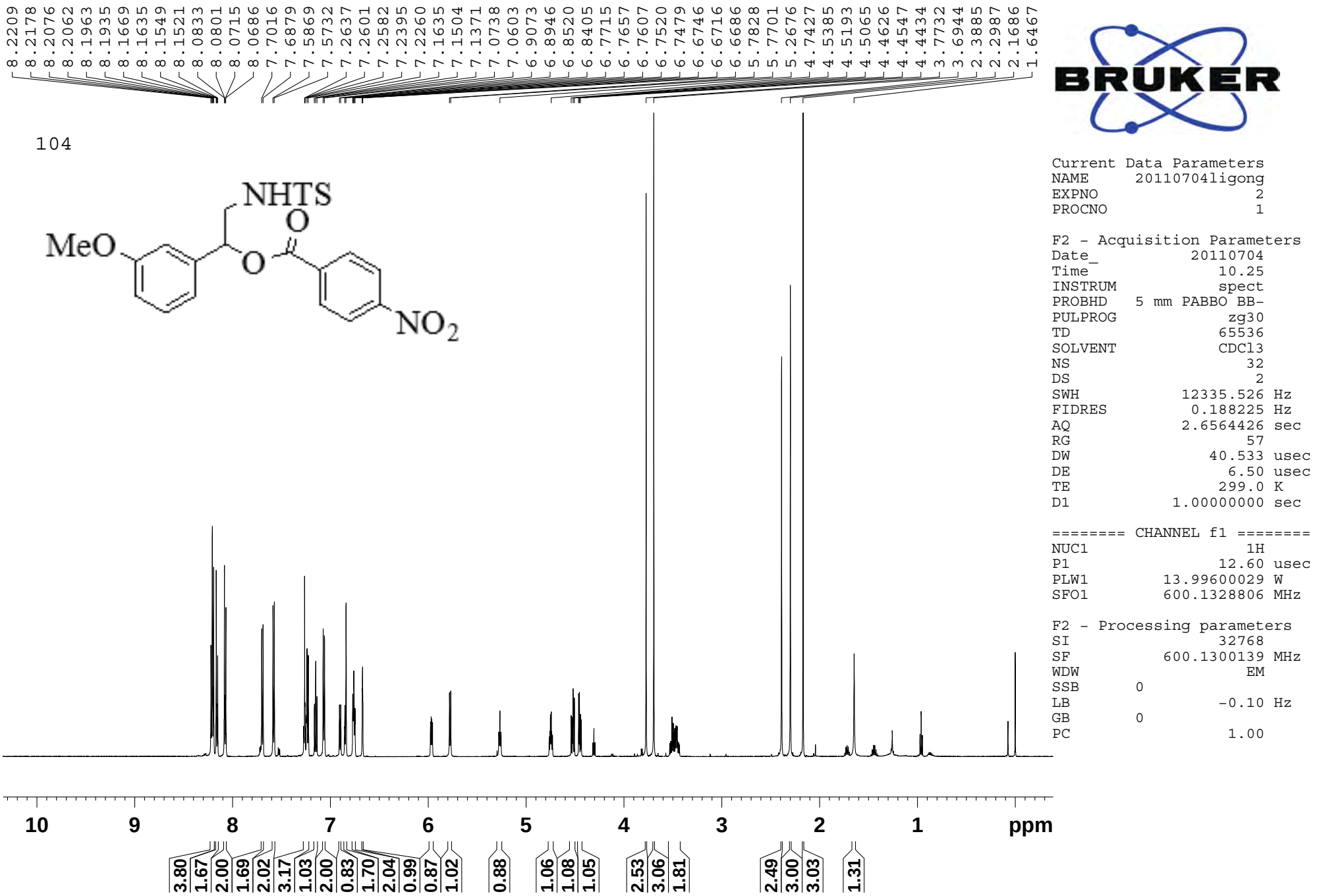
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-14.d	Acquisition Date	7/21/2011 9:36:01 AM
Method	tune_wide.m	Operator	TJU
Sample Name		Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste






```
Current Data Parameters
NAME      20110704ligong
EXPNO                 2
PROCNO                1

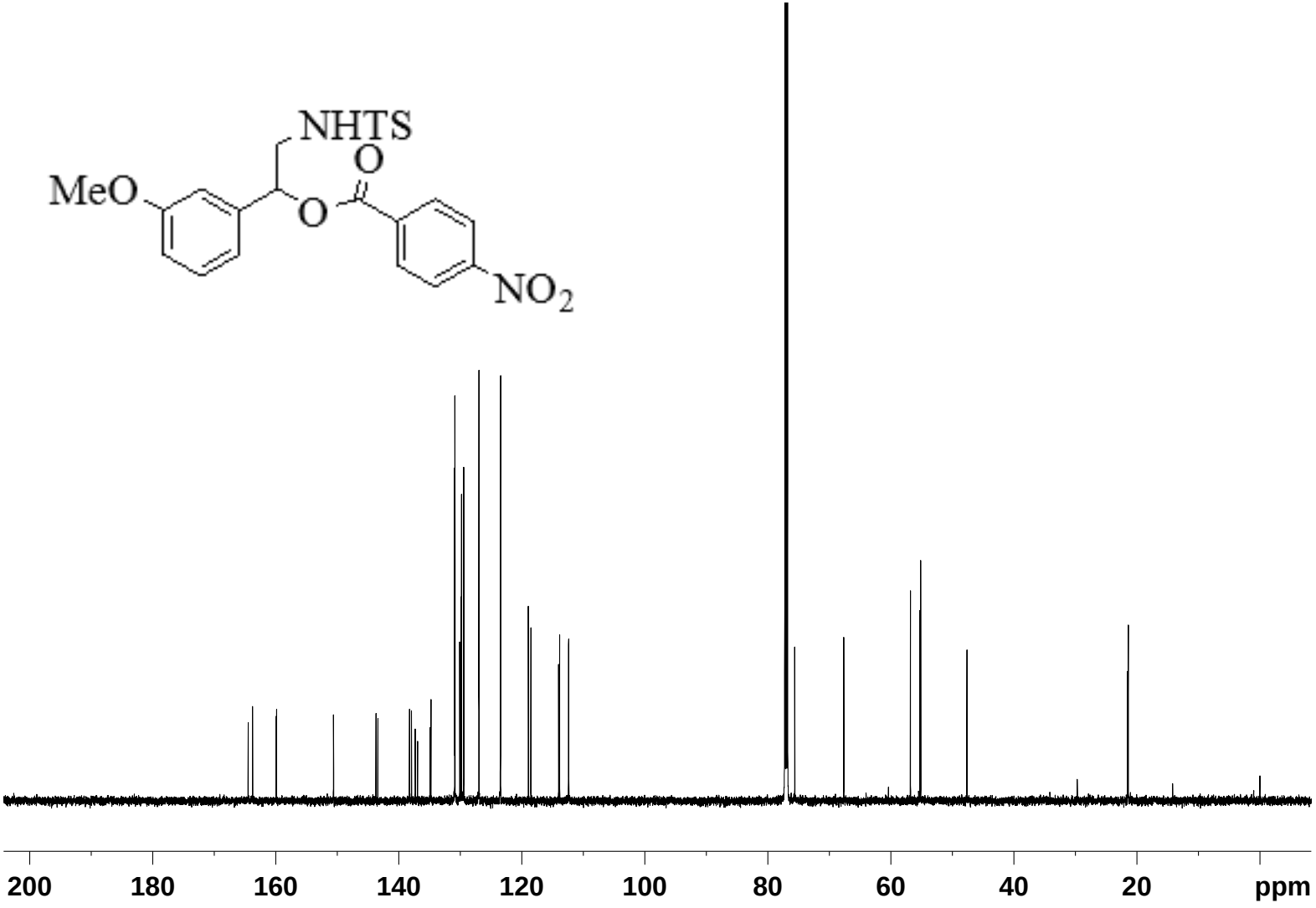
F2 - Acquisition Parameters
Date_          20110704
Time              10.25
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH           12335.526 Hz
FIDRES         0.188225 Hz
AQ             2.6564426 sec
RG                   57
DW               40.533 usec
DE                6.50 usec
TE               299.0 K
D1            1.00000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1               12.60 usec
PLW1        13.99600029 W
SFO1       600.1328806 MHz

F2 - Processing parameters
SI                32768
SF         600.1300139 MHz
WDW                  EM
SSB       0
LB              -0.10 Hz
GB        0
PC               1.00
```

104

164.4610
163.7434
159.9284
159.8373
150.6257
143.7199
143.4168
138.2704
137.9507
137.3418
134.9417
134.7866
130.9212
130.8774
130.0989
129.9081
129.8148
129.4543
126.9845
126.9575
123.4894
123.4544
118.9344
118.5325
114.0208
113.8643
112.4209
112.3764
75.6280
67.6630
56.8206
55.2881
55.1572
47.6326
21.4997
21.4034



Current Data Parameters
NAME 20110727ligong
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110727
Time 10.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2041
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
PLW1 92.68299866 W
SFO1 150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 13.99600029 W
PLW12 0.45346999 W
PLW13 0.22220001 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

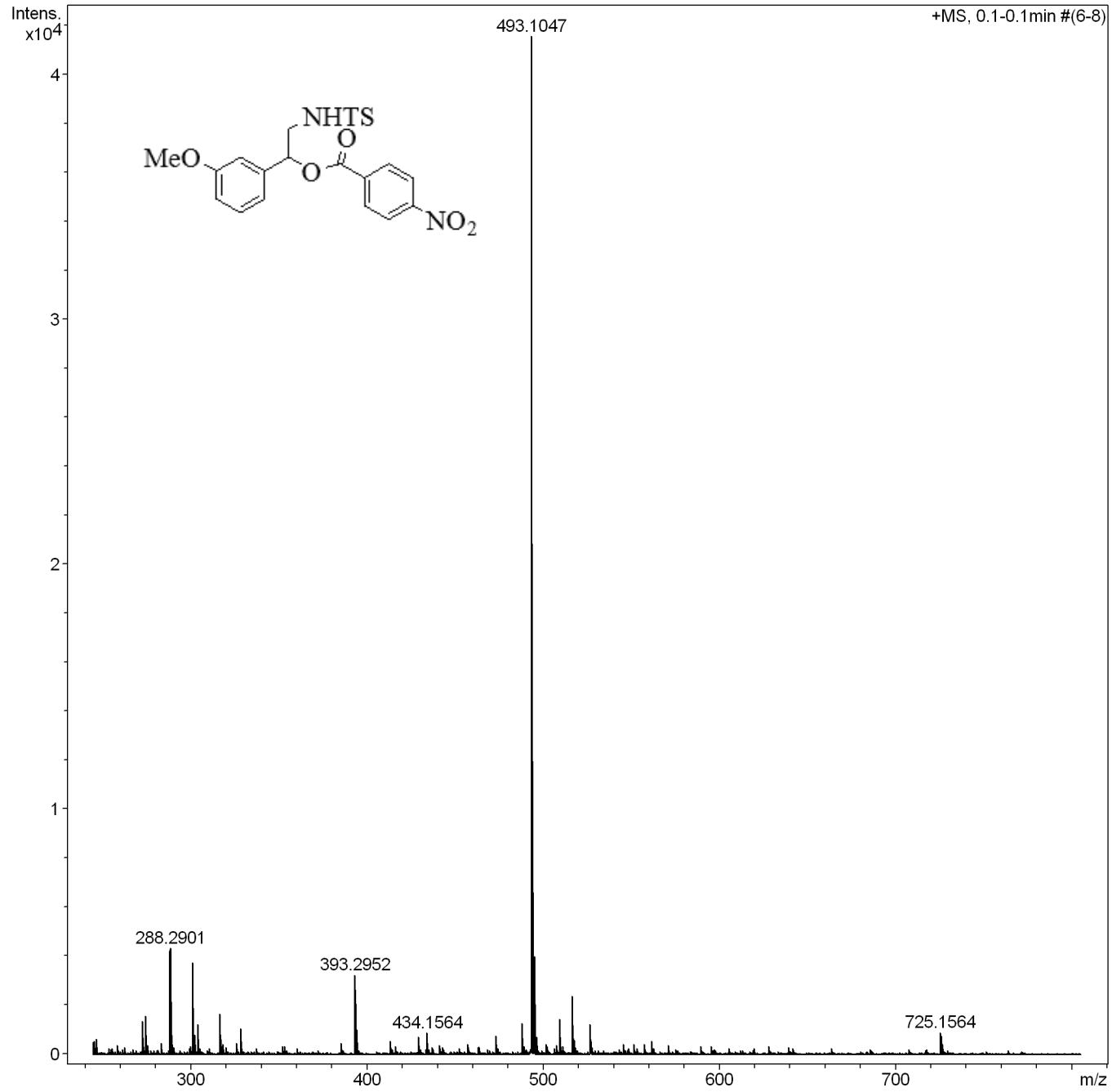
Display Report

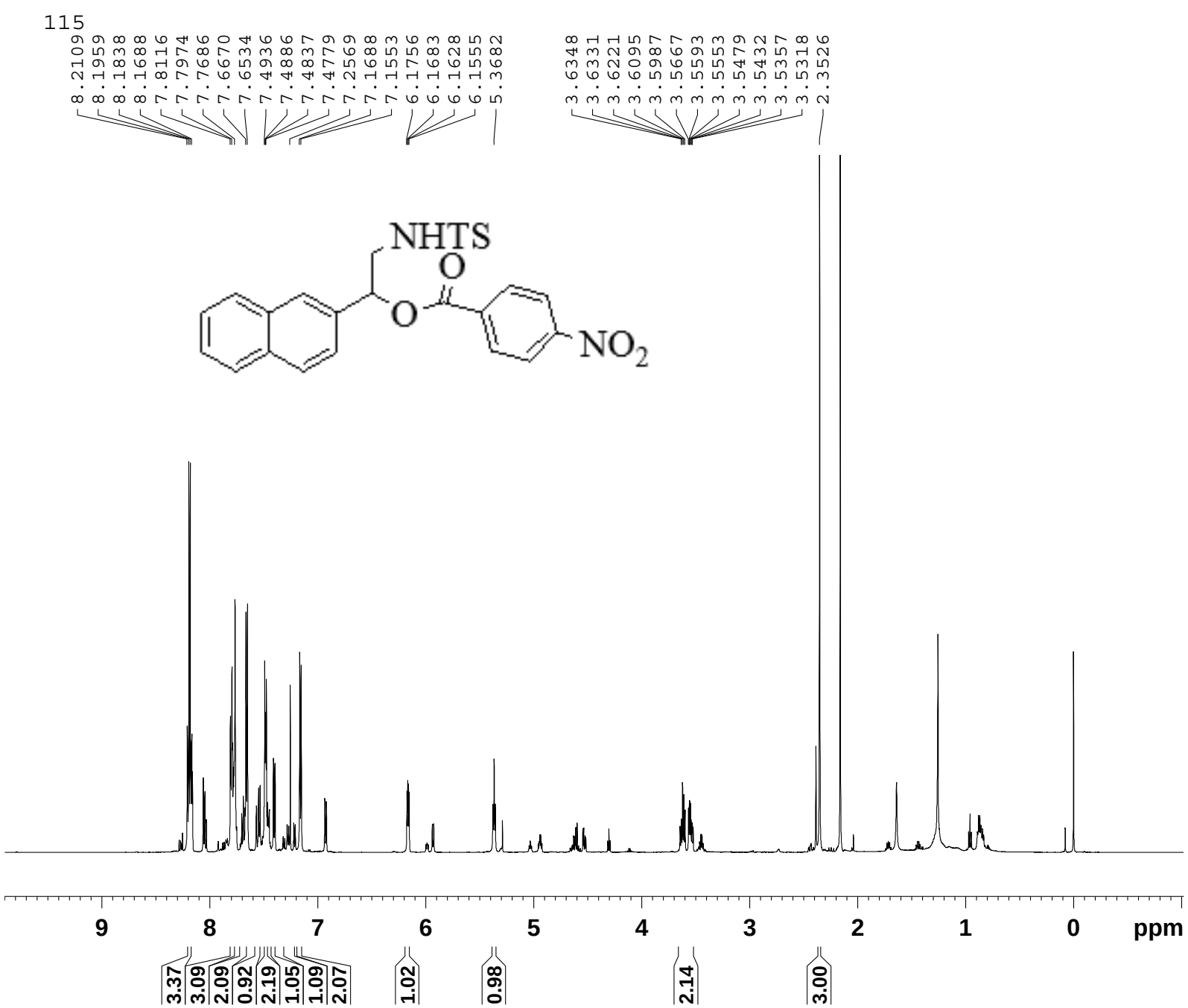
Analysis Info

Analysis Name	D:\Data\20110730_13.d	Acquisition Date	7/30/2011 11:39:30 AM
Method	Na FA_low.m	Operator	TJU
Sample Name	20110707_ZJT_1_3-3_M6	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	250 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	800 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source





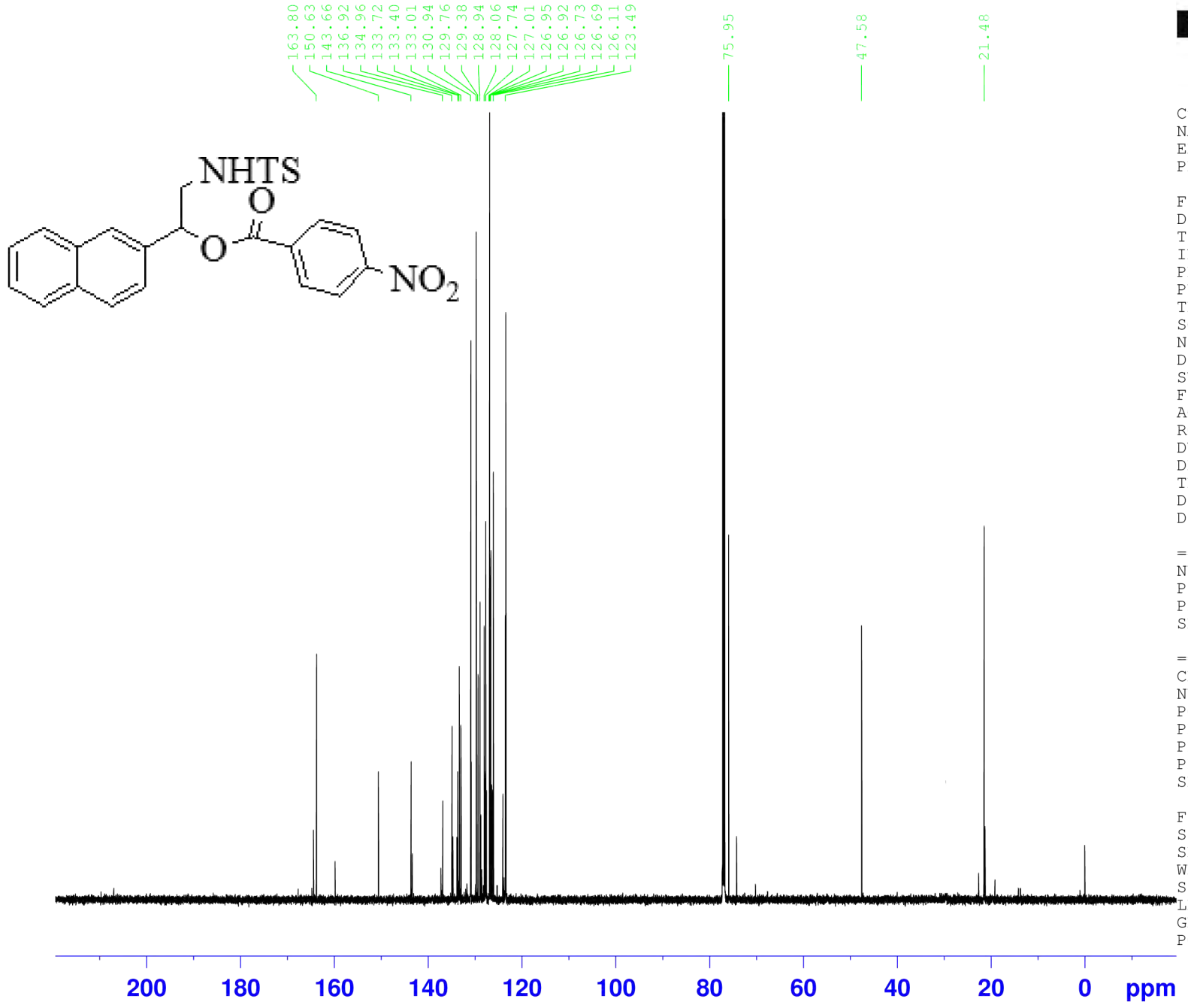
Current Data Parameters
NAME 20110711ligong
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110711
Time 10.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 71.8
DW 40.533 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300181 MHz
WDW GM
SSB 0
LB -0.10 Hz
GB 0.1
PC 1.00

Electronic Supplementary Material (ESI) for RSC Advances




```
Current Data Parameters
NAME      20110718ligong
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20110721
Time              15.07
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                6144
DS                   2
SWH          36057.691 Hz
FIDRES        0.550197 Hz
AQ           0.9088159 sec
RG                 203
DW              13.867 usec
DE                6.50 usec
TE               300.5 K
D1           2.00000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1               13C
P1               11.30 usec
PLW1        92.68299866 W
SFO1       150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            70.00 usec
PLW2        13.99600029 W
PLW12        0.45346999 W
PLW13        0.22220001 W
SFO2       600.1324005 MHz

F2 - Processing parameters
SI                 32768
SF          150.9028096 MHz
WDW                   EM
SSB       0
LB                 0.10 Hz
GB        0
PC                 1.40
```

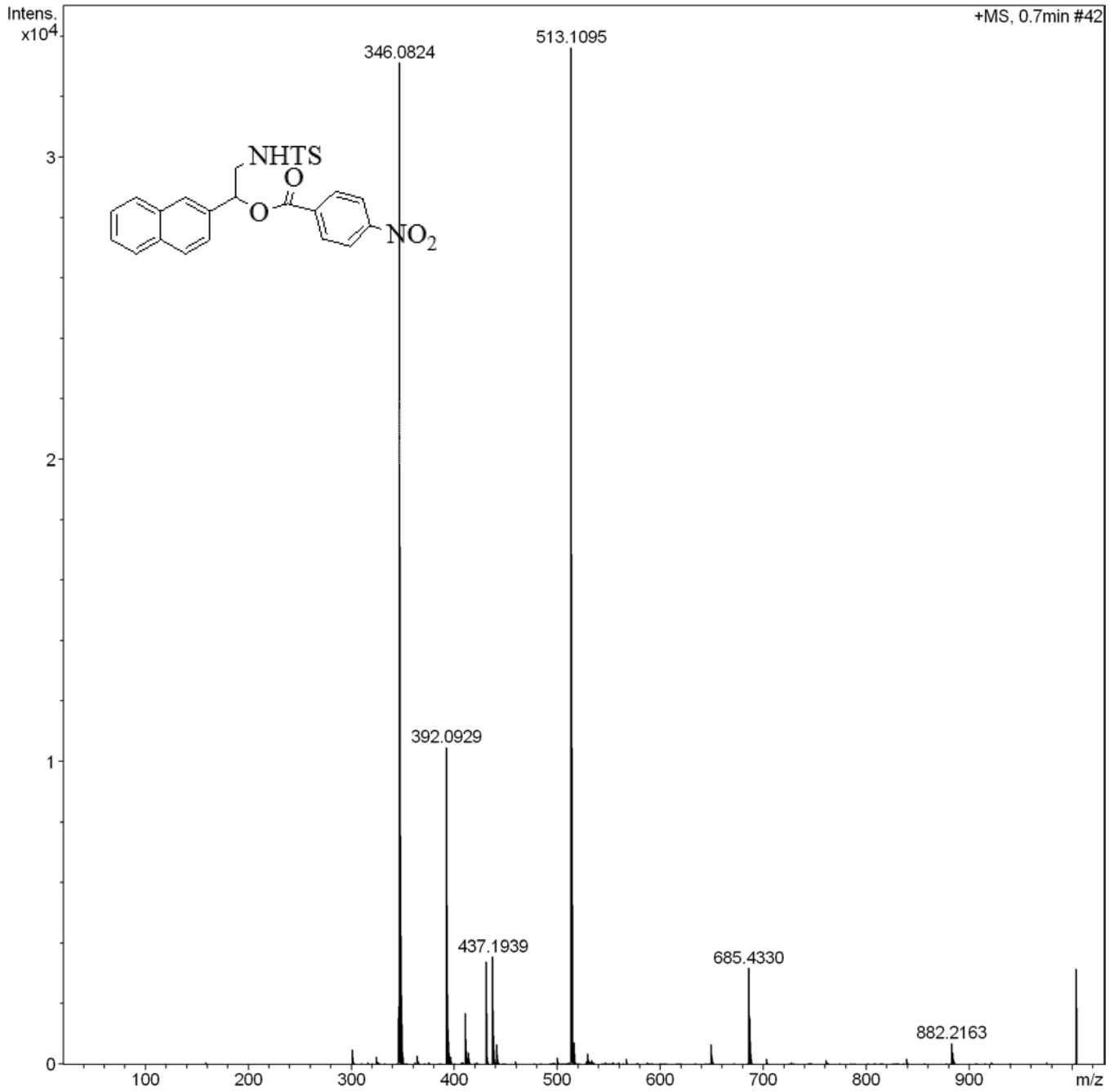
Display Report

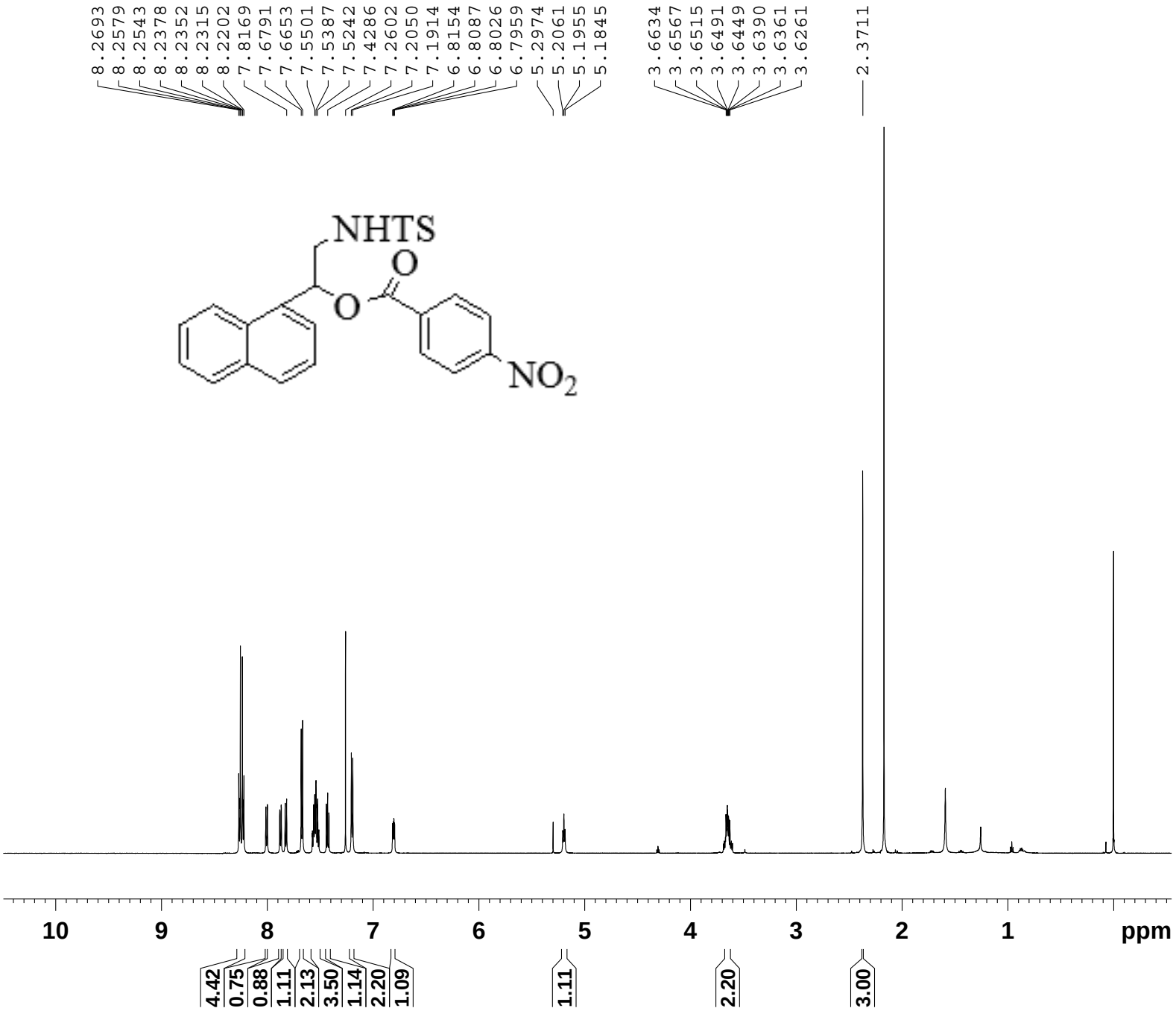
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-16.d	Acquisition Date	7/21/2011 9:55:17 AM
Method	tune_wide.m	Operator	TJU
Sample Name		Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste





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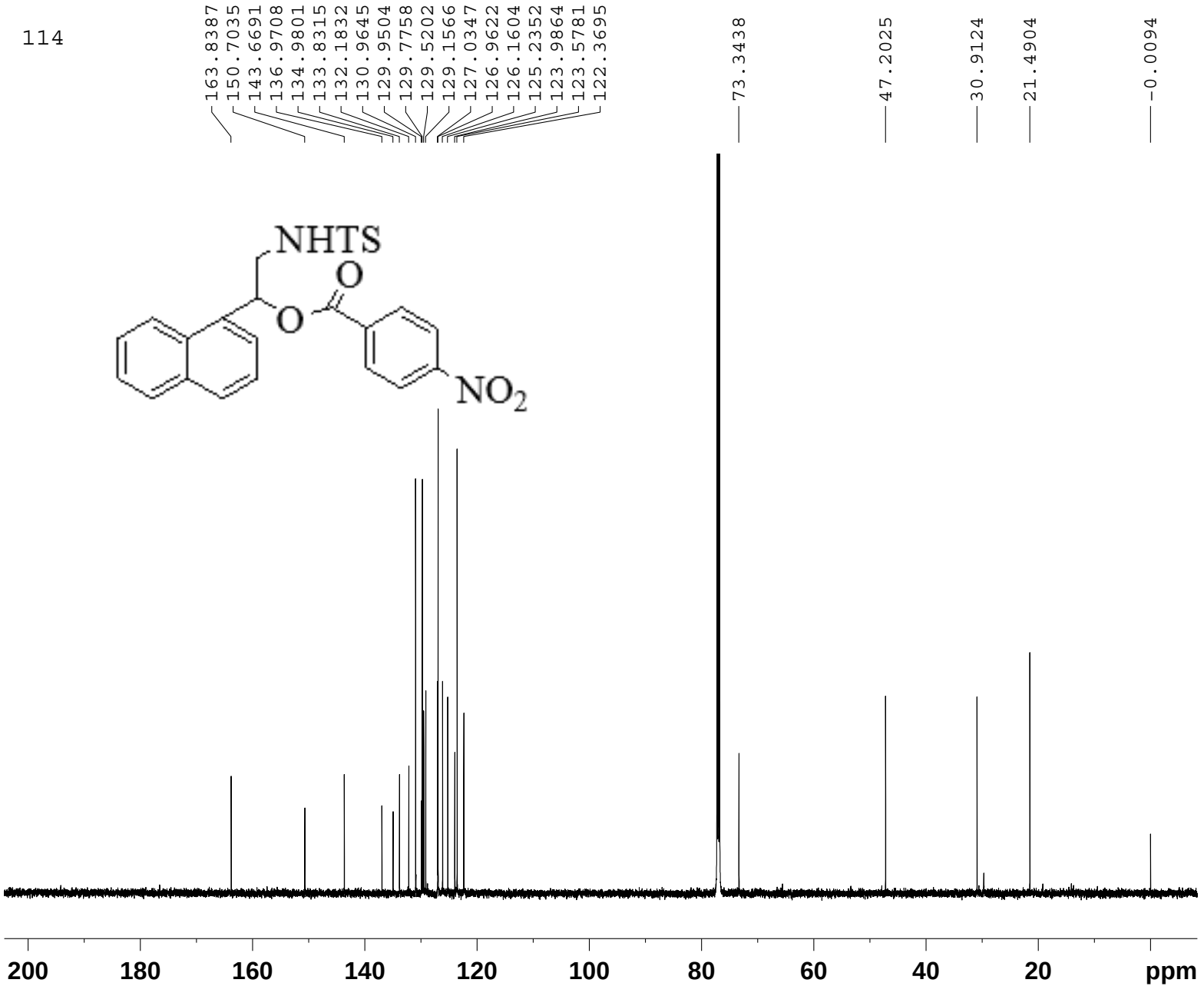
Current Data Parameters
NAME 20110711ligong
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110711
Time 10.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 144
DW 40.533 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300161 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

114



Current Data Parameters
NAME 20110712ligong
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110713
Time 10.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6022
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
PLW1 92.68299866 W
SFO1 150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 13.99600029 W
PLW12 0.45346999 W
PLW13 0.22220001 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

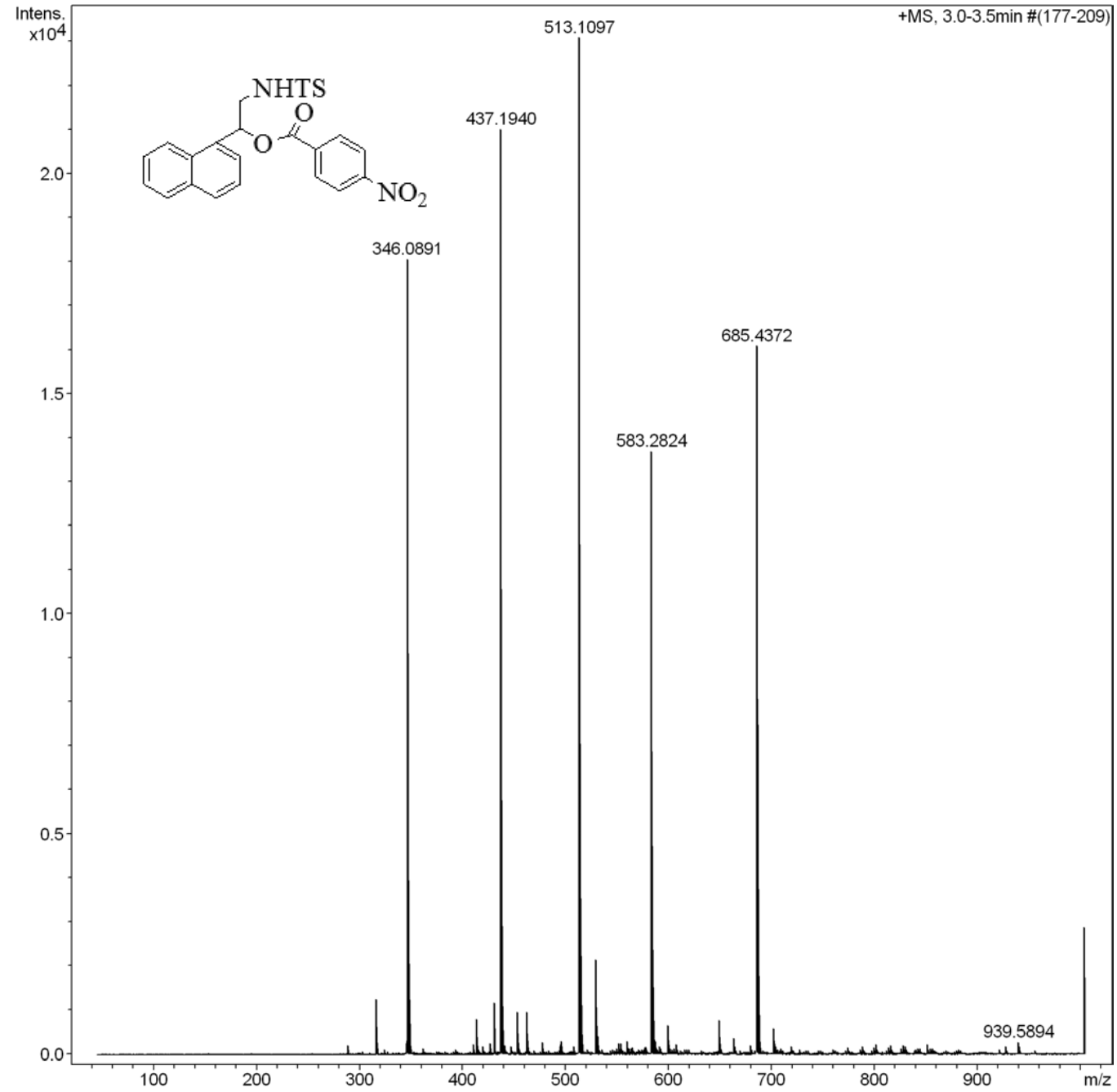
Display Report

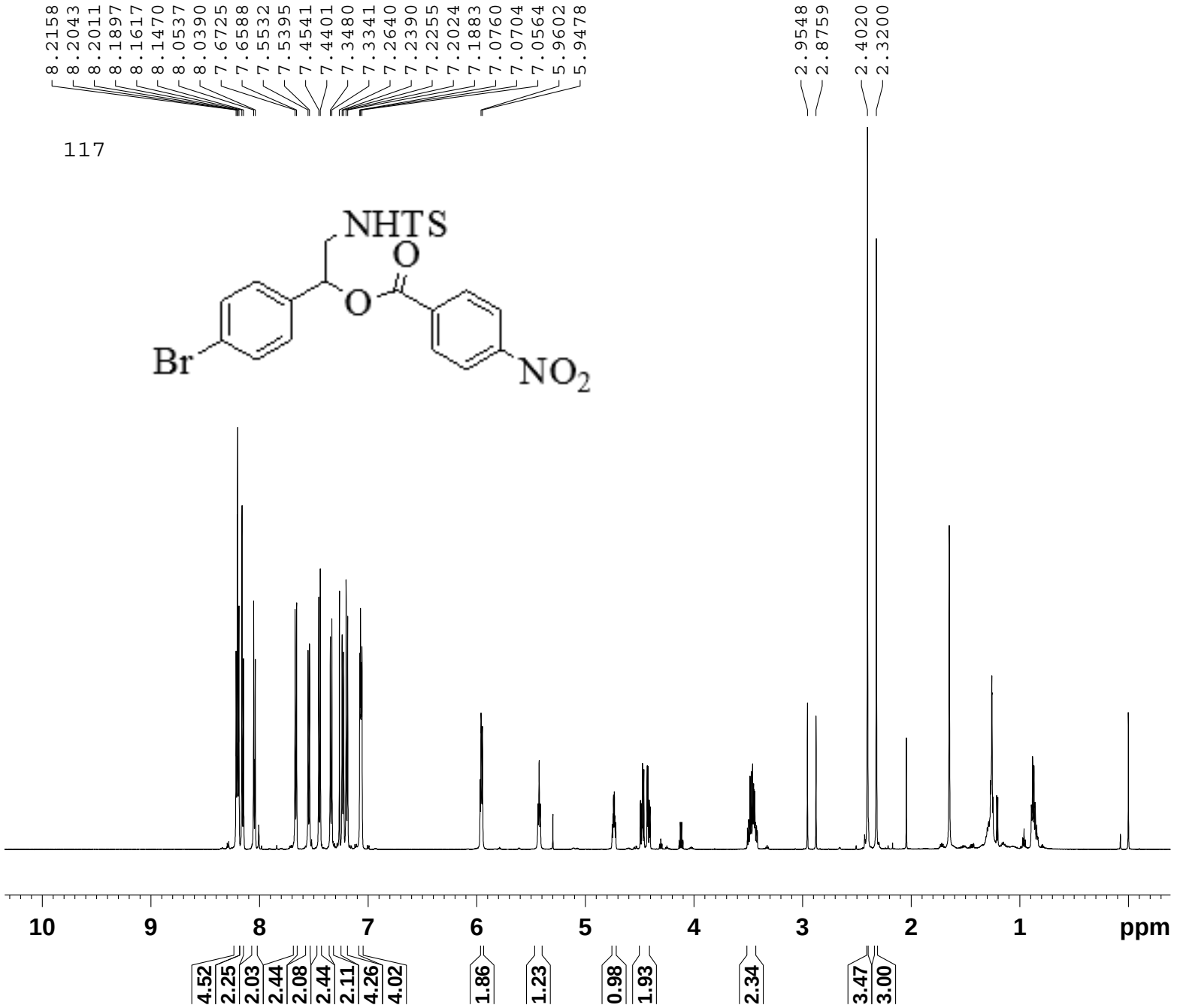
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-15.d	Acquisition Date	7/20/2011 9:52:09 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste





BRUKER

```
Current Data Parameters
NAME      20110711ligong
EXPNO                 11
PROCNO                 1

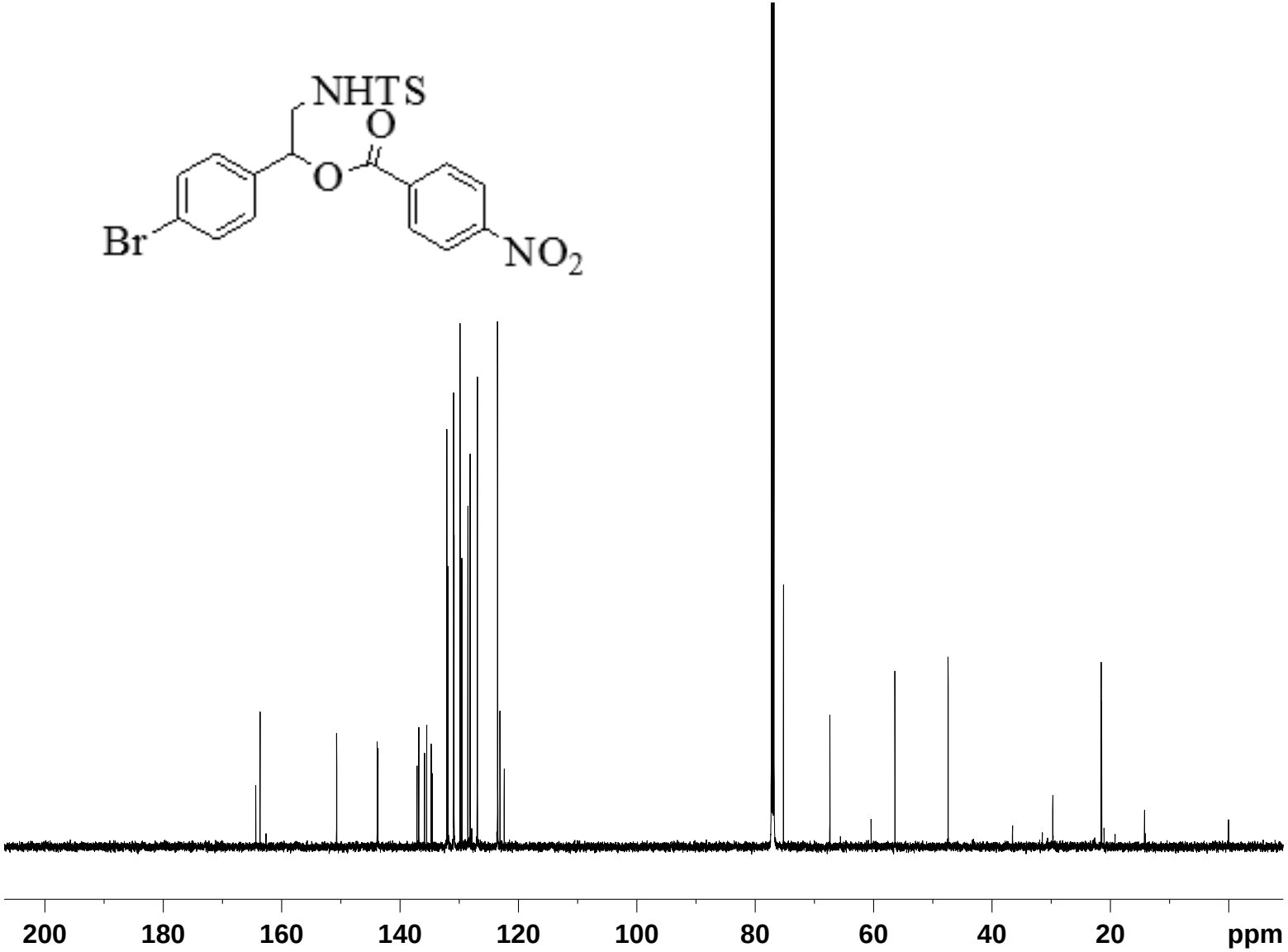
F2 - Acquisition Parameters
Date_           20110711
Time               10.56
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ              2.6564426 sec
RG                  90.5
DW                40.533 usec
DE                 6.50 usec
TE                297.2 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.60 usec
PLW1         13.99600029 W
SFO1         600.1328806 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300137 MHz
WDW                   EM
SSB       0
LB                -0.10 Hz
GB        0
PC                 1.00
```

111

164.3668
163.6413
150.7053
150.6848
143.8466
143.7052
137.1271
136.8215
135.8511
135.4812
134.7118
134.5376
132.0760
131.8974
130.9283
130.8578
129.8354
129.5425
128.5228
128.1390
126.9416
126.9050
123.5131
123.4763
123.0904
122.3766
75.1963
67.3564
56.3536
47.3820
21.5144
21.4328



Current Data Parameters
NAME 20110727ligong
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110727
Time 15.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 301.0 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
PLW1 92.68299866 W
SFO1 150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 13.99600029 W
PLW12 0.45346999 W
PLW13 0.22220001 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

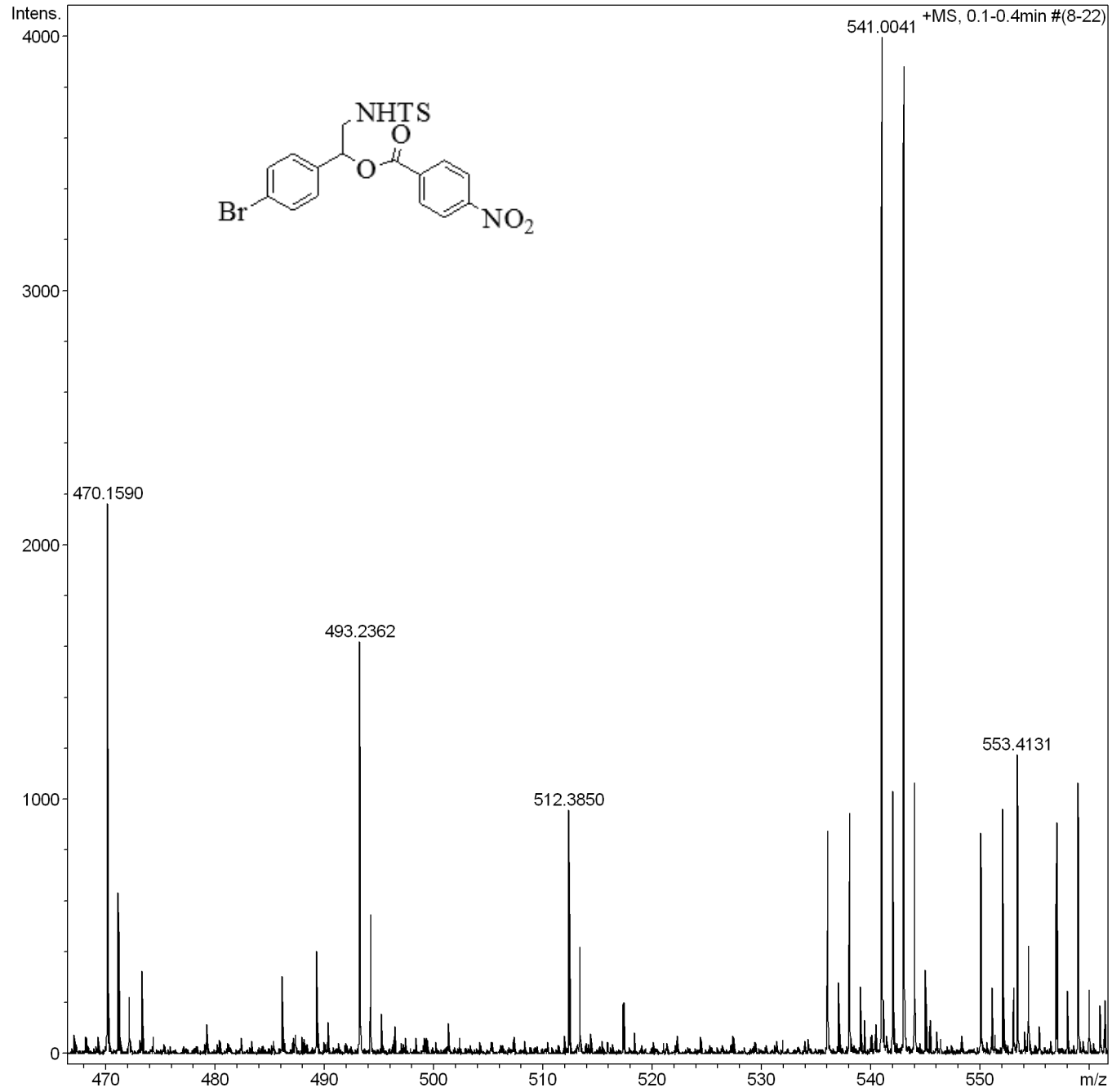
Display Report

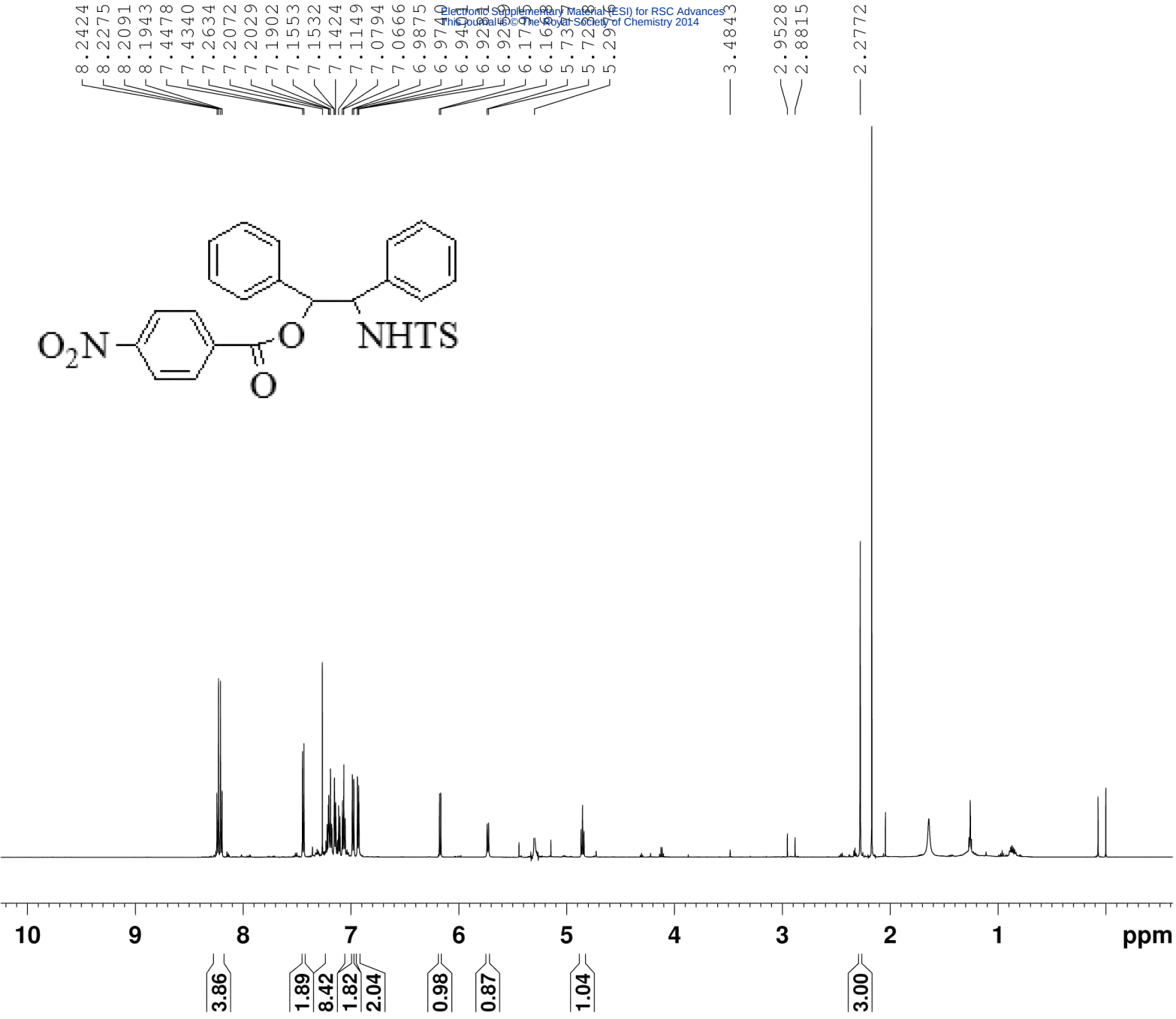
Analysis Info

Analysis Name	D:\Data\20110730_17.d	Acquisition Date	7/30/2011 12:00:10 PM
Method	Na FA_low.m	Operator	TJU
Sample Name	20110707_ZJT_1_3-3_M6	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	250 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	800 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source





BRUKER

```
Current Data Parameters
NAME      20110711ligong
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110711
Time               10.20
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                   114
DW                40.533 usec
DE                 6.50 usec
TE                296.8 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                12.60 usec
PLW1        13.99600029 W
SFO1        600.1328806 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300145 MHz
WDW                   GM
SSB      0
LB               -0.10 Hz
GB                  0.1
PC                 1.00
```

Electronic Supplementary Material (ESI) for RSC Advances
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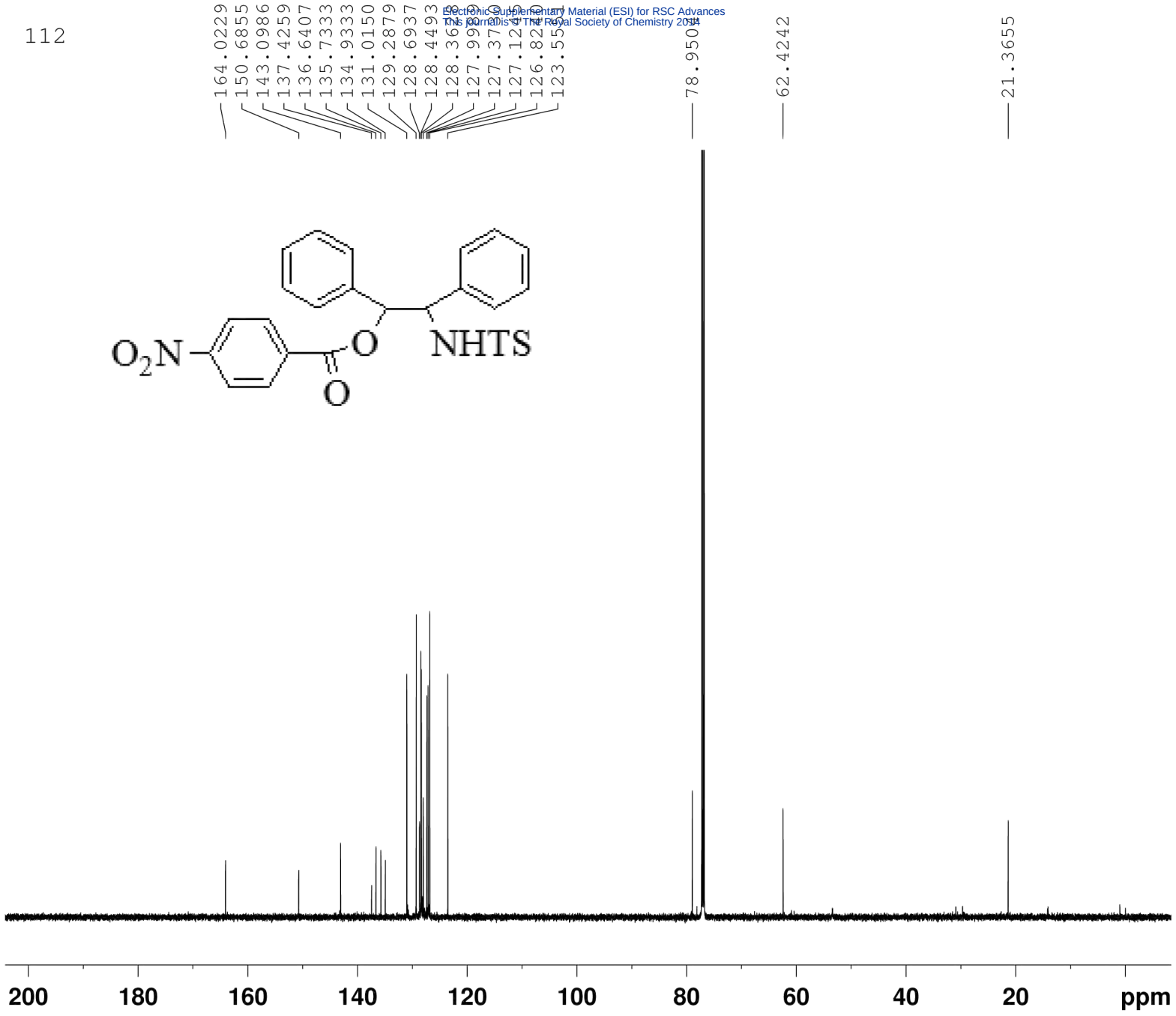



```
Current Data Parameters
NAME      20110718ligong
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20110718
Time               11.45
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 6144
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9088159 sec
RG                  203
DW               13.867 usec
DE                6.50 usec
TE               297.6 K
D1           2.00000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                11.30 usec
PLW1        92.68299866 W
SFO1       150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             70.00 usec
PLW2        13.99600029 W
PLW12        0.45346999 W
PLW13        0.22220001 W
SFO2       600.1324005 MHz

F2 - Processing parameters
SI                32768
SF          150.9028096 MHz
WDW                  EM
SSB       0
LB                0.10 Hz
GB        0
PC                1.40
```

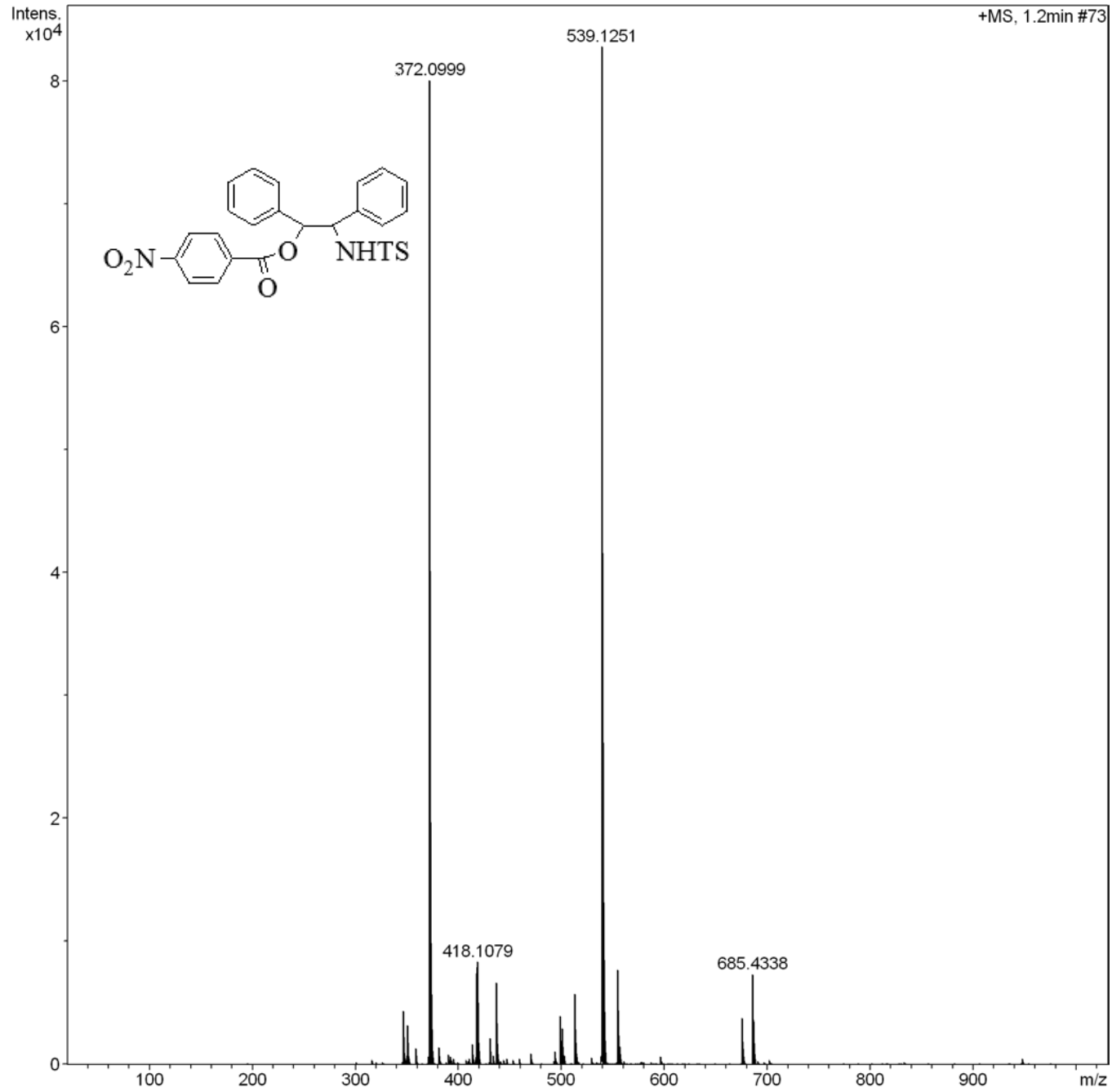
Display Report

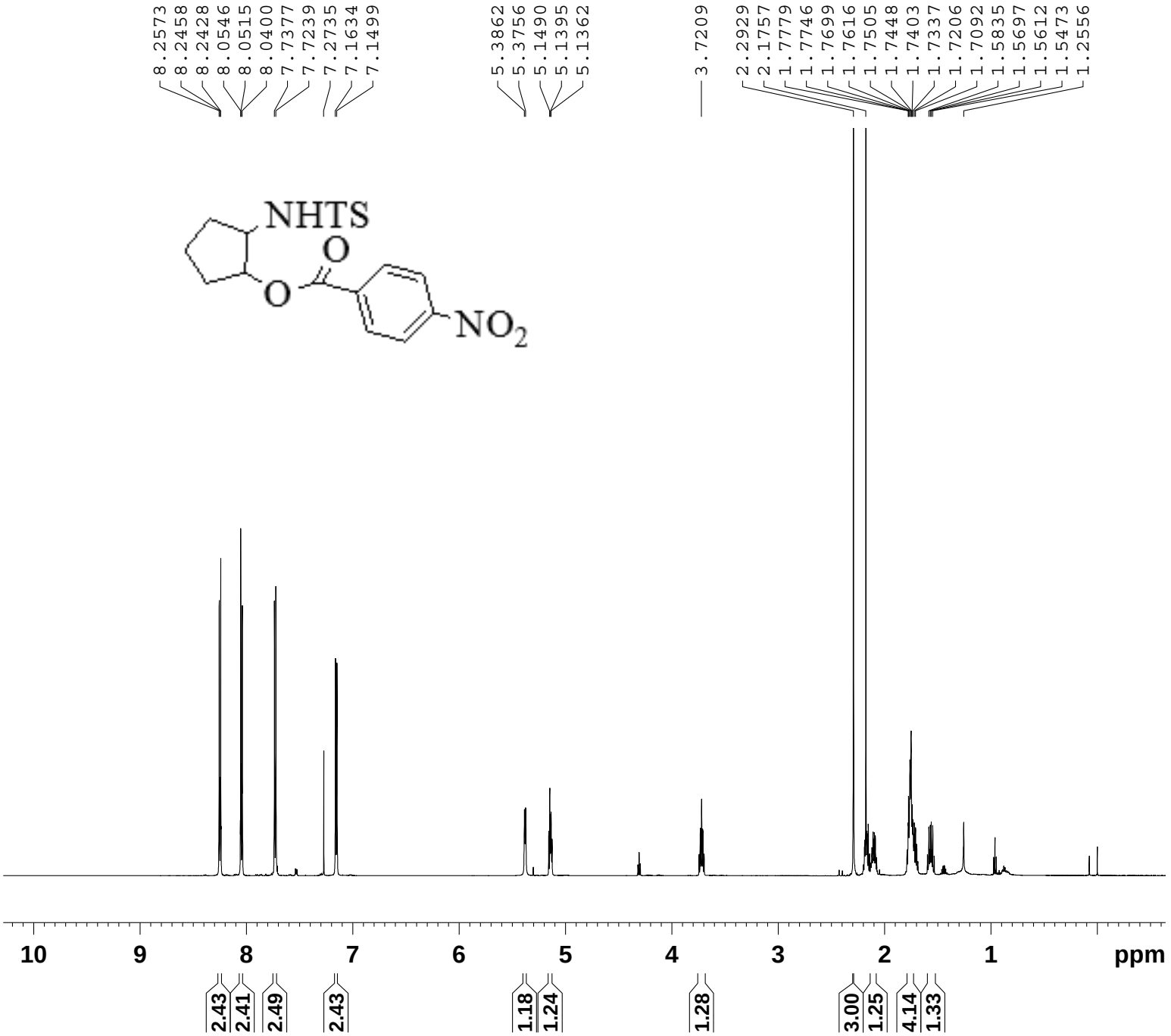
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-18.d	Acquisition Date	7/21/2011 10:00:35 AM
Method	tune_wide.m	Operator	TJU
Sample Name		Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste





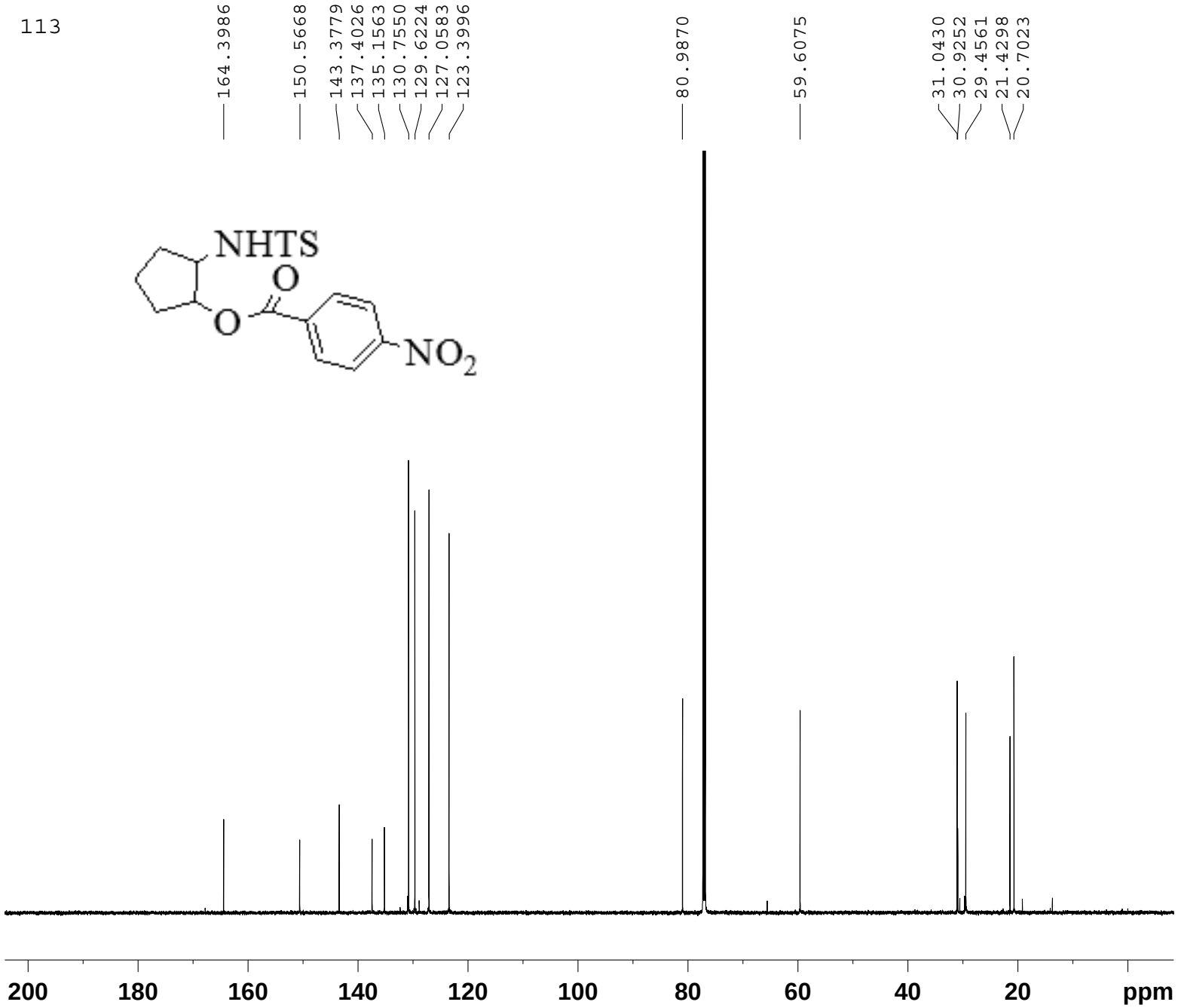
Current Data Parameters
NAME 20110711ligong
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110711
Time 10.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 64
DW 40.533 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300084 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

113



Current Data Parameters
NAME 20110712ligong
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110713
Time 8.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1740
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
PLW1 92.68299866 W
SFO1 150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 13.99600029 W
PLW12 0.45346999 W
PLW13 0.22220001 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

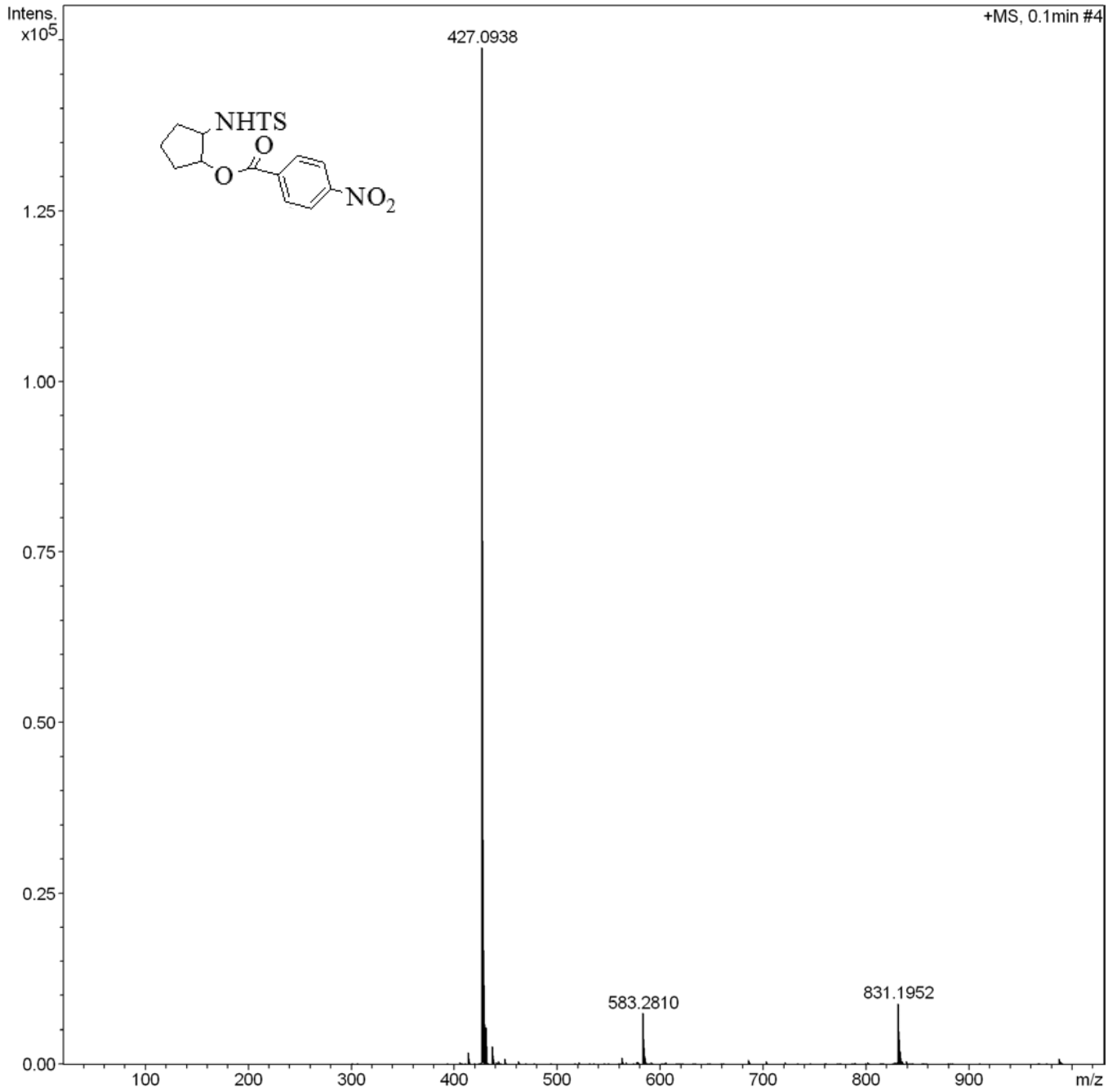
Display Report

Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-19.d	Acquisition Date	7/20/2011 9:45:38 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



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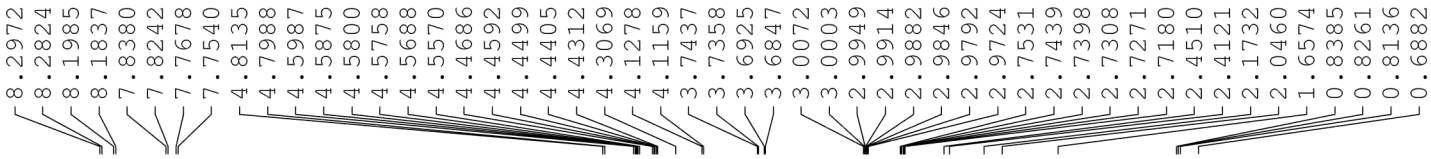
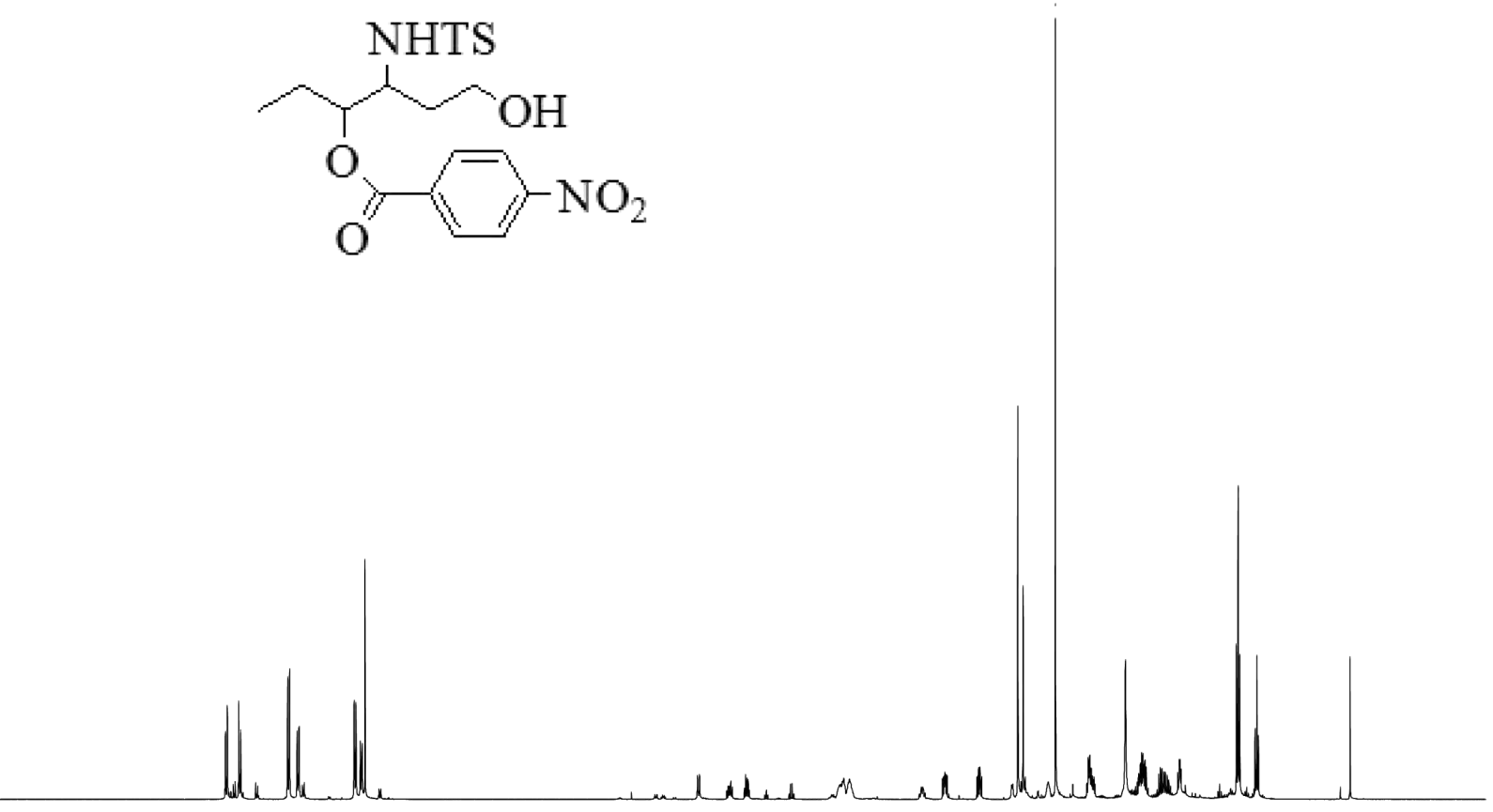
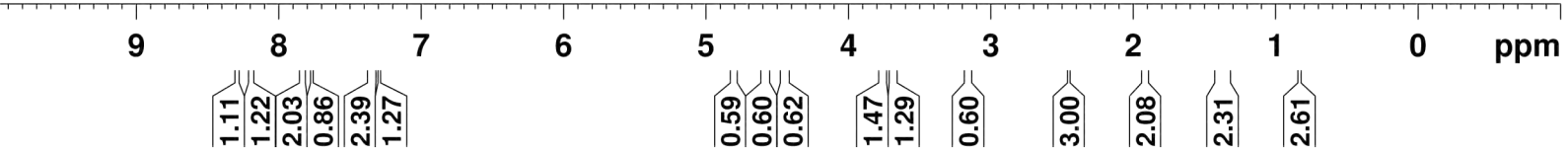




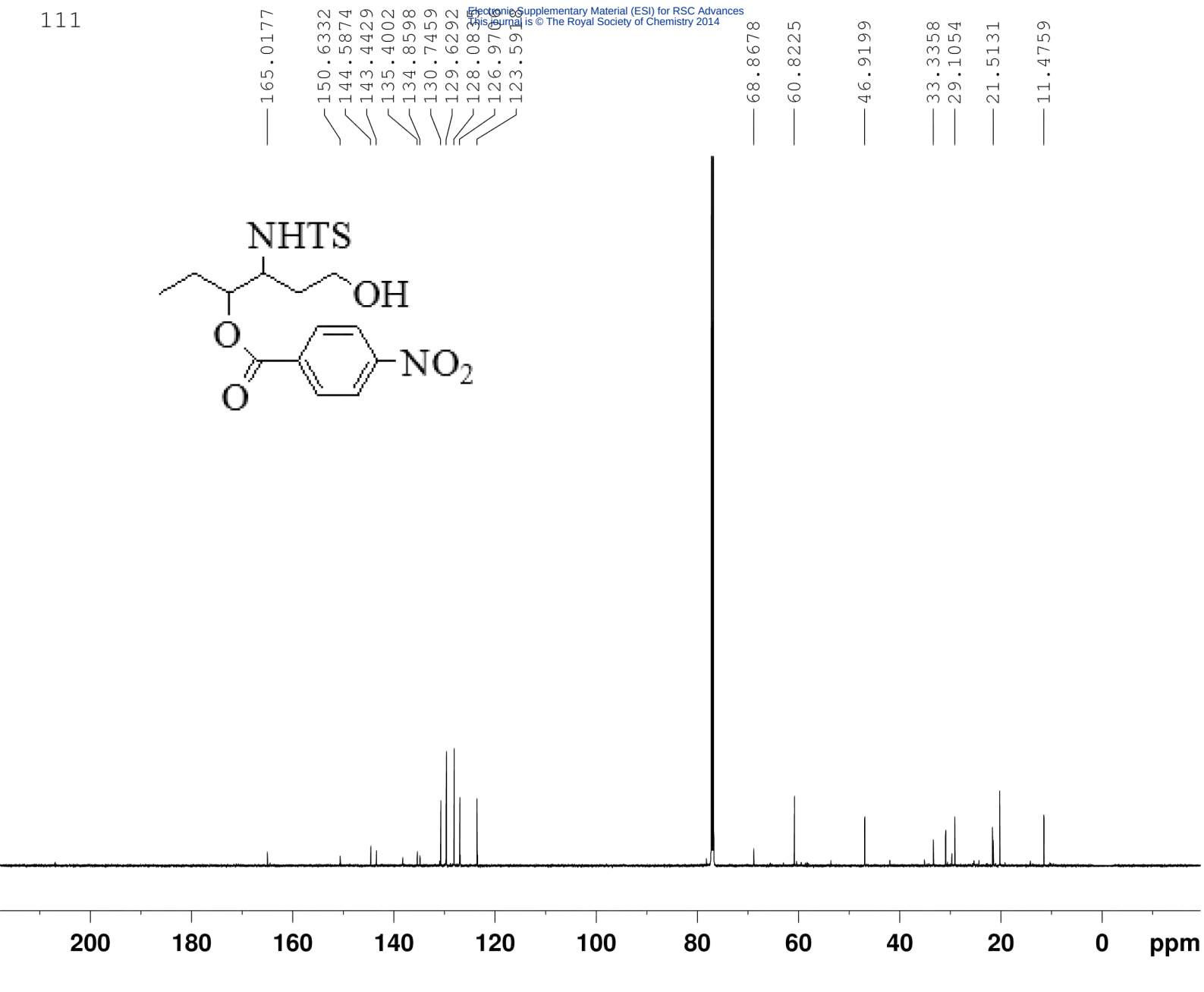


Current Data Parameters
NAME 20110711ligong
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110711
Time 10.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 114
DW 40.533 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300123 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00



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```
Current Data Parameters
NAME      20110718ligong
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110726
Time                8.43
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 7960
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9088159 sec
RG                  203
DW               13.867 usec
DE                6.50 usec
TE               296.8 K
D1           2.00000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                11.30 usec
PLW1        92.68299866 W
SFO1       150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            70.00 usec
PLW2        13.99600029 W
PLW12        0.45346999 W
PLW13        0.22220001 W
SFO2       600.1324005 MHz

F2 - Processing parameters
SI                 32768
SF          150.9028096 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

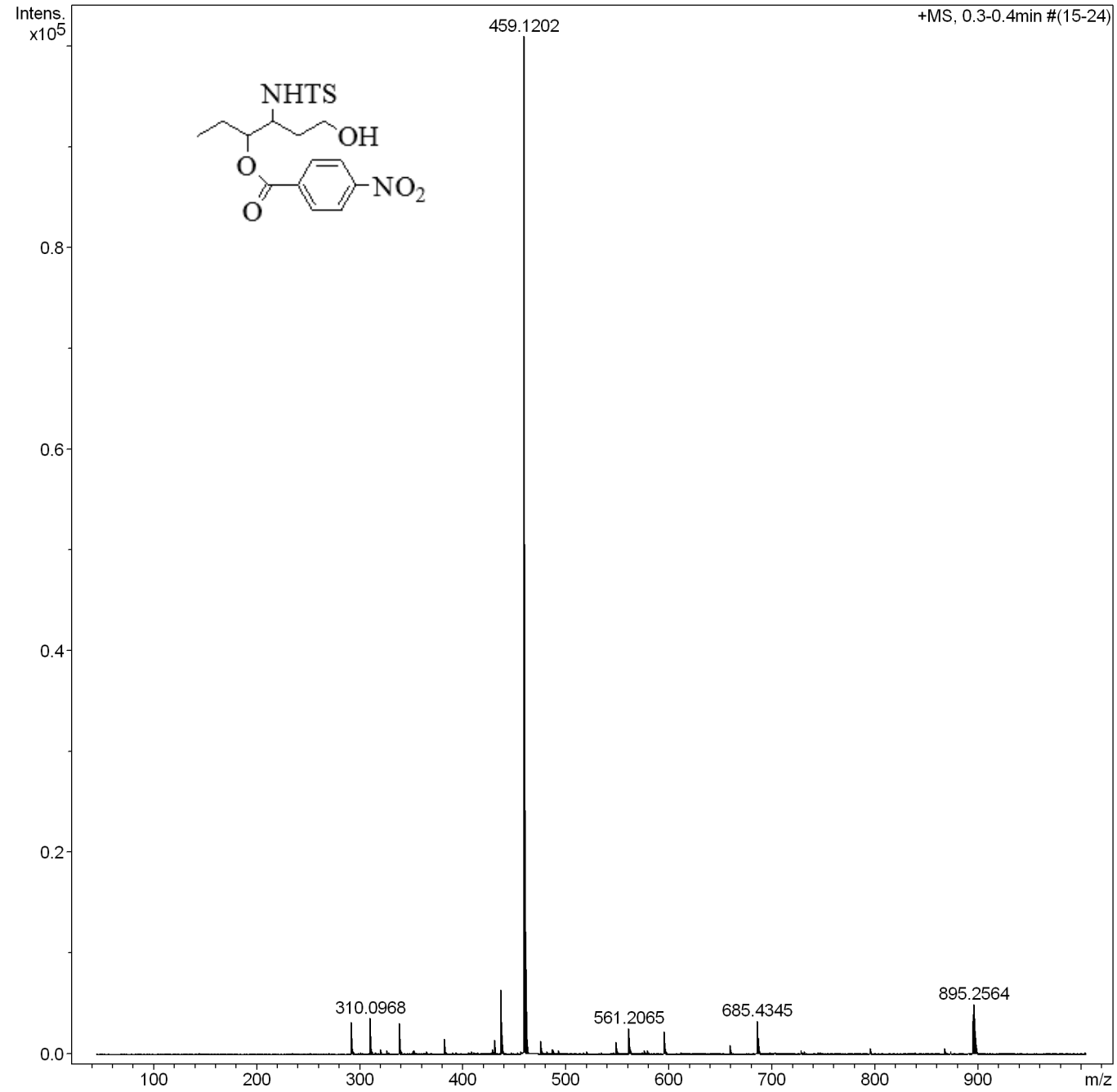
Display Report

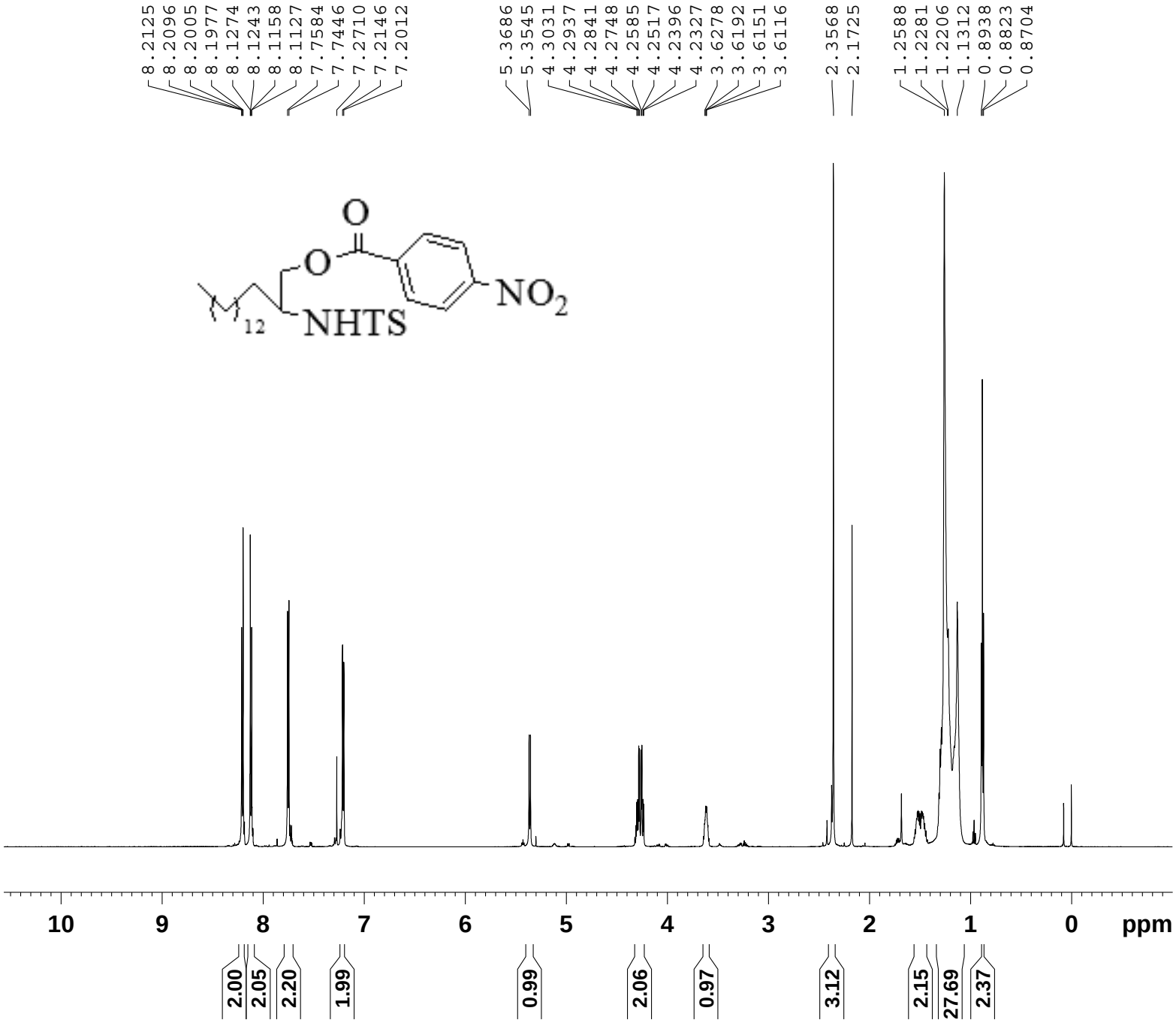
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-22.d	Acquisition Date	7/21/2011 9:41:54 AM
Method	tune_wide.m	Operator	TJU
Sample Name		Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste





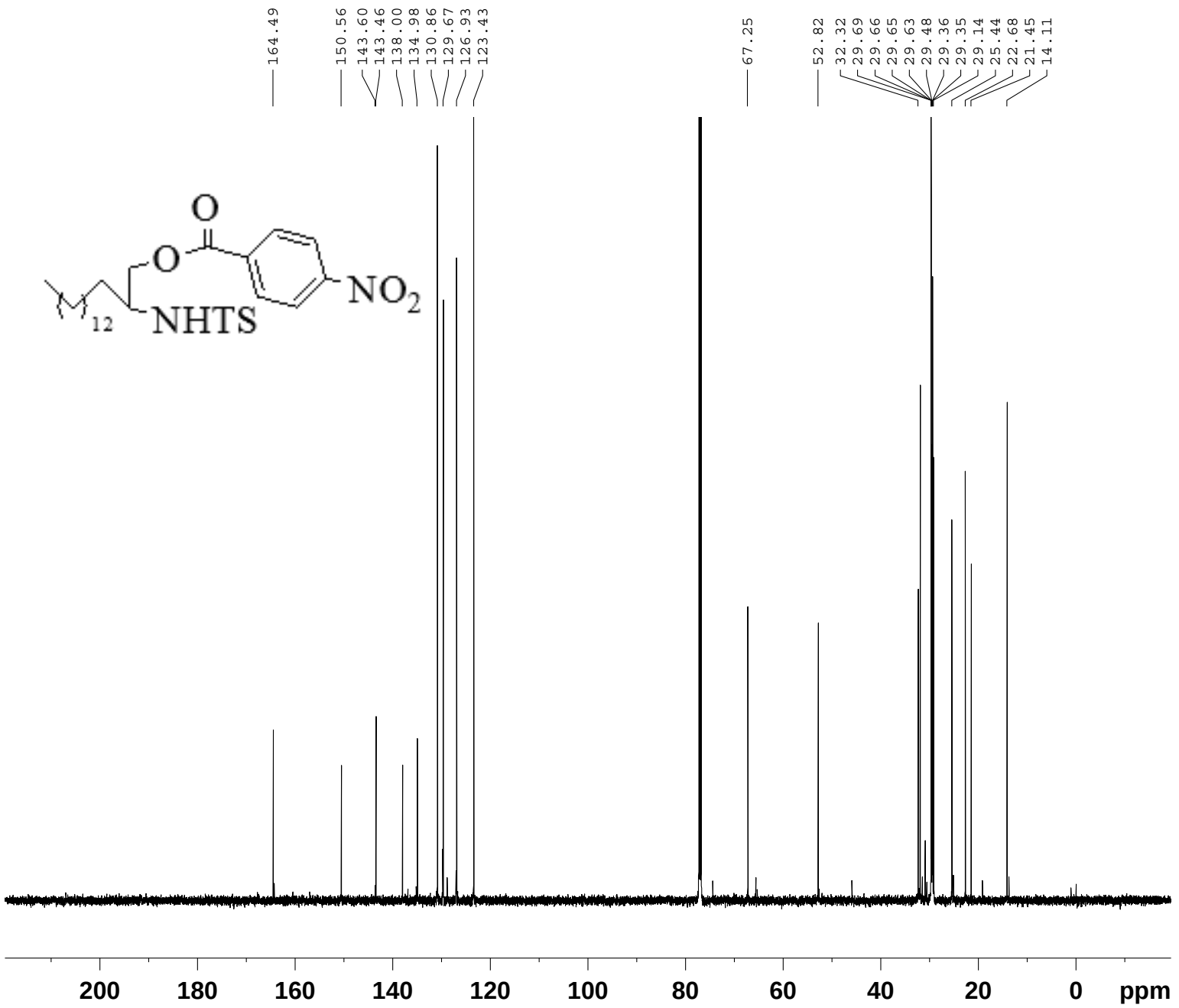

```
Current Data Parameters
NAME      20110629ligong
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110629
Time               10.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                  40.3
DW                40.533 usec
DE                 6.50 usec
TE                300.1 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.60 usec
PLW1         13.99600029 W
SFO1         600.1328806 MHz

F2 - Processing parameters
SI                 32768
SF          600.1300098 MHz
WDW                   EM
SSB       0
LB                -0.10 Hz
GB        0
PC                 1.00
```

100



BRUKER

```
Current Data Parameters
NAME      20110629ligong
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20110630
Time               9.27
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD              65536
SOLVENT         CDCl3
NS                860
DS                  2
SWH         36057.691 Hz
FIDRES       0.550197 Hz
AQ           0.9088159 sec
RG                203
DW             13.867 usec
DE              6.50 usec
TE              297.5 K
D1          2.00000000 sec
D11         0.03000000 sec

======== CHANNEL f1 ========
NUC1               13C
P1               11.30 usec
PLW1        92.68299866 W
SFO1       150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2               1H
PCPD2            70.00 usec
PLW2        13.99600029 W
PLW12        0.45346999 W
PLW13        0.22220001 W
SFO2       600.1324005 MHz

F2 - Processing parameters
SI                32768
SF         150.9028096 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

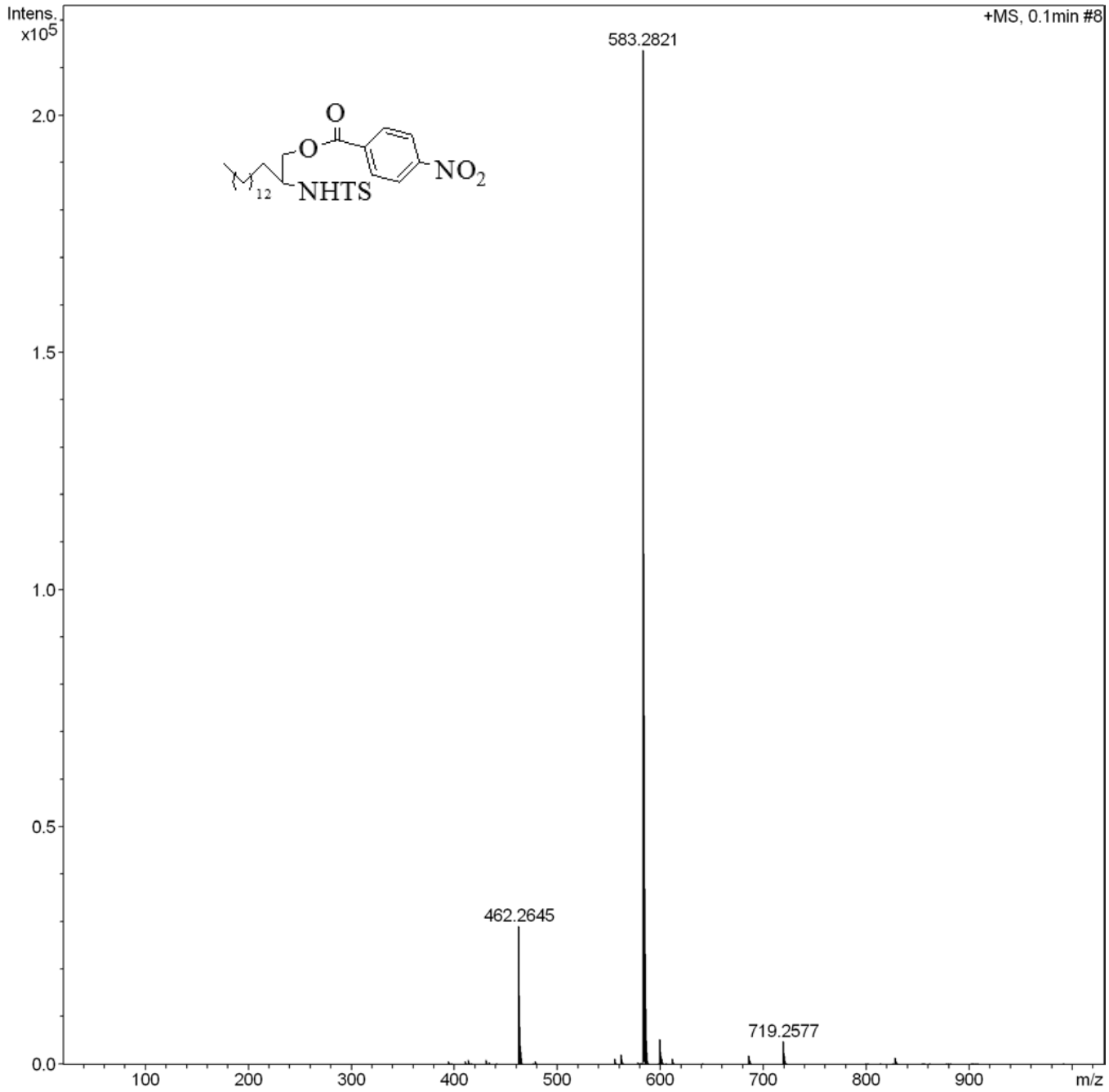
Display Report

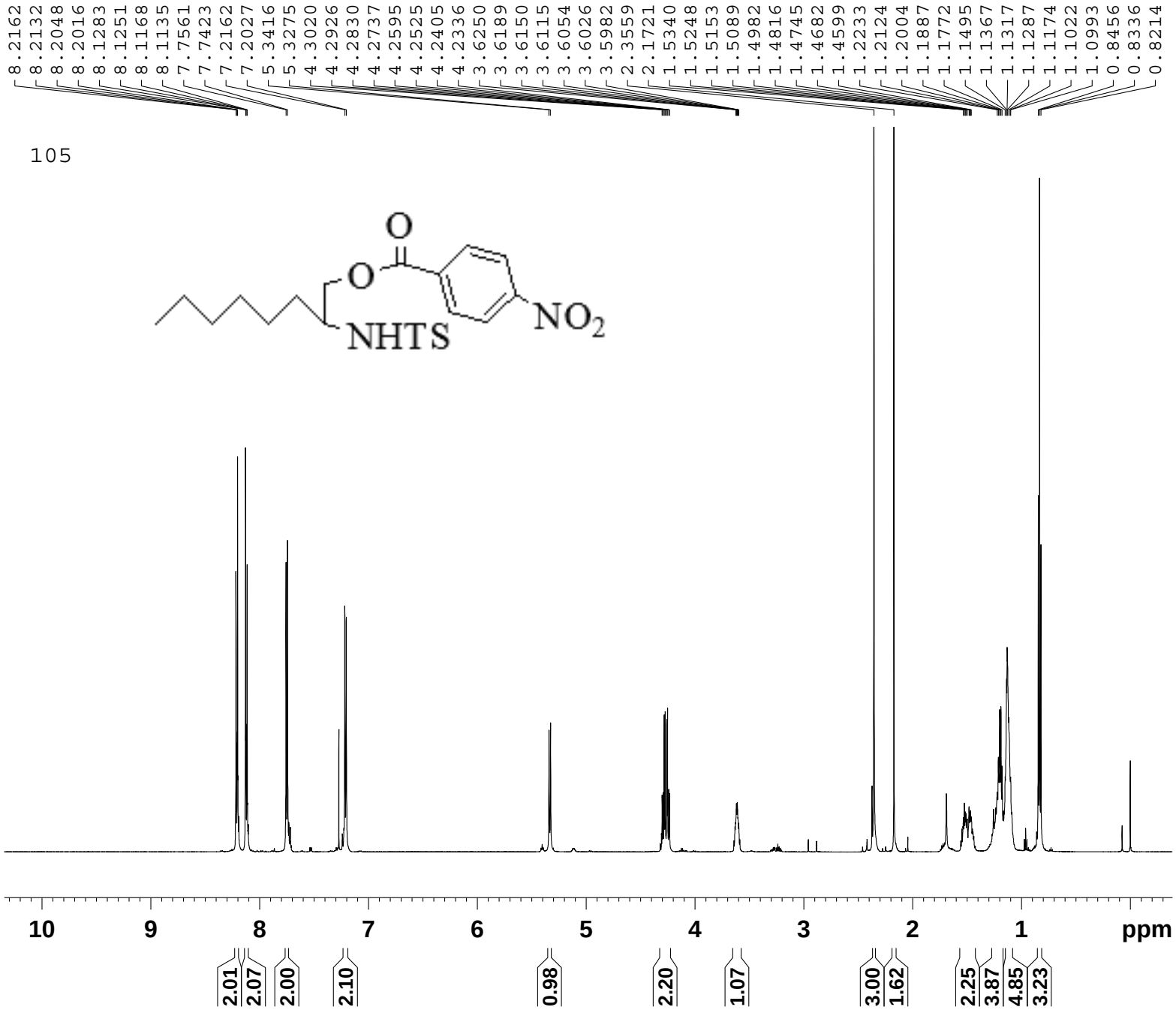
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-21.d	Acquisition Date	7/20/2011 9:36:57 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste





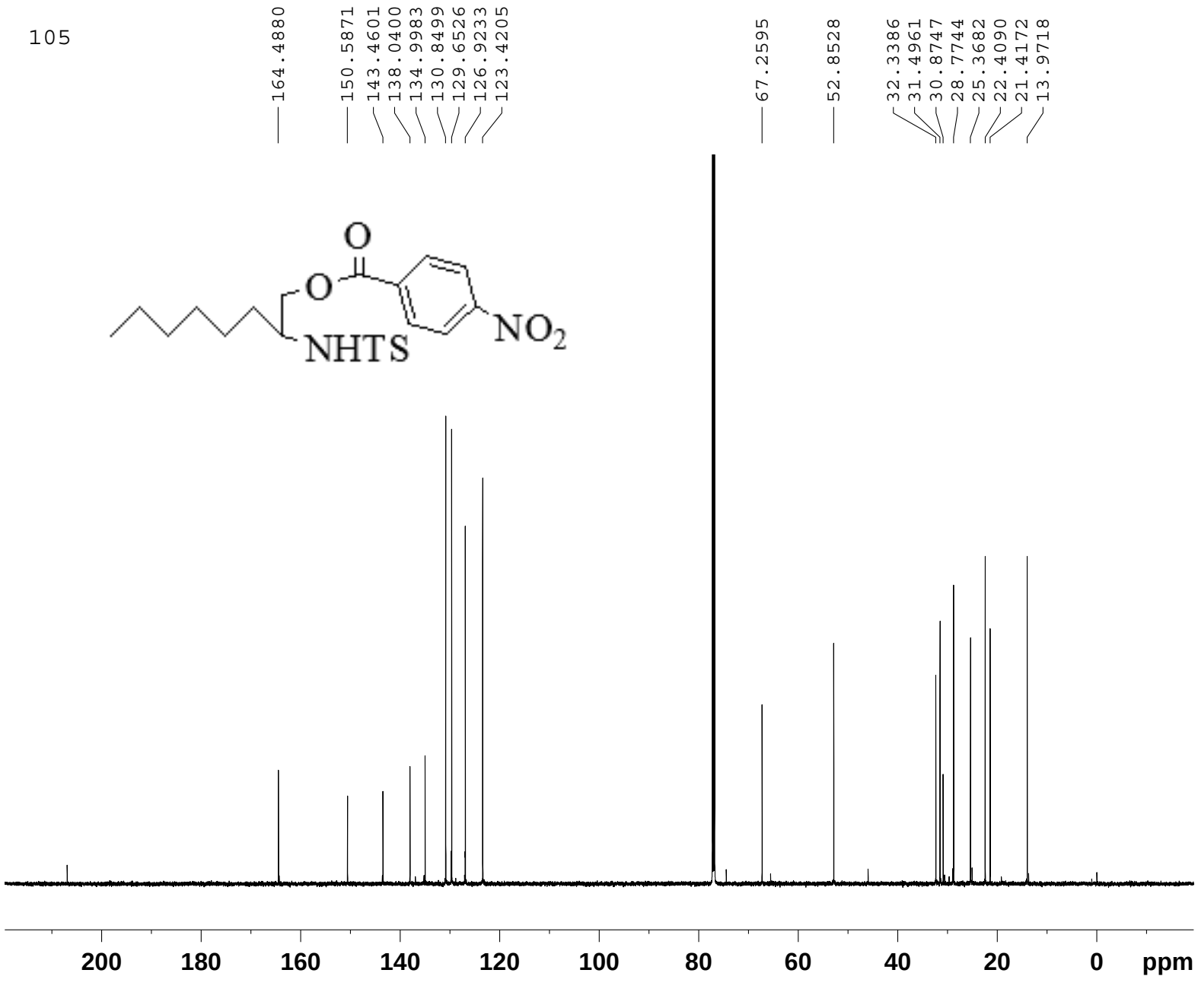
Current Data Parameters
NAME 20110704ligong
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110704
Time 10.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 57
DW 40.533 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300096 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

105




```
Current Data Parameters
NAME      20110712ligong
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20110712
Time              16.33
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1536
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9088159 sec
RG                  203
DW               13.867 usec
DE                6.50 usec
TE                301.9 K
D1           2.00000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                11.30 usec
PLW1        92.68299866 W
SFO1       150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             70.00 usec
PLW2        13.99600029 W
PLW12        0.45346999 W
PLW13        0.22220001 W
SFO2       600.1324005 MHz

F2 - Processing parameters
SI                32768
SF          150.9028096 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

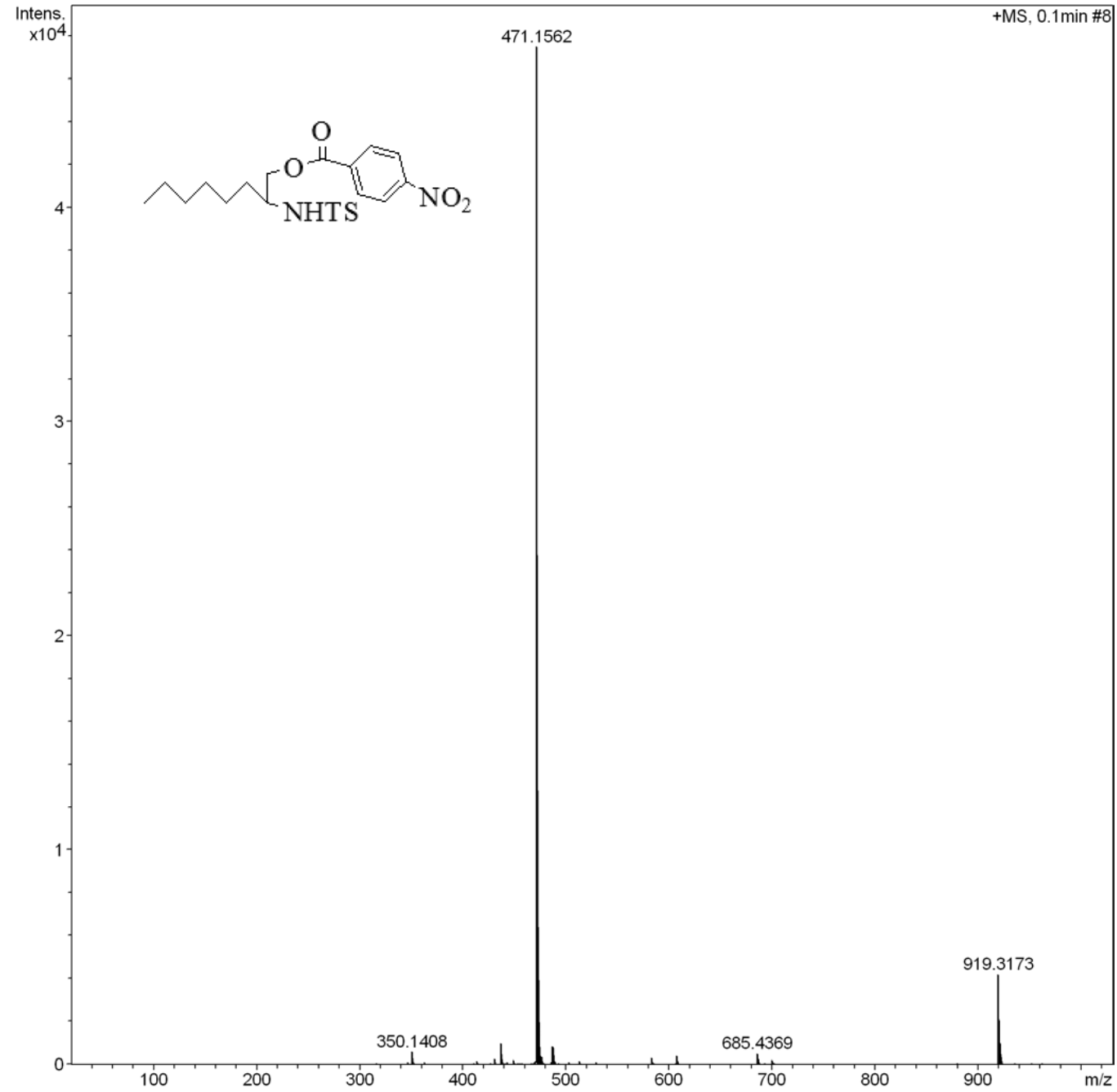
Display Report

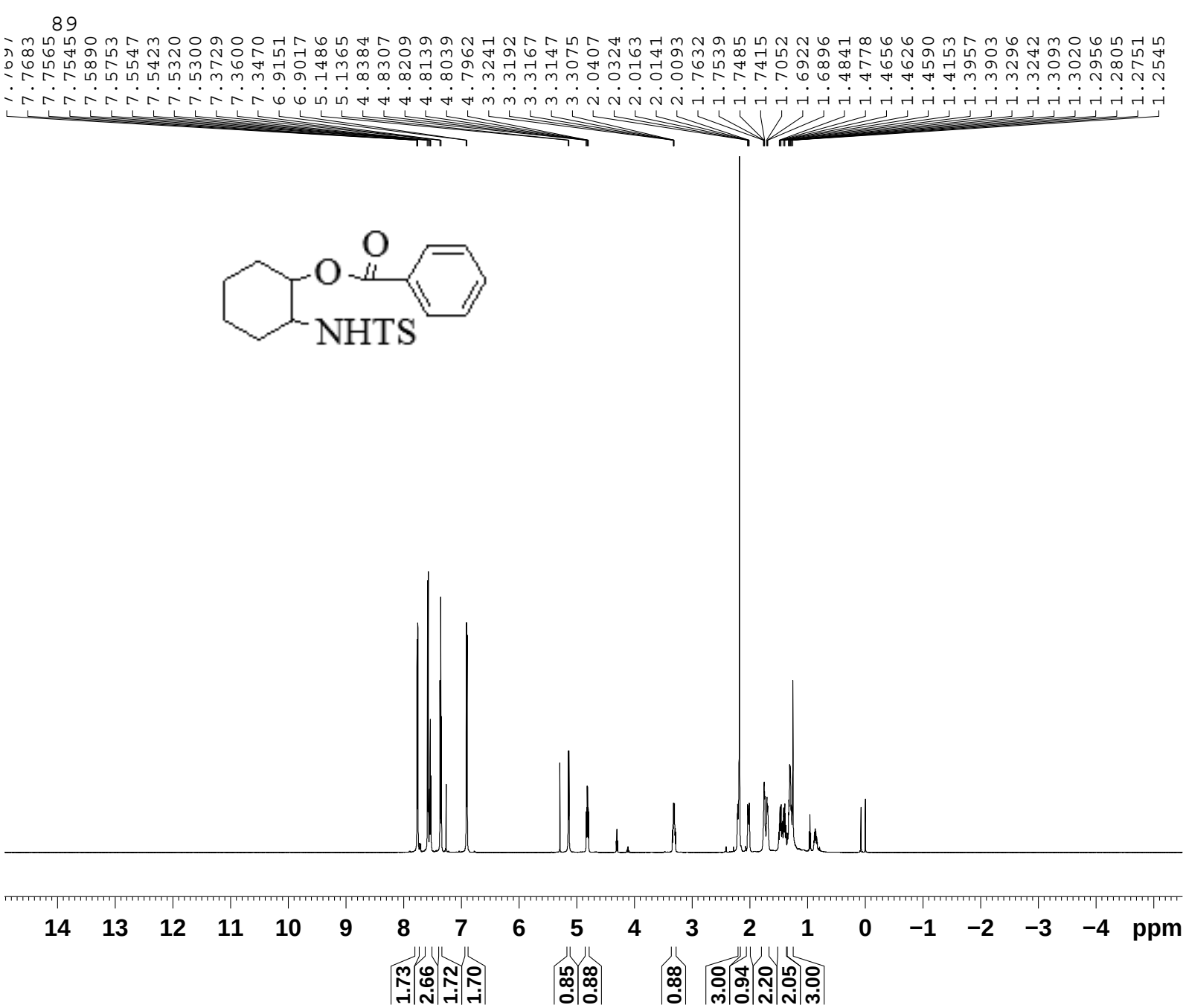
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-20.d	Acquisition Date	7/20/2011 9:58:33 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



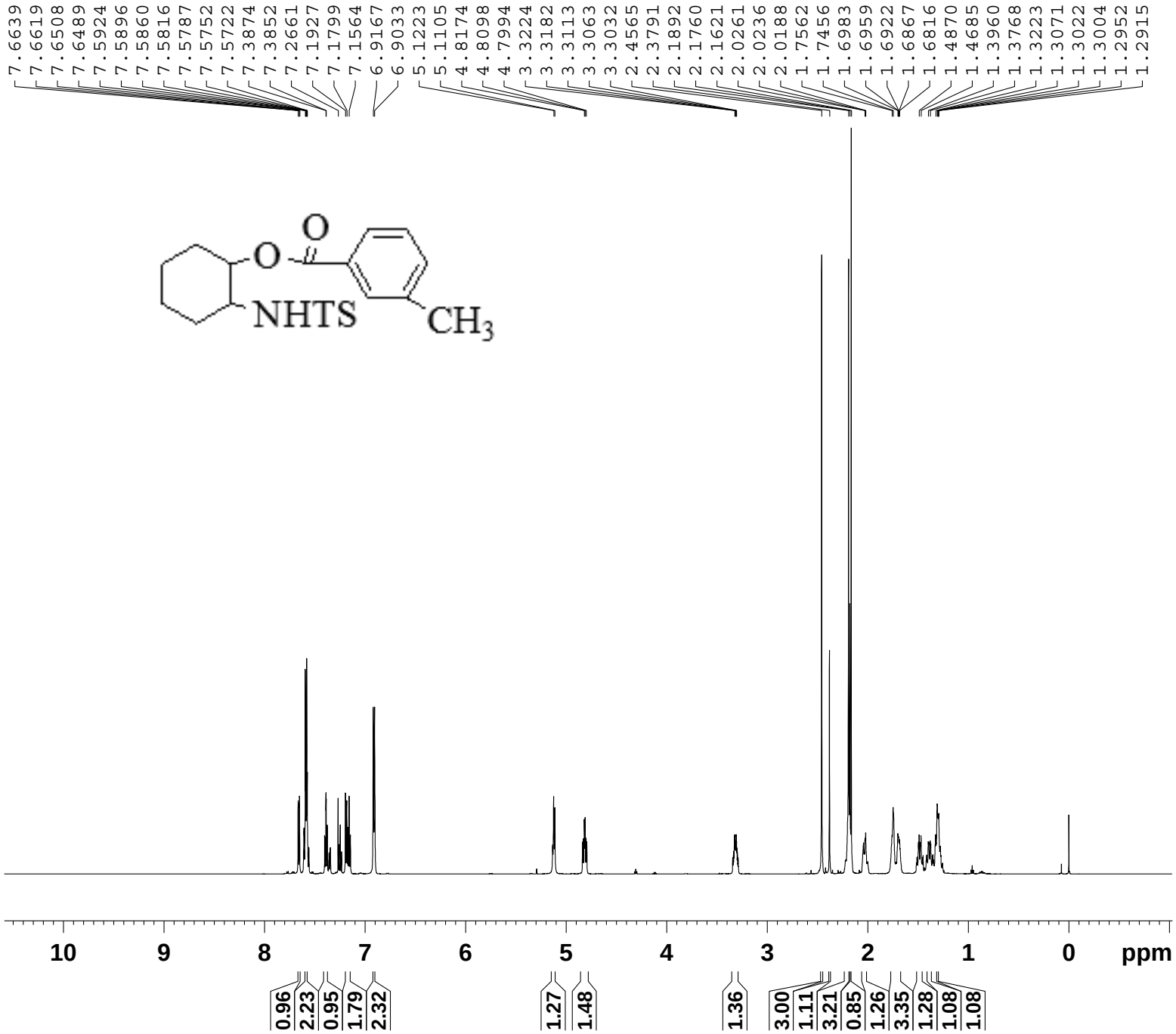


Current Data Parameters
NAME 20110620ligong
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110620
Time 9.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 11
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 40.3
DW 40.533 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300128 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00



BRUKER

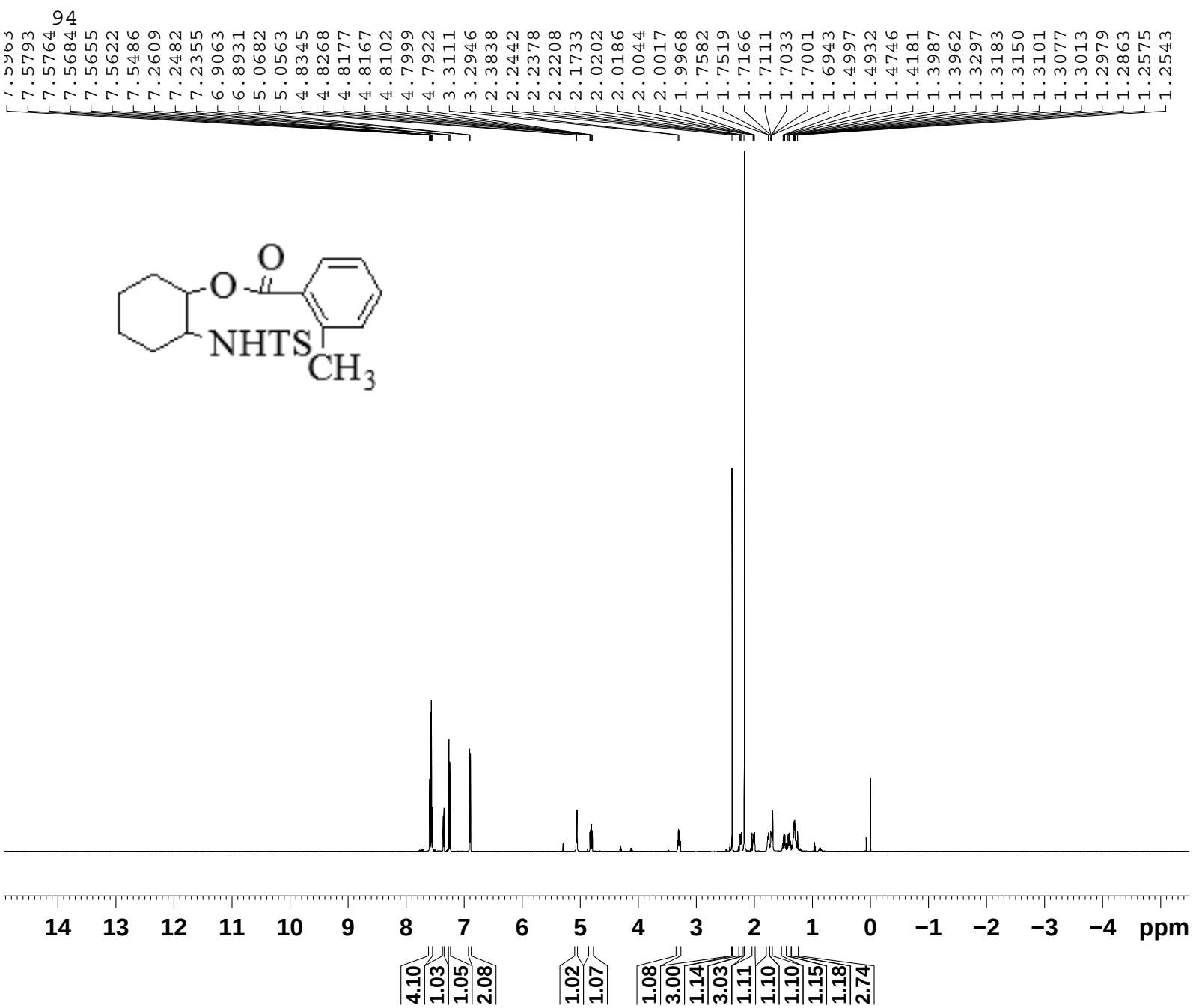
Current Data Parameters
NAME 20110629ligong
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110629
Time 9.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 40.3
DW 40.533 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300127 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

94



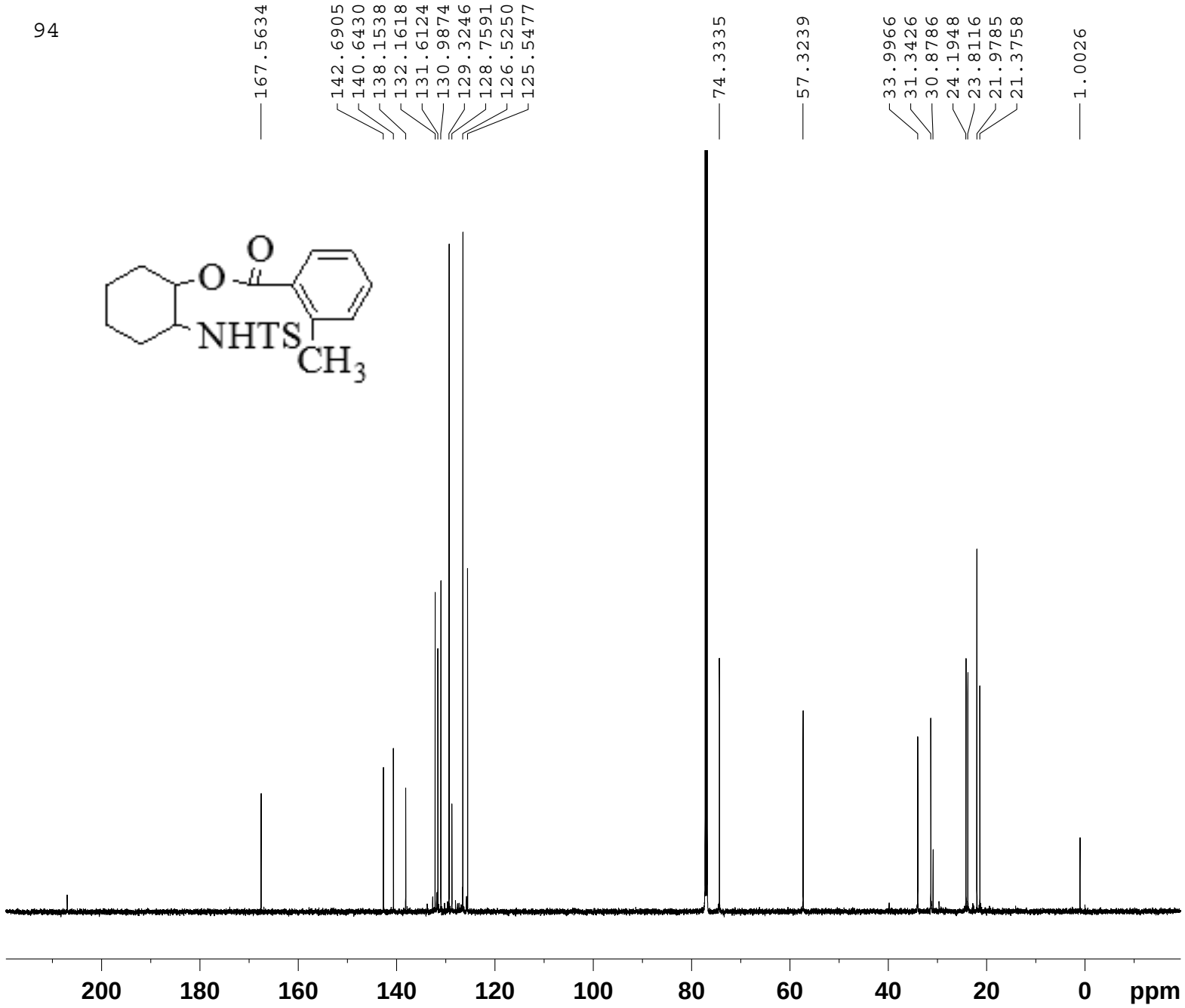
Current Data Parameters
NAME 20110620ligong
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110620
Time 10.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 71.8
DW 40.533 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300120 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

94



BRUKER

Current Data Parameters
NAME 20110712ligong
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110712
Time 15.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1250
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 301.4 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
PLW1 92.68299866 W
SFO1 150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 13.99600029 W
PLW12 0.45346999 W
PLW13 0.22220001 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

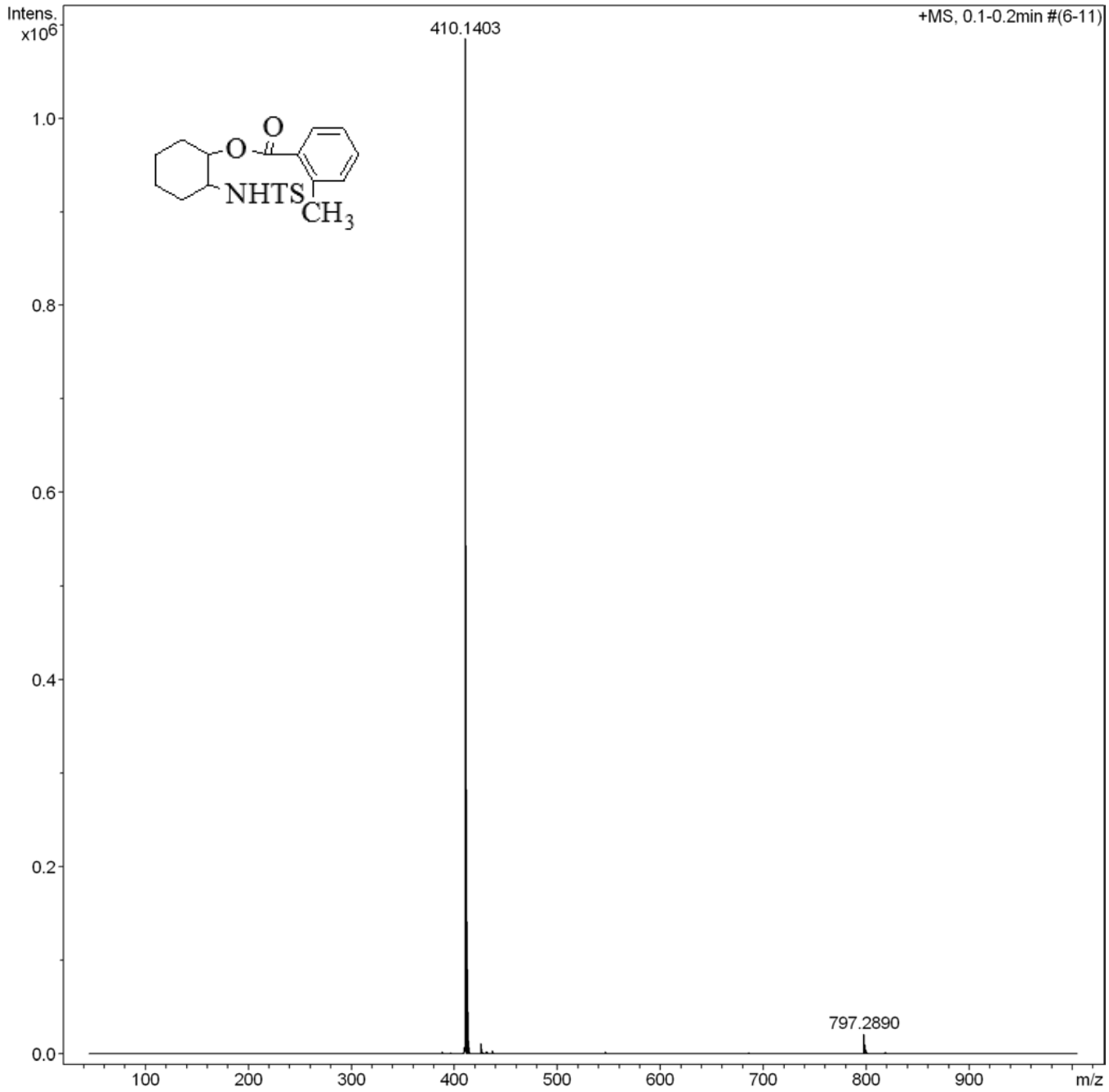
Display Report

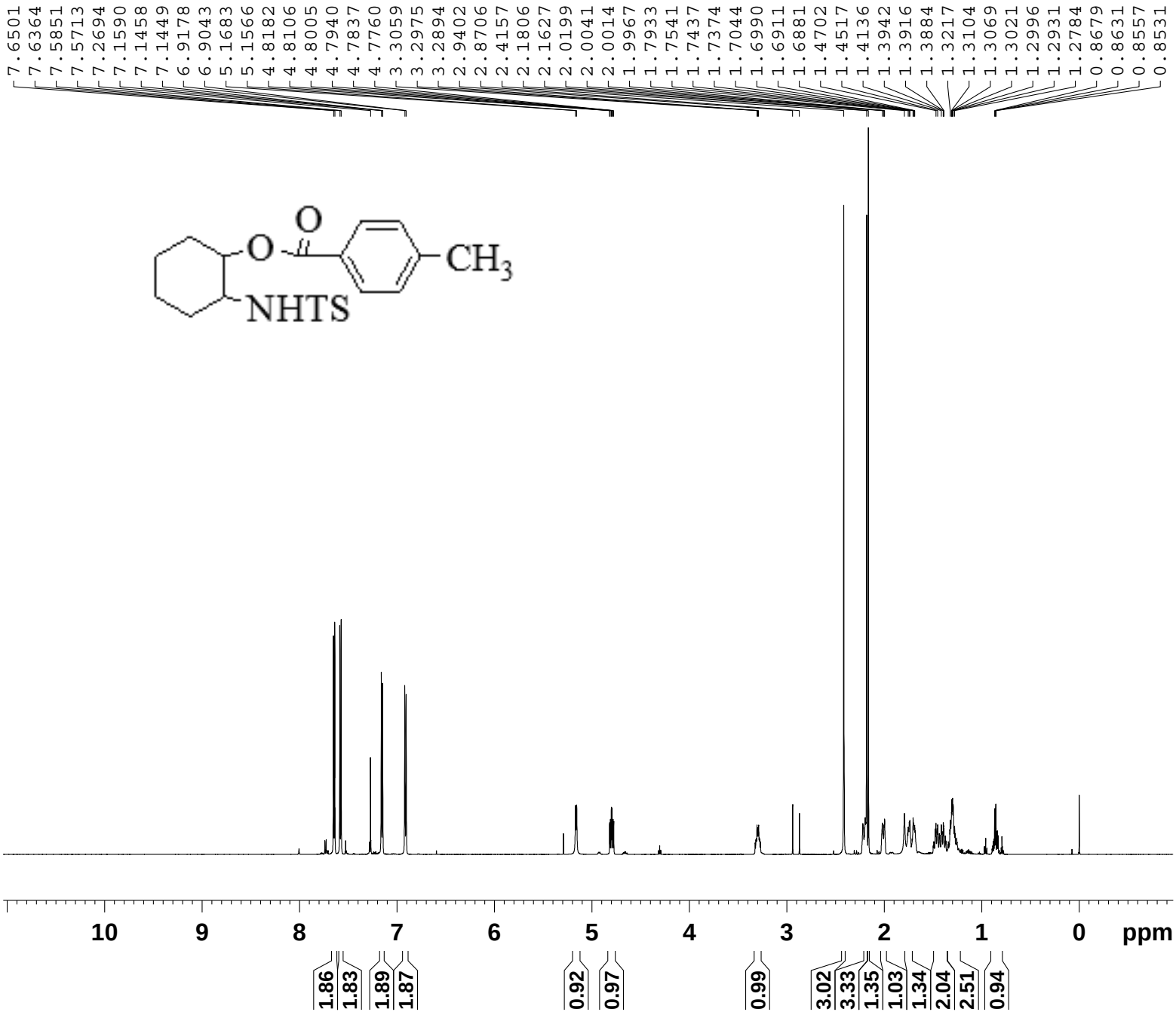
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-6.d	Acquisition Date	7/20/2011 8:59:22 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste





BRUKER

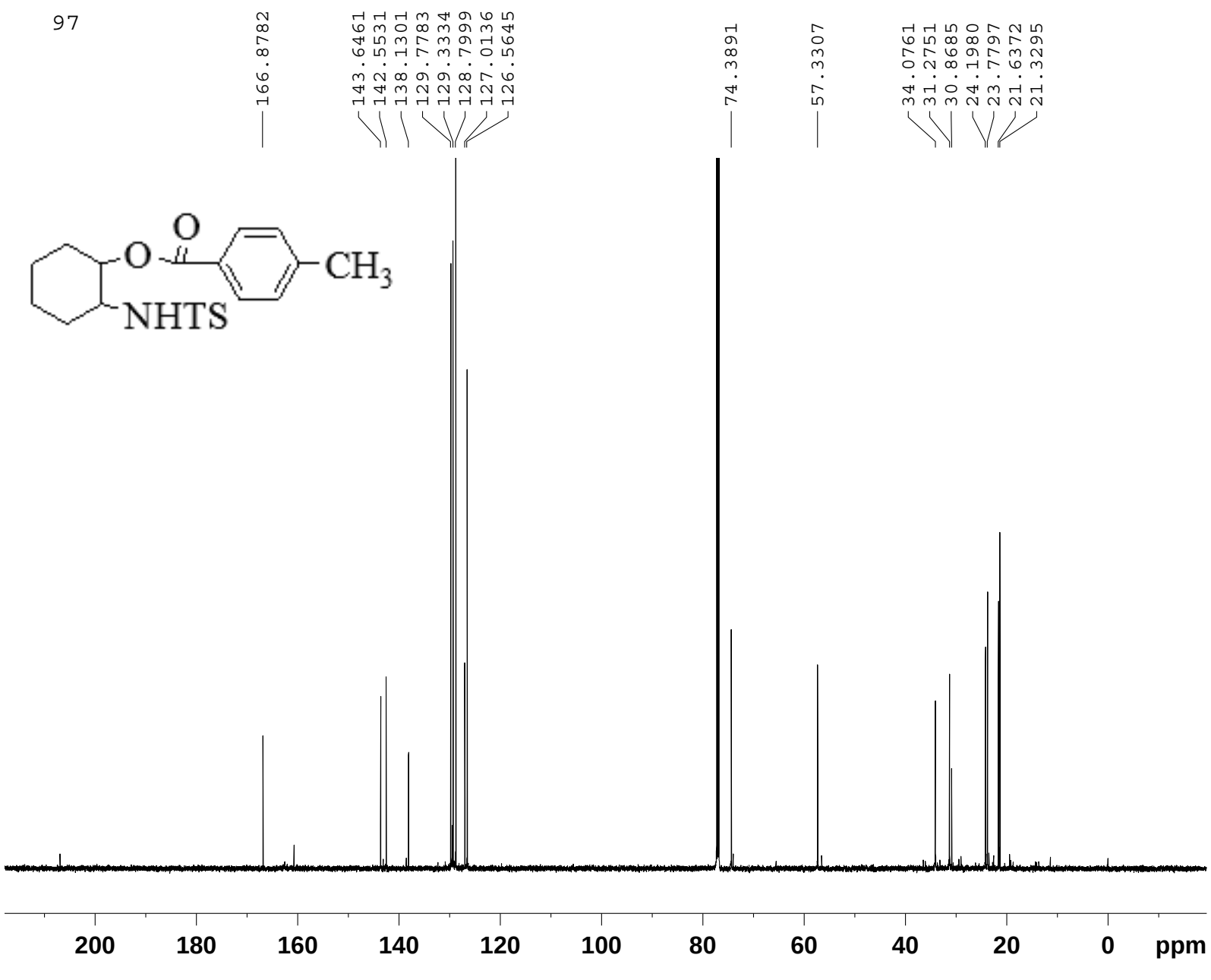
Current Data Parameters
NAME 20110629ligong
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110629
Time 9.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 40.3
DW 40.533 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300104 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

97



Current Data Parameters
NAME 20110629ligong
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110629
Time 15.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 873
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 302.6 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
PLW1 92.68299866 W
SFO1 150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 13.99600029 W
PLW12 0.45346999 W
PLW13 0.22220001 W
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

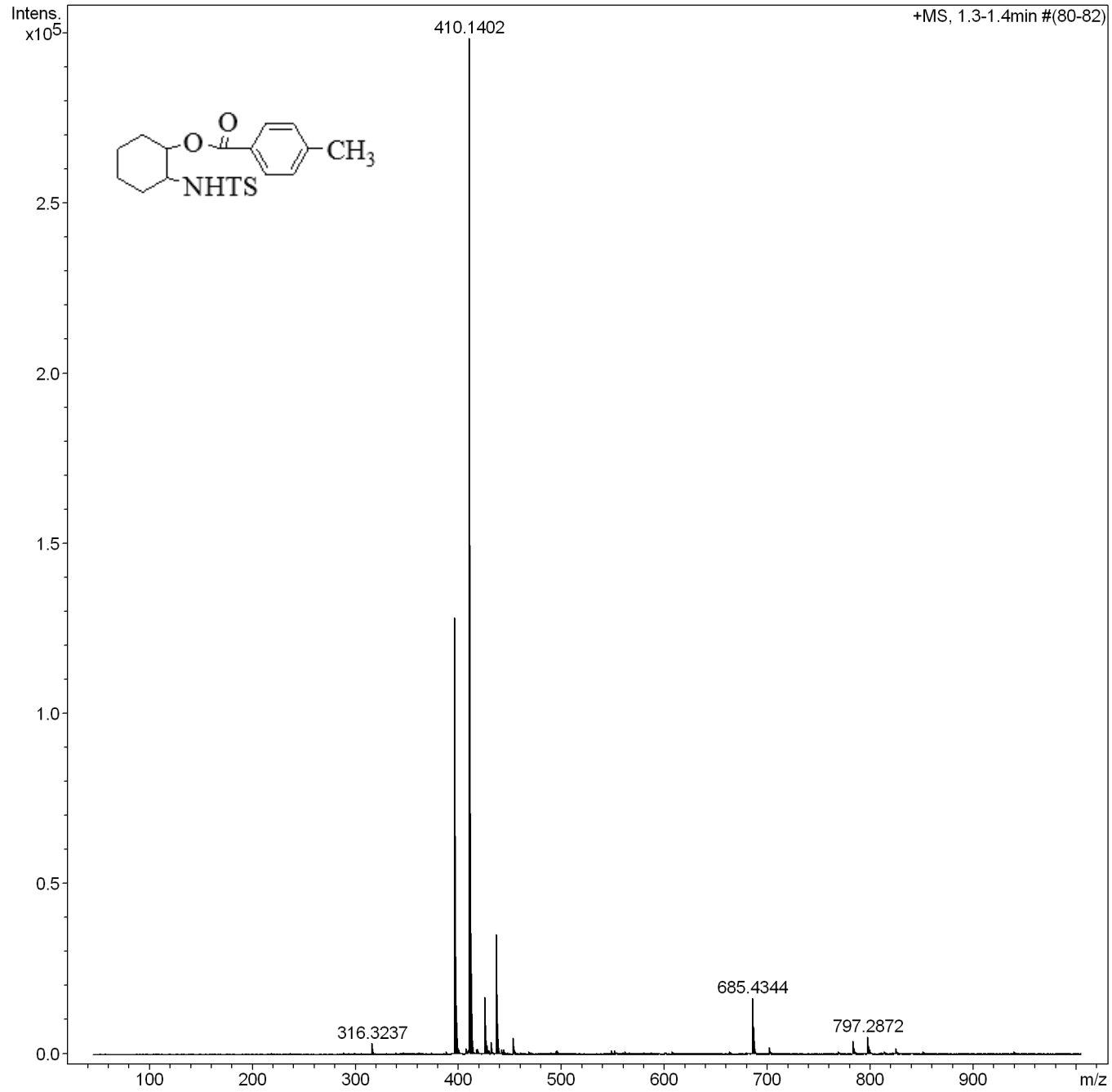
Display Report

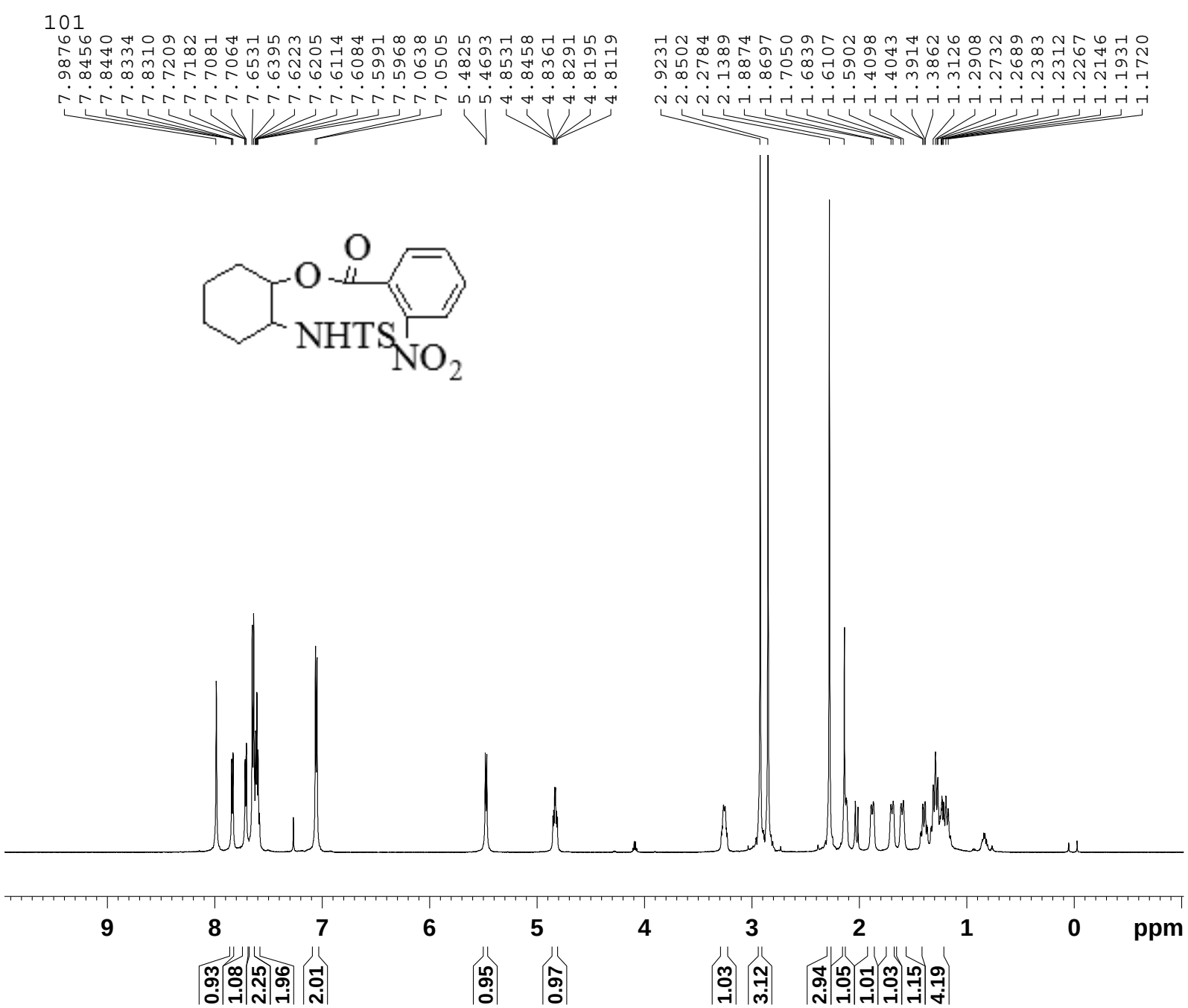
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-4.d	Acquisition Date	7/20/2011 10:03:53 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste





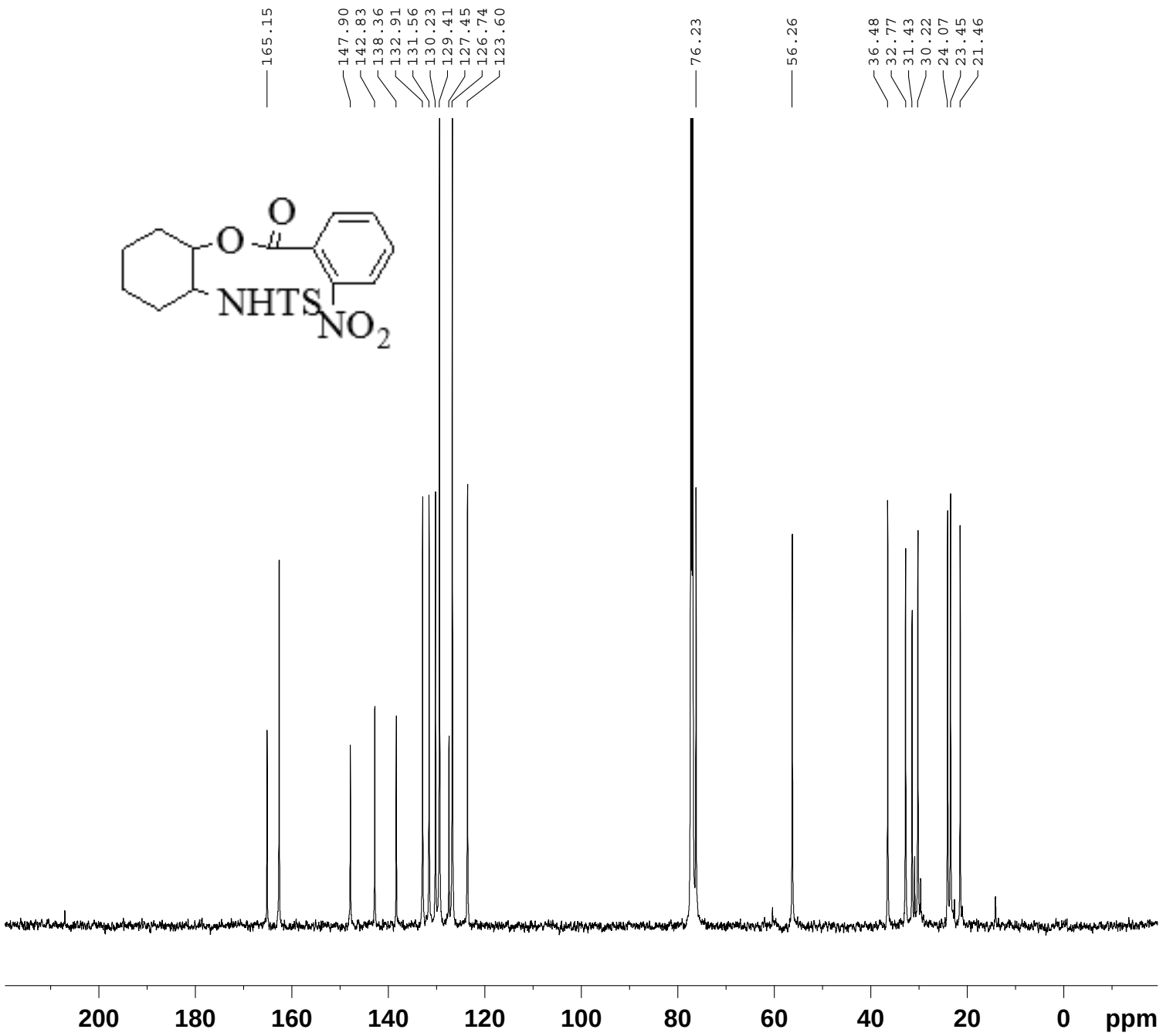
Current Data Parameters
NAME 20110629ligong
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110629
Time 10.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 3
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 40.3
DW 40.533 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300098 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

101




```
Current Data Parameters
NAME      20110629ligong
EXPNO                 13
PROCNO                 1

F2 - Acquisition Paramete
Date_           20110630
Time              10.17
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  860
DS                    2
SWH           36057.691 H
FIDRES         0.550197 H
AQ             0.9088159 s
RG                  203
DW                13.867 u
DE                 6.50 u
TE                297.9 K
D1            2.00000000 s
D11           0.03000000 s

======== CHANNEL f1 =====
NUC1                13C
P1                11.30 u
PLW1         92.68299866 W
SFO1        150.9178988 M

======== CHANNEL f2 =====
CPDPRG2         waltz16
NUC2                1H
PCPD2             70.00 u
PLW2         13.99600029 W
PLW12         0.45346999 W
PLW13         0.22220001 W
SFO2         600.1324005 M

F2 - Processing parameter
SI                32768
SF           150.9028096 M
WDW                  EM
SSB       0
LB                10.00 H
GB        0
PC                 1.40
```

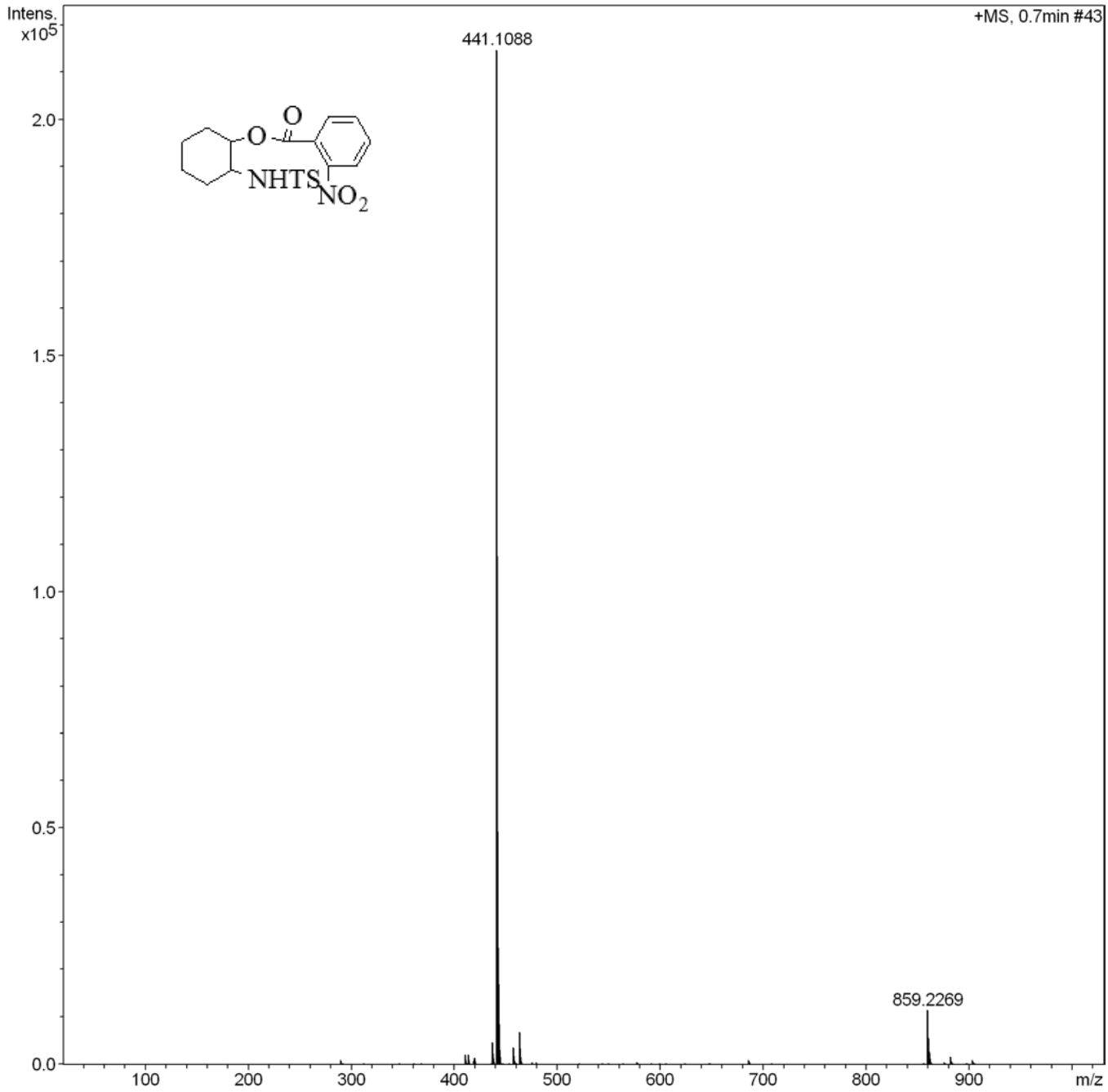
Display Report

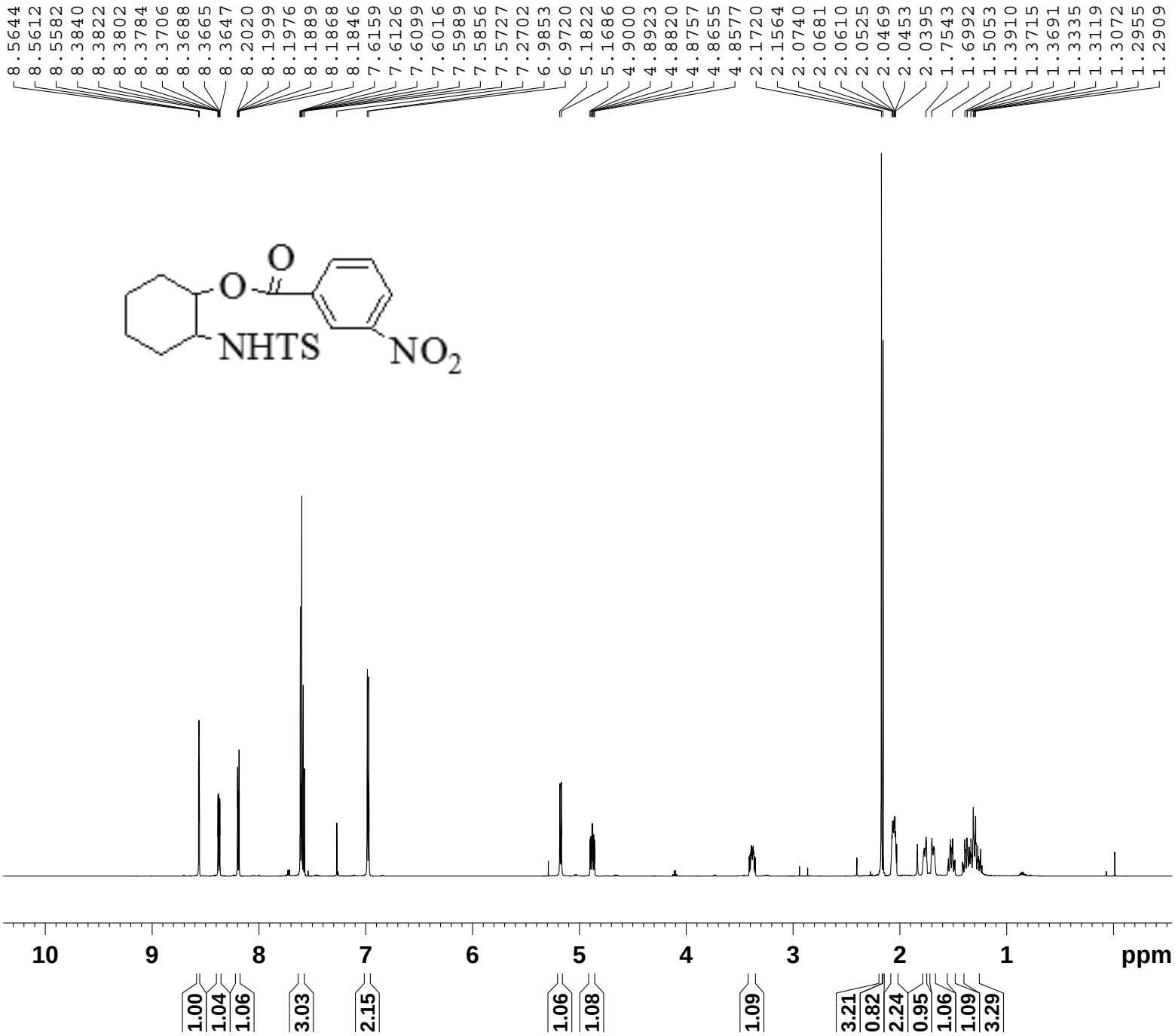
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-2.d	Acquisition Date	7/20/2011 9:09:34 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste





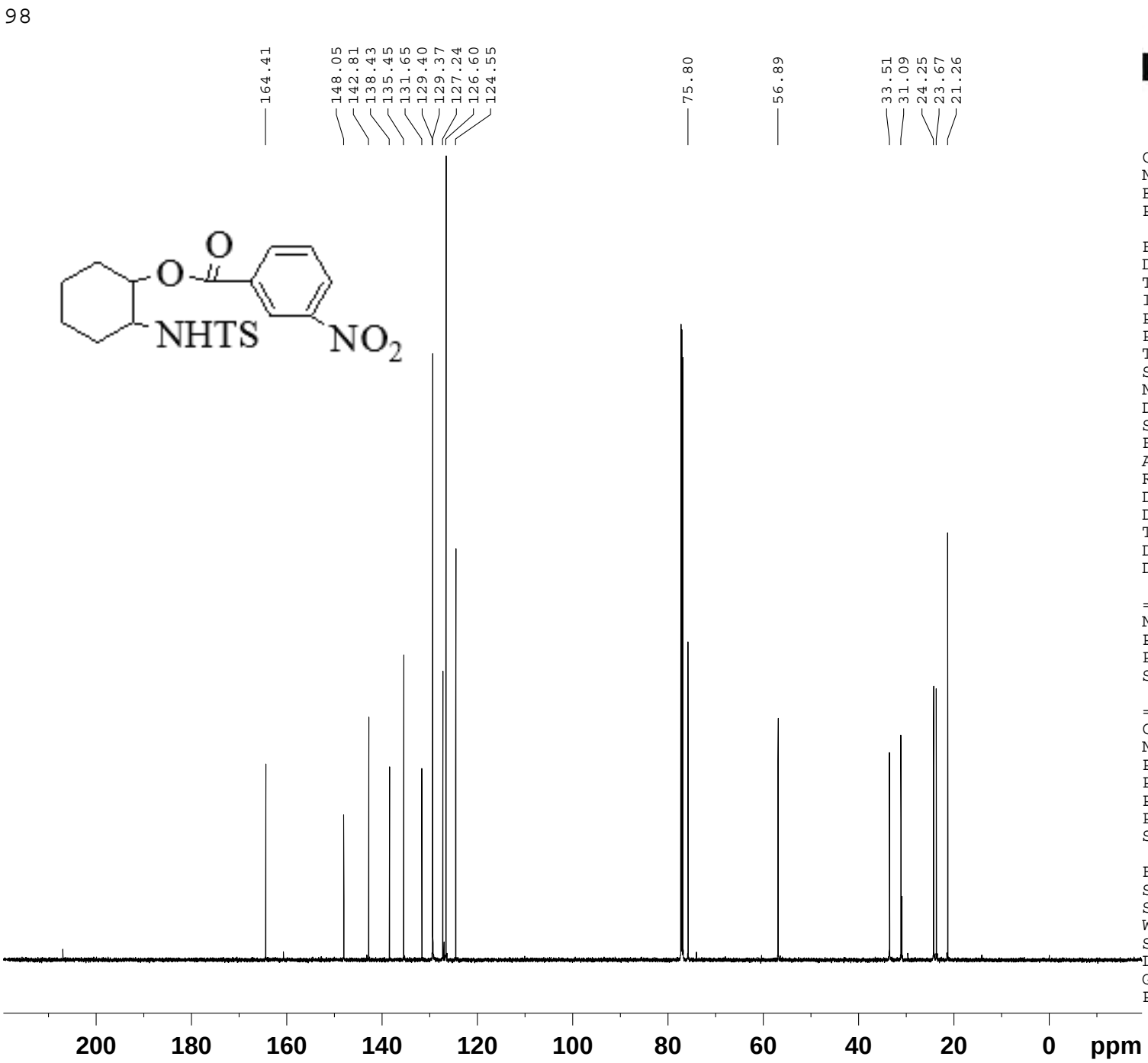
Current Data Parameters
NAME 20110629ligong
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110629
Time 9.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 40.3
DW 40.533 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300098 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

98




```
Current Data Parameters
NAME      20110629ligong
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110629
Time              16.01
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD              65536
SOLVENT           CDCl3
NS                  860
DS                    2
SWH          36057.691 Hz
FIDRES        0.550197 Hz
AQ           0.9088159 sec
RG                  203
DW              13.867 usec
DE               6.50 usec
TE               302.0 K
D1          2.00000000 sec
D11         0.03000000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                11.30 usec
PLW1        92.68299866 W
SFO1        150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            70.00 usec
PLW2        13.99600029 W
PLW12        0.45346999 W
PLW13        0.22220001 W
SFO2        600.1324005 MHz

F2 - Processing parameters
SI                32768
SF          150.9028096 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

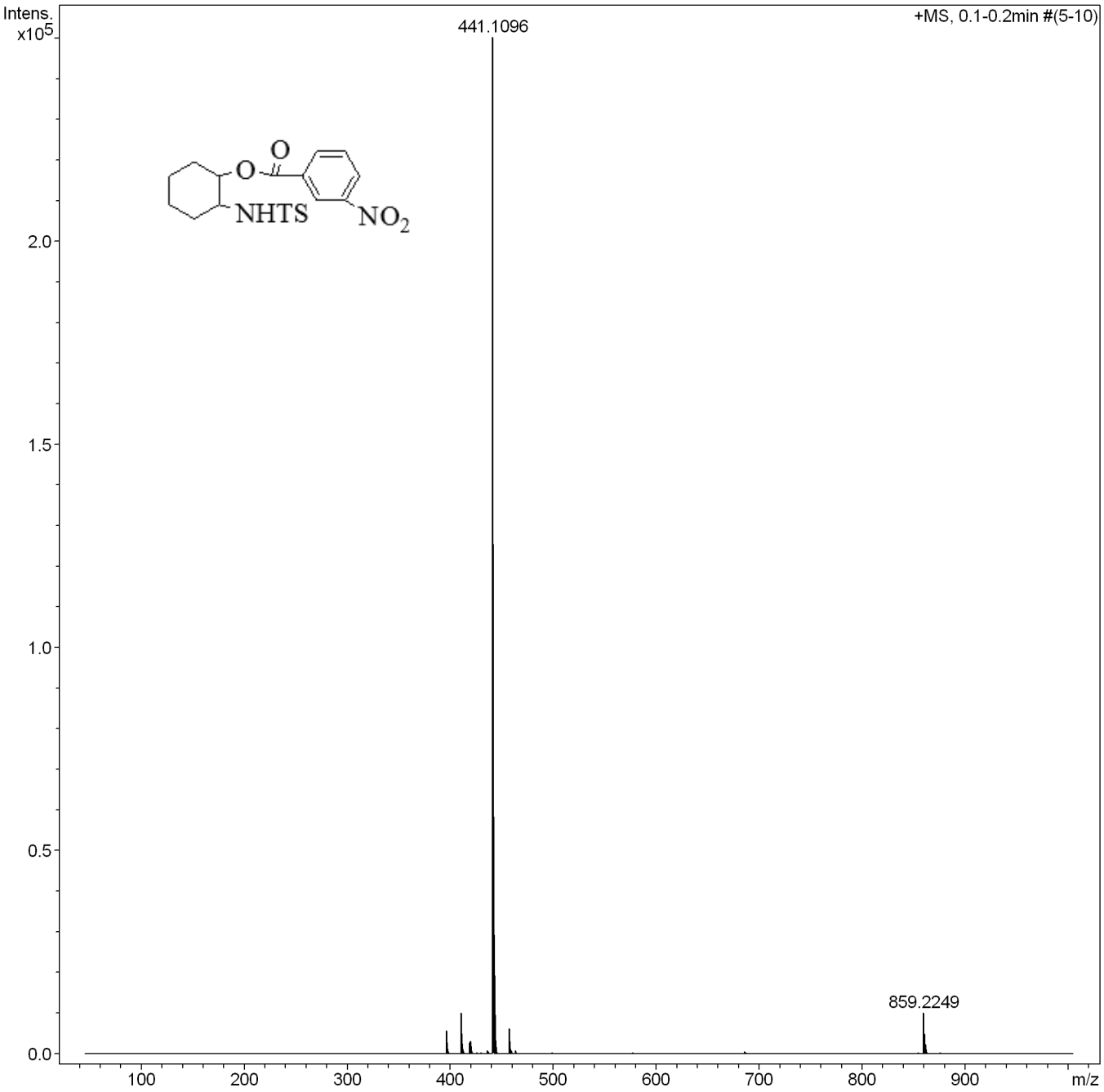
Display Report

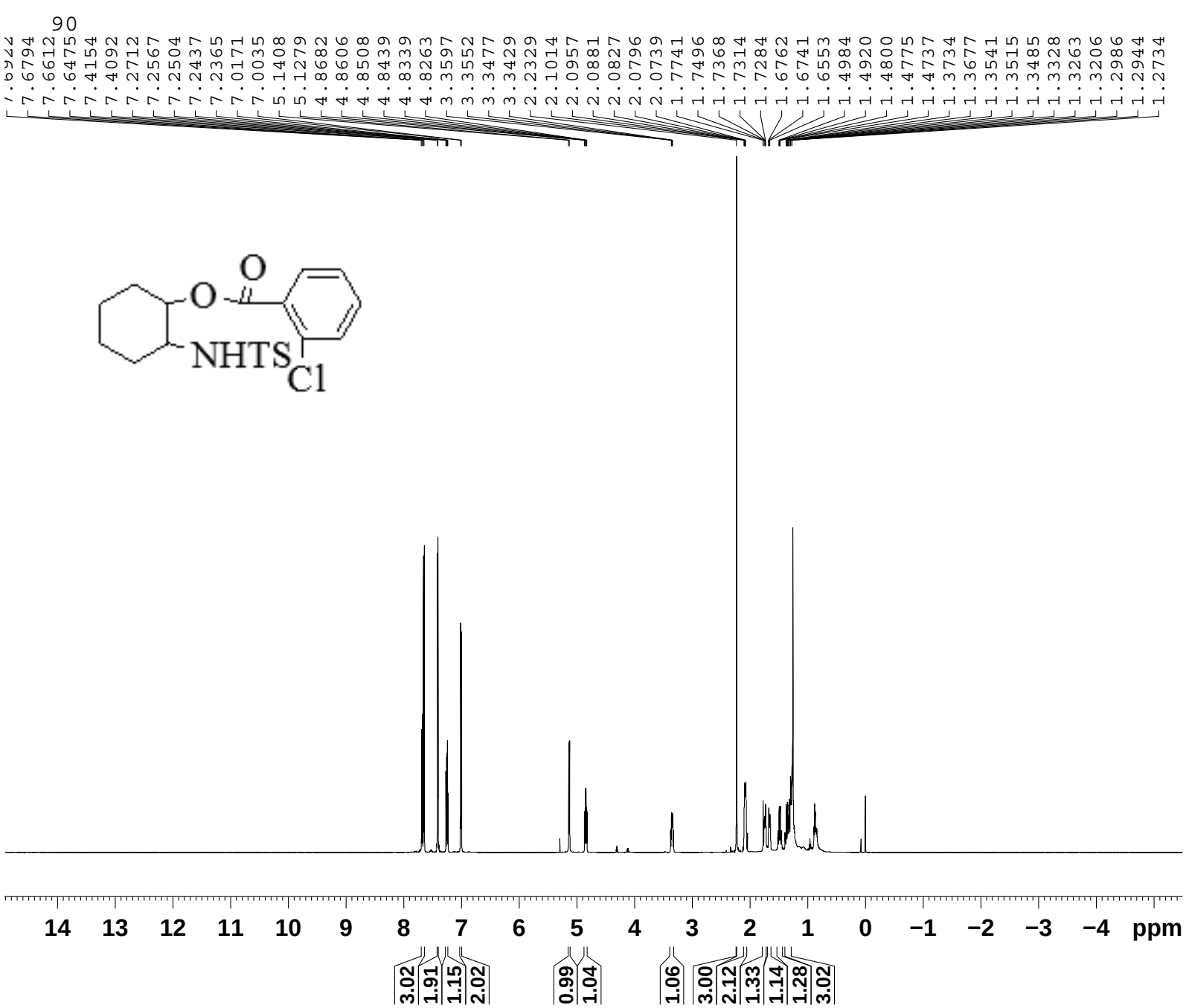
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-3.d	Acquisition Date	7/20/2011 10:06:45 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



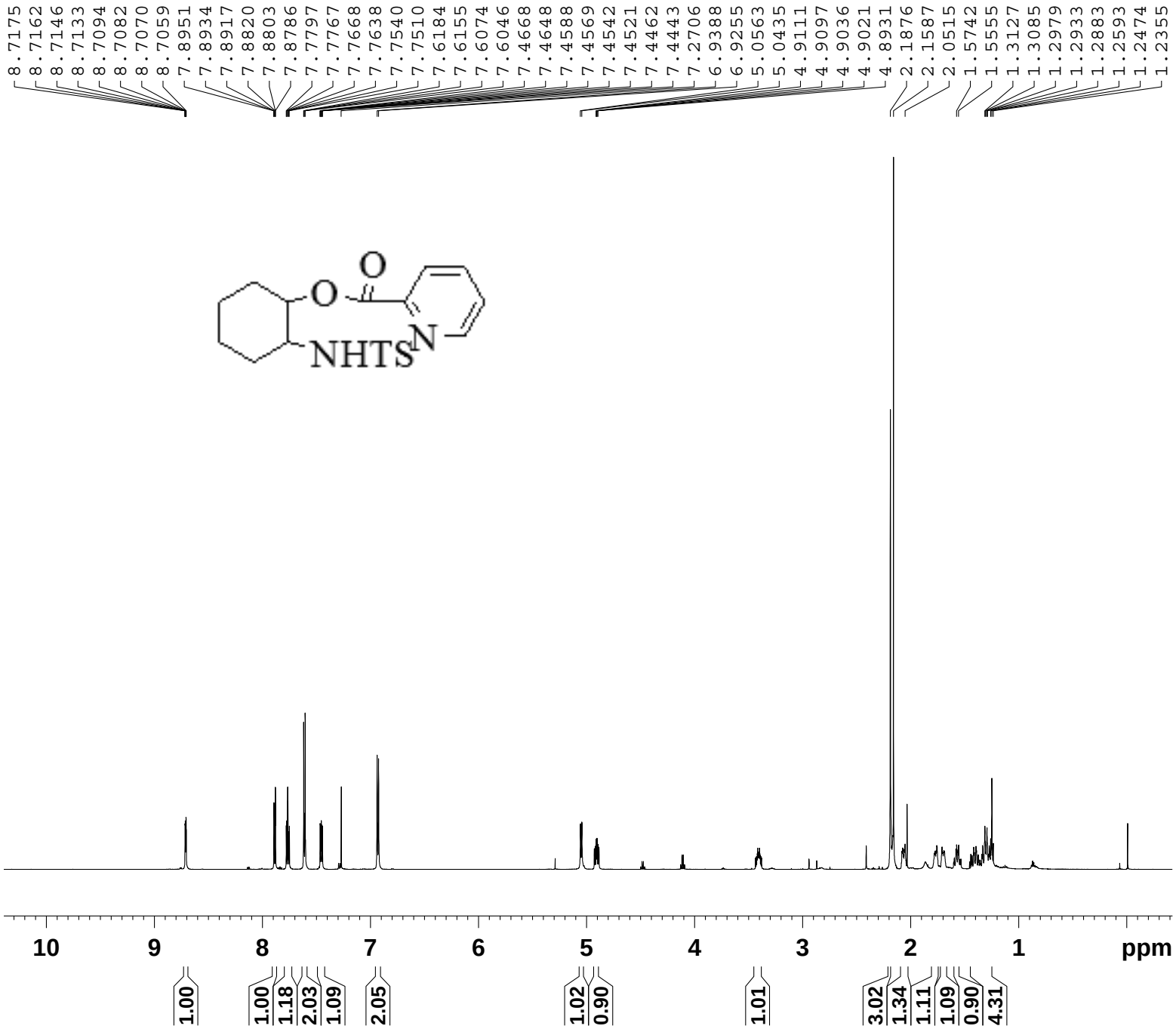


Current Data Parameters
NAME 20110620ligong
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110620
Time 9.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 40.3
DW 40.533 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300098 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00



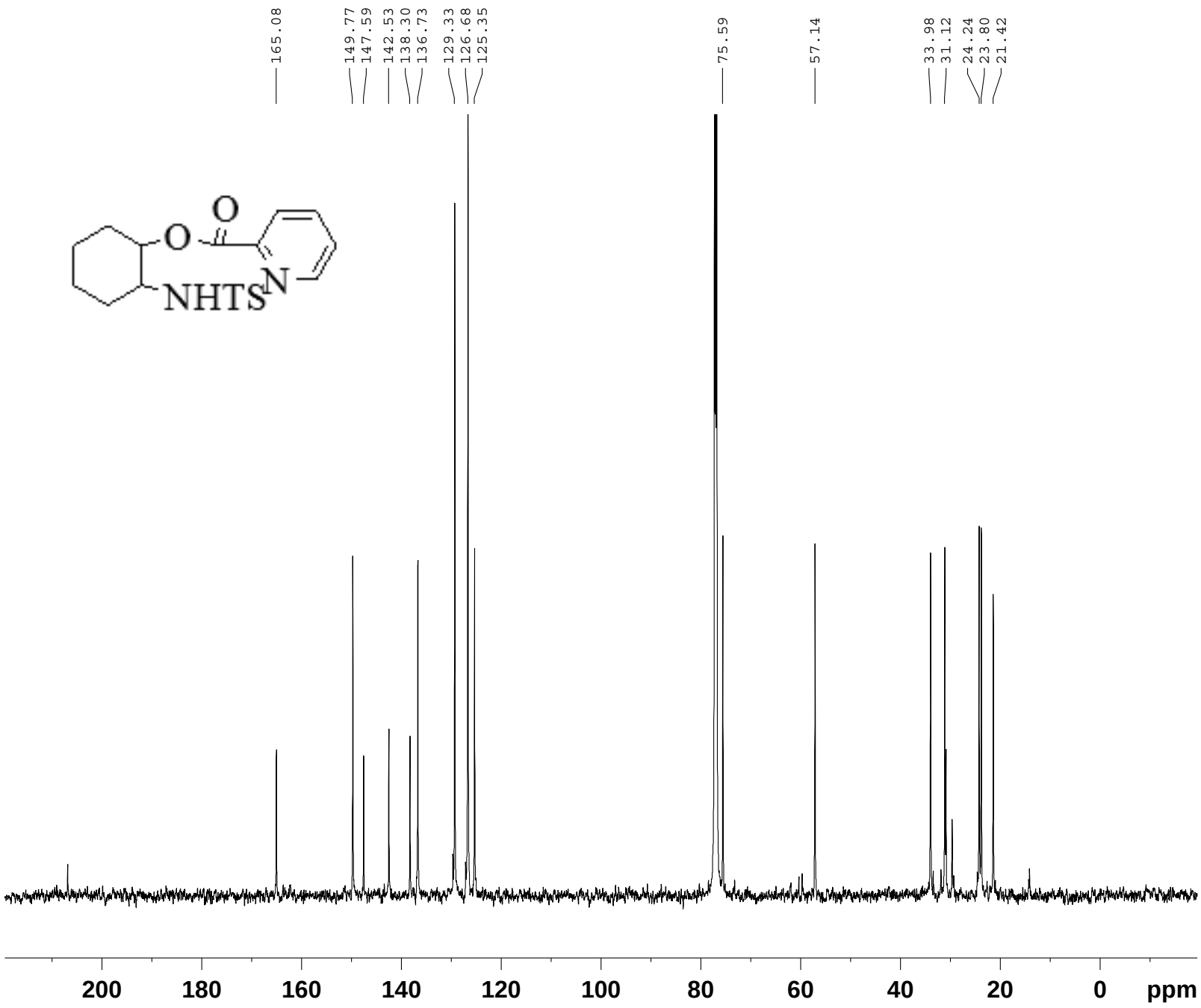
Current Data Parameters
NAME 20110629ligong
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110629
Time 10.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 40.3
DW 40.533 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300098 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

99



BRUKER

```
Current Data Parameters
NAME      20110629ligong
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110629
Time              16.57
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  860
DS                    2
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ             0.9088159 sec
RG                  203
DW                13.867 usec
DE                 6.50 usec
TE                301.8 K
D1            2.00000000 sec
D11           0.03000000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                11.30 usec
PLW1         92.68299866 W
SFO1        150.9178988 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             70.00 usec
PLW2         13.99600029 W
PLW12         0.45346999 W
PLW13         0.22220001 W
SFO2         600.1324005 MHz

F2 - Processing parameters
SI                32768
SF          150.9028096 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

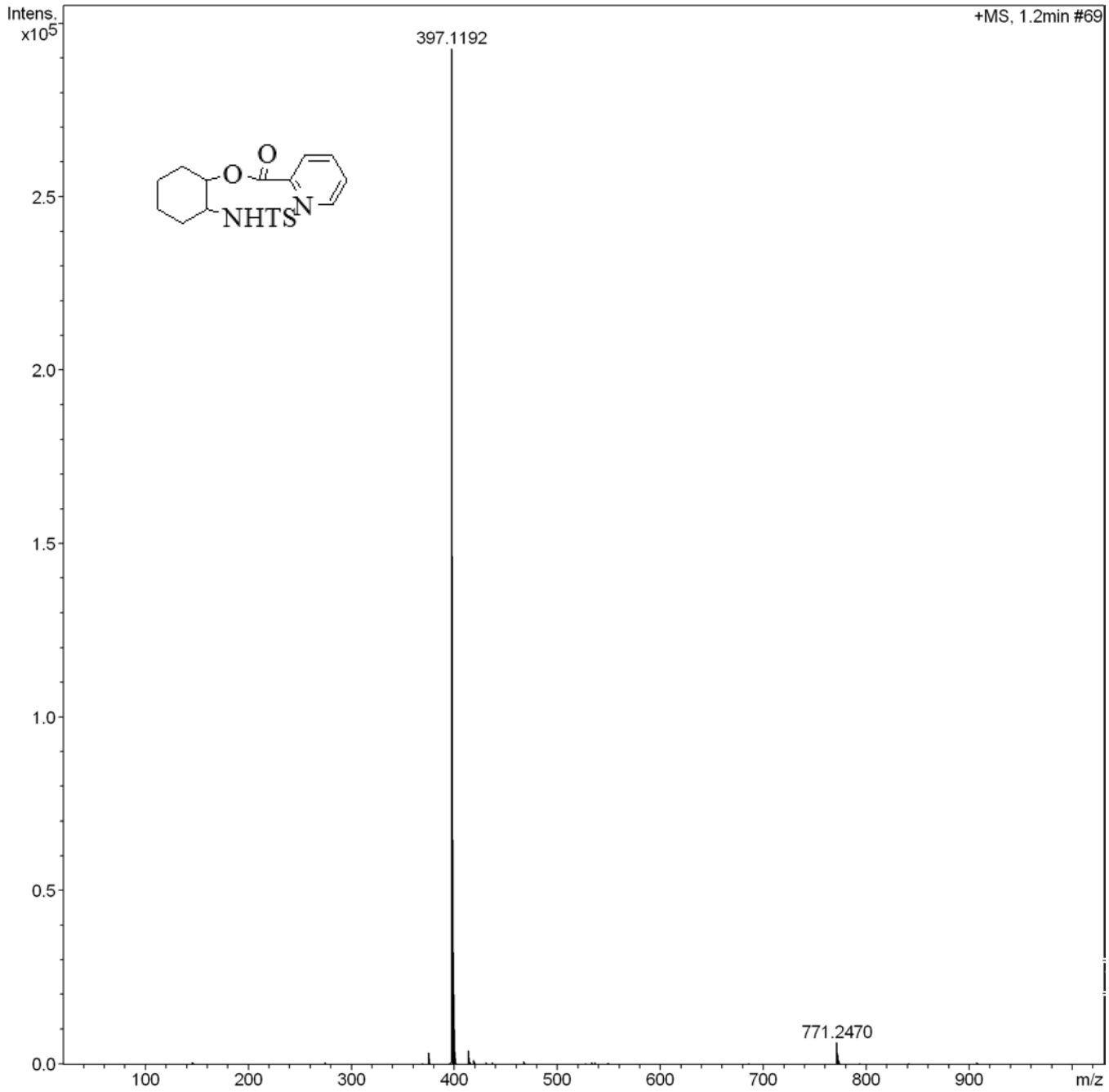
Display Report

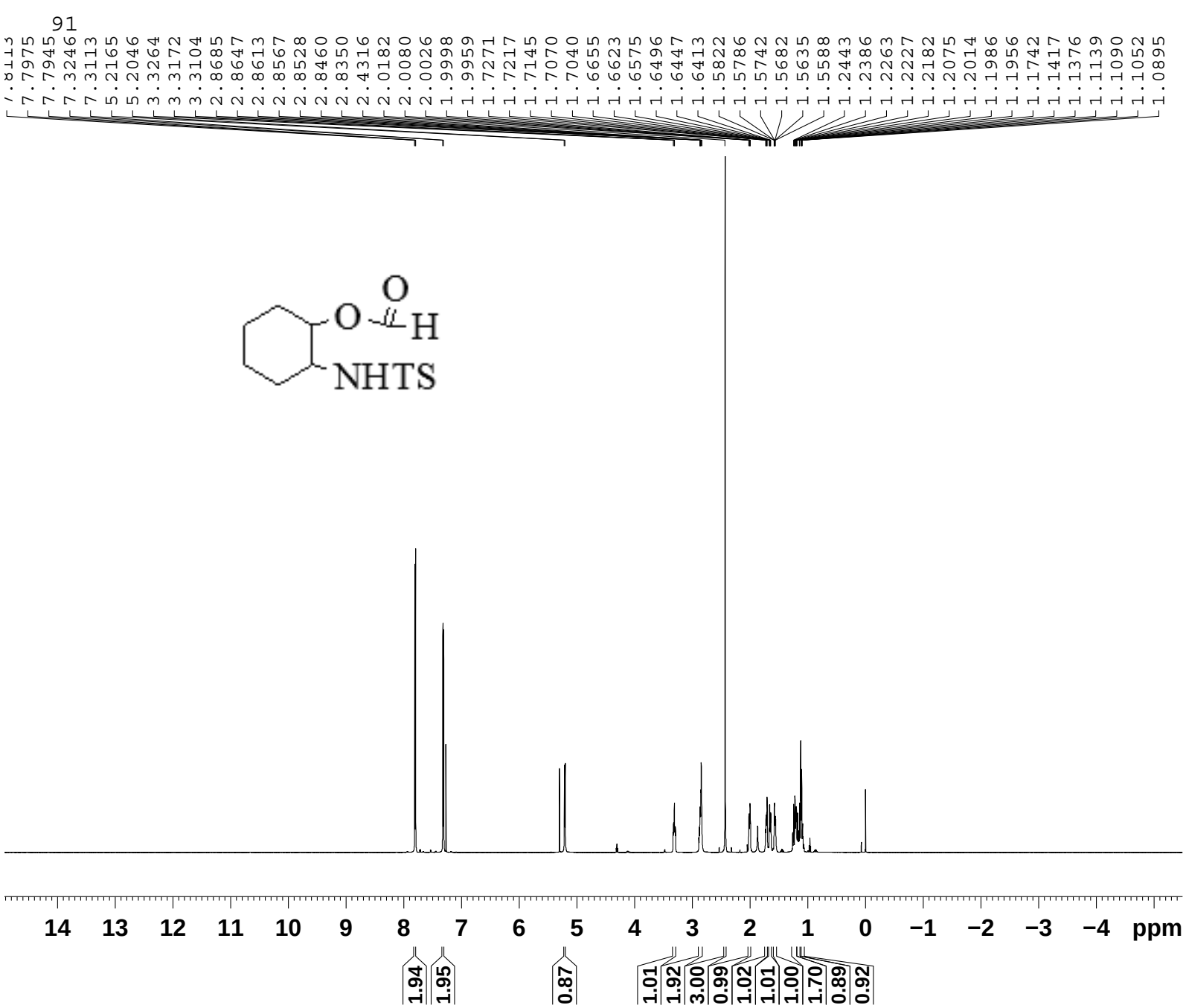
Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110720-5.d	Acquisition Date	7/20/2011 8:23:45 PM
Method	tune_wide.m	Operator	TJU
Sample Name	20110718-1M-NH4Cl	Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



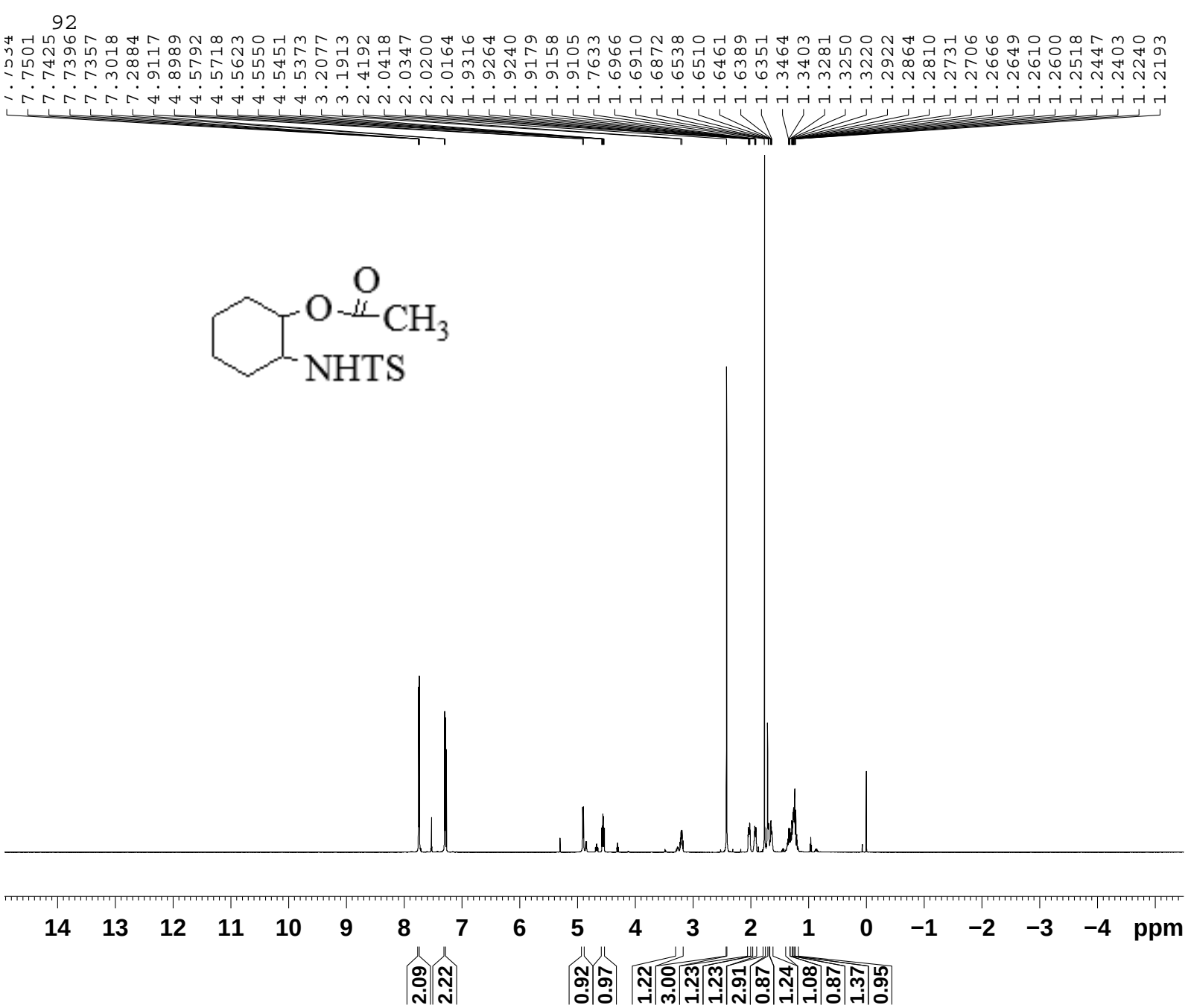


Current Data Parameters
NAME 20110620ligong
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110620
Time 9.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 40.3
DW 40.533 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300094 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

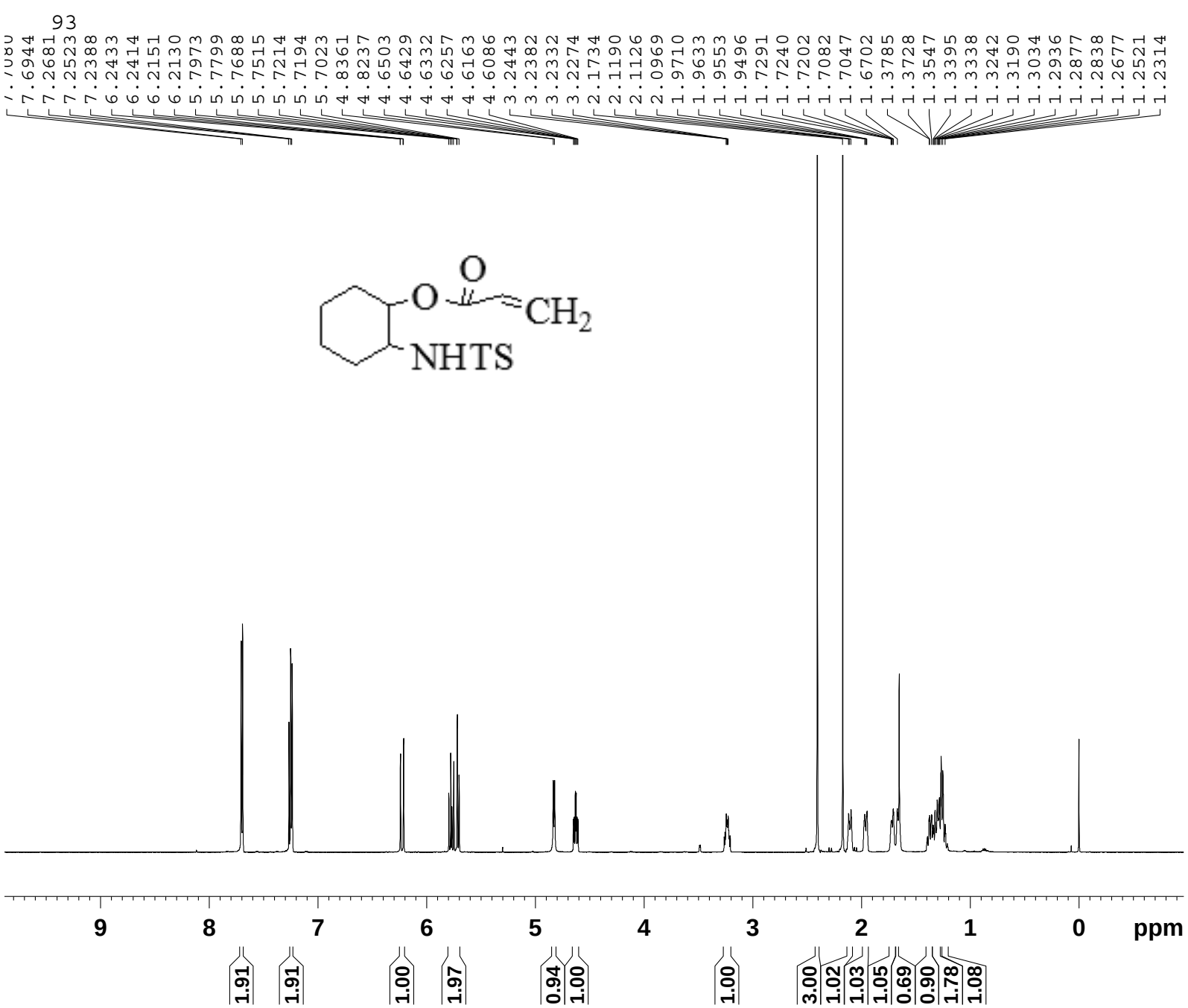


Current Data Parameters
NAME 20110620ligong
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110620
Time 9.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 71.8
DW 40.533 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300099 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20110620ligong
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110620
Time 10.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 71.8
DW 40.533 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 13.99600029 W
SFO1 600.1328806 MHz

F2 - Processing parameters
SI 32768
SF 600.1300125 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00