Electronic Supplementary Material (ESI) for Chemical Communications

A Palladium-Catalyzed Three-Component Reaction for the Preparation of Quinazolin-4(3H)-imines

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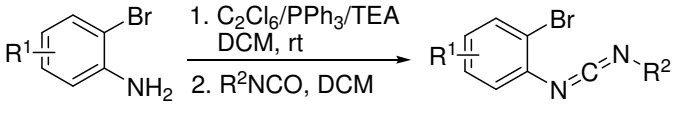
Supporting Information

General experimental methods:

Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr at 25–35°C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constants quoted in Hz. High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF II Instrument.

The carbodiimides **1** were synthesized according to literature method (F. Zeng and H. Alper, *Org. Lett.* 2010, **12**, 1188.)



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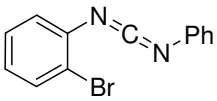
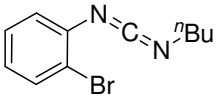


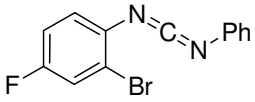
2-Bromo-N-((phenylimino)methylene)aniline **1a** (X. Lv and W. Bao, *J. Org. Chem.* 2009, **74**, 5618.)

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.85 (t, J = 7.2 Hz, 1H), 7.16-7.22 (m, 4H), 7.27-7.34 (m, 3H), 7.79 (d, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 93.6, 124.5, 124.7, 125.7, 126.7, 129.2, 129.4, 132.6, 137.6, 139.5, 140.9. LC-MS (ESI): 273 (M^{+}+H).



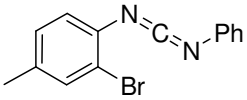
2-Bromo-N-((butylimino)methylene)aniline **1b**

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.93 (t, *J* = 7.2 Hz Hz, 3H), 1.42-1.44 (m, 2H), 1.64-1.67 (m, 2H), 3.44 (t, *J* = 6.4 Hz Hz, 2H), 6.76-6.79 (m, 1H), 7.15 (d, *J* = 7.6 Hz, 1H), 7.23-7.27 (m, 1H), 7.75 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.5, 19.8, 33.0, 46.2, 93.1, 123.5, 125.6, 129.0, 138.0, 139.2, 142.9. LC-MS (ESI): 253 (M^++H); HRMS Calcd for $C_{11}H_{14}BrN_2$ (ESI, M^++H): 253.0340; Found: 253.0346.



2-Bromo-4-fluoro-N-((phenylimino)methylene)aniline **1c**

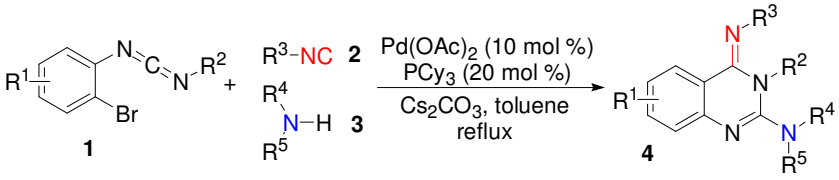
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.96-7.00 (m, 1H), 7.16-7.22 (m, 4H), 7.30-7.34 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 115.4 (d, *J* = 14 Hz), 120.2 (d, *J* = 25 Hz), 124.1, 124.4, 125.6, 125.7, 126.2, 129.5, 137.6, 138.3, 159.8 (d, *J* = 259 Hz). LC-MS (ESI): 291 (M^++H); HRMS Calcd for $C_{13}H_9BrFN_2$ (ESI, M^++H): 290.9933; Found: 290.9947.



2-Bromo-4-methyl-N-((phenylimino)methylene)aniline **1d** (X. Lv and W. Bao, *J. Org. Chem.* 2009, **74**, 5618.)

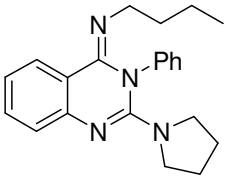
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.28 (s, 3H), 7.10-7.13 (m, 2H), 7.15 (m, 3H), 7.30-7.34 (m, 2H), 7.63 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.4, 93.4, 124.3, 124.4, 125.6, 129.4, 130.0, 136.9, 137.9, 139.7. LC-MS (ESI): 287 (M^++H).

General Procedure for the Palladium-Catalyzed Three-Component Reaction of Carbodiimide 1, Isocyanide 2, and Nucleophile 3



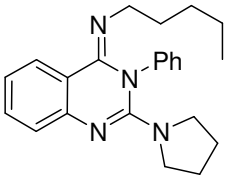
$Pd(OAc)_2$ (10 mol %), PCy_3 (20 mol %), and Cs_2CO_3 (2 equiv) were added into a solution of carbodiimide **1** (0.2 mmol) in dry toluene (3.0 mL). Subsequently nucleophile **2** (3 equiv) and isocyanide **3** (1.5 equiv) were added. The mixture was

stirred at reflux under N_2. After completion of the reaction as indicated by TLC, the solvent was evaporated and the residue was purified on silica gel to provide the desired product **4.**



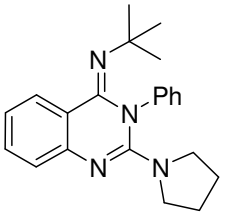
N-(3-Phenyl-2-(pyrrolidin-1-yl)quinazolin-4(3*H*)-ylidene)butan-1-amine **4a**

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.89 (t, *J* = 7.2 Hz, 3H), 1.35-1.42 (m, 2H), 1.57-1.75 (m, 6H), 3.04-3.15 (m, 3H), 3.48-3.74 (m, 3H), 6.97 (t, *J* = 6.8 Hz, 7.2 Hz, 1H), 7.23-7.45 (m, 7H), 7.70 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.9, 20.4, 25.4, 35.0, 49.1, 50.7, 118.1, 120.4, 123.4, 124.6, 126.3, 127.6, 127.9, 129.5, 131.2, 141.6, 148.8, 154.4; LC-MS (ESI): 347 (M^++H); HRMS Calcd for $C_{22}H_{27}N_4$ (ESI, M^++H): 347.2236; Found: 347.2236.



N-(3-Phenyl-2-(pyrrolidin-1-yl)quinazolin-4(3*H*)-ylidene)pentan-1-amine **4b**

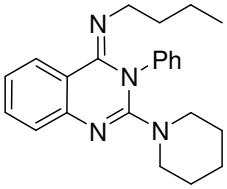
^{1}H NMR (400 MHz, $CDCl_3$) δ 0.0725 (m, 3H), 0.78-0.87 (m, 3H), 1.59-1.67 (m, 4H), 1.84-1.97 (m, 1H), 2.99-3.23 (m, 4H), 3.54-3.71 (m, 4H), 6.97 (t, *J* = 6.8 Hz, 7.2 Hz, 1H), 7.18-7.45 (m, 7H), 7.70 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 1.11, 14.3, 22.6, 25.4, 32.6, 49.3, 51.1, 118.3, 120.5, 123.6, 124.7, 126.5, 127.8, 128.0, 129.7, 131.4, 141.7, 148.9, 153.4; LC-MS (ESI): 361 (M^++H); HRMS Calcd for $C_{23}H_{29}N_4$ (ESI, M^++H): 361.2392; Found: 361.2392.



2-Methyl-*N*-(3-phenyl-2-(pyrrolidin-1-yl)quinazolin-4(3*H*)-ylidene)propan-2-amine

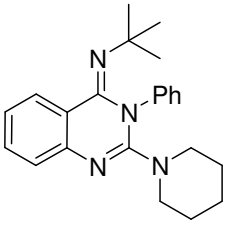
4c

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.41 (s, 9H), 1.79-1.85 (m, 4H), 3.30-3.38 (m, 4H), 6.92 (t, *J* = 7.2 Hz, 7.6 Hz, 1H), 7.05-7.28 (m, 7H), 7.61 (d, *J* = 8.0 Hz, 1H); ^{13}CNMR (100 MHz, $CDCl_3$) δ 25.4, 31.4, 48.4, 55.4, 121.0, 122.7, 123.2, 123.6, 124.2, 127.4, 128.6, 130.8, 141.9, 145.6, 148.1, 153.6; LC-MS (ESI): 347 (M^++H); HRMS Calcd for $C_{22}H_{27}N_4$ (ESI, M^++H): 347.2236; Found: 347.2240.



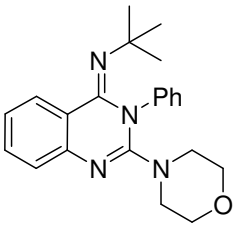
N-(3-Phenyl-2-(piperidin-1-yl)quinazolin-4(3*H*)-ylidene)butan-1-amine **4d**

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.90 (t, *J* = 7.2 Hz, 3H), 1.10-1.21 (m, 3H), 1.35-1.40 (m, 3H), 1.57-1.62 (m, 4H), 3.09-3.19 (m, 3H), 3.34-3.38 (m, 1H), 3.38-3.48 (m, 1H), 3.69-3.72 (m, 1H), 7.04-7.11 (m, 2H), 7.30-7.37 (m, 4H), 7.46-7.48 (m, 2H), 7.69 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.4, 21.0, 24.5, 25.4, 31.0, 48.1, 55.5, 122.1, 122.5, 123.6, 123.9, 126.5, 128.5, 130.6, 142.5, 145.5, 146.6, 155.4; LC-MS (ESI): 361 (M^++H); HRMS Calcd for $C_{23}H_{29}N_4$ (ESI, M^++H): 361.2392; Found: 361.2388.



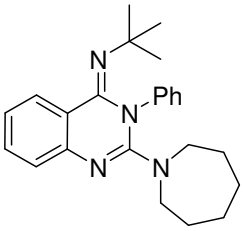
2-Methyl-*N*-(3-phenyl-2-(piperidin-1-yl)quinazolin-4(3*H*)-ylidene)propan-2-amine **4e**

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.36 (s, 9H), 1.42-1.58 (m, 6H), 3.45-3.50 (m, 4H), 6.97-7.29 (m, 8H), 7.66 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.6, 25.4, 31.0, 48.1, 55.5, 122.1, 122.5, 123.7, 123.9, 126.7, 128.5, 130.6, 142.7, 145.2, 146.9, 155.5; LC-MS (ESI): 361 (M^++H); HRMS Calcd for $C_{23}H_{29}N_4$ (ESI, M^++H): 361.2392; Found: 361.2392.



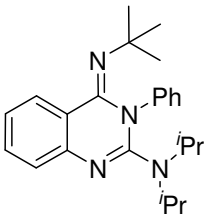
2-Methyl-*N*-(2-morpholino-3-phenylquinazolin-4(3*H*)-ylidene)propan-2-amine **4f**

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.35 (s, 9H), 3.44-3.46 (m, 4H), 3.56-3.57 (m, 4H), 7.04 (t, *J* = 7.6 Hz, 1H), 7.11 (t, *J* = 7.2 Hz, 1H), 7.19-7.34 (m, 6H), 7.68 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.0, 47.8, 55.1, 66.4, 122.4, 123.3, 124.1, 124.4, 124.9, 127.3, 128.4, 130.8, 142.3, 144.8, 146.8, 155.3; LC-MS (ESI): 363 (M^++H); HRMS Calcd for $C_{22}H_{27}N_4O$ (ESI, M^++H): 363.2185; Found: 363.2182.



N-(2-(Azepan-1-yl)-3-phenylquinazolin-4(3*H*)-ylidene)-2-methylpropan-2-amine **4g**

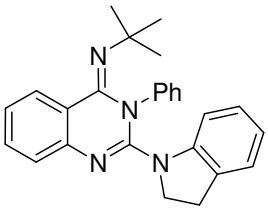
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.42 (s, 9H), 1.55-1.59 (m, 4H), 1.60-1.71 (m, 4H), 3.59-3.70 (m, 4H), 6.91 (t, *J* = 7.2 Hz, 7.6 Hz, 1H), 6.97 (t, *J* = 6.8 Hz, 7.2 Hz, 1H), 7.05-7.09 (m, 3H), 7.18-7.24 (m, 3H), 7.59 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.6, 28.3, 31.1, 48.7, 56.1, 119.8, 121.5, 123.0, 123.3, 124.4, 126.6, 128.7, 130.6, 142.3, 145.6, 147.4, 155.0; LC-MS (ESI): 375 (M^++H); HRMS Calcd for $C_{24}H_{31}N_4$ (ESI, M^++H): 375.2549; Found: 375.2556.



4-(*tert*-Butylimino)-*N*,*N*-diisopropyl-3-phenyl-3,4-dihydroquinazolin-2-amine **4h**

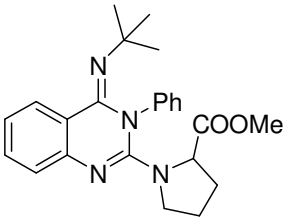
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.27 (d, *J* = 6.8 Hz, 12 H), 1.42 (s, 9H), 3.87-3.91 (m, 2H), 6.90 (t, *J* = 7.2 Hz, 1H), 6.97 (t, *J* = 4.0 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 1H), 7.19-7.20 (m, 4H), 7.23-7.30 (m, 1H), 7.53 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.2, 31.1, 48.3, 55.6, 121.7, 123.6, 123.9, 124.0, 126.8, 128.4, 130.3, 142.9,

146.1, 147.7, 153.5; LC-MS (ESI): 377 (M^++H); HRMS Calcd for $C_{24}H_{33}N_4$ (ESI, M^++H): 377.2705; Found: 377.2699.



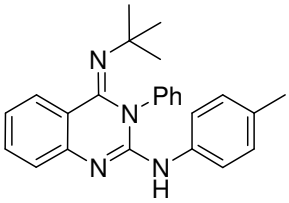
N-(2-(Indolin-1-yl)-3-phenylquinazolin-4(3*H*)-ylidene)-2-methylpropan-2-amine **4l**

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.42 (s, 9H), 2.94 (t, *J* = 8.4 Hz, 2H), 3.60 (t, *J* = 8.0 Hz, 8.4 Hz, 2H), 6.86 (t, *J* = 7.2, 7.6 Hz, 1H), 7.07-7.24 (m, 6H), 7.37-7.42 (m, 4H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.7, 31.1, 50.7, 54.7, 115.4, 121.5, 122.0, 122.2, 124.5, 124.6, 125.6, 125.7, 127.0, 127.9, 128.2, 130.8, 131.3, 141.3, 144.5, 147.4, 151.2; LC-MS (ESI): 395 (M^++H); HRMS Calcd for $C_{26}H_{27}N_4$ (ESI, M^++H): 395.2236; Found: 395.2224.



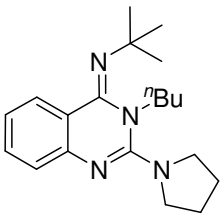
Methyl 1-(4-(*tert*-butylimino)-3-phenyl-3,4-dihydroquinazolin-2-yl)pyrrolidine-2-carboxylate **4j**

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.38 (s, 9H), 1.72-2.19 (m, 4H), 2.79-2.81 (m, 1H), 3.10-3.20 (m, 1H), 3.76 (s, 3H), 4.66 (t, *J* = 6.4 Hz, 7.2 Hz, 1H), 6.93 (t, *J* = 7.2, 7.6 Hz, 1H), 7.12 (t, *J* = 8.4 Hz, 1H), 7.25-7.31 (m, 3H), 7.46-7.52 (m, 3H), 7.59 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.2, 29.4, 31.1, 49.0, 51.9, 54.5, 61.0, 120.7, 122.4, 124.0, 125.2, 126.4, 128.0, 128.1, 141.4, 148.2, 152.6, 174.1; LC-MS (ESI): 405 (M^++H); HRMS Calcd for $C_{24}H_{29}N_4O_2$ (ESI, M^++H): 405.2291; Found: 405.2297.



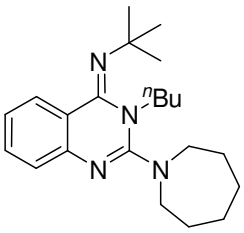
4-(*tert*-Butylimino)-3-phenyl-*N*-(*p*-tolyl)-3,4-dihydroquinazolin-2-amine **4l**

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.23 (s, 9H), 2.26 (s, 3H), 7.03-7.85 (m, 13H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.6, 29.6, 31.4, 111.6, 119.3, 120.6, 122.3, 123.0, 125.3, 126.6, 128.6, 129.1, 129.5, 129.7, 130.3, 131.3, 133.0, 141.4, 148.4; LC-MS (ESI): 383 (M^++H); HRMS Calcd for $C_{25}H_{27}N_4$ (ESI, M^++H): 383.2236; Found: 383.2242.



N-(3-Butyl-2-(pyrrolidin-1-yl)quinazolin-4(3*H*)-ylidene)-2-methylpropan-2-amine **4m**

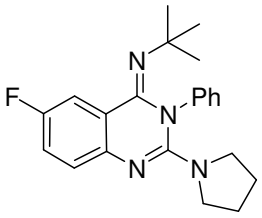
^{1}H NMR (400 MHz, $CDCl_3$) δ 0.75 (t, *J* = 7.2 Hz, 7.6 Hz, 3H), 1.04-1.09 (m, 2H), 1.33-1.35 (m, 2H), 1.46 (s, 9H), 1.87 (m, 4H), 3.50-3.58 (m, 6H), 6.98 (t, *J* = 7.2 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 1H), 7.26-7.31 (m, 1H), 7.85 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.6, 19.8, 25.5, 29.7, 30.2, 30.8, 48.4, 54.4, 122.0, 123.5, 125.3, 130.3, 139.5, 145.3, 146.6, 155.5; LC-MS (ESI): 327 (M^++H); HRMS Calcd for $C_{20}H_{31}N_4$ (ESI, M^++H): 327.2549; Found: 327.2549.



N-(2-(Azepan-1-yl)-3-butylquinazolin-4(3*H*)-ylidene)-2-methylpropan-2-amine **4n**

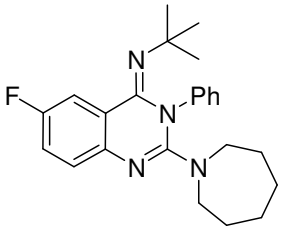
^{1}H NMR (400 MHz, $CDCl_3$) δ 0.74 (t, *J* = 6.8 Hz, 7.2 Hz, 3H), 1.04-1.09 (m, 2H), 1.18-1.34 (m, 4H), 1.41 (s, 9H), 1.44-1.90 (m, 6H), 3.49-3.53 (m, 6H), 6.98 (t, *J* = 7.2 Hz, 8.0 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 1H), 7.25-7.30 (m, 1H), 7.83 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.5, 19.8, 27.4, 27.7, 28.7, 30.1, 30.7, 49.7, 54.5, 122.2, 123.7, 125.2, 130.3, 145.6, 146.6, 157.5; LC-MS (ESI): 355 (M^++H); HRMS

Calcd for $C_{22}H_{35}N_4$ (ESI, M^++H): 355.2862; Found: 355.2857.



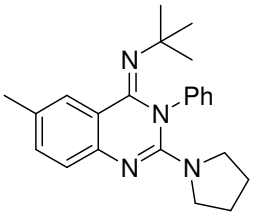
N-(6-Fluoro-3-phenyl-2-(pyrrolidin-1-yl)quinazolin-4(3*H*)-ylidene)-2-methylpropan-2-amine **4o**

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.41 (s, 9H), 1.86-1.88 (m, 4H), 3.43-3.44 (m, 4H), 6.96-7.11 (m, 5H), 7.24 (t, *J* = 6.4 Hz, 7.2 Hz, 2H), 7.31-7.34 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.2, 31.1, 48.1, 55.7, 112.9 (d, $^2J_{CF}$ = 23Hz), 117.8 (d, $^2J_{CF}$ = 23Hz), 121.6, 123.9, 124.5, 124.6, 128.7, 141.6, 143.7, 144.4, 153.1, 157.8 (d, $^1J_{CF}$ = 284Hz); LC-MS (ESI): 365 (M^++H); HRMS Calcd for $C_{22}H_{26}FN_4$ (ESI, M^++H): 365.2142; Found: 365.2144.



N-(2-(Azepan-1-yl)-6-fluoro-3-phenylquinazolin-4(3*H*)-ylidene)-2-methylpropan-2-amine **4p**

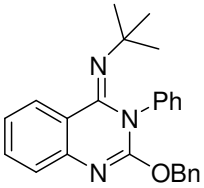
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.42 (s, 9H), 1.52-1.58 (m, 4H), 1.59-1.74 (m, 5H), 3.63-3.65 (m, 3H), 6.92-6.99 (m, 5H), 7.19-7.24 (m, 2H), 7.30-7.32 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.6, 28.4, 31.0, 48.6, 55.6, 112.4 (d, $^2J_{CF}$ = 24 Hz), 117.6 (d, $^2J_{CF}$ = 23 Hz), 119.0, 123.0, 124.4, 128.9, 142.1, 143.2, 144.5, 154.5, 158.2 (d, $^1J_{CF}$ = 284 Hz); LC-MS (ESI): 393 (M^++H); HRMS Calcd for $C_{24}H_{30}FN_4$ (ESI, M^++H): 393.2455; Found: 393.2447.



2-Methyl-*N*-(6-methyl-3-phenyl-2-(pyrrolidin-1-yl)quinazolin-4(3*H*)-ylidene)propan-

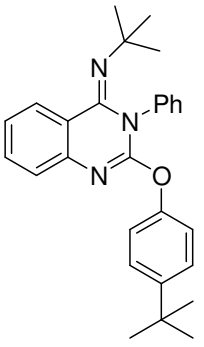
2-amine **4q**

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.42 (s, 9H), 1.85-1.88 (m, 4H), 2.28 (s, 3H), 3.43-3.46 (m, 4H), 7.00-7.12 (m, 5H), 7.20-7.25 (m, 2H), 7.41 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.9, 25.3, 31.2, 48.0, 55.6, 121.6, 123.2, 123.6, 127.0, 128.9, 130.7, 131.7, 141.9, 145.2, 145.8, 153.1; LC-MS (ESI): 361 (M^++H); HRMS Calcd for $C_{23}H_{29}N_4$ (ESI, M^++H): 361.2392; Found: 361.2376.



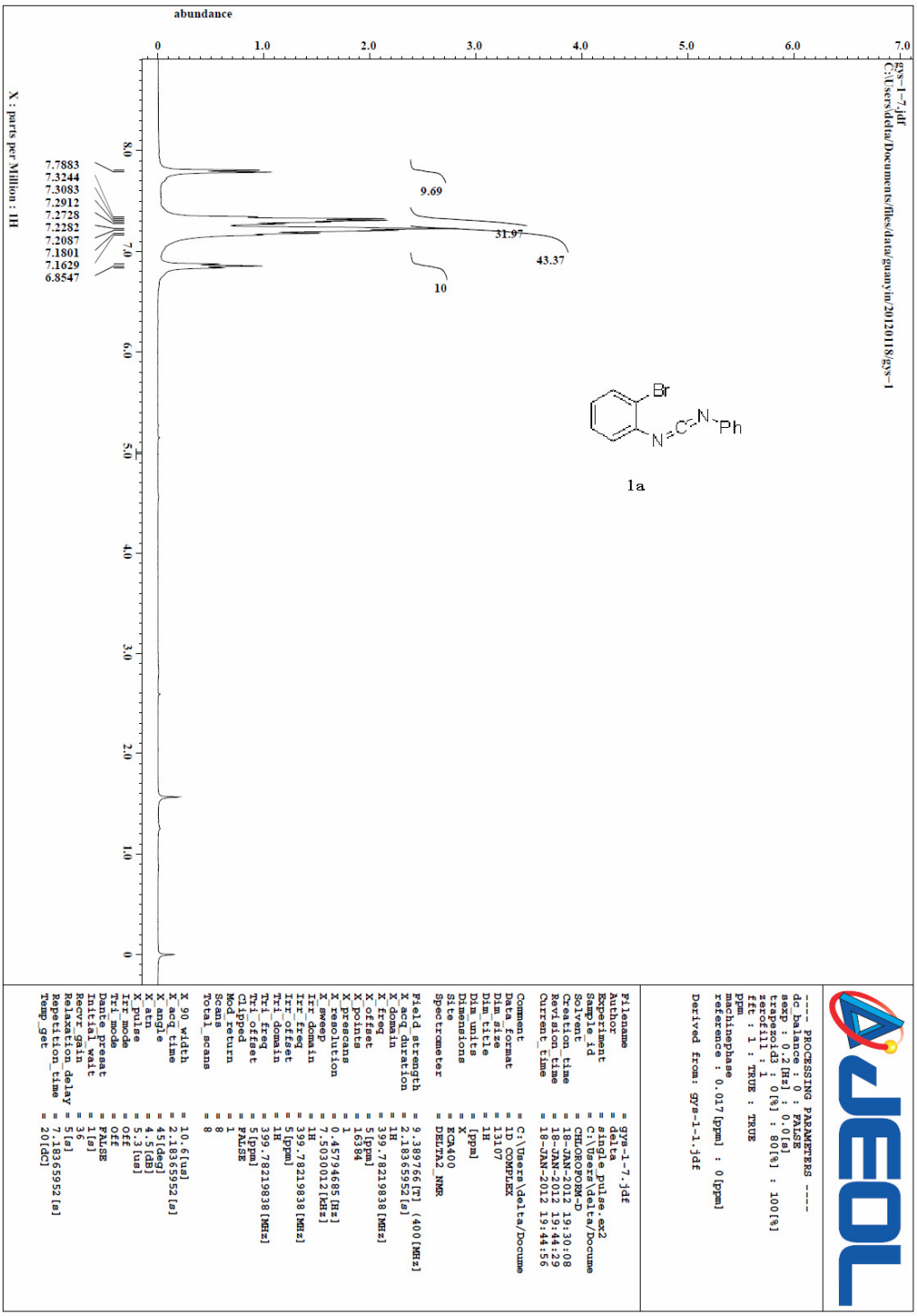
N-(2-(Benzyloxy)-3-phenylquinazolin-4(3*H*)-ylidene)-2-methylpropan-2-amine **4r**

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.18 (s, 9H), 5.37 (s, 2H), 7.11-7.16 (m, 4H), 7.22-7.28 (m, 3H), 7.26-7.30 (m, 2H), 7.34-7.36 (m, 3H), 7.41-7.45 (m, 1H), 7.94 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.1, 53.3, 68.4, 120.4, 122.3, 125.3, 126.8, 126.9, 127.5, 127.9, 128.2, 129.0, 129.6, 131.3, 136.5, 139.8, 142.9, 146.8, 154.0; LC-MS (ESI): 384 (M^++H); HRMS Calcd for $C_{25}H_{26}N_3O$ (ESI, M^++H): 384.2076; Found: 384.2083.



N-(2-(4-(*tert*-Butyl)phenoxy)-3-phenylquinazolin-4(3*H*)-ylidene)-2-methylpropan-2-amine **4s**

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.22 (s, 9H), 1.29 (s, 9H), 7.01 (d, *J* = 8.4 Hz, 2H), 7.07-7.15 (m, 2H), 7.24-7.39 (m, 8H), 7.94 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.0, 31.4, 34.4, 53.3, 120.5, 120.7, 122.7, 125.8, 126.0, 126.9, 128.3, 129.0, 129.4, 131.2, 139.8, 142.9, 146.6, 147.7, 150.0, 154.1; LC-MS (ESI): 426 (M^++H); HRMS Calcd for $C_{28}H_{32}N_3O$ (ESI, M^++H): 426.2545; Found: 426.2551.


abundance
gys-1-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20120118\gys-1
X : parts per Million : 1H
7.7883
7.3244
7.3083
7.2912
7.2728
7.2282
7.2087
7.1801
7.1629
6.8547
9.69
31.97
43.37
10
Br
N
C
N
Ph
1a
JEOL
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
exp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1 : TRUE : TRUE
fft : 1 : TRUE : TRUE
ppm
machinephase : 0.017[ppm] : 0[ppm]
reference : 0.017[ppm] : 0[ppm]
Derived from: gys-1-1.jdf
Filename = gys-1-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = C:\Users\delta\Docume
Solvent = CHLOROFORM-D
Creation_time = 18-JAN-2012 19:30:08
Revision_time = 18-JAN-2012 19:44:29
Current_time = 18-JAN-2012 19:44:56
Comment = C:\Users\delta\Docume
Data_format = 1D COMPLEX
Dim_size = 131072
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
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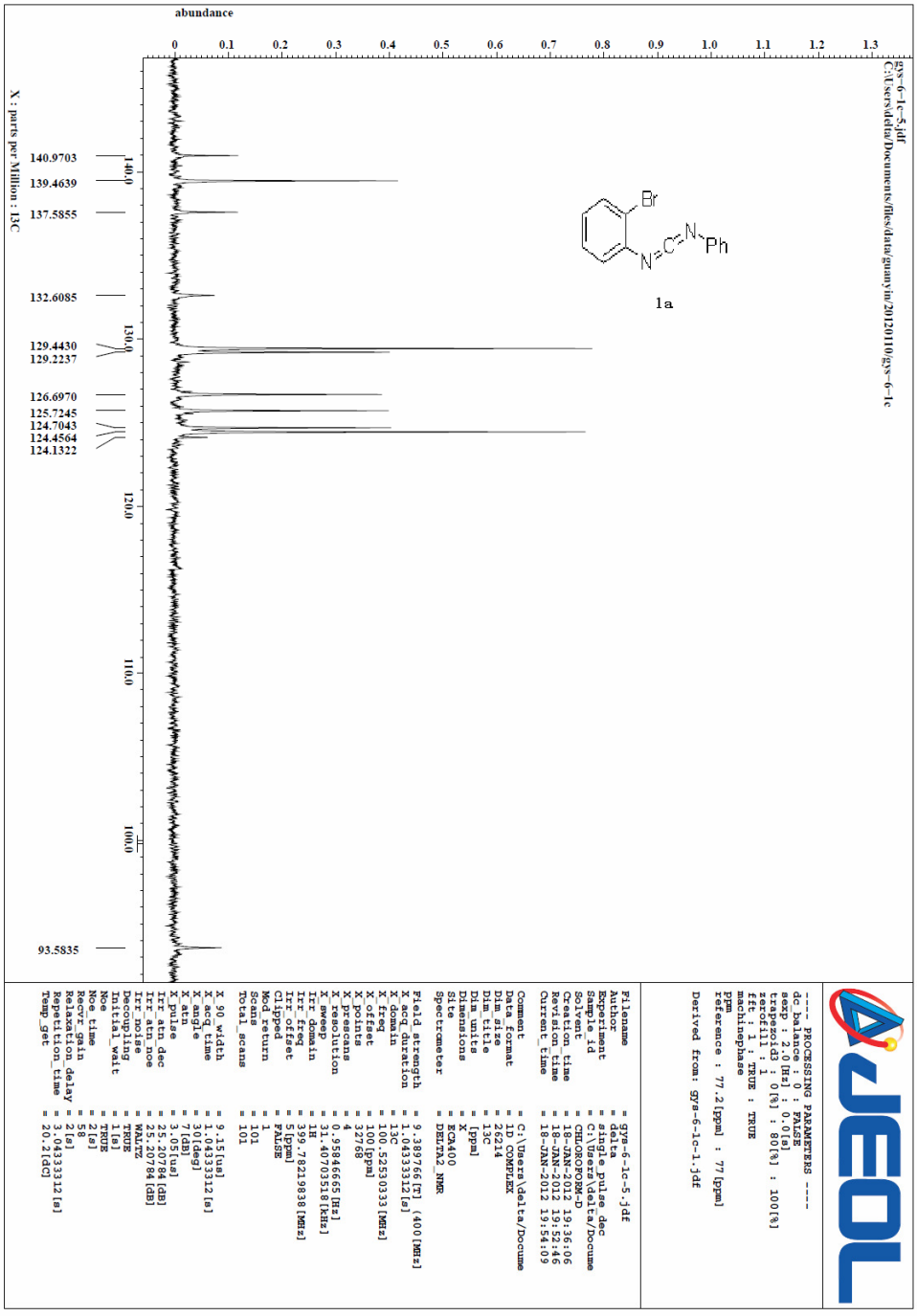
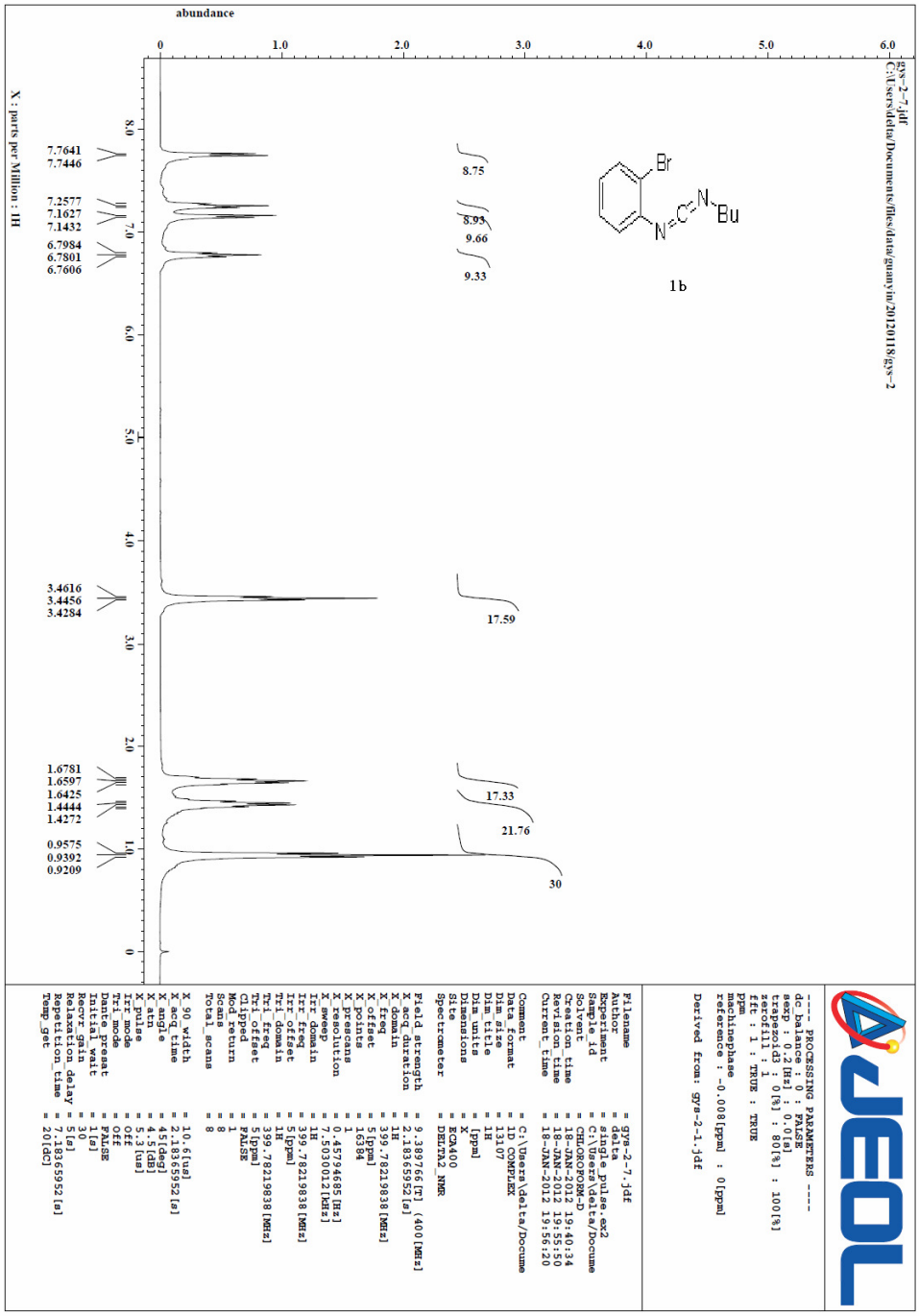
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.183655952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.50300012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scan_return = 8
Total_scans = 8
X_90_width = 10.6[us]
X_acq_time = 2.183655952[s]
X_angle = 45[deg]
X_atn = 4.5[dB]
X_pulse = 5.3[us]
Irr_mode = off
Tri_mode = off
Decpl_presat = FALSE
Initial_wait = 1[s]
Relaxation_delay = 5[s]
Repetition_time = 7.183655952[s]
Temp_get = 20[dC]


abundance
gys-6-1c-5.jdf
C:\Users\delta\Documents\files\data\guanyin\20120110\gys-6-1c
X : parts per Million : 13C
140.9703
139.4639
137.5855
132.6085
129.4430
129.2237
126.6970
125.7245
124.7043
124.4564
124.1322
93.5835
1a
JEOL
---- PROCESSING PARAMETERS ----
dc balance : 0 ; FALSE
exsp : 2.0 [Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm_ref
reference : 77.2[ppm] : 77[ppm]
Derived from: gys-6-1c-1.jdf
Filename = gys-6-1c-5.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = C:\Users\delta\Docume
Solvent = CHLOROFORM-D
Creation_time = 18-JAN-2012 19:36:06
Revision_time = 18-JAN-2012 19:52:46
Current_time = 18-JAN-2012 19:54:09
Comment = C:\Users\delta\Docume
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Site = X
Dimensions = X
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.043333312[s]
X_domain = 13C
X_freq = 100.5253033[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.9584666[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.7821938[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 101
Total_scans = 101
X_90_width = 9.15[us]
X_acq_time = 1.043333312[s]
X_angle = 30[deg]
X_atn = 7[dB]
X_pulse = 3.05[us]
Irr_atn_dec = 25.20784[dB]
Irr_atn_noe = 25.20784[dB]
Irr_mode = WALTZ16
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recyc_gain = 58
Relaxation_delay = 2[s]
Repetition_time = 3.043333312[s]
Temp_get = 20.2[dC]


gys-2-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20120118\gys-2
abundance
X : parts per Million : 1H
7.7641
7.7446
7.2577
7.1627
7.1432
6.7984
6.7801
6.7606
3.4616
3.4456
3.4284
1.6781
1.6597
1.6425
1.4444
1.4272
0.9575
0.9392
0.9209
8.75
8.93
9.66
9.33
17.59
17.33
21.76
30
Br
N
C
N
Bu
1b
JEOL
Filename = gys-2-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = C:\Users\delta\Docume
Solvent = CHLOROFORM-D
Creation_time = 18-JAN-2012 19:40:34
Revision_time = 18-JAN-2012 19:55:50
Current_time = 18-JAN-2012 19:56:20
Comment = C:\Users\delta\Docume
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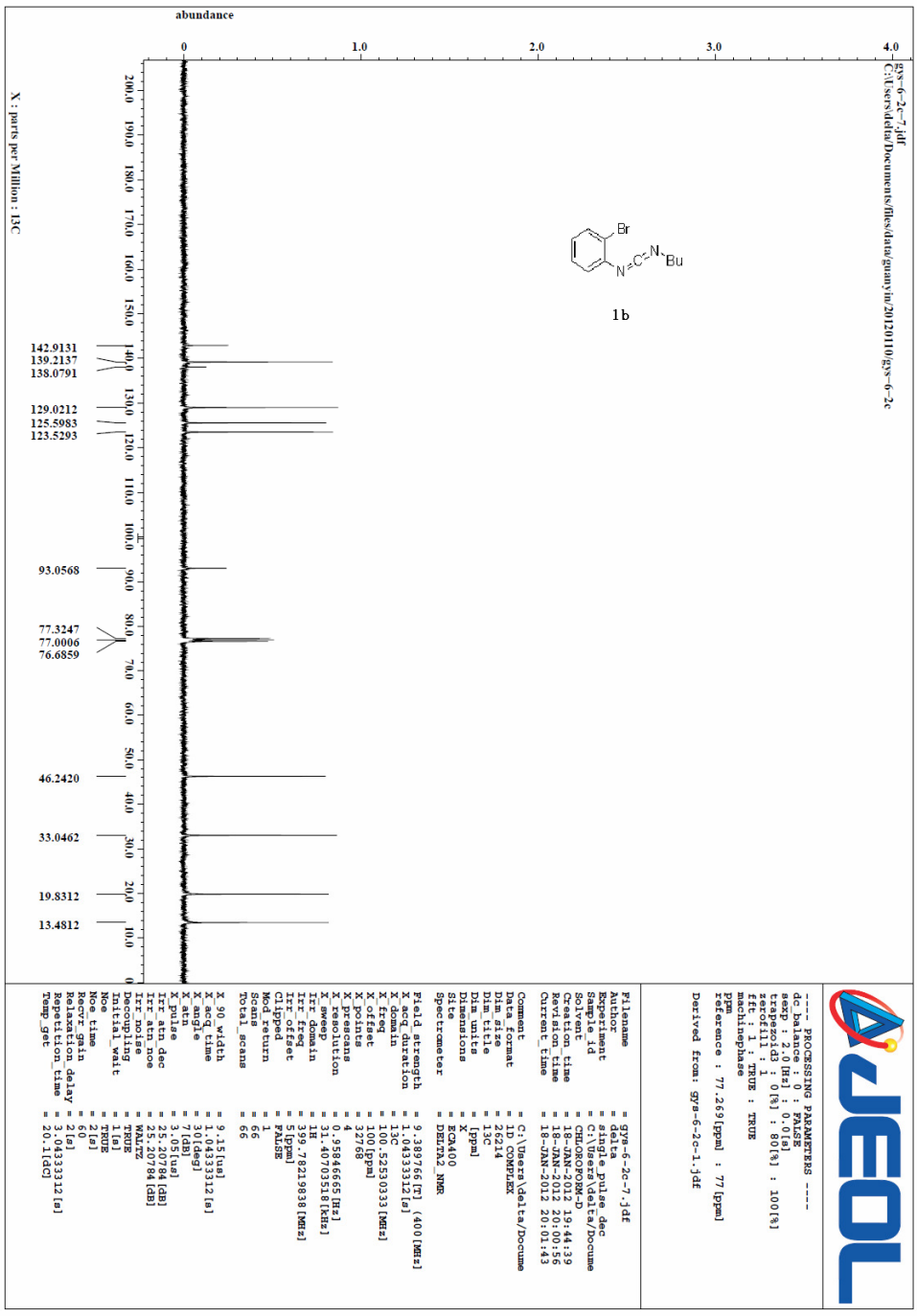
Dim_size = 16107
Dim_title = [ppm]
Dim_units = X
Dimensions = ECA400
Site = DELTA2_NMR
Spectrometer
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.50300121[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Magnitude
Scans = 8
Total_scans = 8
X_90_width = 10.6[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atten = 5.3[dB]
X_pulse = off
Irr_mode = off
Tri_mode = off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 7.13[s]
Repetition_time = 20[sec]
Temp_get
---- PROCESSING PARAMETERS ----
do_baseline : 0 ; FALSE
expd : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
phase
mechinephase
reference : -0.008[ppm] : 0[ppm]
Derived from: gys-2-1.jdf


abundance
X : parts per Million : 13C
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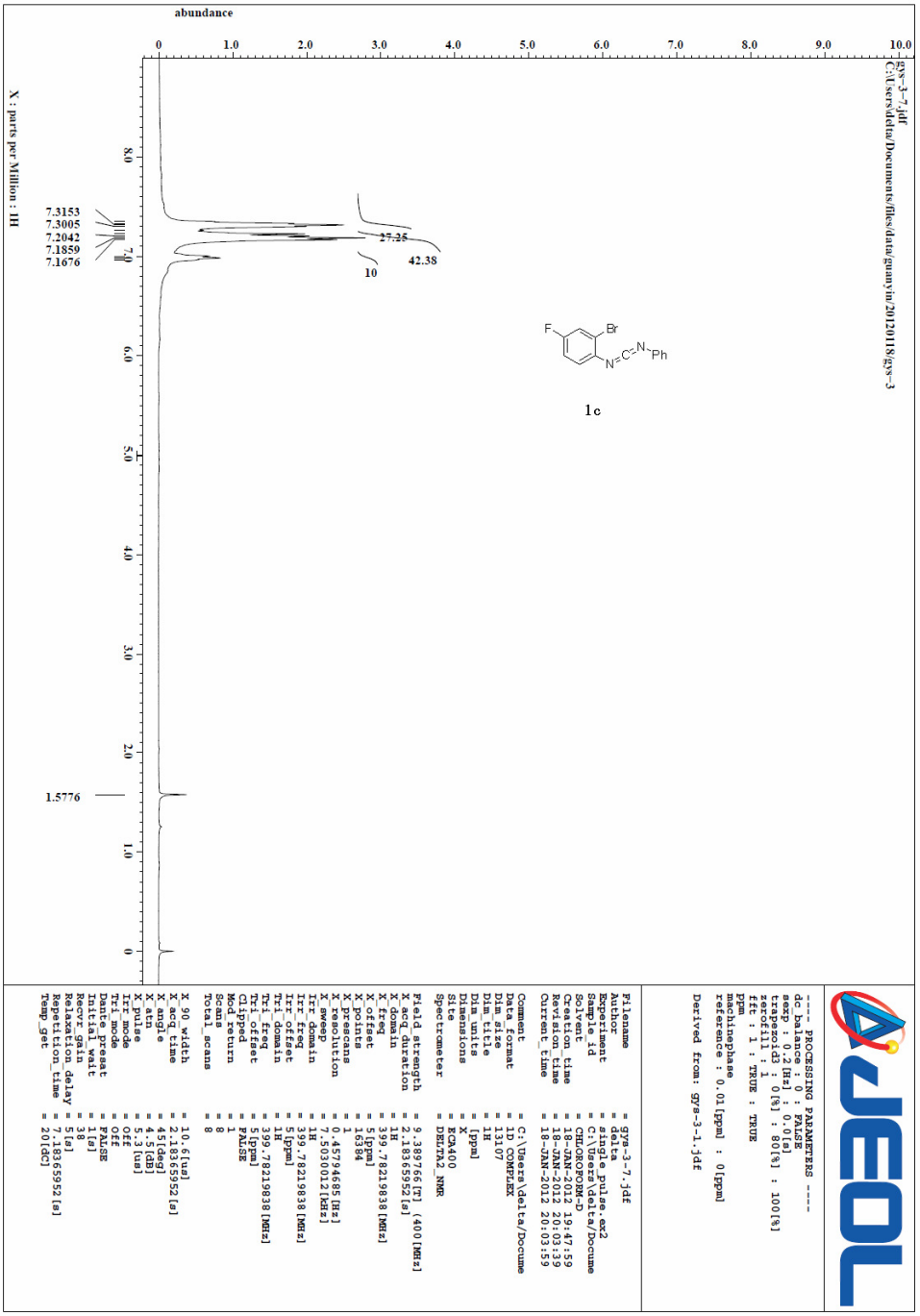
139.2137
138.0791
129.0212
125.5983
123.5293
93.0568
77.3247
77.0006
76.6859
46.2420
33.0462
19.8312
13.4812
Br
N
Bu
1b



---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
escp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1 : TRUE : TRUE
fft : 1 : TRUE
phase
machinephase
reference : 0.01[ppm] : 0[ppm]

Derived from: gys-3-1.jdf

Filename = gys-3-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = C:\Users\delta\Docume
Solvent = CDCl3
Creation_time = 18-JAN-2012 19:47:59
Revision_time = 18-JAN-2012 20:03:39
Current_time = 18-JAN-2012 20:03:59

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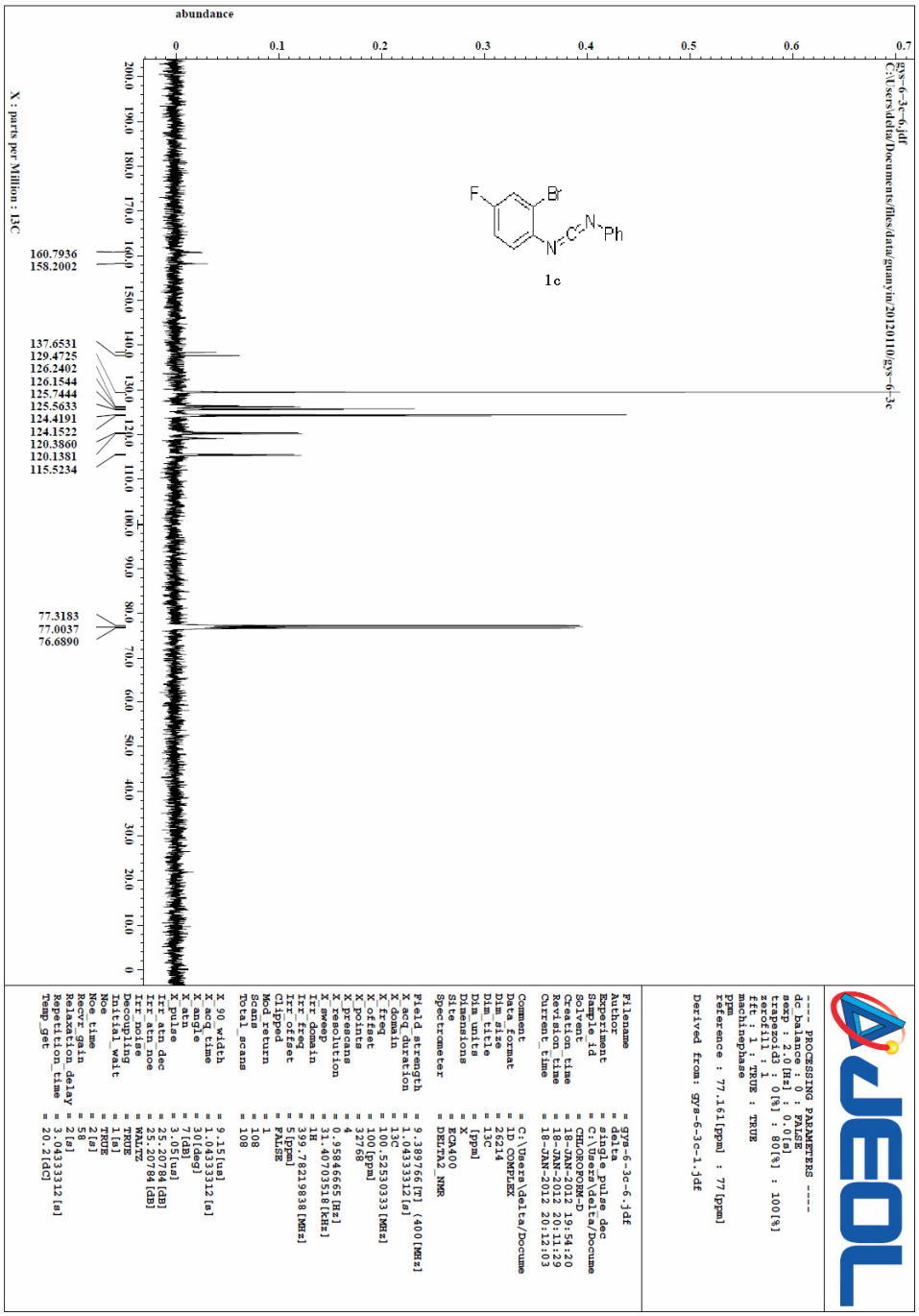
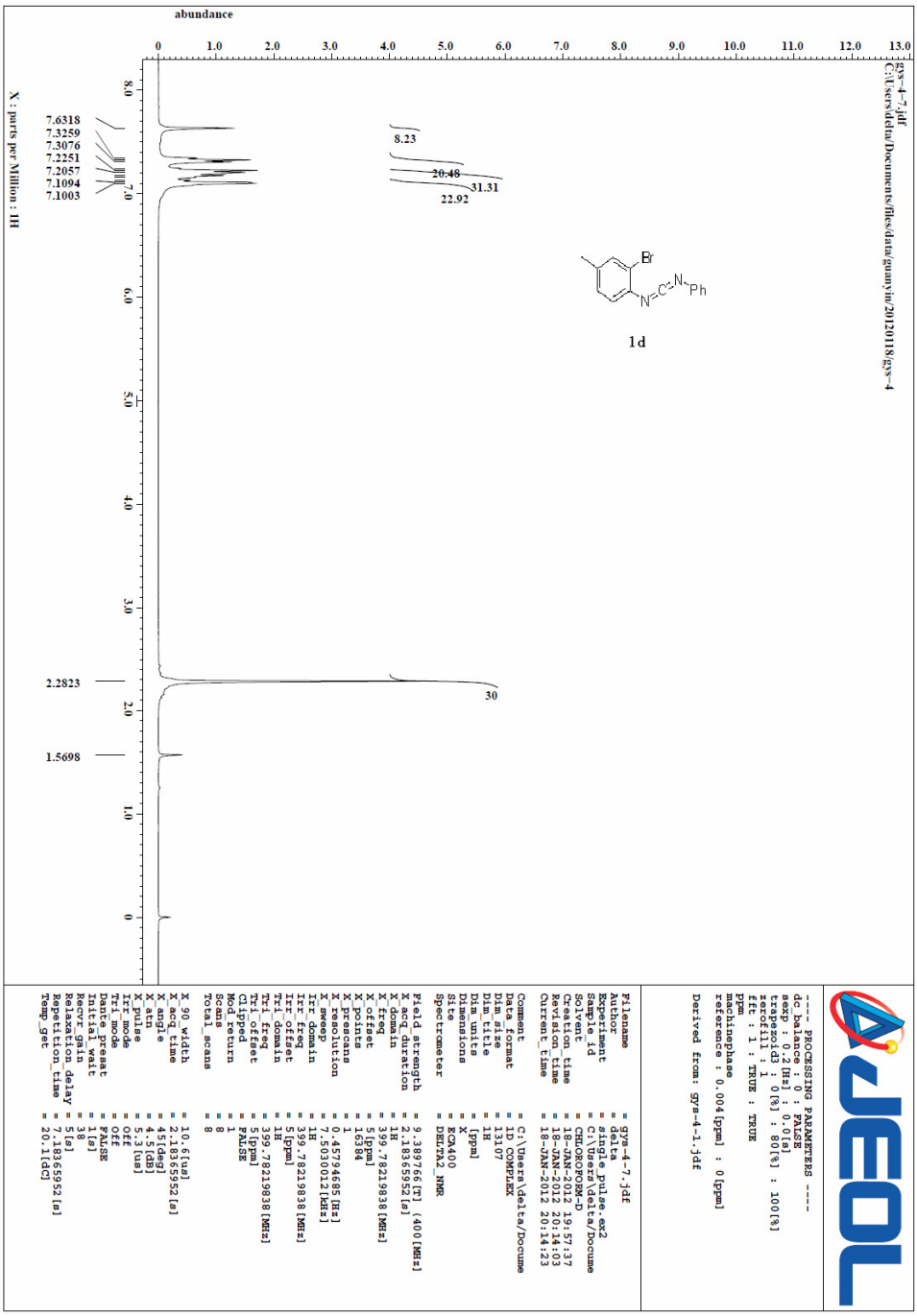
Data_format = 1D COMPLEX
Data_type = 1D
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA400
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz]
X_channel_nucleus = 2:1.83659[e]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794695[Hz]
X_sweep = 7.45030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_pattern = 1
Scans = 8
Total_scans = 8

X_90_width = 10.6[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_pulse = 5.3[us]
X_plus = Off
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
Temp_get_time = 20[dC]


abundance
X : parts per Million : 13C
160.7936
158.2002
137.6531
129.4725
126.2402
126.1544
125.7444
125.5633
124.4191
124.1522
120.3860
120.1381
115.5234
77.3183
77.0037
76.6890
F
Br
N
C
N
Ph
1c
gys-6-3c-6.jdf
C:\Users\delta\Documents\files\data\guanyin\20120110\gys-6-3c
JEOL
Filename = gys-6-3c-6.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = C:\Users\delta\Docume
Solvent = CHLOROFORM-D
Creation_time = 18-JAN-2012 19:54:20
Revision_time = 18-JAN-2012 20:11:29
Current_time = 18-JAN-2012 20:12:03
Comment = C:\Users\delta\Docume
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = KCH400
Spectrometer = DELTA2_NMR
Field_strength = 9.389766 [T] (400 [MHz]
X_acq_duration = 1.043333312[s]
X_domain = 13C
X_freq = 100.5253033 [MHz]
X_offset = 100.0 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.9584665 [Hz]
X_sweep = 31.40703518[KHz]
Irr_domain = 1H
Irr_freq = 399.7821903 [MHz]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 108
Total_scans = 108
X_90_width = 9.15[us]
X_acq_time = 1.043333312[s]
X_angle = 30[deg]
X_atn = 7[dB]
X_pulse = 3.05[us]
Irr_atn_dec = 25.20784 [dB]
Irr_atn_noe = 25.20784 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = TRUE
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 58
Relaxation_delay = 2[s]
Repetition_time = 3.043333312[s]
Temp_get = 20.2[dC]
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
exp : 0.0[Hz] : 80[%] : 100[%]
gaussian : 0.0[s] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
reference : 77.161[ppm] : 77[ppm]
Derived from: gys-6-3c-1.jdf


gys-4-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20120118\gys-4
abundance
X : parts per Million : 1H
7.6318
7.3259
7.3076
7.2251
7.2057
7.1094
7.1003
8.23
20.48
31.31
22.92
2.2823
1.5698
30
1d
Br
N
C
N
Ph
JEOL
Filename = gys-4-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = C:\Users\delta\Docume
Solvent = CHLOROFORM-D
Creation_time = 18-JAN-2012 19:57:37
Revision_time = 18-JAN-2012 20:14:03
Current_time = 18-JAN-2012 20:14:23
Comment = C:\Users\delta\Docume
Data_format = 1D COMPLEX
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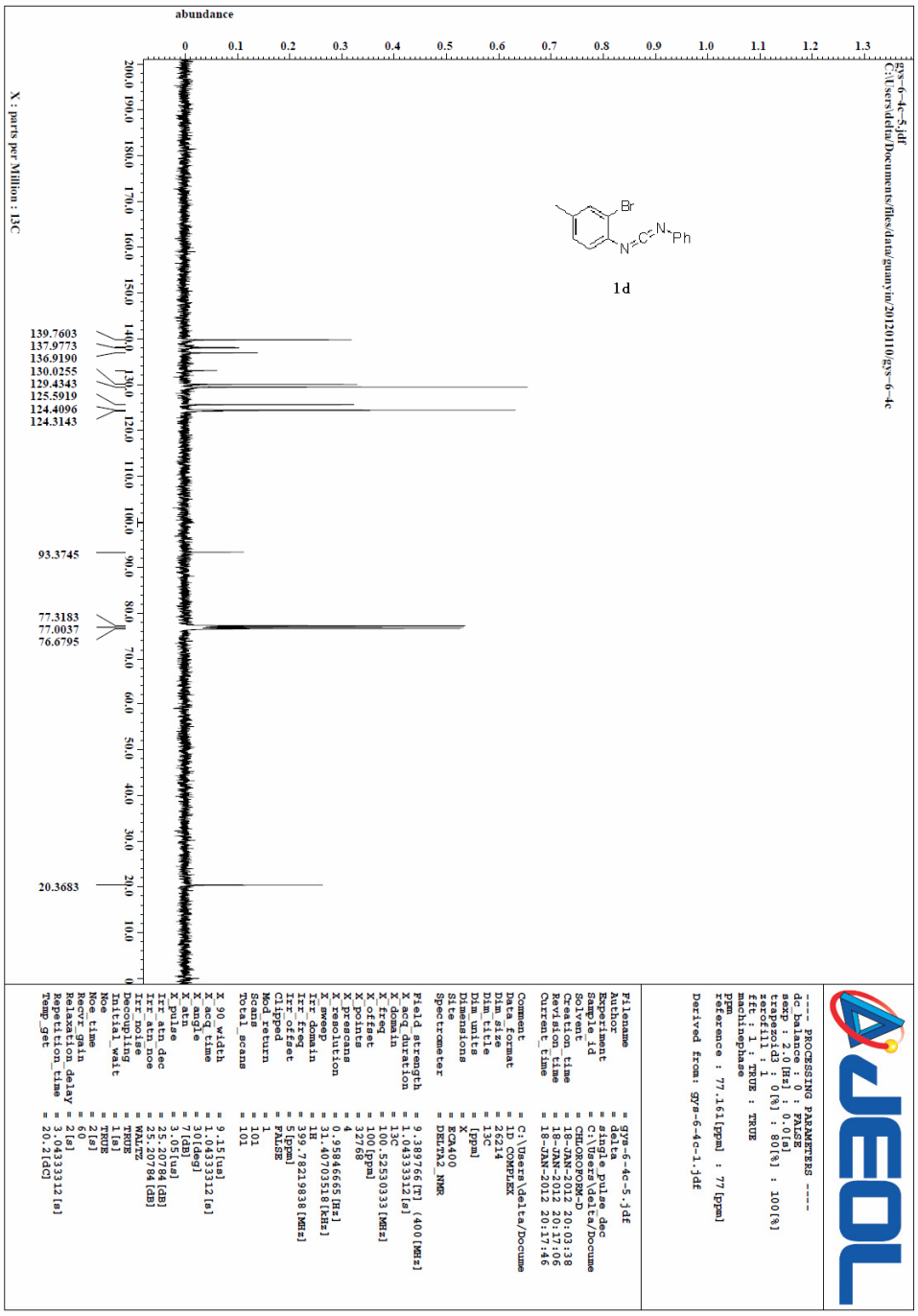
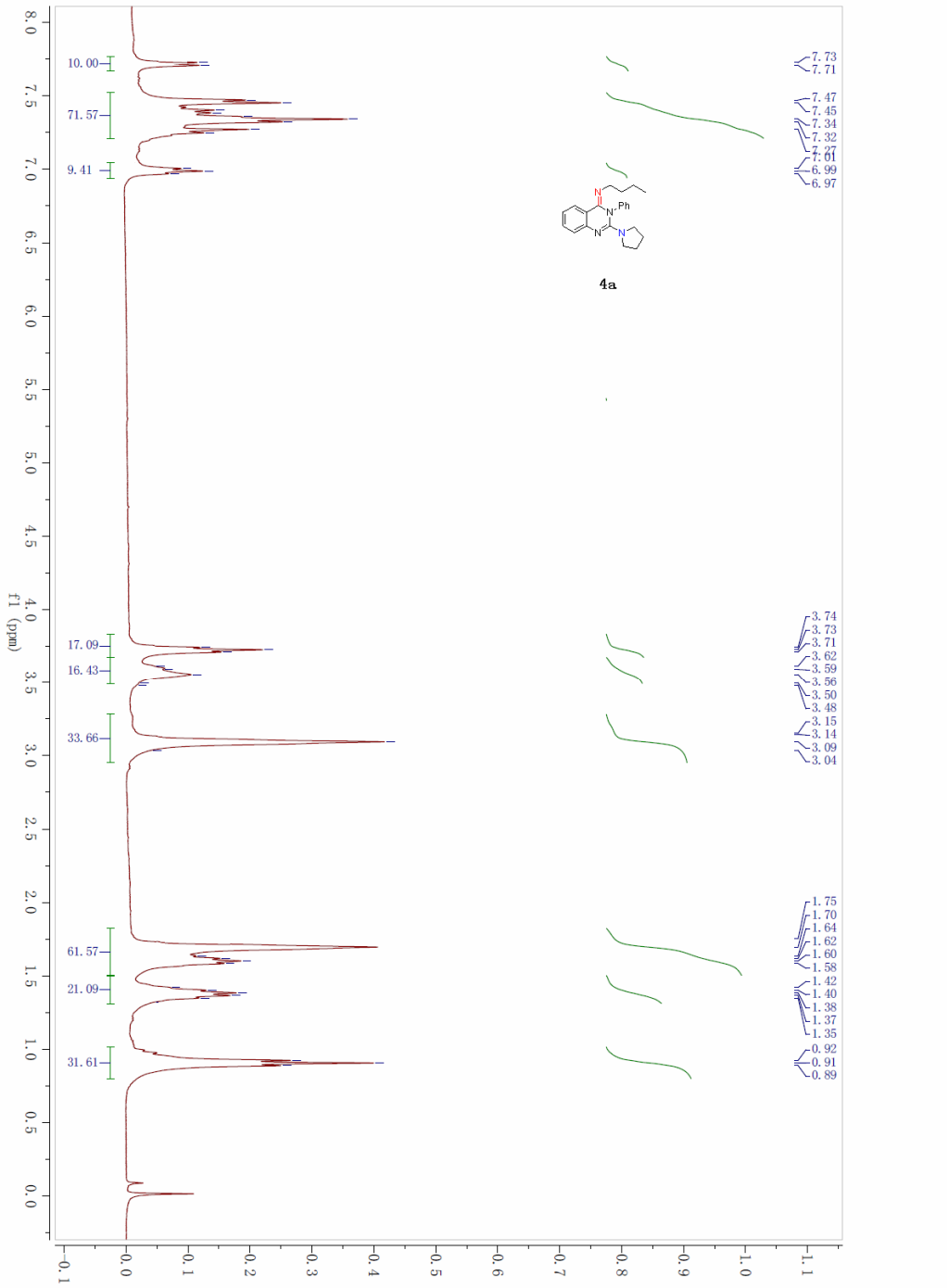
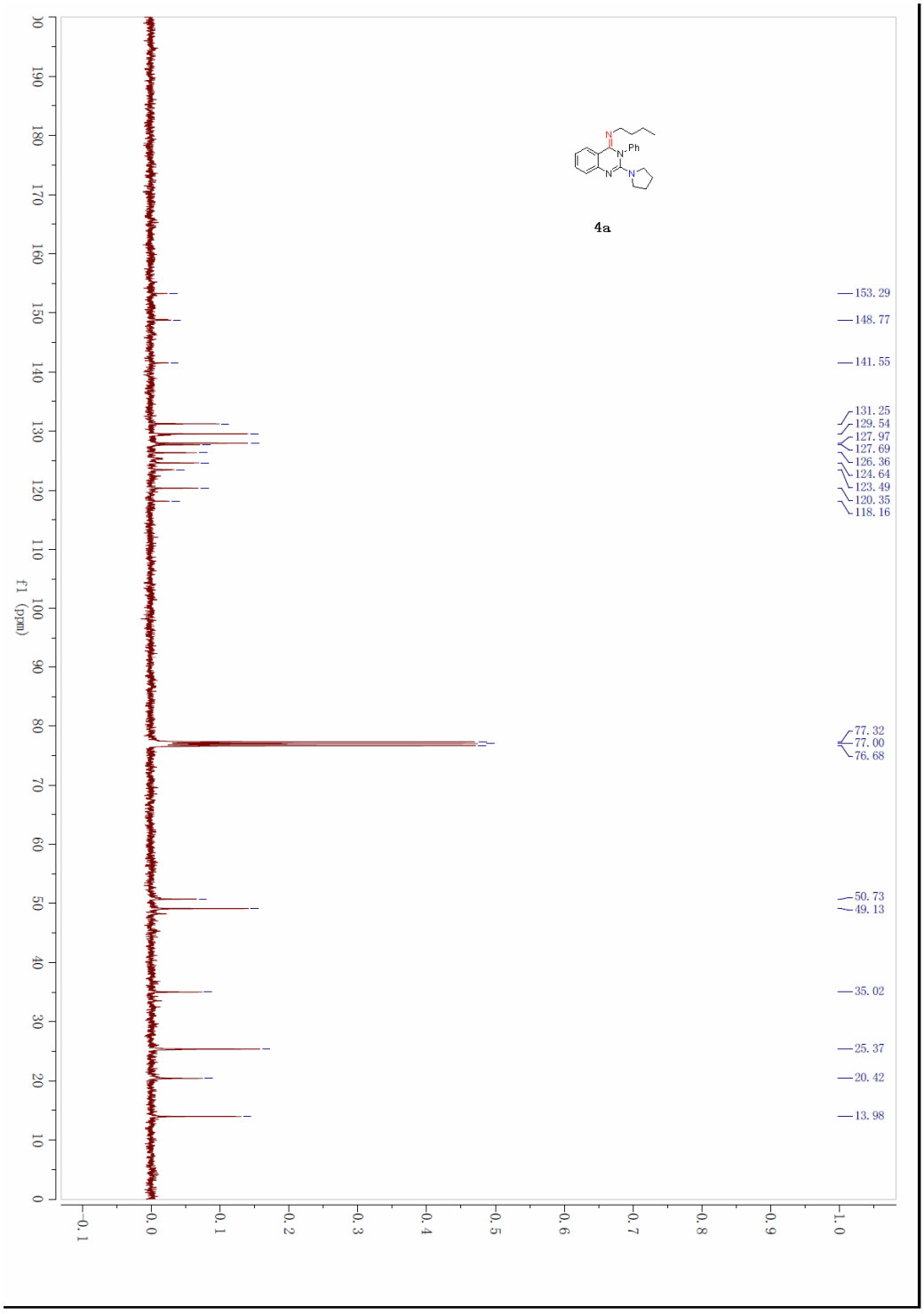
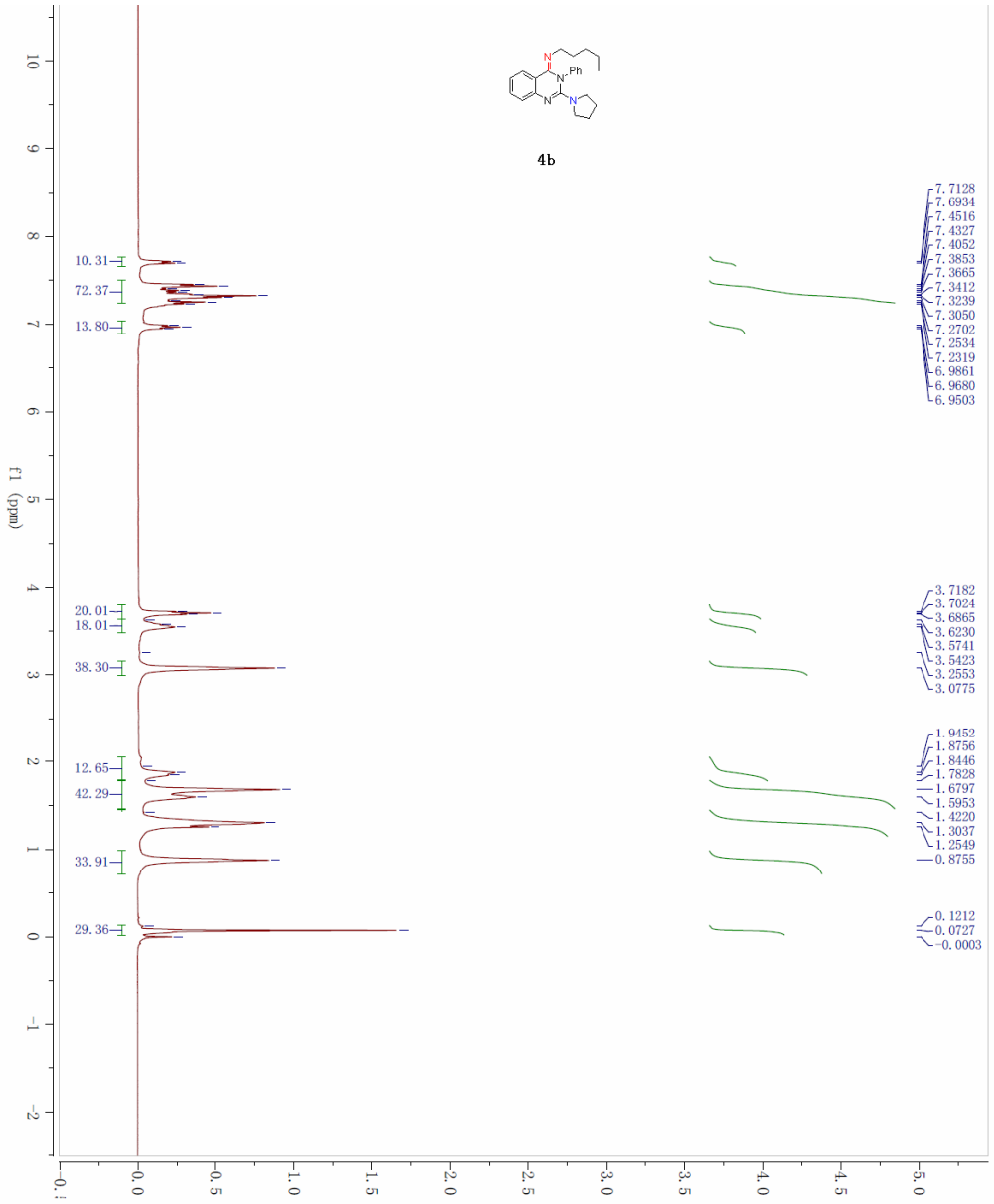
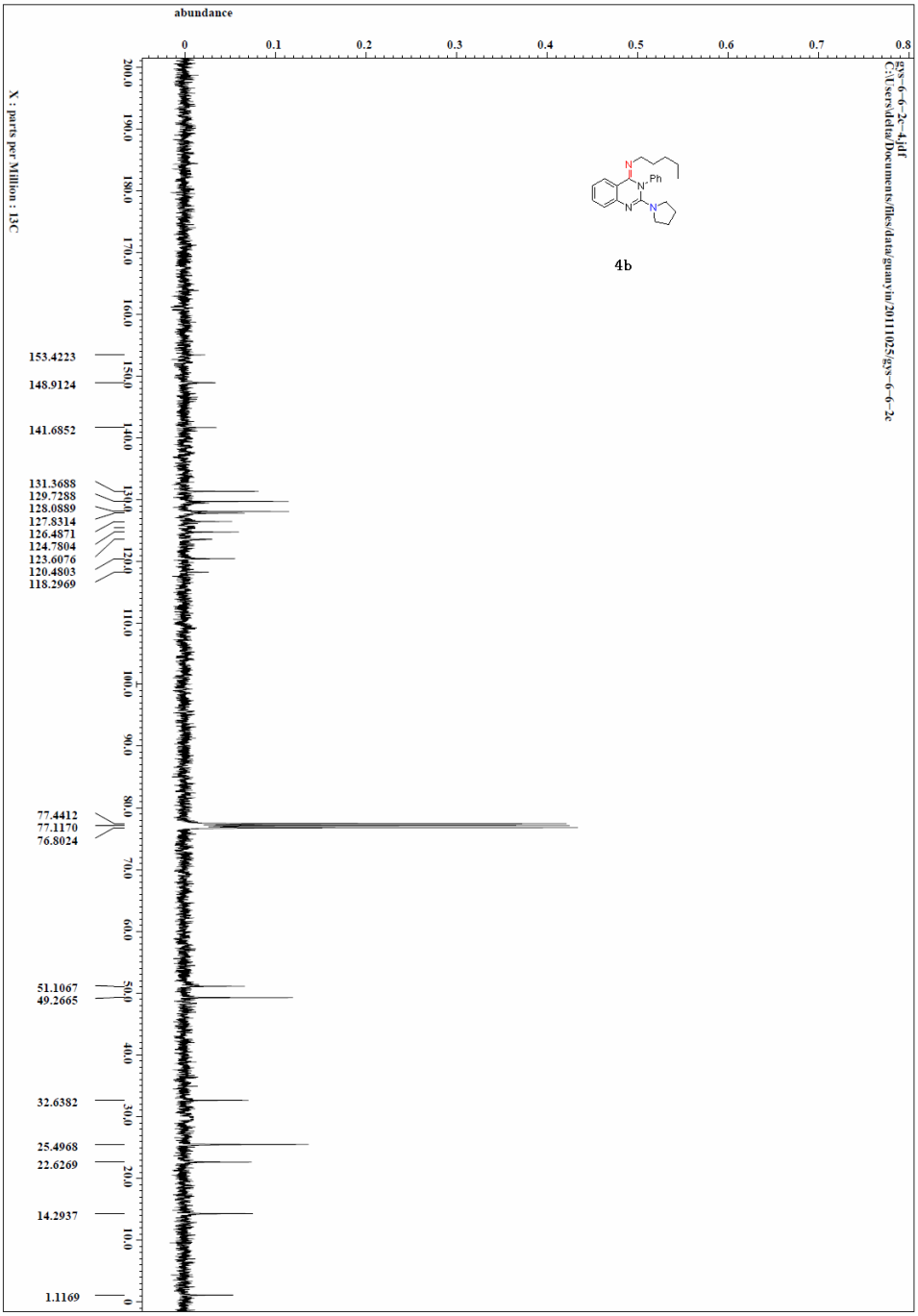
Dim_title = [ppm]
Dim_units = X
Dimensions = ECA400
Site = DELTA2_NMR
Spectrometer
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.50301012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.6[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atten = 5.3[dB]
X_pulse = 5[us]
Tri_mode = off
Tri_power = off
Dante_preset = FALSE
Initial_wait = 1[s]
Recyr_gain = 38
Relaxation_delay = 5[s]
Repetition_time = 7.68365952[s]
Temp_get = 20.1[dC]
---- PROCESSING PARAMETERS ----
dc-balance : 0 : FALSE
expp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
phase
manualphase
reference : 0.004[ppm] : 0[ppm]
Derived from: gys-4-1.jdf

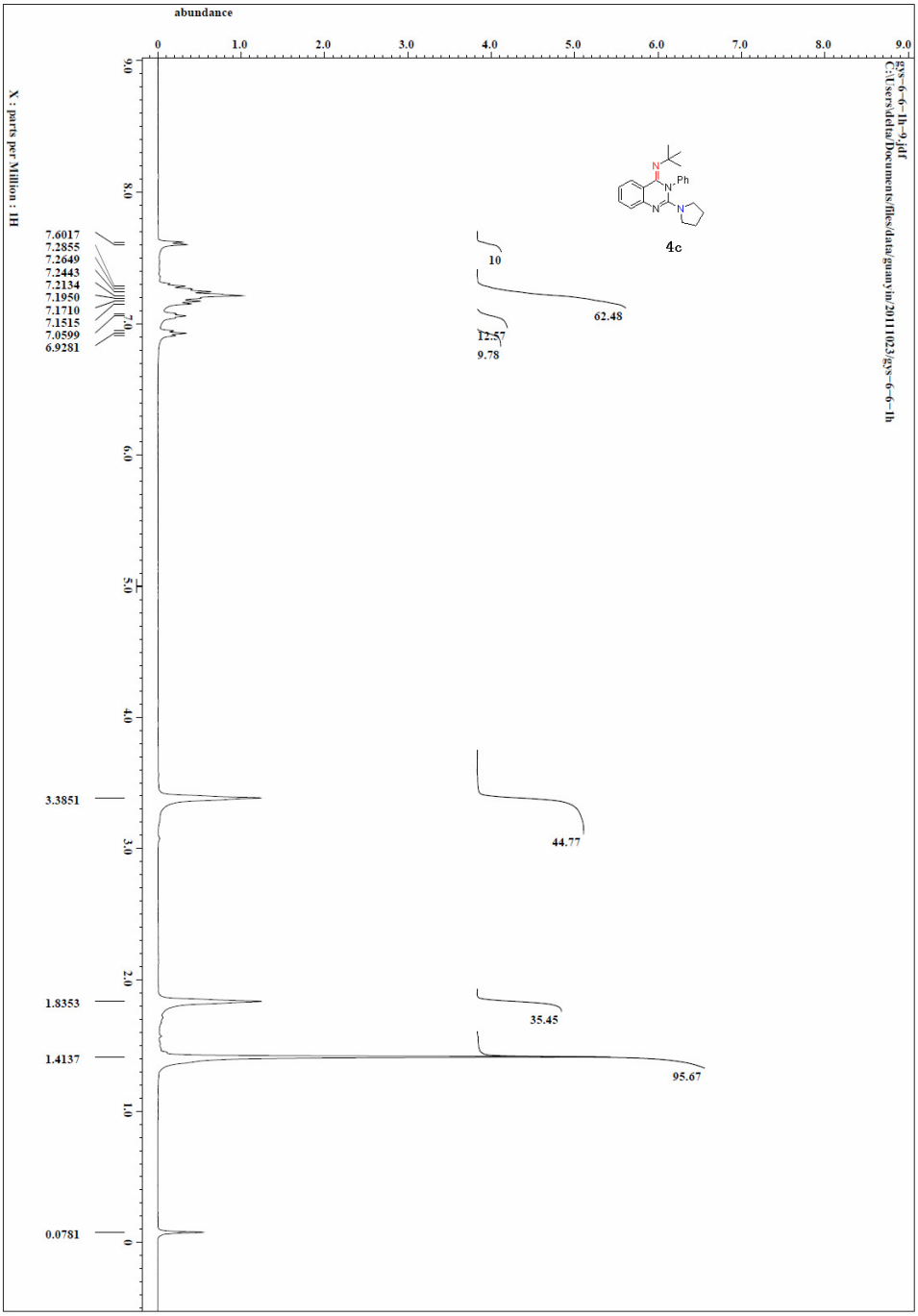

abundance
X : parts per Million : 13C
139.7603
137.9773
136.9190
130.0255
129.4343
125.5919
124.4096
124.3143
93.3745
77.3183
77.0037
76.6795
20.3683
Br
N
N
Ph
1d

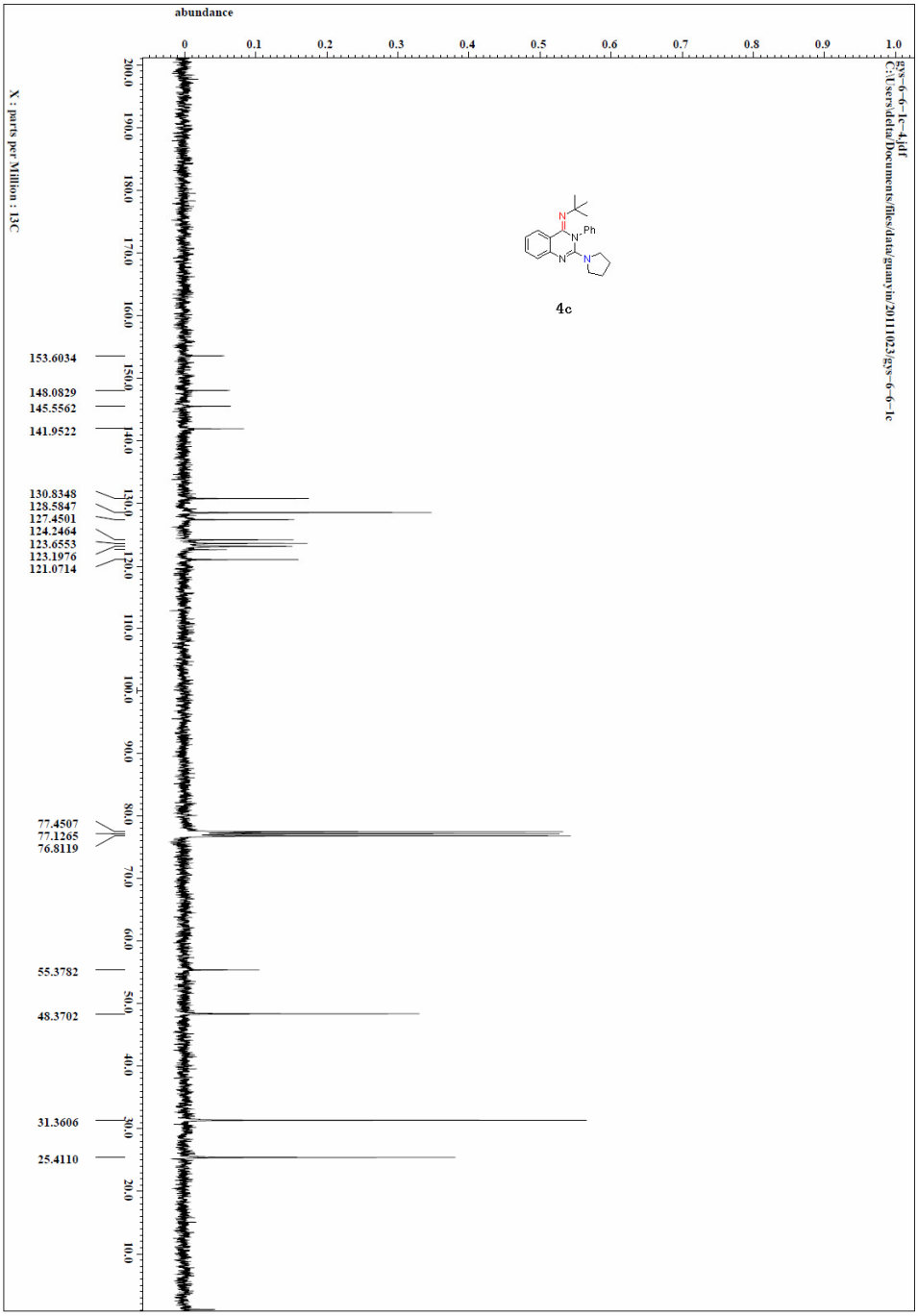

10.00
71.57
9.41
17.09
16.43
33.66
61.57
21.09
31.61
7.73
7.71
7.47
7.45
7.34
7.32
7.27
7.01
6.99
6.97
3.74
3.73
3.71
3.62
3.59
3.56
3.50
3.48
3.15
3.14
3.09
3.04
1.75
1.70
1.64
1.62
1.60
1.58
1.42
1.40
1.38
1.37
1.35
0.92
0.91
0.89
f1 (ppm)
Ph
4a

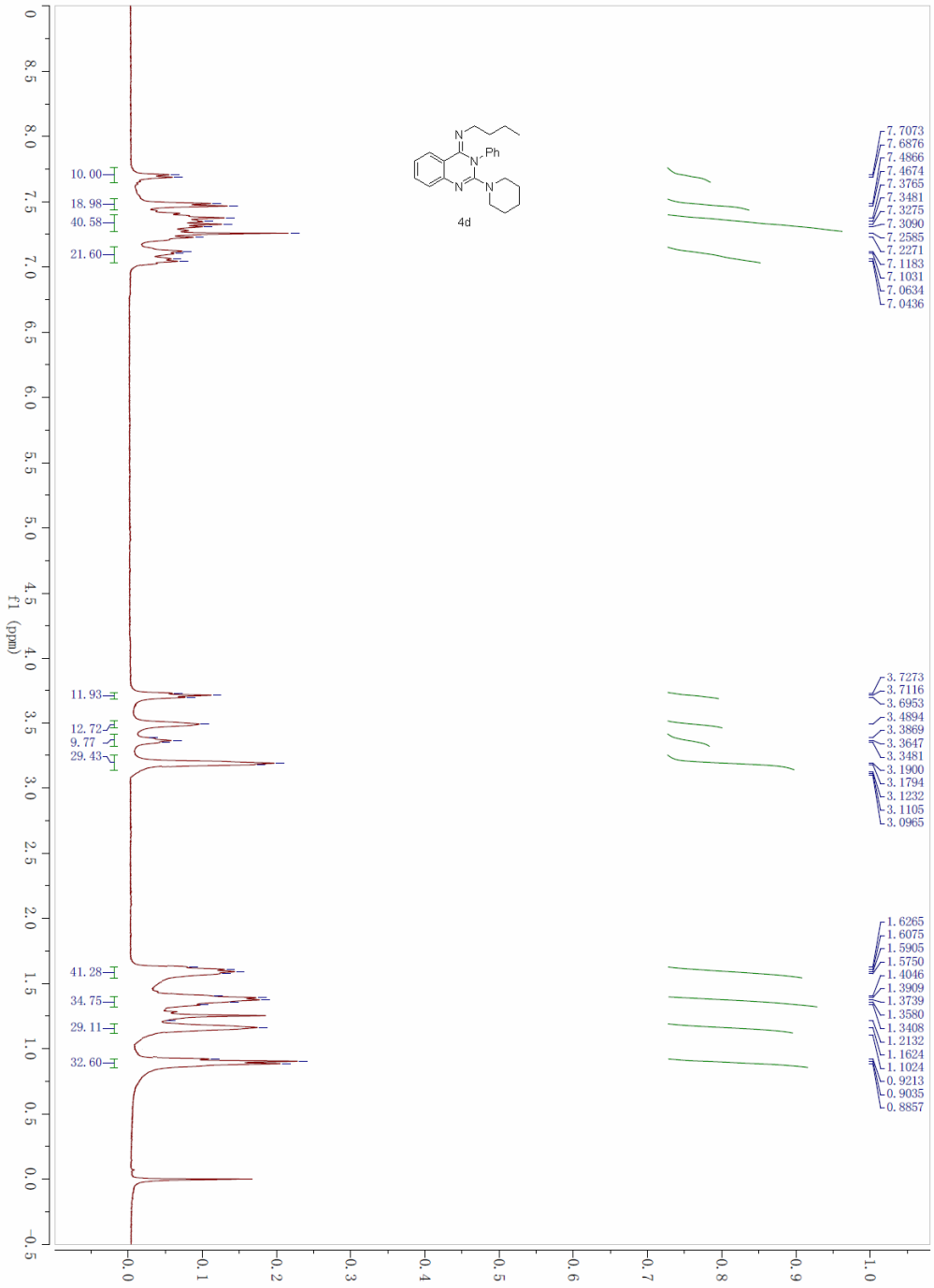

4a
153.29
148.77
141.55
131.25
129.54
127.97
127.69
126.36
124.64
123.49
120.35
118.16
77.32
77.00
76.68
50.73
49.13
35.02
25.37
20.42
13.98
f1 (ppm)

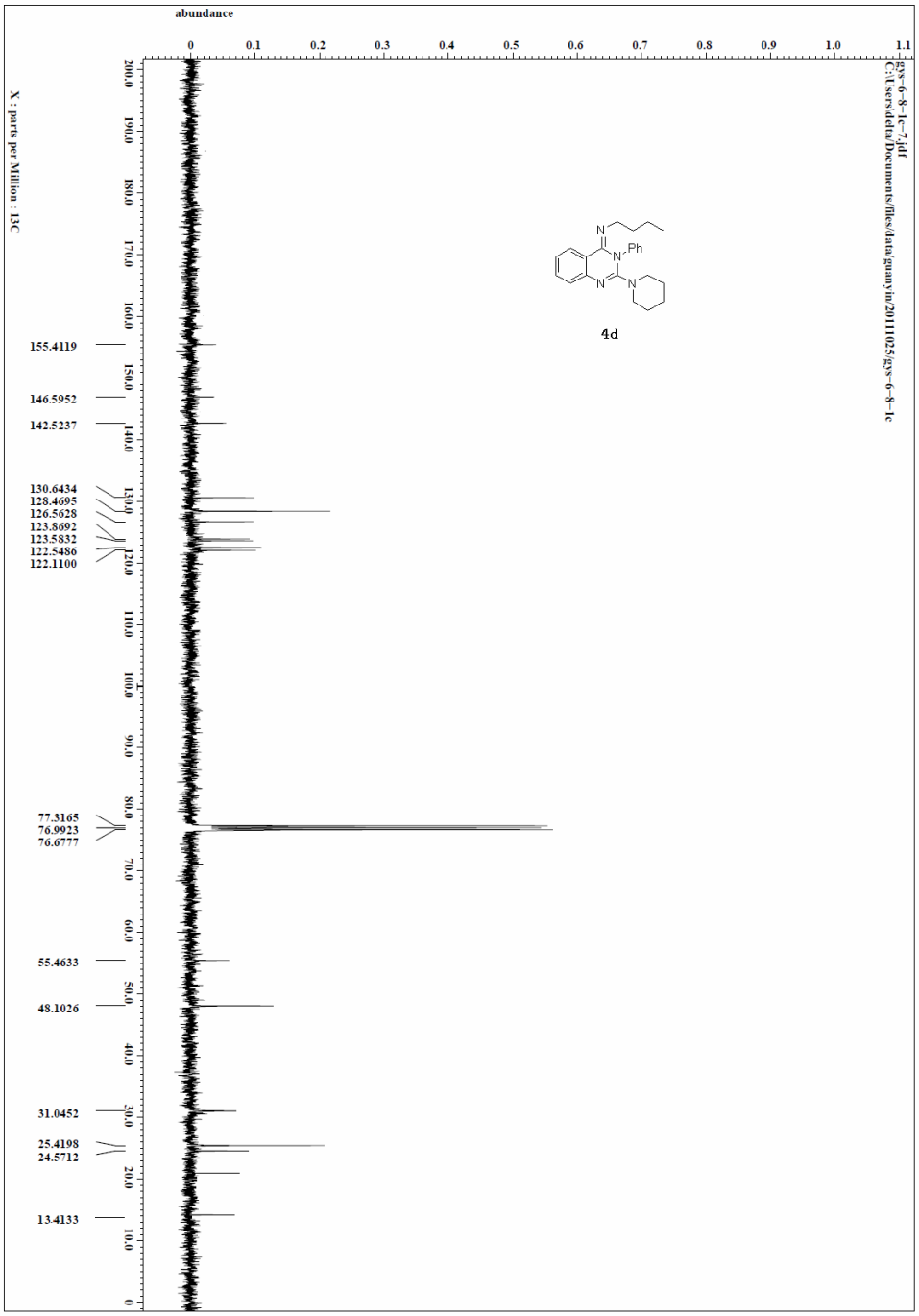

4b
f1 (ppm)
10.31
72.37
13.80
20.01
18.01
38.30
12.65
42.29
33.91
29.36
7.7128
7.6934
7.4516
7.4327
7.4052
7.3853
7.3665
7.3412
7.3239
7.3050
7.2702
7.2534
7.2319
6.9861
6.9680
6.9503
3.7182
3.7024
3.6865
3.6230
3.5741
3.5423
3.2553
3.0775
1.9452
1.8756
1.8446
1.7828
1.6797
1.5953
1.4220
1.3037
1.2549
0.8755
0.1212
0.0727
-0.0003

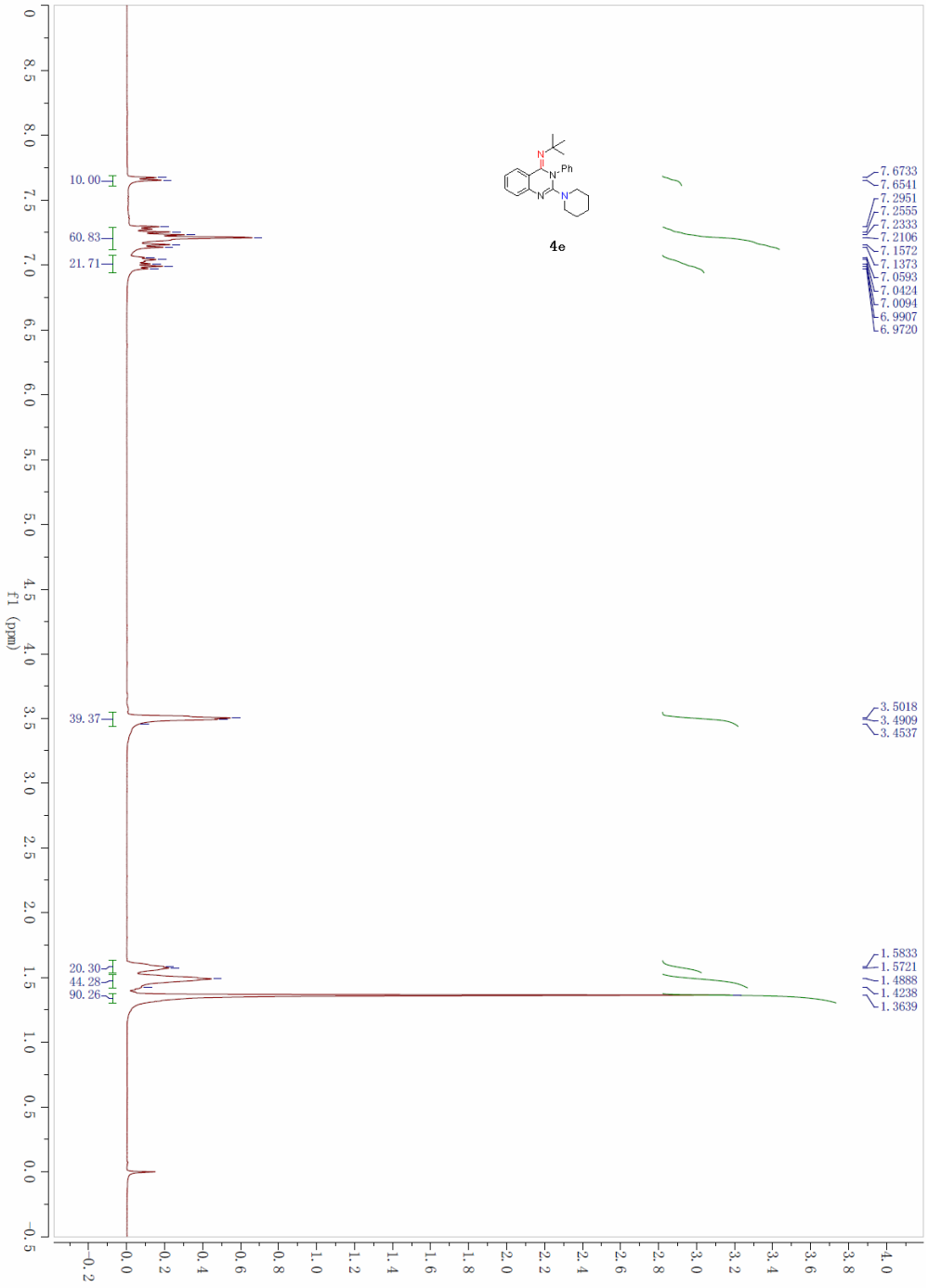

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
X : parts per Million : 13C
C:\Users\data\Documents\files\data\guanyin\20111025\gys-6-6-2c
153.4223
148.9124
141.6852
131.3688
129.7288
128.0889
127.8314
126.4871
124.7804
123.6076
120.4803
118.2969
77.4412
77.1170
76.8024
51.1067
49.2665
32.6382
25.4968
22.6269
14.2937
1.1169
Ph
4b

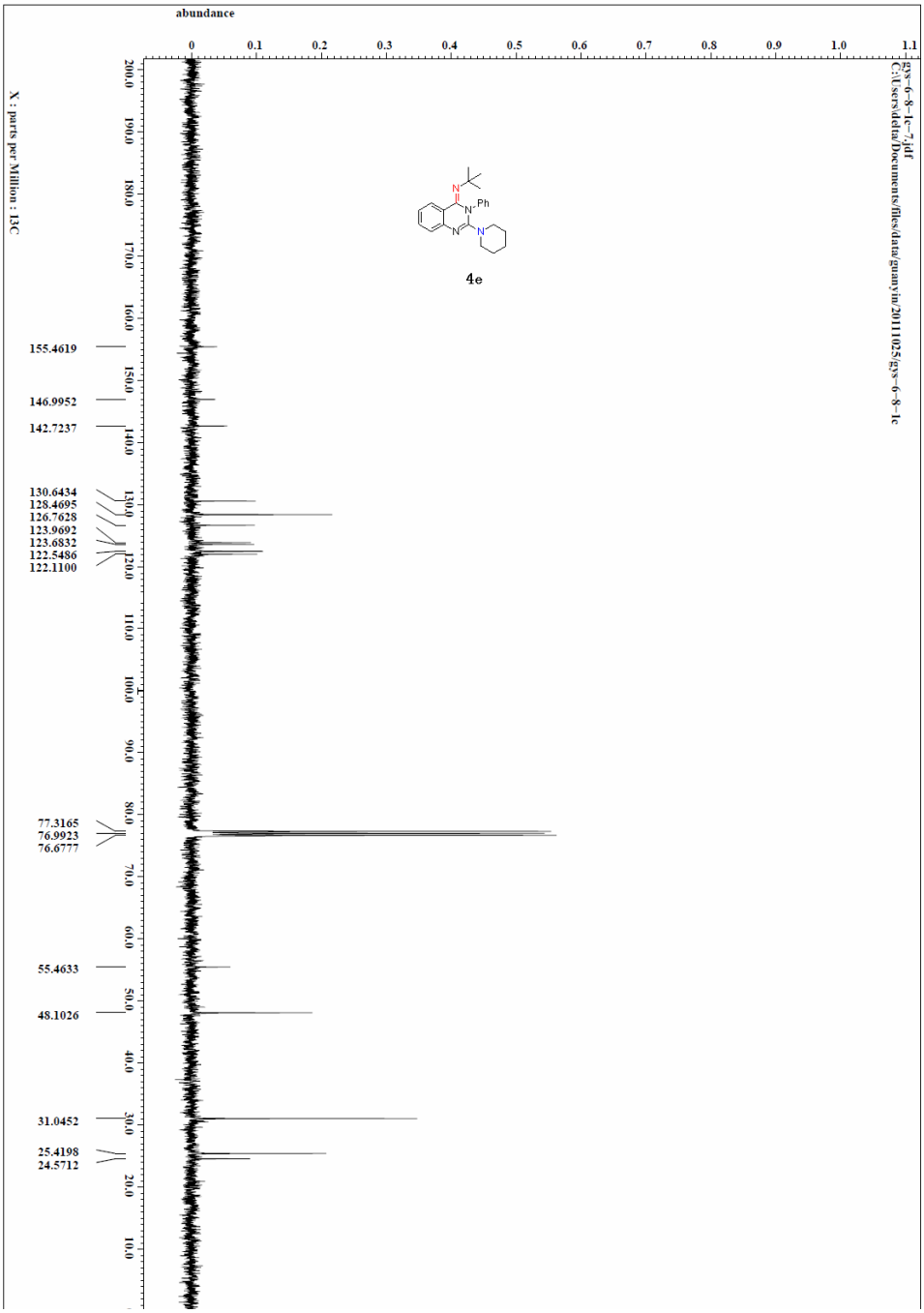

abundance
X : parts per Million : 1H
C:\Users\data\Documents\files\data\guanyin\20111023\gys-6-6-1h
gys-6-6-1h-9.jdf
7.6017
7.2855
7.2649
7.2443
7.2134
7.1950
7.1710
7.1515
7.0599
6.9281
3.3851
1.8353
1.4137
0.0781
10
62.48
12.57
9.78
44.77
35.45
95.67
Ph
4c

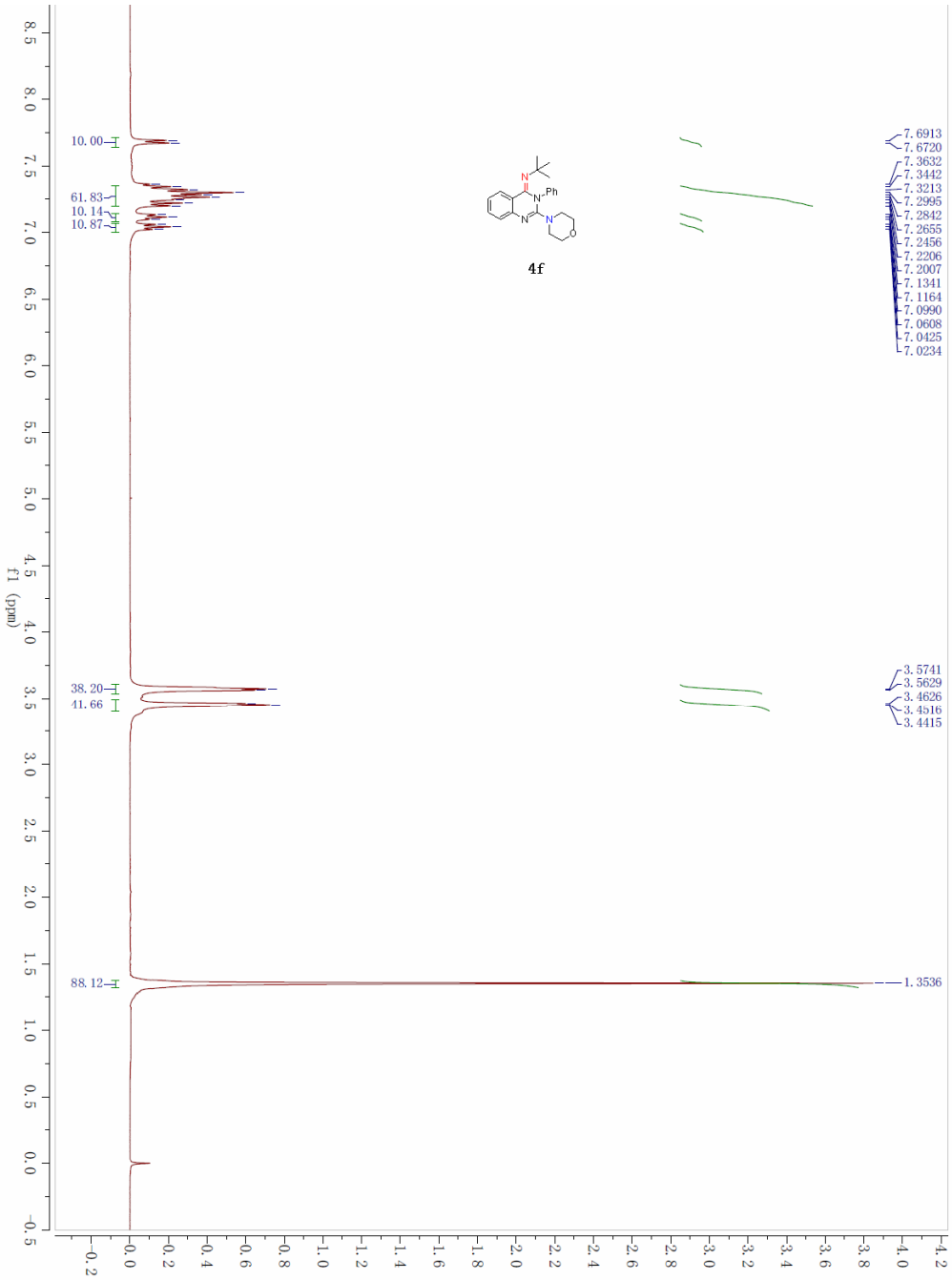

abundance
X : parts per Million : 13C
gss-6-6-1c-4.jdf
C:\Users\ddzu\Documents\files\data\guanyin\20111023\gss-6-6-1c
Ph
4c
153.6034
148.0829
145.5562
141.9522
130.8348
128.5847
127.4501
124.2464
123.6553
123.1976
121.0714
77.4507
77.1265
76.8119
55.3782
48.3702
31.3606
25.4110


4d
10.00
18.98
40.58
21.60
11.93
12.72
9.77
29.43
41.28
34.75
29.11
32.60
7.7073
7.6876
7.4866
7.4674
7.3765
7.3481
7.3275
7.3090
7.2585
7.2271
7.1183
7.1031
7.0634
7.0436
3.7273
3.7116
3.6953
3.4894
3.3869
3.3647
3.3481
3.1900
3.1794
3.1232
3.1105
3.0965
1.6265
1.6075
1.5905
1.5750
1.4046
1.3909
1.3739
1.3580
1.3408
1.2132
1.1624
1.1024
0.9213
0.9035
0.8857
f1 (ppm)

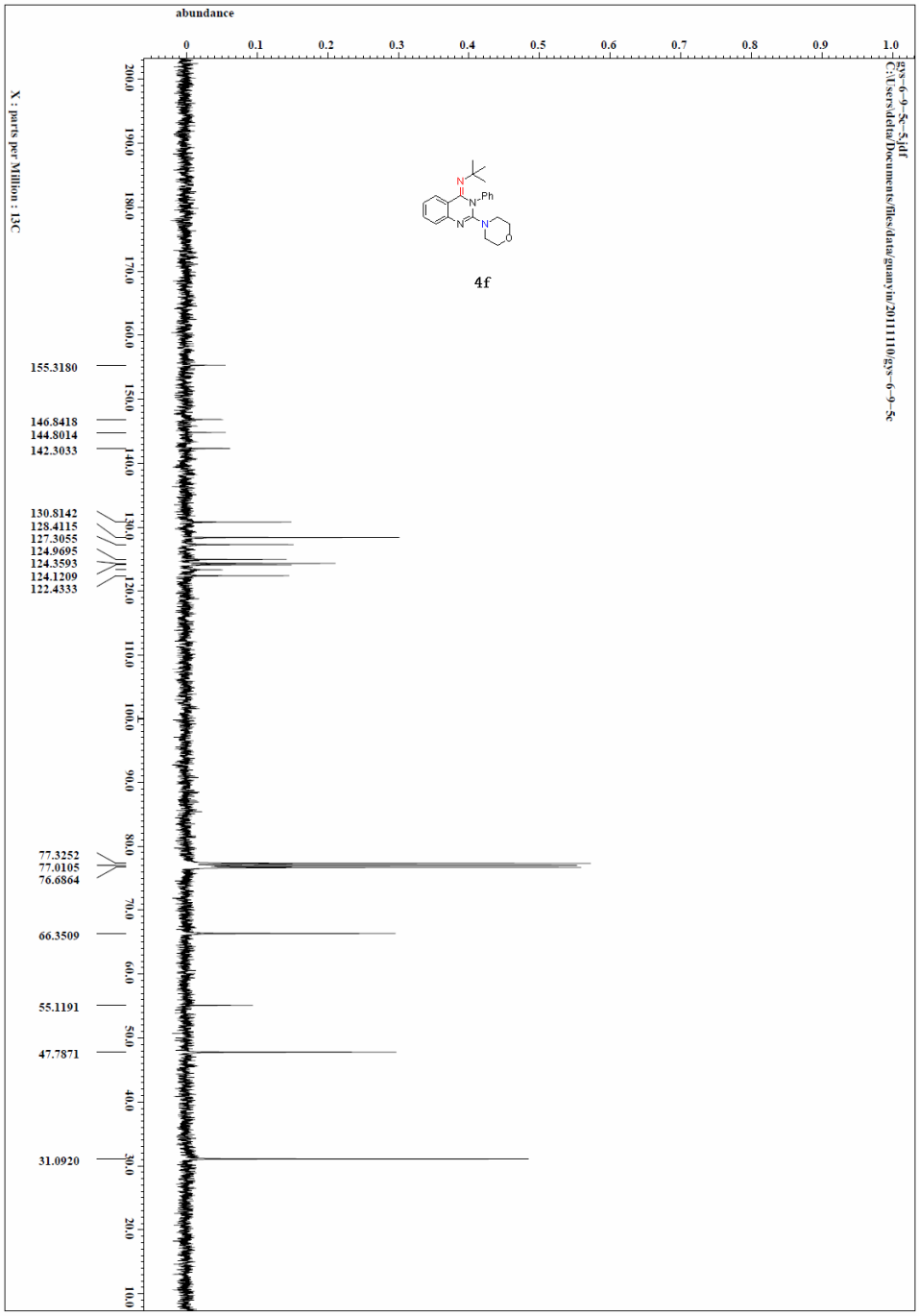

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
155.4119
146.5952
142.5237
130.6434
128.4695
126.5628
123.8692
123.5832
122.5486
122.1100
77.3165
76.9923
76.6777
55.4633
48.1026
31.0452
25.4198
24.5712
13.4133
N
N
Ph
N
N
4d
gsy-6-8-1c-7.jdf
C:\Users\delta\Documents\files\data\guanyi\nr\20111025\gsy-6-8-1c


4e
10.00
60.83
21.71
39.37
20.30
44.28
90.26
7.6733
7.6541
7.2951
7.2555
7.2333
7.2106
7.1572
7.1373
7.0593
7.0424
7.0094
6.9907
6.9720
3.5018
3.4909
3.4537
1.5833
1.5721
1.4888
1.4238
1.3639
f1 (ppm)

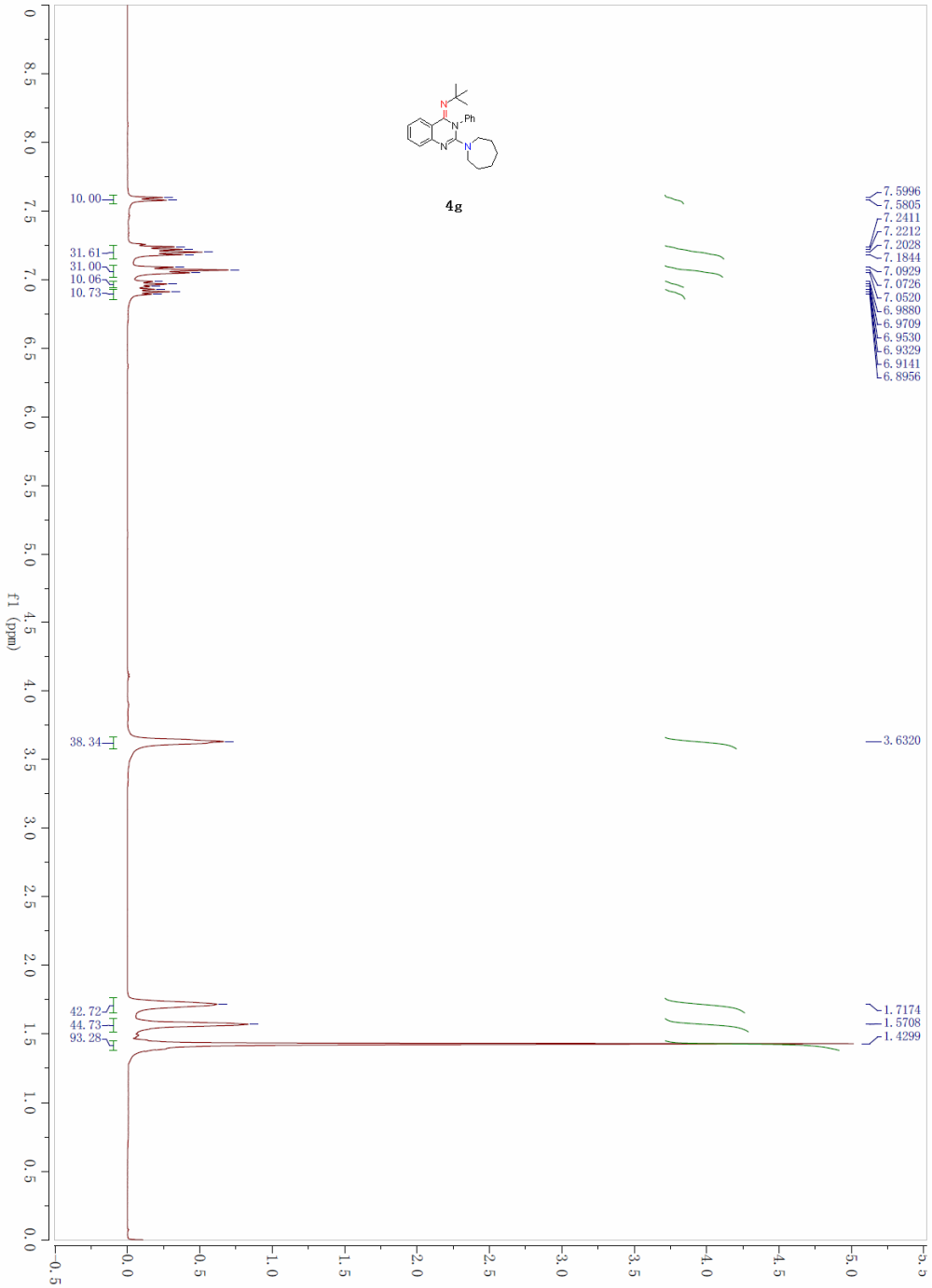

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
155.4619
146.9952
142.7237
130.6434
128.4695
126.7628
123.9692
123.6832
122.5486
122.1100
77.3165
76.9923
76.6777
55.4633
48.1026
31.0452
25.4198
24.5712
N
Ph
N
N
4e
gss-6-8-1c-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20111025\gss-6-8-1c

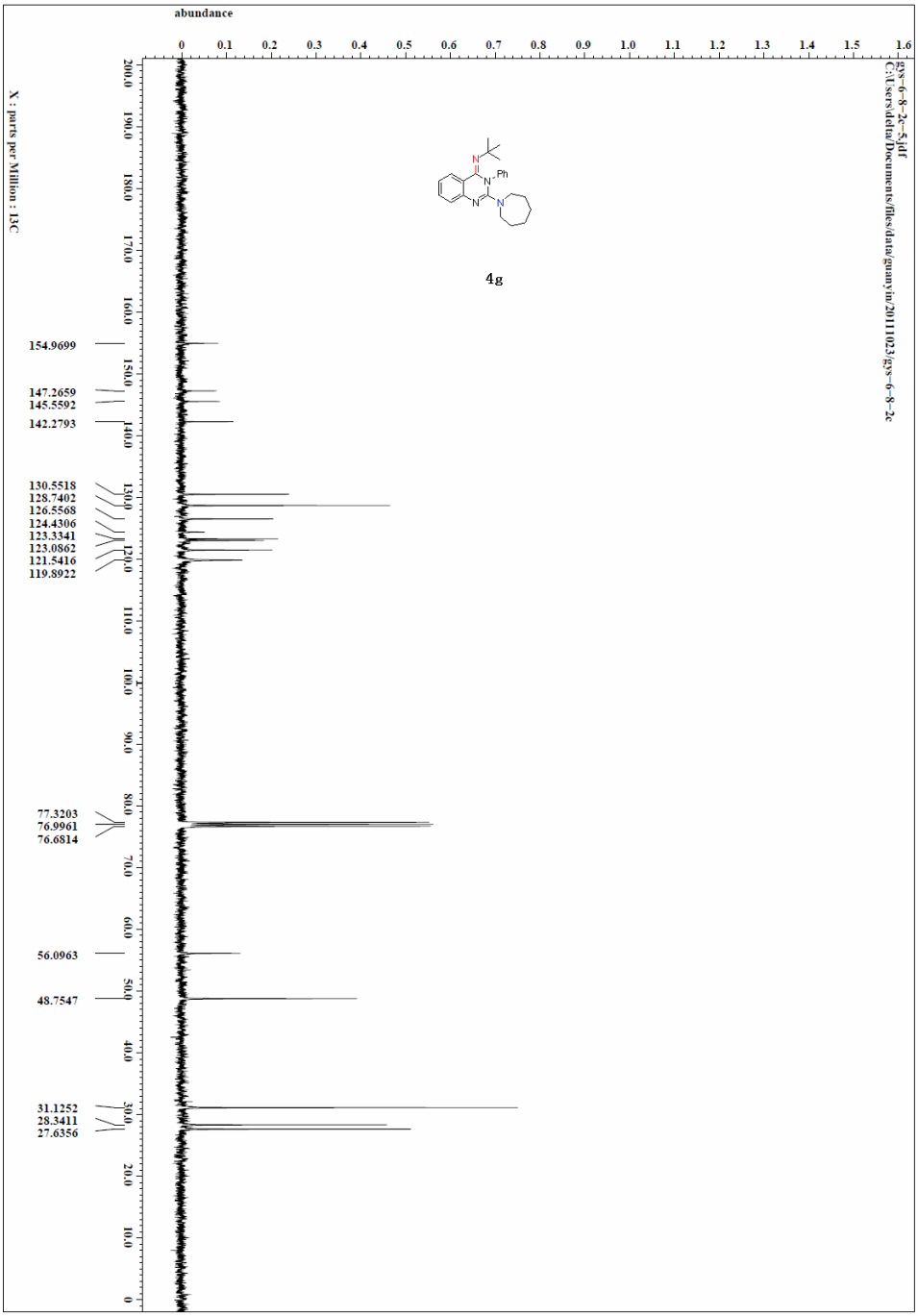

10.00
61.83
10.14
10.87
38.20
41.66
88.12
7.6913
7.6720
7.3632
7.3442
7.3213
7.2995
7.2842
7.2655
7.2456
7.2206
7.2007
7.1341
7.1164
7.0990
7.0608
7.0425
7.0234
3.5741
3.5629
3.4626
3.4516
3.4415
1.3536
f1 (ppm)

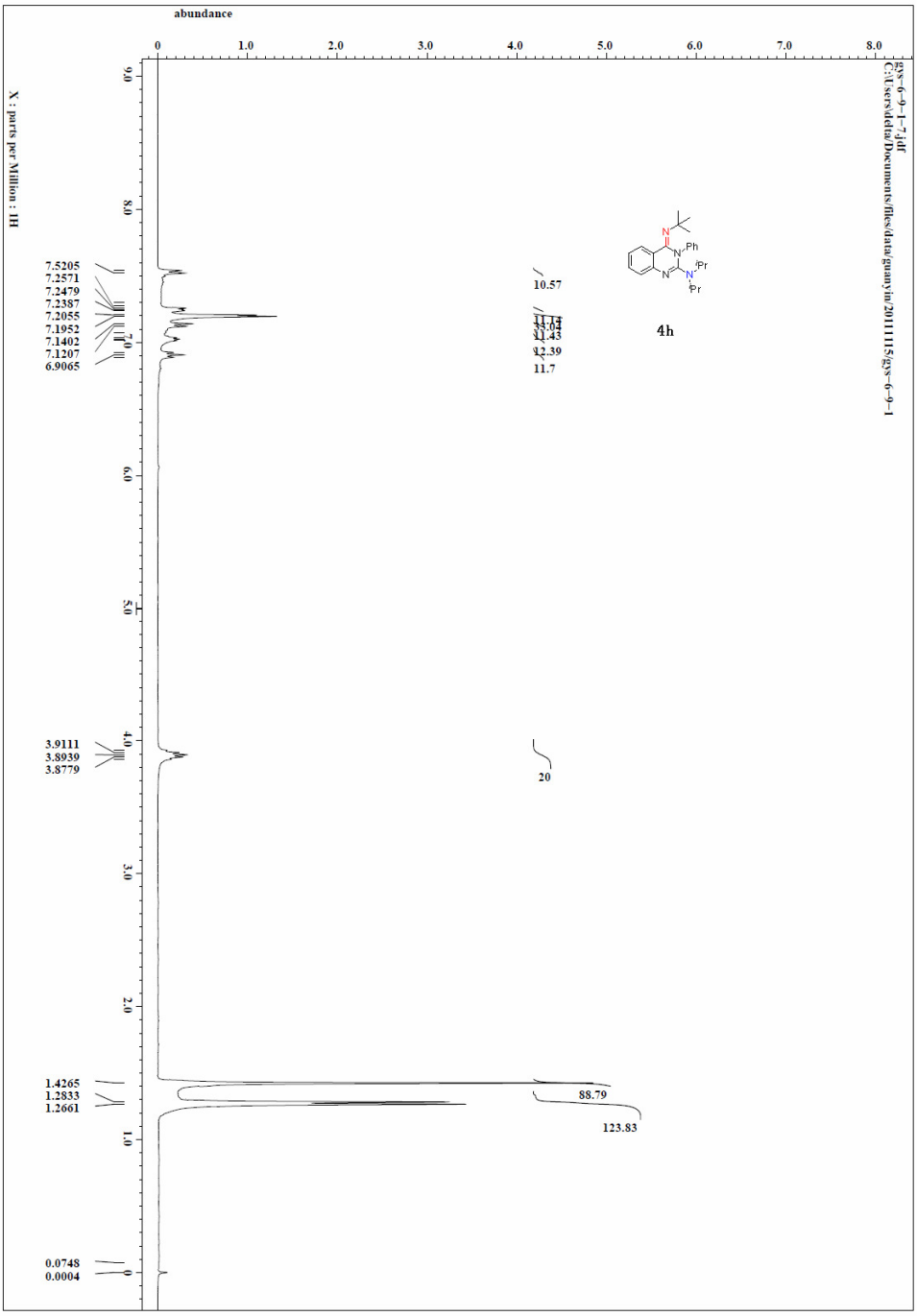
4f

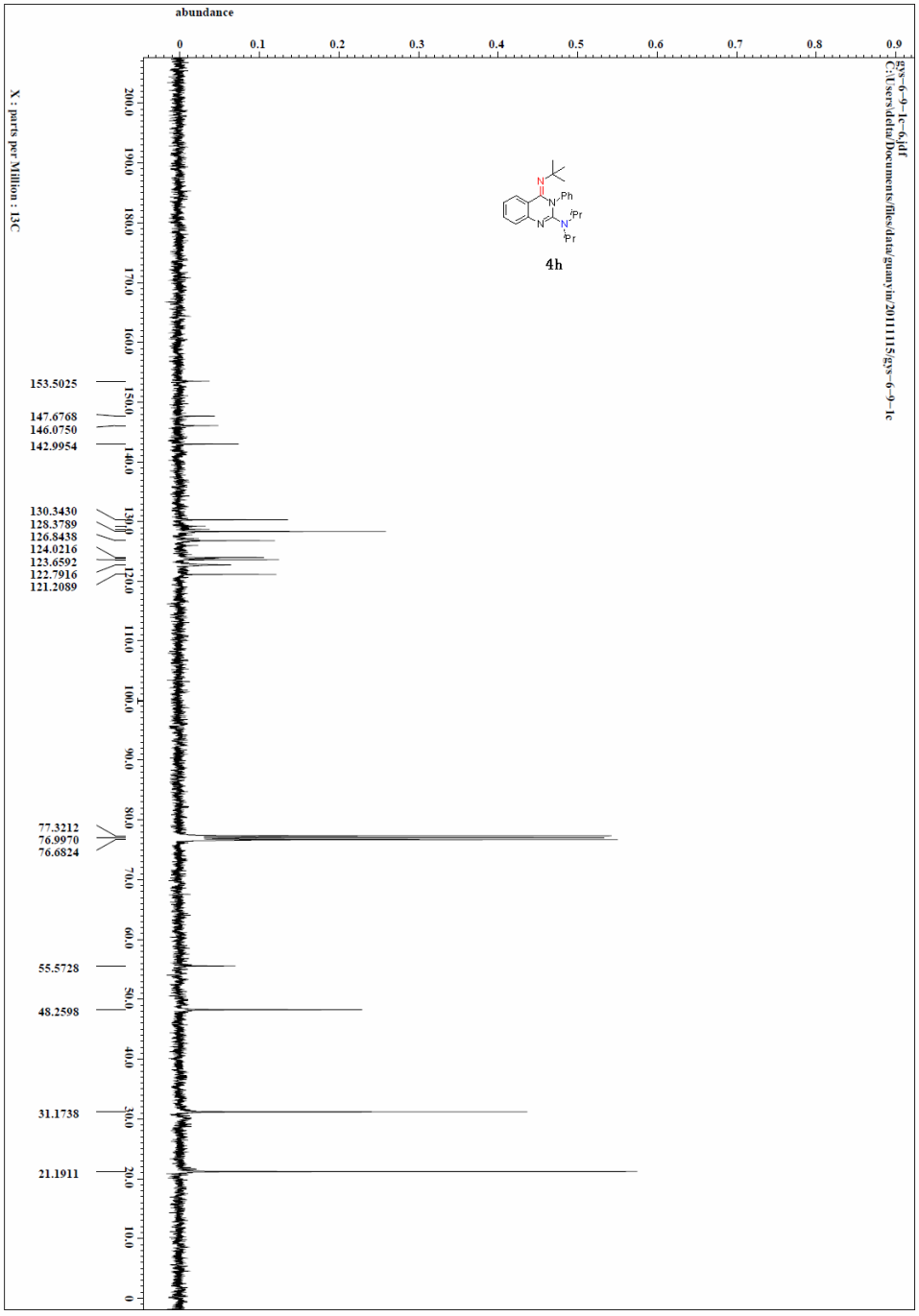

abundance
X : parts per Million : 13C
gsx-6-9-5c-5.jdf
C:\Users\delta\Documents\files\data\guanyin\20111110\gsx-6-9-5c
155.3180
146.8418
144.8014
142.3033
130.8142
128.4115
127.3055
124.9695
124.3593
124.1209
122.4333
77.3252
77.0105
76.6864
66.3509
55.1191
47.7871
31.0920
Ph
N
O

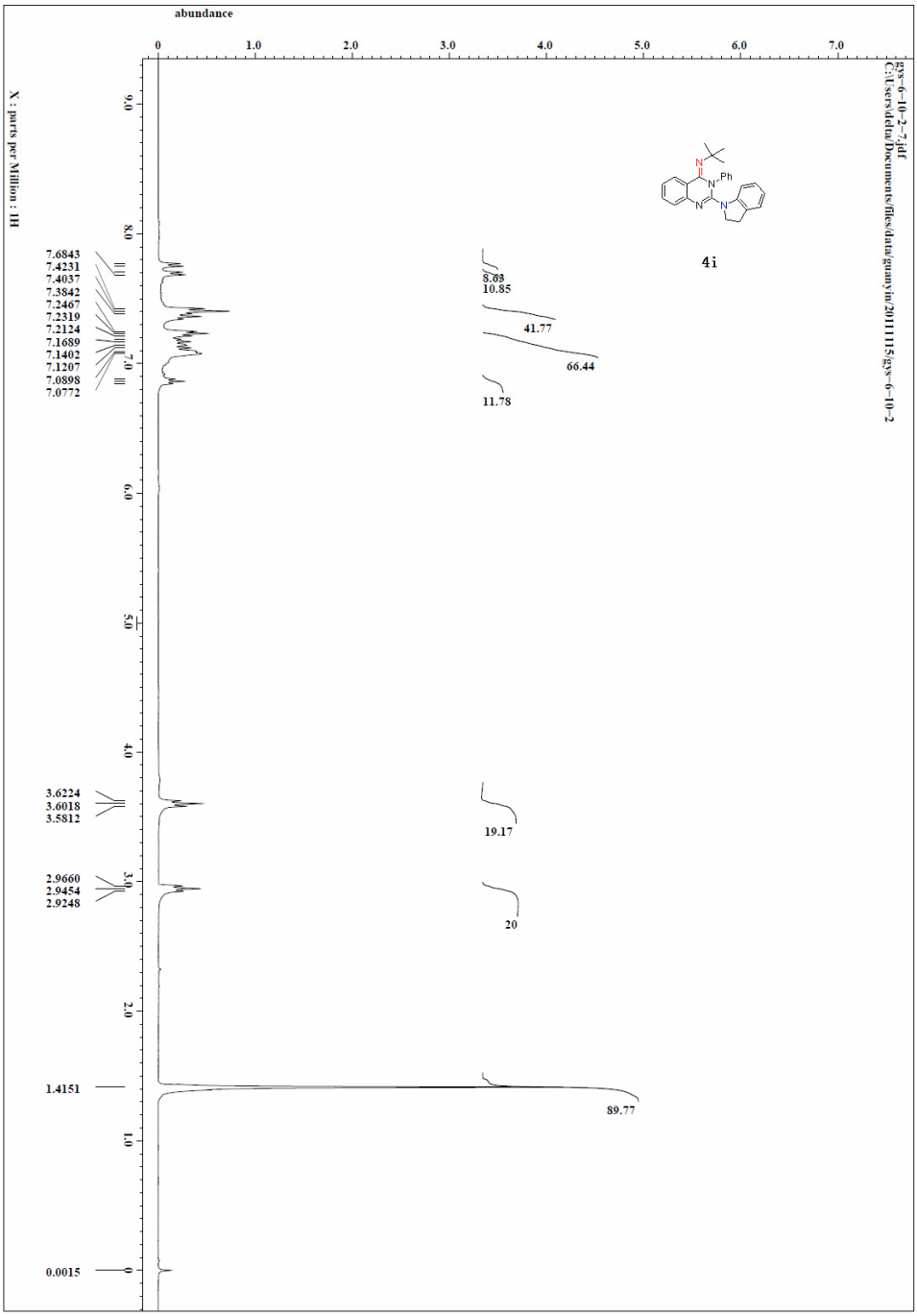
4f

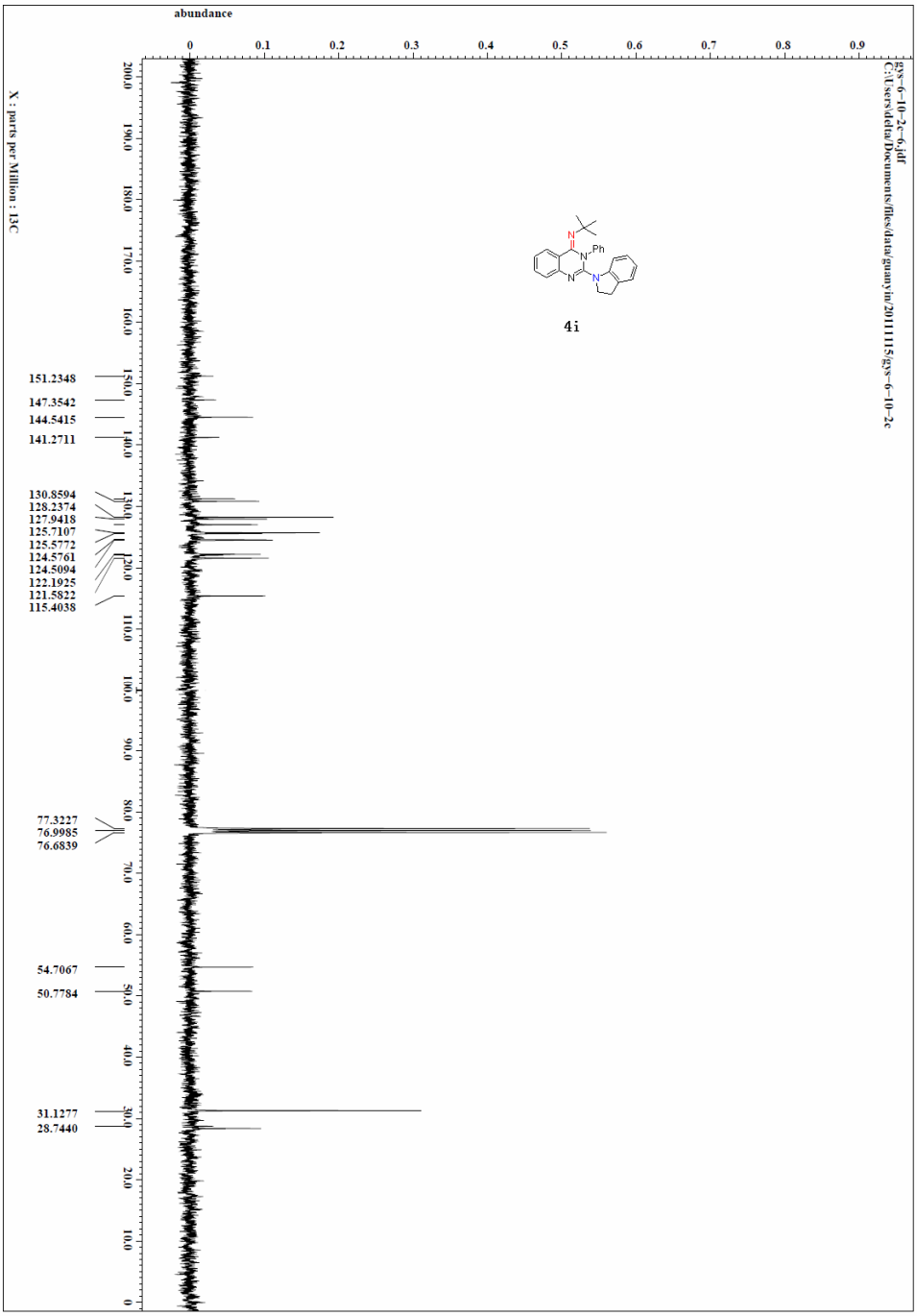

4g
10.00
31.61
31.00
10.06
10.73
38.34
42.72
44.73
93.28
7.5996
7.5805
7.2411
7.2212
7.2028
7.1844
7.0929
7.0726
7.0520
6.9880
6.9709
6.9530
6.9329
6.9141
6.8956
3.6320
1.7174
1.5708
1.4299
f1 (ppm)

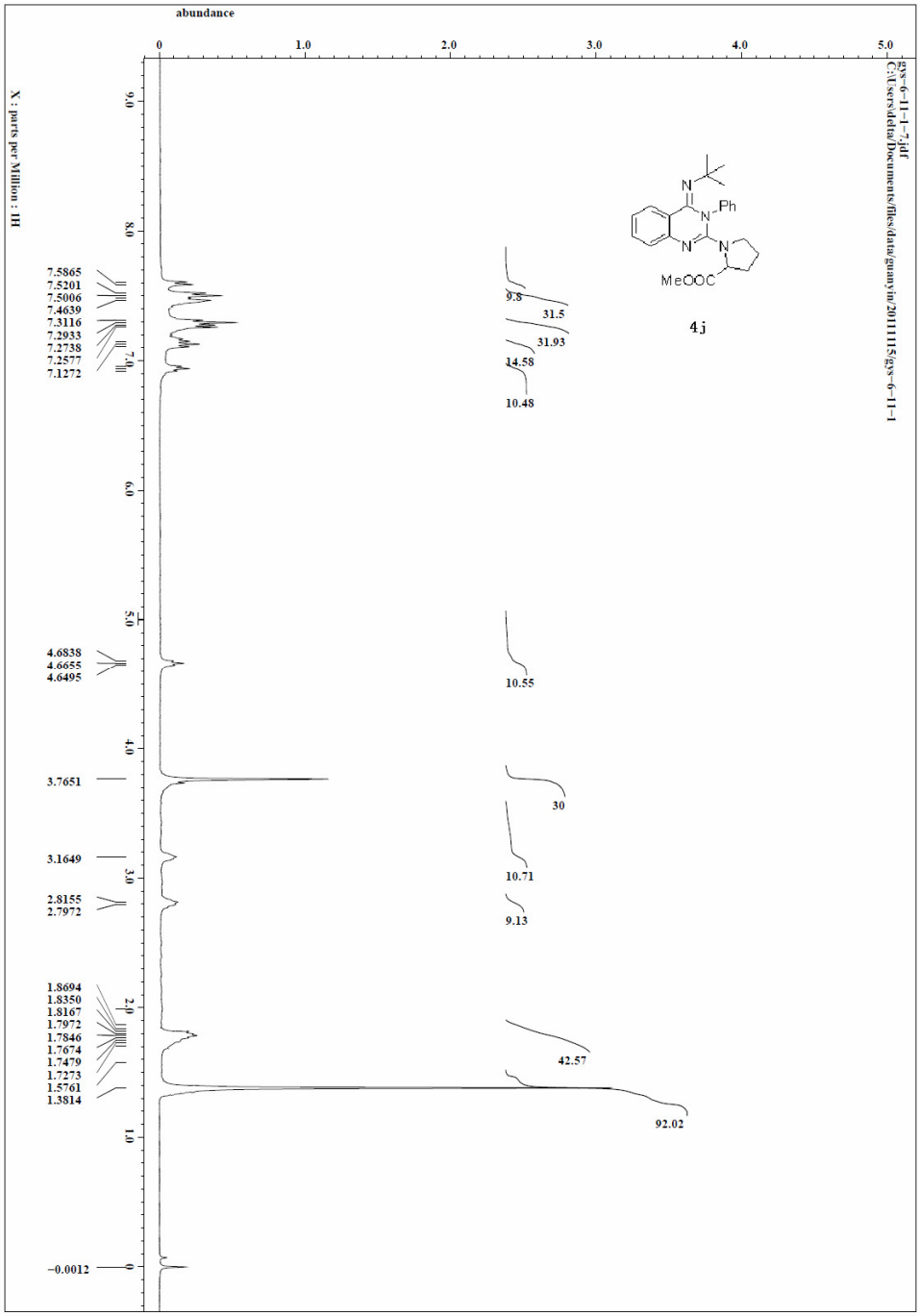

abundance
X : parts per Million : 13C
gys-6-8-2c--5.jdf
C:\Users\delta\Documents\files\data\guanyin\20111023\gys-6-8-2c
Ph
4g
154.9699
147.2659
145.5592
142.2793
130.5518
128.7402
126.5568
124.4306
123.3341
123.0862
121.5416
119.8922
77.3203
76.9961
76.6814
56.0963
48.7547
31.1252
28.3411
27.6356

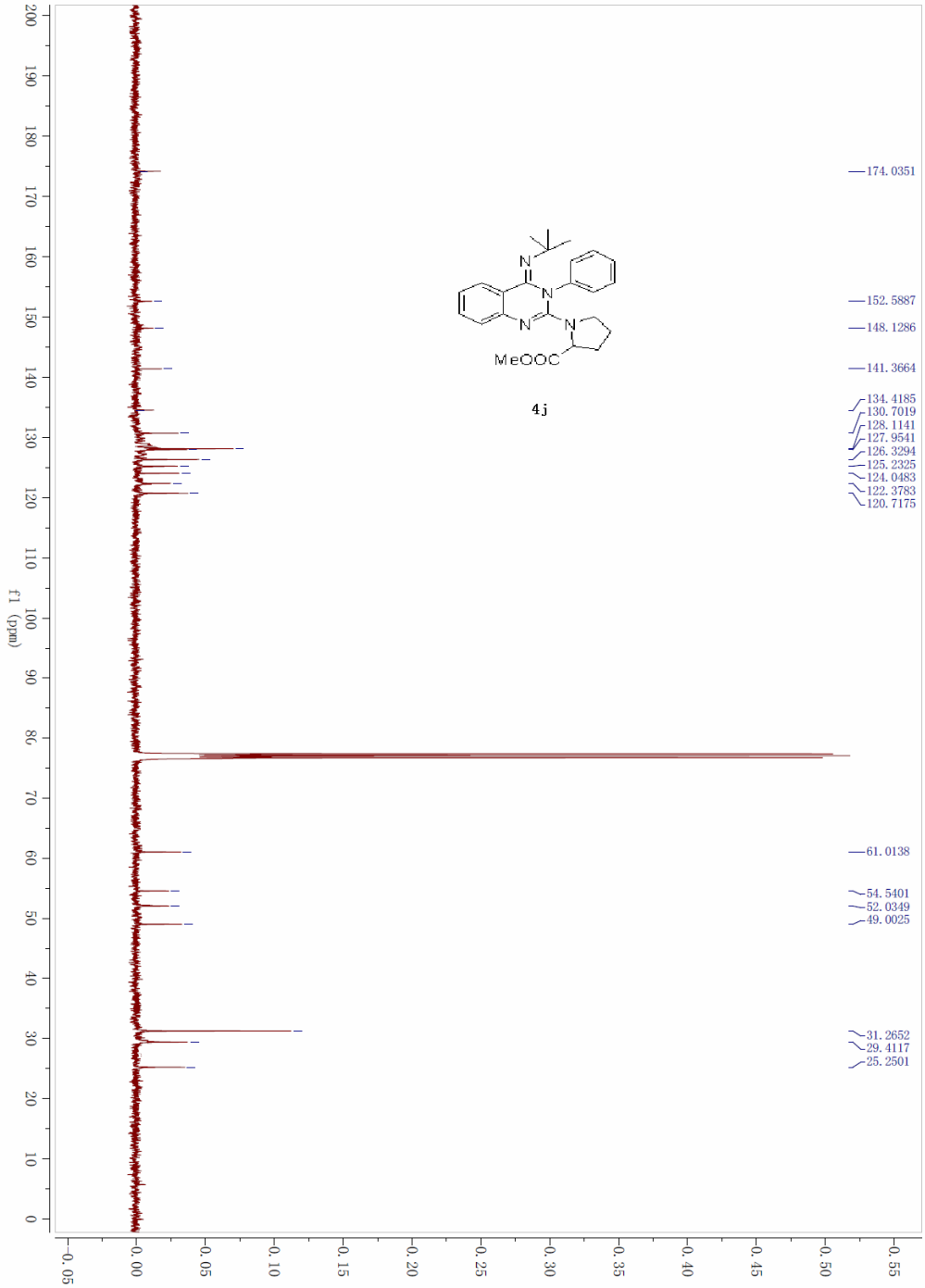

abundance
X : parts per Million : 1H
7.5205
7.2571
7.2479
7.2387
7.2055
7.1952
7.1402
7.1207
6.9065
3.9111
3.8939
3.8779
1.4265
1.2833
1.2661
0.0748
0.0004
10.57
12.39
11.7
20
88.79
123.83
4h
Ph
iPr
iPr

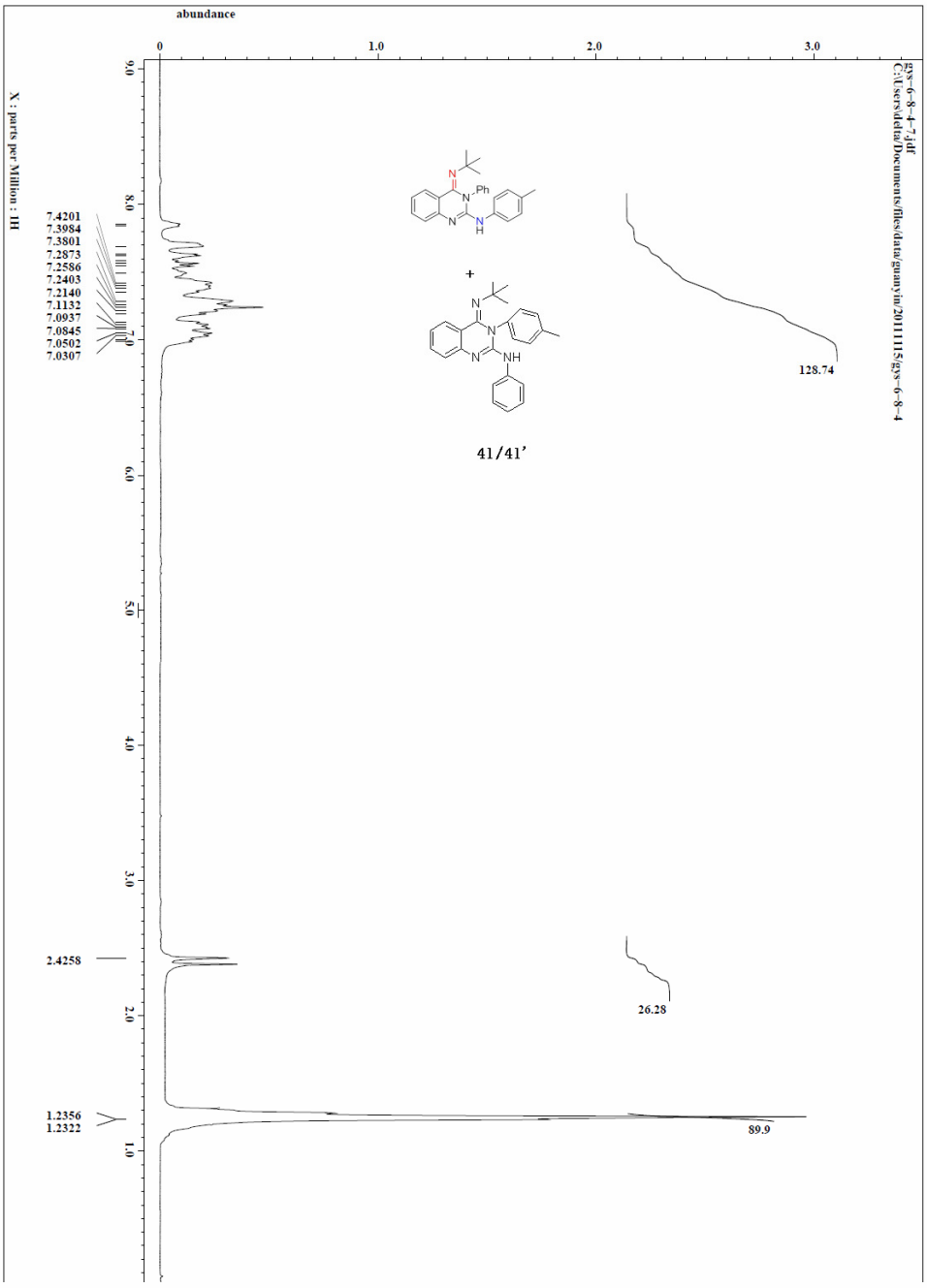

abundance
X : parts per Million : 13C
gys-6-9-1c-6.jdf
C:\Users\data\Documents\files\data\guanyin\20111115\gys-6-9-1c
153.5025
147.6768
146.0750
142.9954
130.3430
128.3789
126.8438
124.0216
123.6592
122.7916
121.2089
77.3212
76.9970
76.6824
55.5728
48.2598
31.1738
21.1911
4h

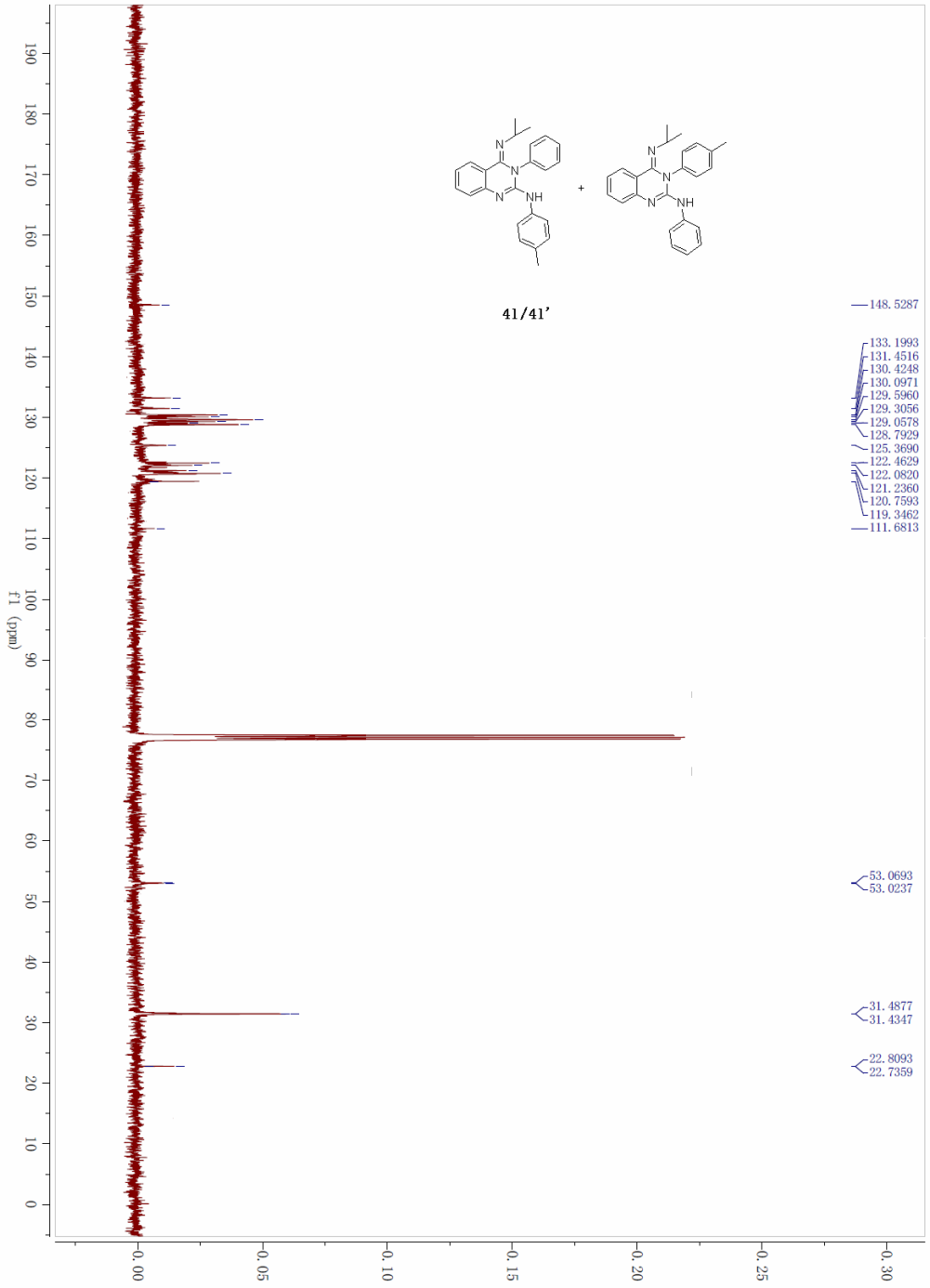

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
X : parts per Million : 1H
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.6843
7.4231
7.4037
7.3842
7.2467
7.2319
7.2124
7.1689
7.1402
7.1207
7.0898
7.0772
3.6224
3.6018
3.5812
2.9660
2.9454
2.9248
1.4151
0.0015
8.03
10.85
41.77
66.44
11.78
19.17
20
89.77
Ph
4i
gys-6-10-2-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20111115\gys-6-10-2

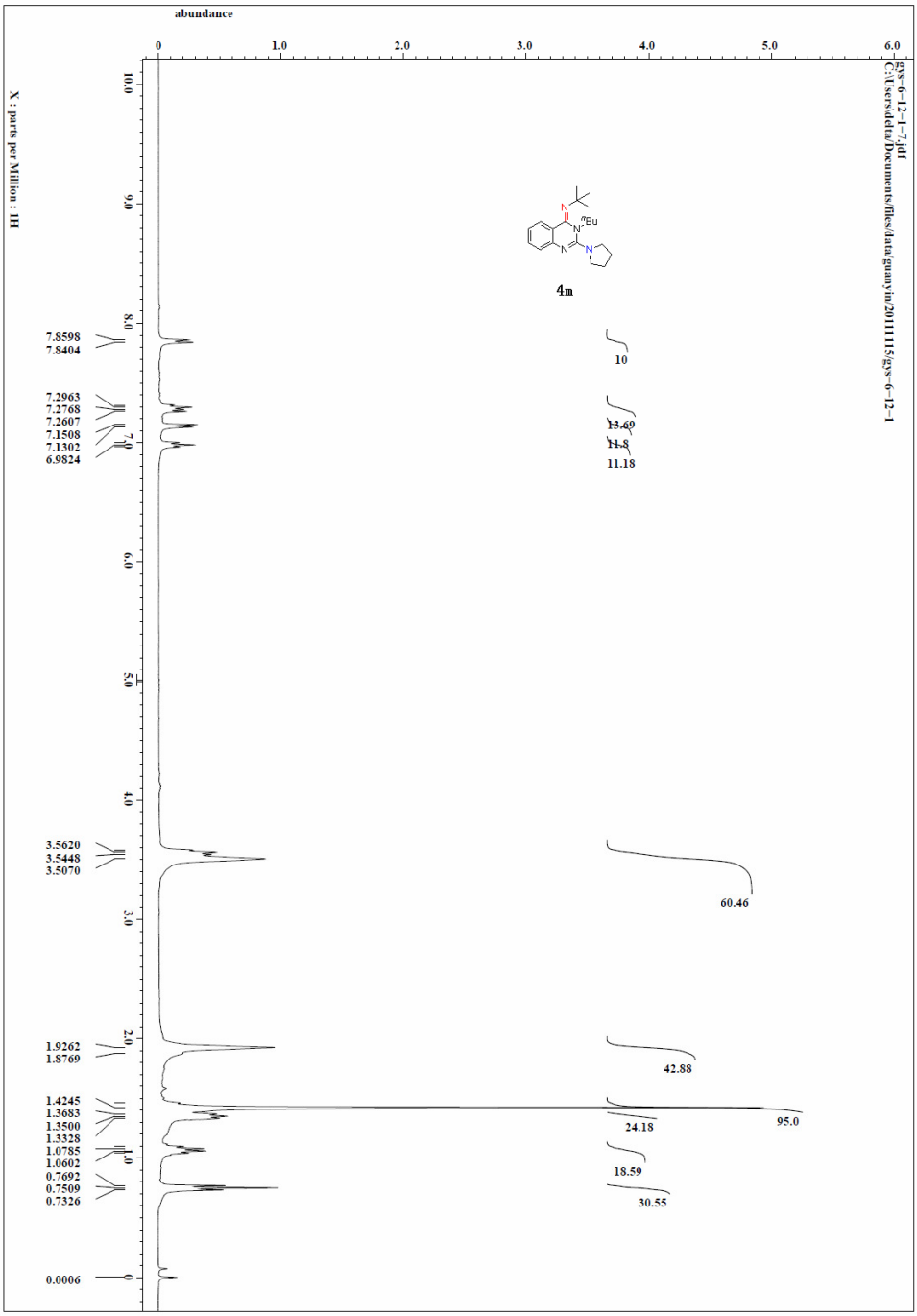

abundance
X : parts per Million : 13C
gsx-6-10-2c-6.jdf
C:\Users\delta\Documents\files\data\guanyin\20111115\gsx-6-10-2c
151.2348
147.3542
144.5415
141.2711
130.8594
128.2374
127.9418
125.7107
125.5772
124.5761
124.5094
122.1925
121.5822
115.4038
77.3227
76.9985
76.6839
54.7067
50.7784
31.1277
28.7440
Ph
4i

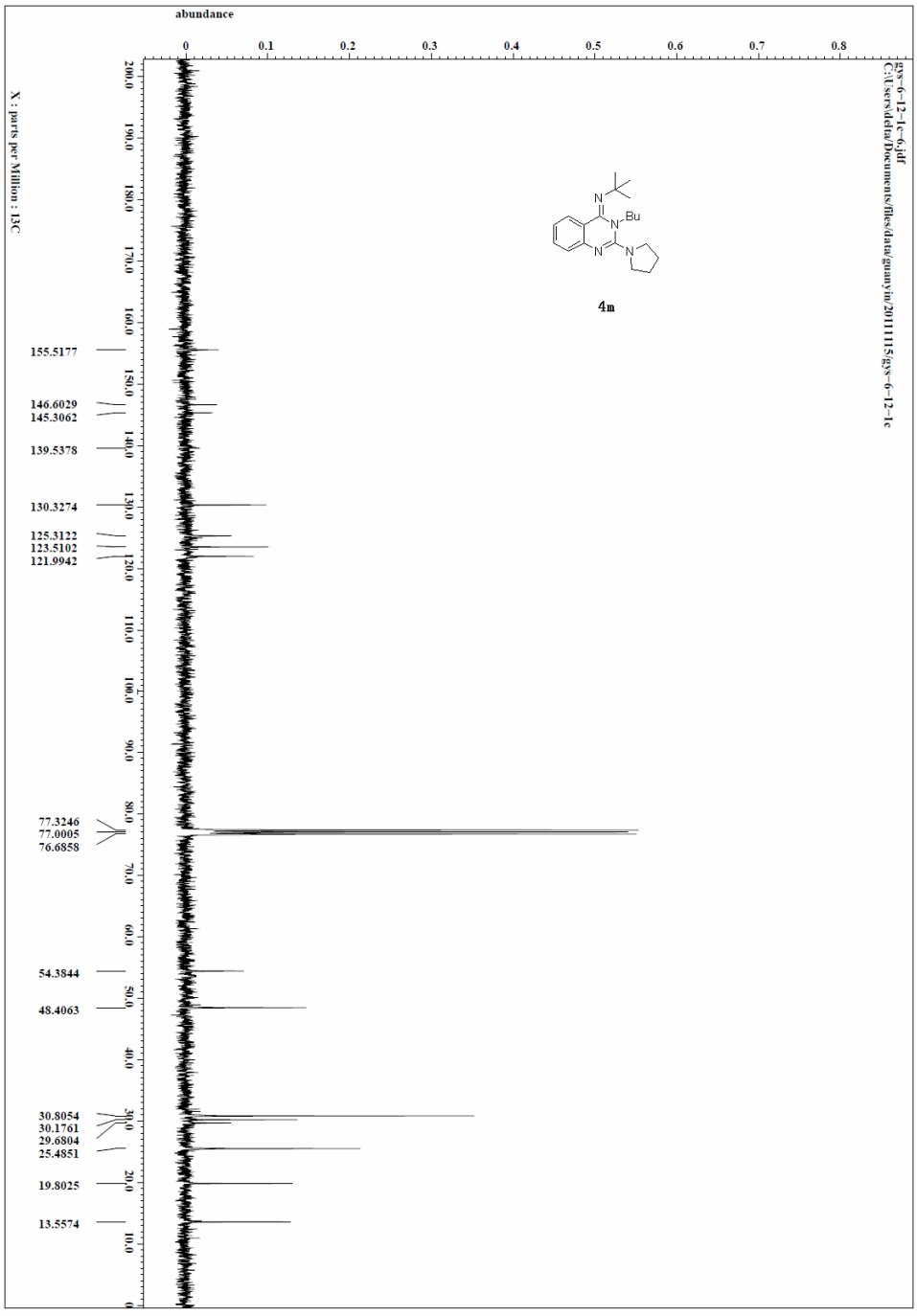

abundance
X : parts per Million : 1H
gyx-6-11-7.jdf
C:\Users\delta\Documents\flex\data\guanyin\20111115\gyx-6-11-1
7.5865
7.5201
7.5006
7.4639
7.3116
7.2933
7.2738
7.2577
7.1272
4.6838
4.6655
4.6495
3.7651
3.1649
2.8155
2.7972
1.8694
1.8350
1.8167
1.7972
1.7846
1.7674
1.7479
1.7273
1.5761
1.3814
−0.0012
9.8
31.5
31.93
14.58
10.48
10.55
30
10.71
9.13
42.57
92.02
Ph
MeOOC
4j

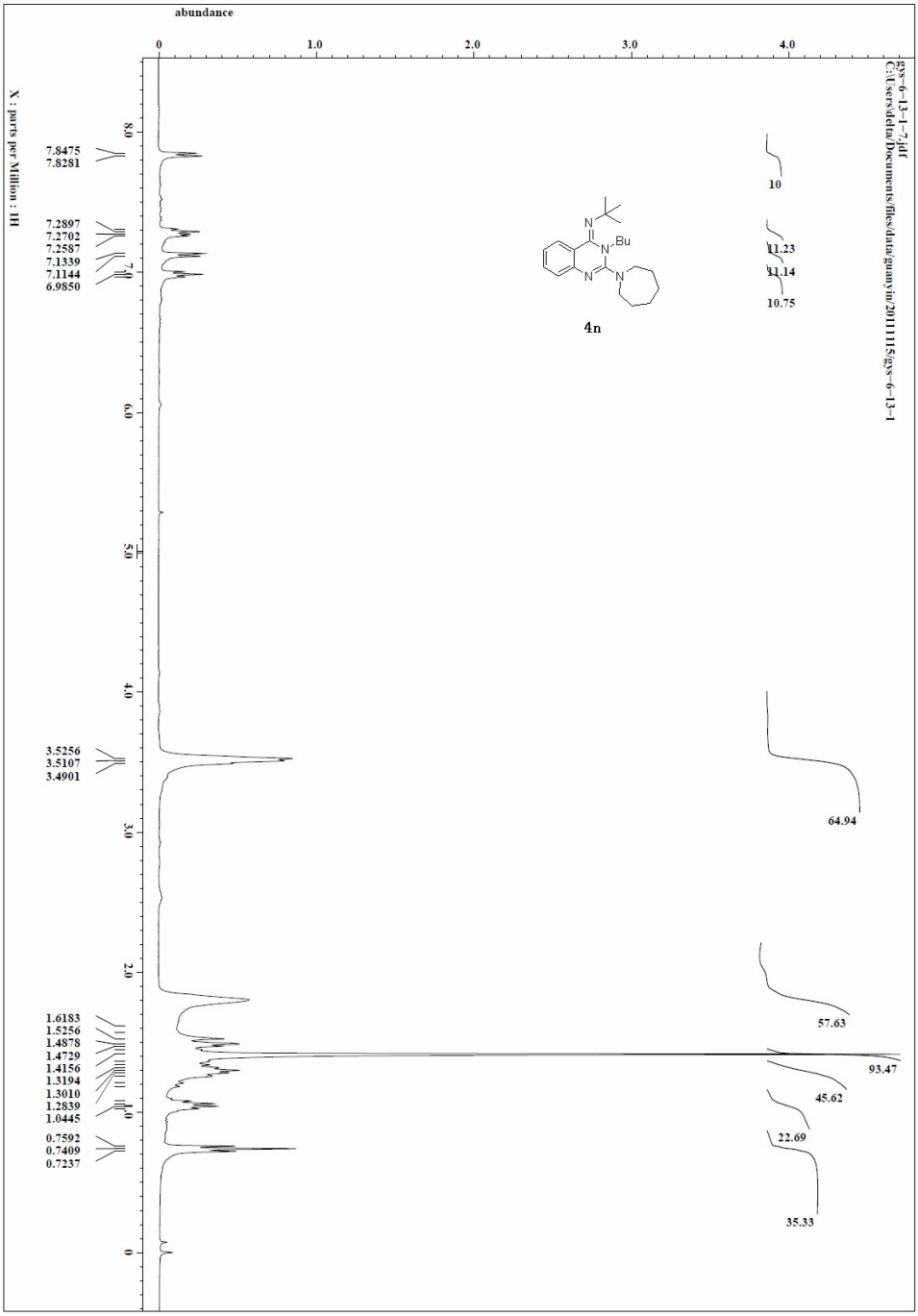

174.0351
152.5887
148.1286
141.3664
134.4185
130.7019
128.1141
127.9541
126.3294
125.2325
124.0483
122.3783
120.7175
61.0138
54.5401
52.0349
49.0025
31.2652
29.4117
25.2501
MeOOC
4j
f1 (ppm)

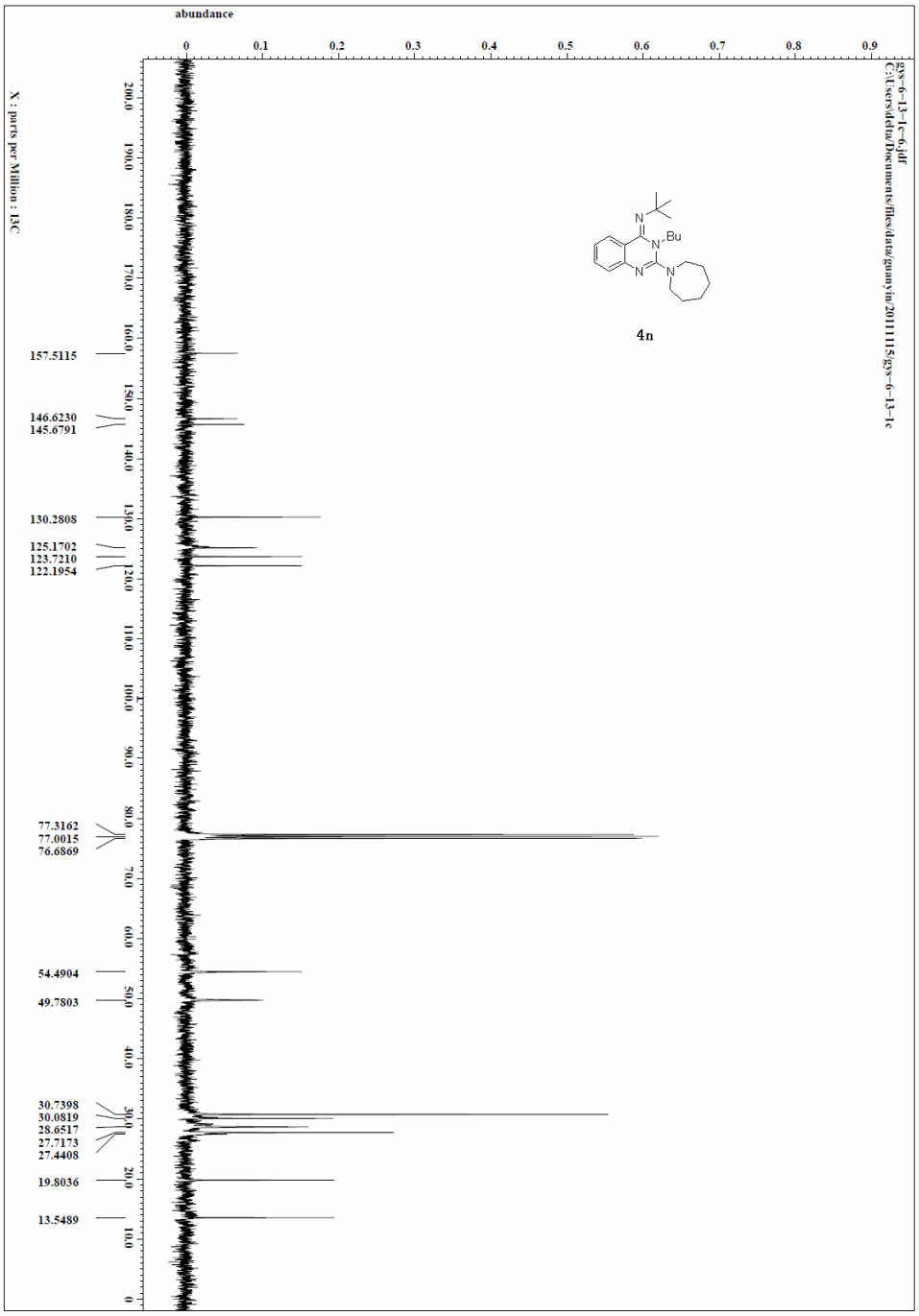

abundance
0
1.0
2.0
3.0
X : parts per Million : 1H
7.4201
7.3984
7.3801
7.2873
7.2586
7.2403
7.2140
7.1132
7.0937
7.0845
7.0502
7.0307
2.4258
1.2356
1.2322
128.74
26.28
89.9
Ph
NH
41/41'
gys-6-8-4-1.jdf
C:\Users\ldfu\Documents\files\data\guanyin\20111115\gys-6-8-4

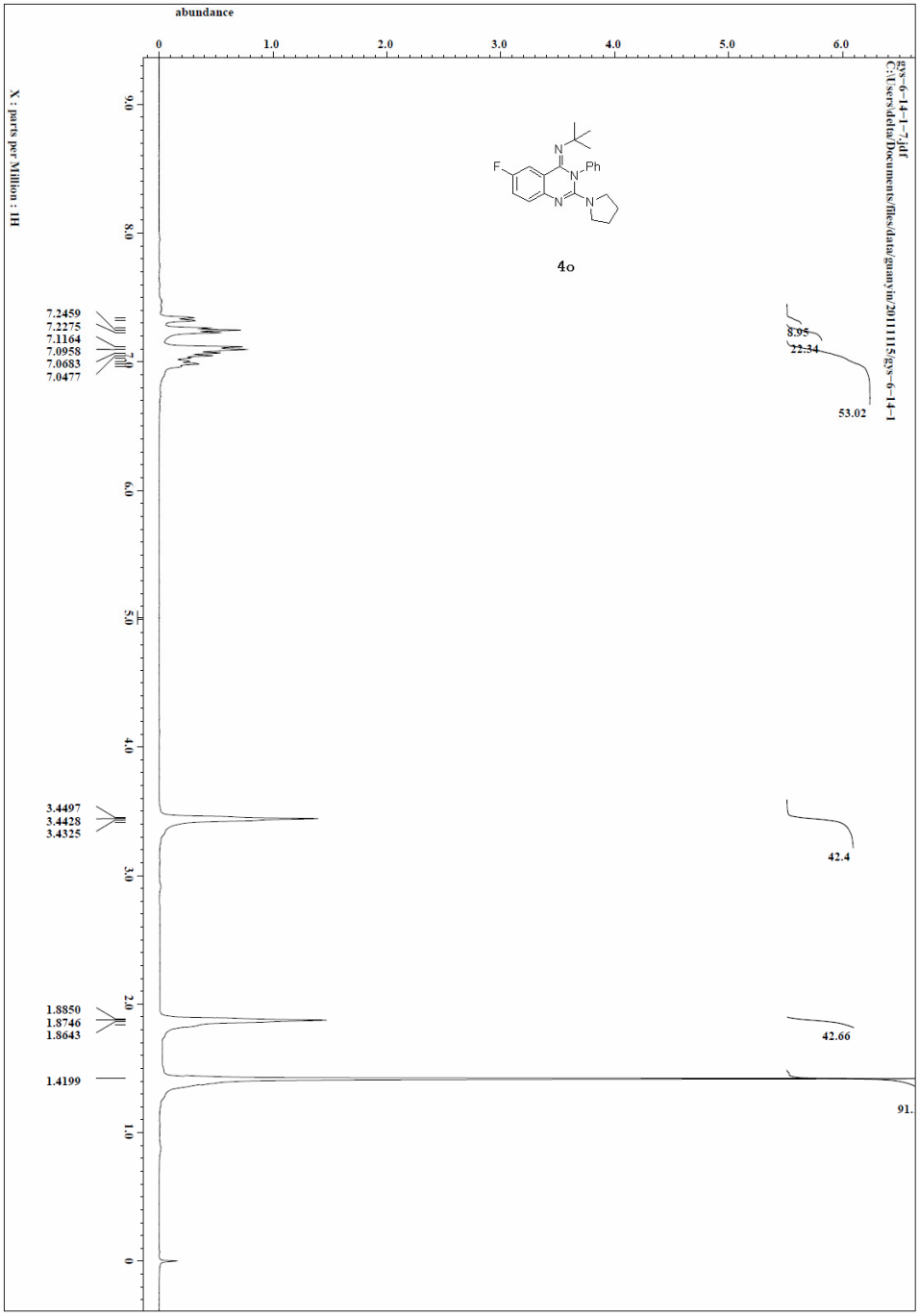

41/41'
148.5287
133.1993
131.4516
130.4248
130.0971
129.5960
129.3056
129.0578
128.7929
125.3690
122.4629
122.0820
121.2360
120.7593
119.3462
111.6813
53.0693
53.0237
31.4877
31.4347
22.8093
22.7359
f1 (ppm)

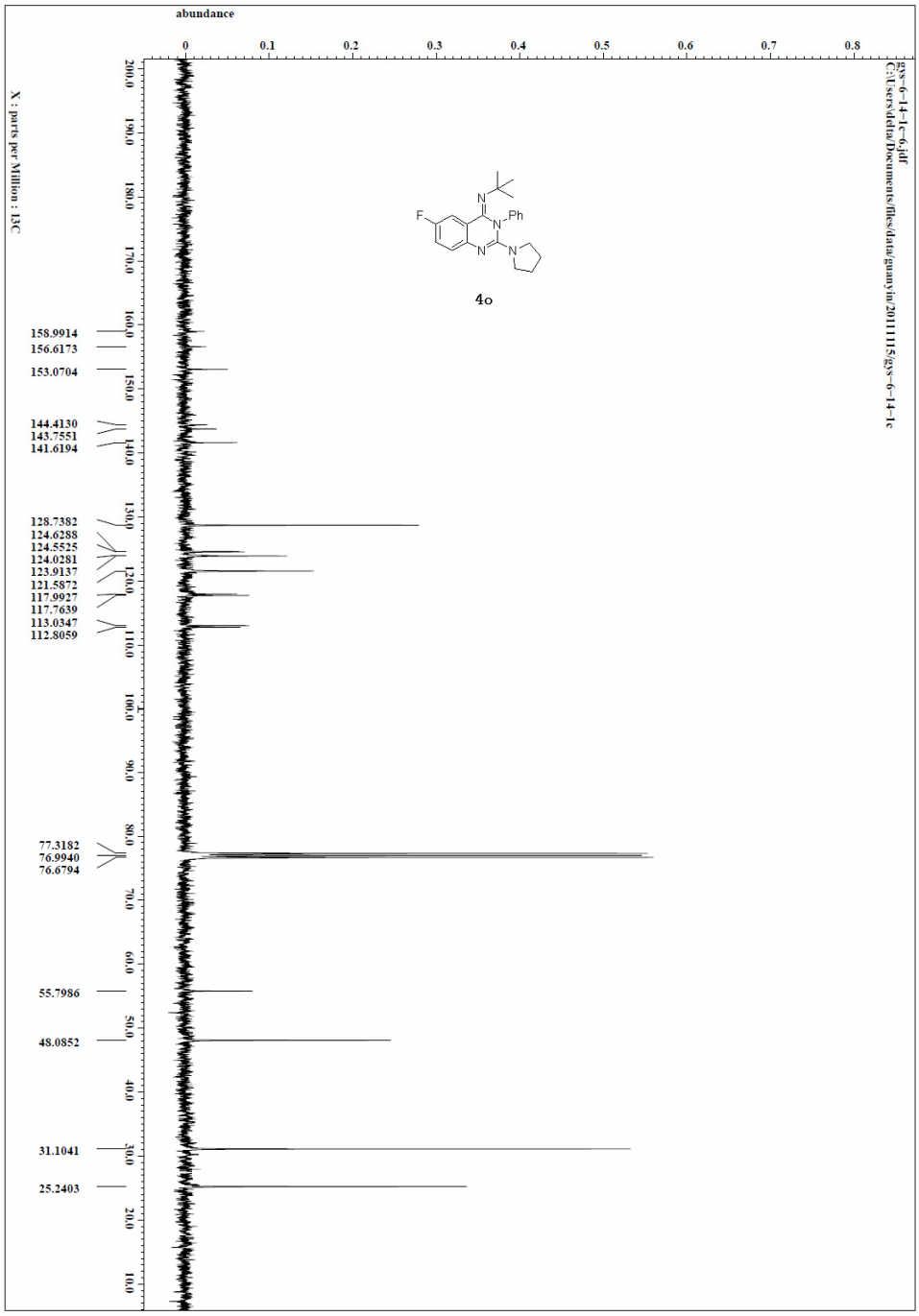

abundance
X : parts per Million : 1H
gys-6-12-1-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20111115\gys-6-12-1
4m
7.8598
7.8404
7.2963
7.2768
7.2607
7.1508
7.1302
6.9824
3.5620
3.5448
3.5070
1.9262
1.8769
1.4245
1.3683
1.3500
1.3328
1.0785
1.0602
0.7692
0.7509
0.7326
0.0006
10
13.69
11.18
60.46
42.88
95.0
24.18
18.59
30.55

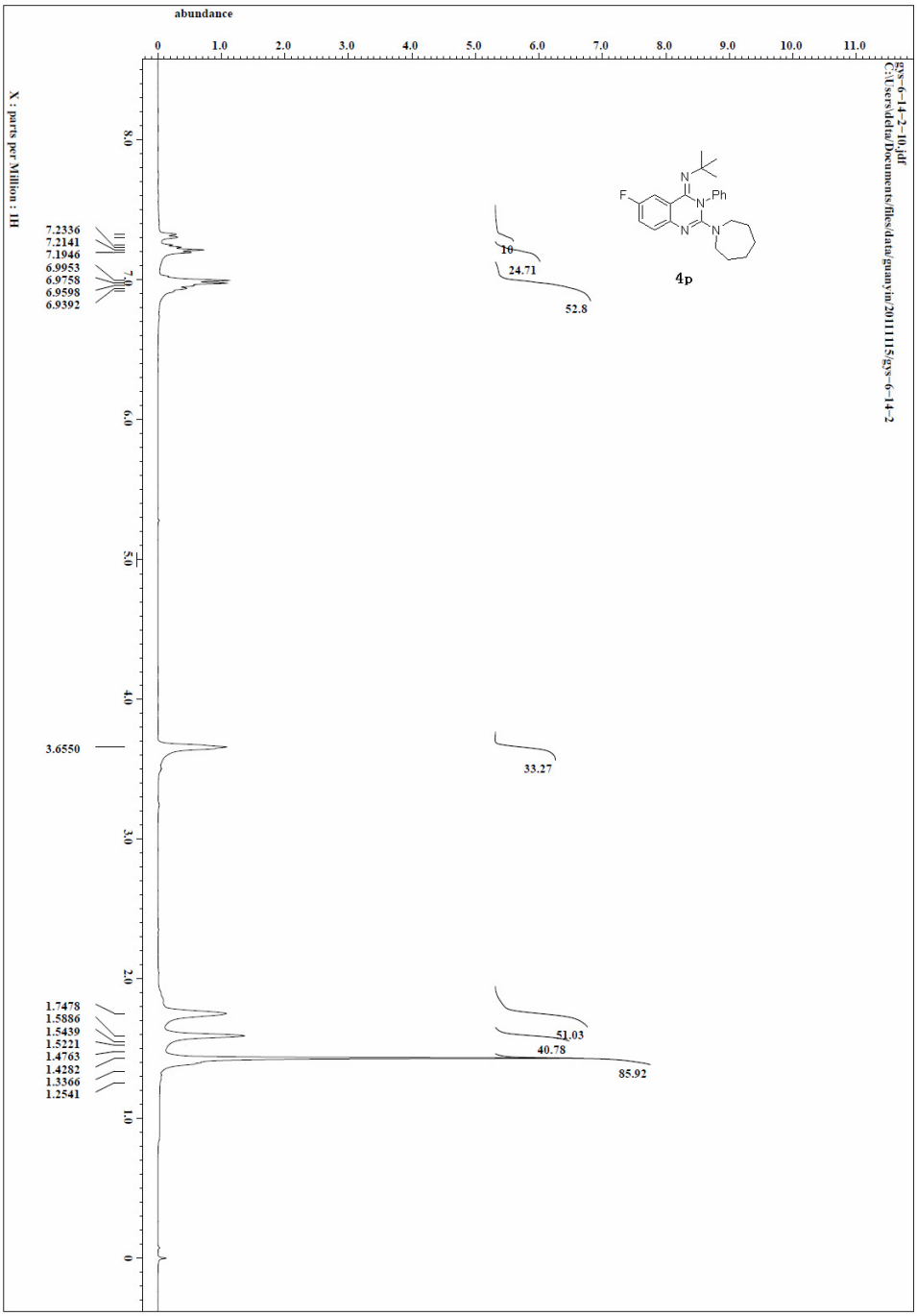

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
X : parts per Million : 13C
gys-6-12-1c-6.jdf
C:\Users\ddtu\Documents\files\data\guanyin\20111115\gys-6-12-1c
Bu
4m
155.5177
146.6029
145.3062
139.5378
130.3274
125.3122
123.5102
121.9942
77.3246
77.0005
76.6858
54.3844
48.4063
30.8054
30.1761
29.6804
25.4851
19.8025
13.5574

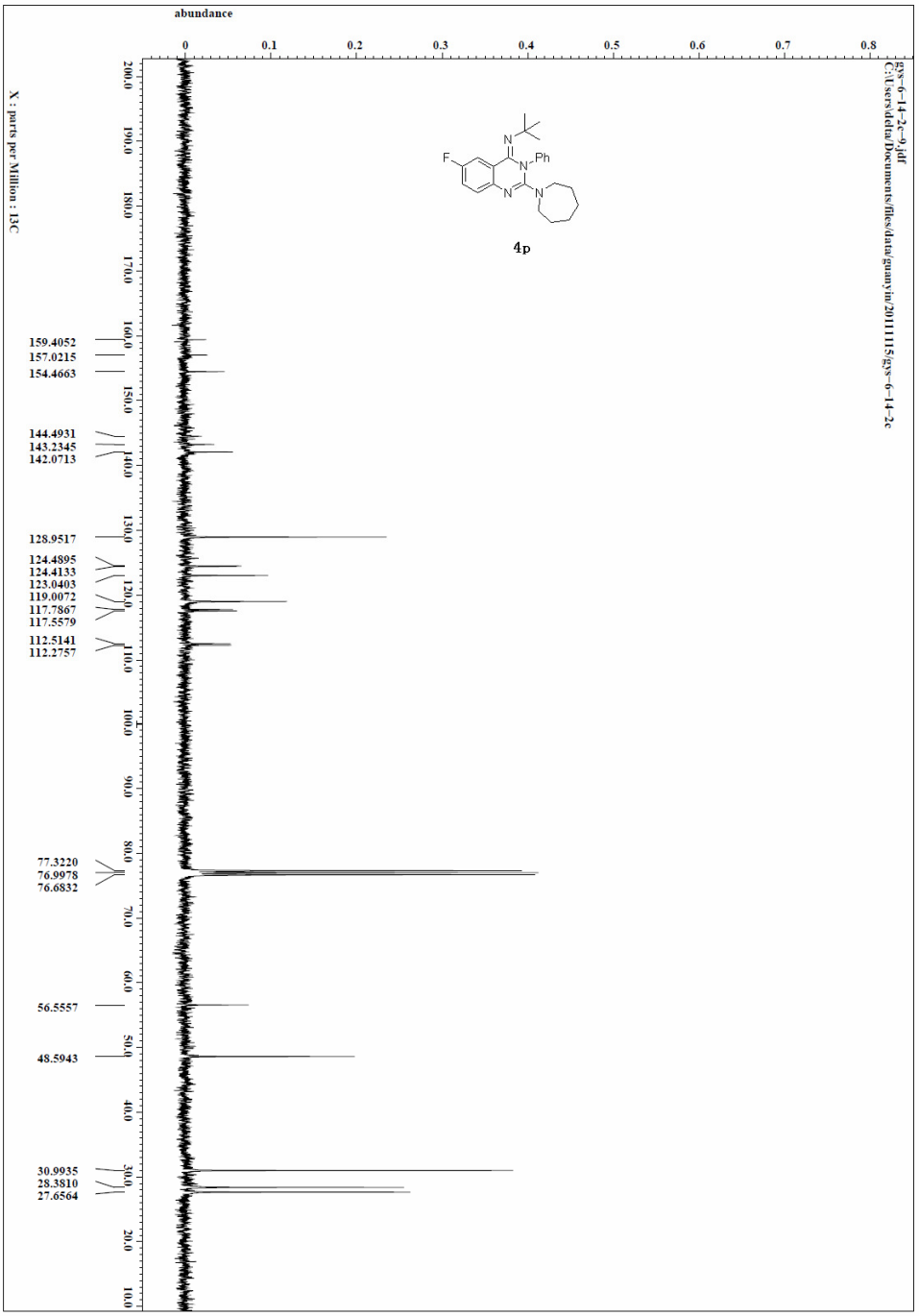

abundance
X : parts per Million : 1H
gss-6-13-1-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20111115\gss-6-13-1
7.8475
7.8281
7.2897
7.2702
7.2587
7.1339
7.1144
6.9850
3.5256
3.5107
3.4901
1.6183
1.5256
1.4878
1.4729
1.4156
1.3194
1.3010
1.2839
1.0445
0.7592
0.7409
0.7237
10
11.23
11.14
10.75
64.94
57.63
93.47
45.62
22.69
35.33
4n


abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
157.5115
146.6230
145.6791
130.2808
125.1702
123.7210
122.1954
77.3162
77.0015
76.6869
54.4904
49.7803
30.7398
30.0819
28.6517
27.7173
27.4408
19.8036
13.5489
gys-6-13-1c-6.jdf
C:\Users\delta\Documents\files\data\guanyin\20111115\gys-6-13-1c
N
N
Bu
N
N
4n

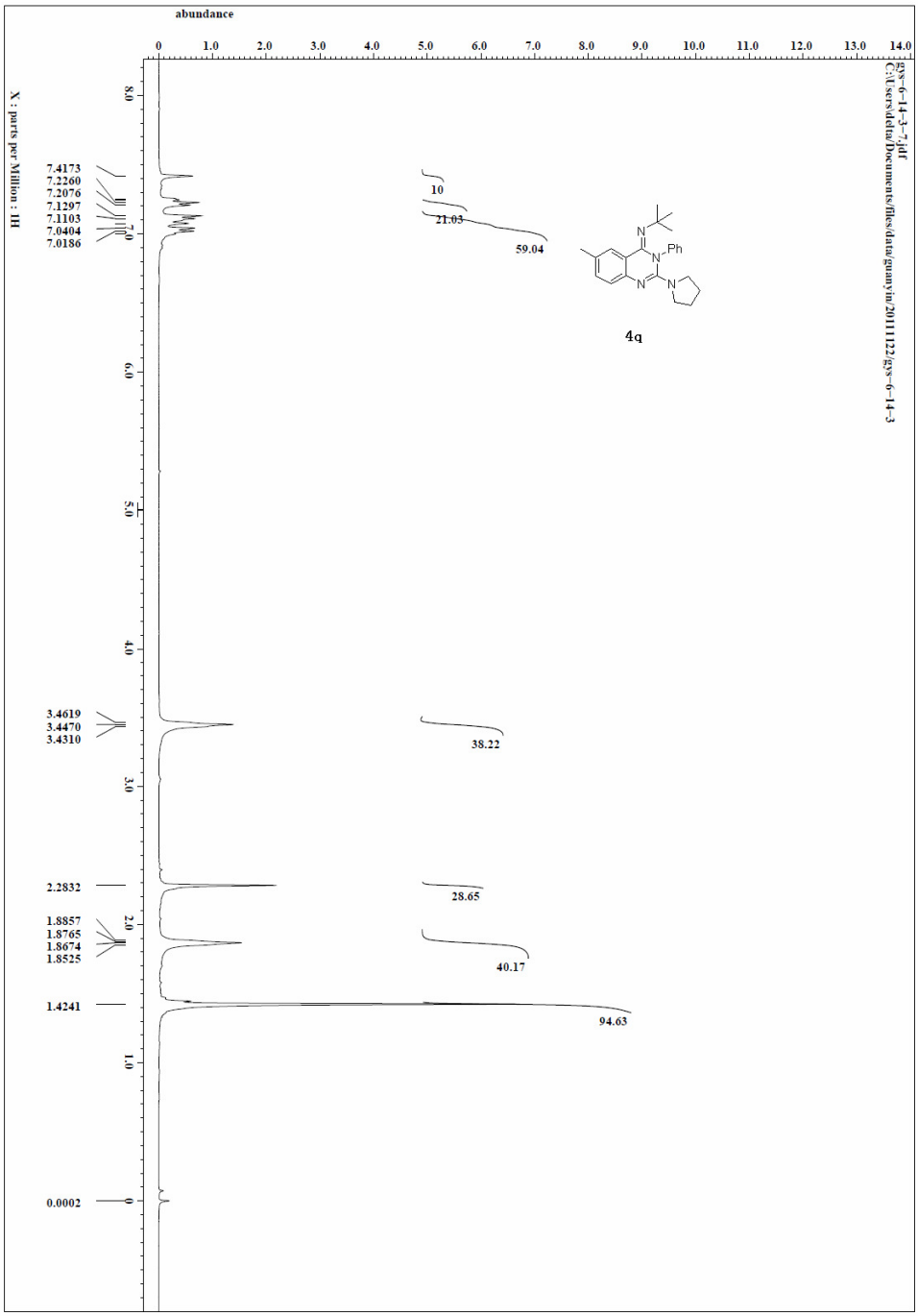

abundance
X : parts per Million : 1H
gys-6-14-1-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20111115\gys-6-14-1
4o
7.2459
7.2275
7.1164
7.0958
7.0683
7.0477
3.4497
3.4428
3.4325
1.8850
1.8746
1.8643
1.4199
8.95
22.34
53.02
42.4
42.66
91.

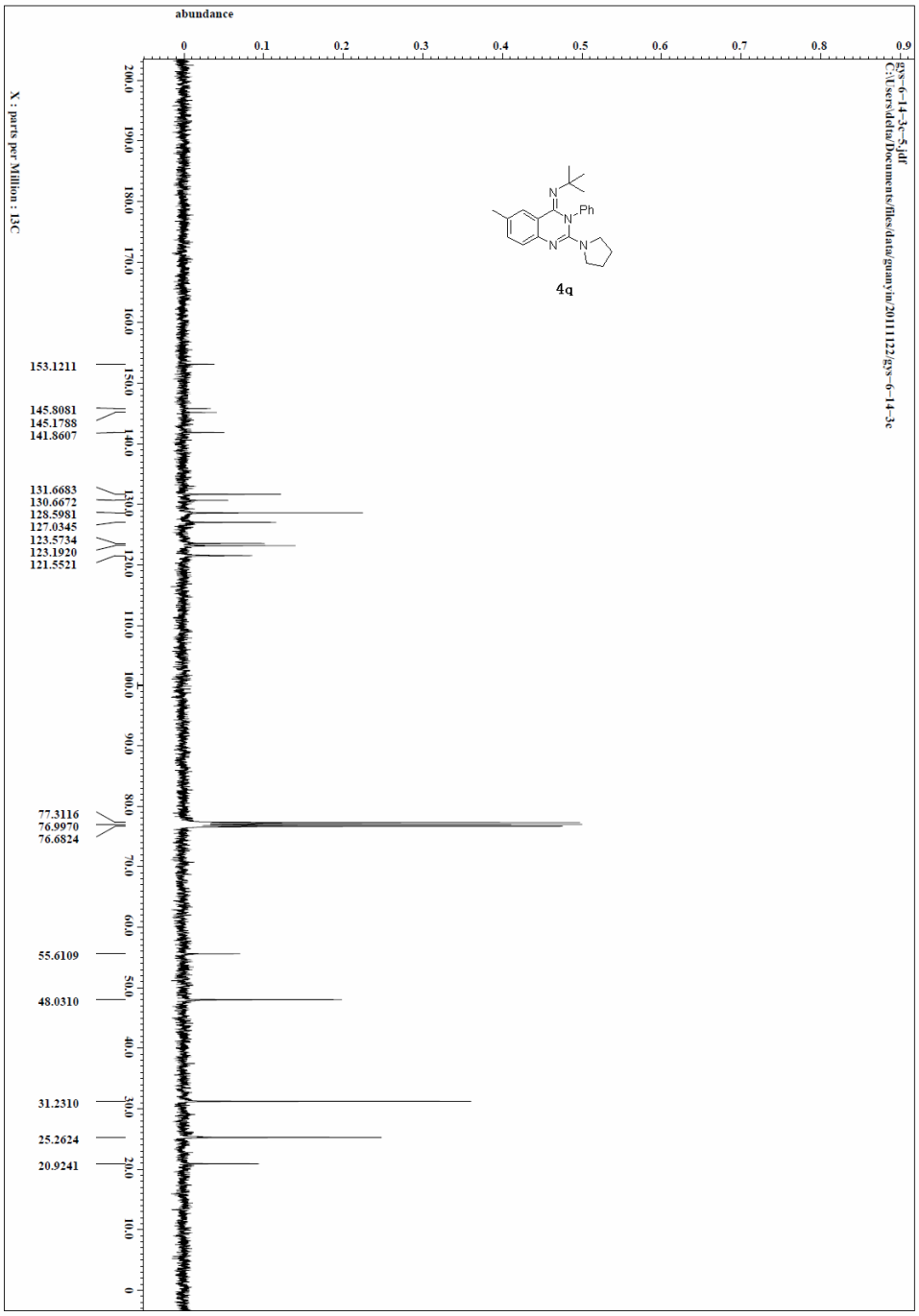

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
gys-6-14-1c-6.jdf
C:\Users\dell\a\Documents\files\data\guanyin\20111115\gys-6-14-1c
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
158.9914
156.6173
153.0704
144.4130
143.7551
141.6194
128.7382
124.6288
124.5525
124.0281
123.9137
121.5872
117.9927
117.7639
113.0347
112.8059
77.3182
76.9940
76.6794
55.7986
48.0852
31.1041
25.2403
F
N
Ph
N
N
N
4o

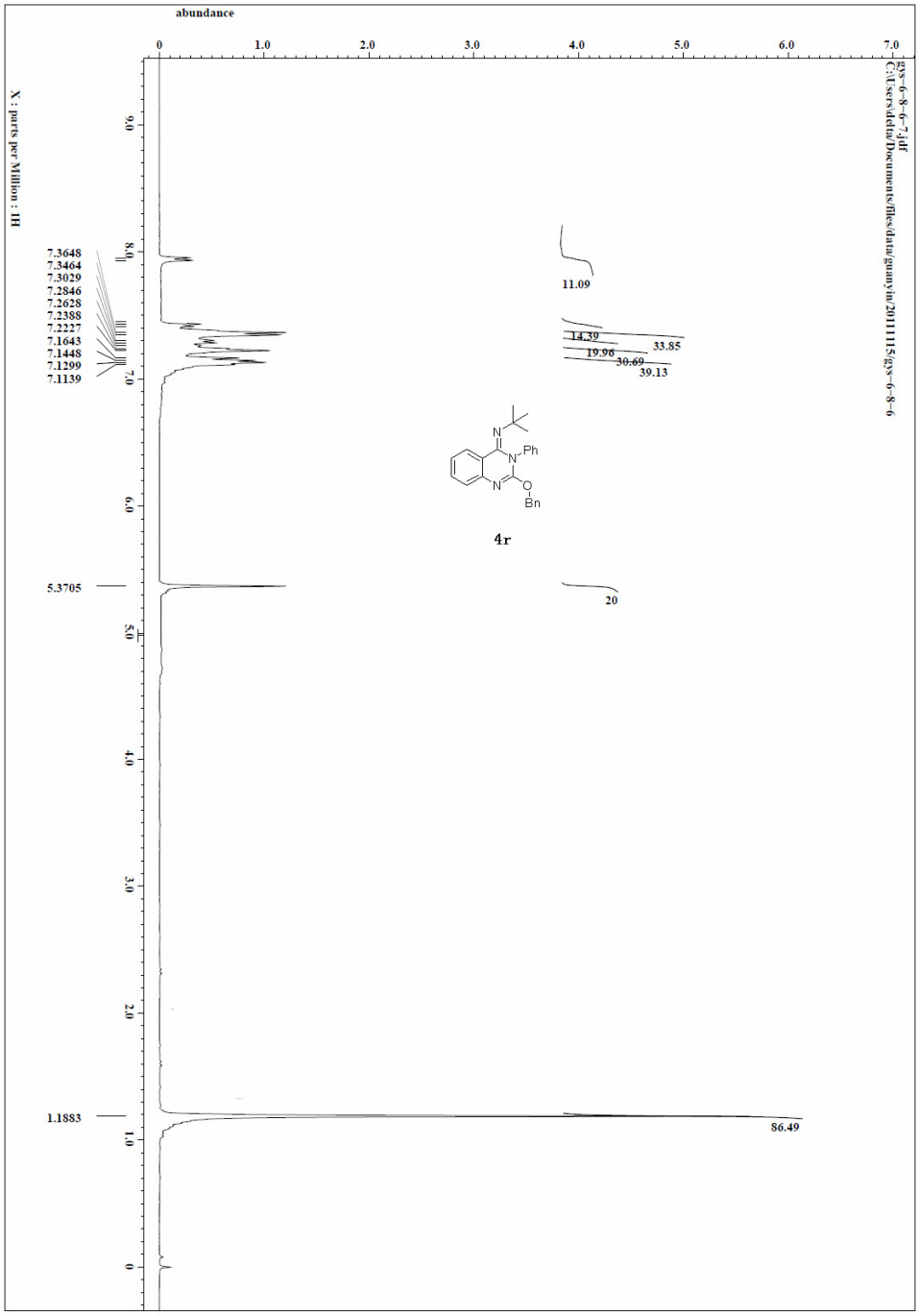

abundance
X : parts per Million : 1H
7.2336
7.2141
7.1946
6.9953
6.9758
6.9598
6.9392
3.6550
1.7478
1.5886
1.5439
1.5221
1.4763
1.4282
1.3366
1.2541
10
24.71
52.8
33.27
51.03
40.78
85.92
4p
gzs-6-14-2-10.jdf
C:\Users\delta\Documents\files\data\guanyin\20111115\gzs-6-14-2

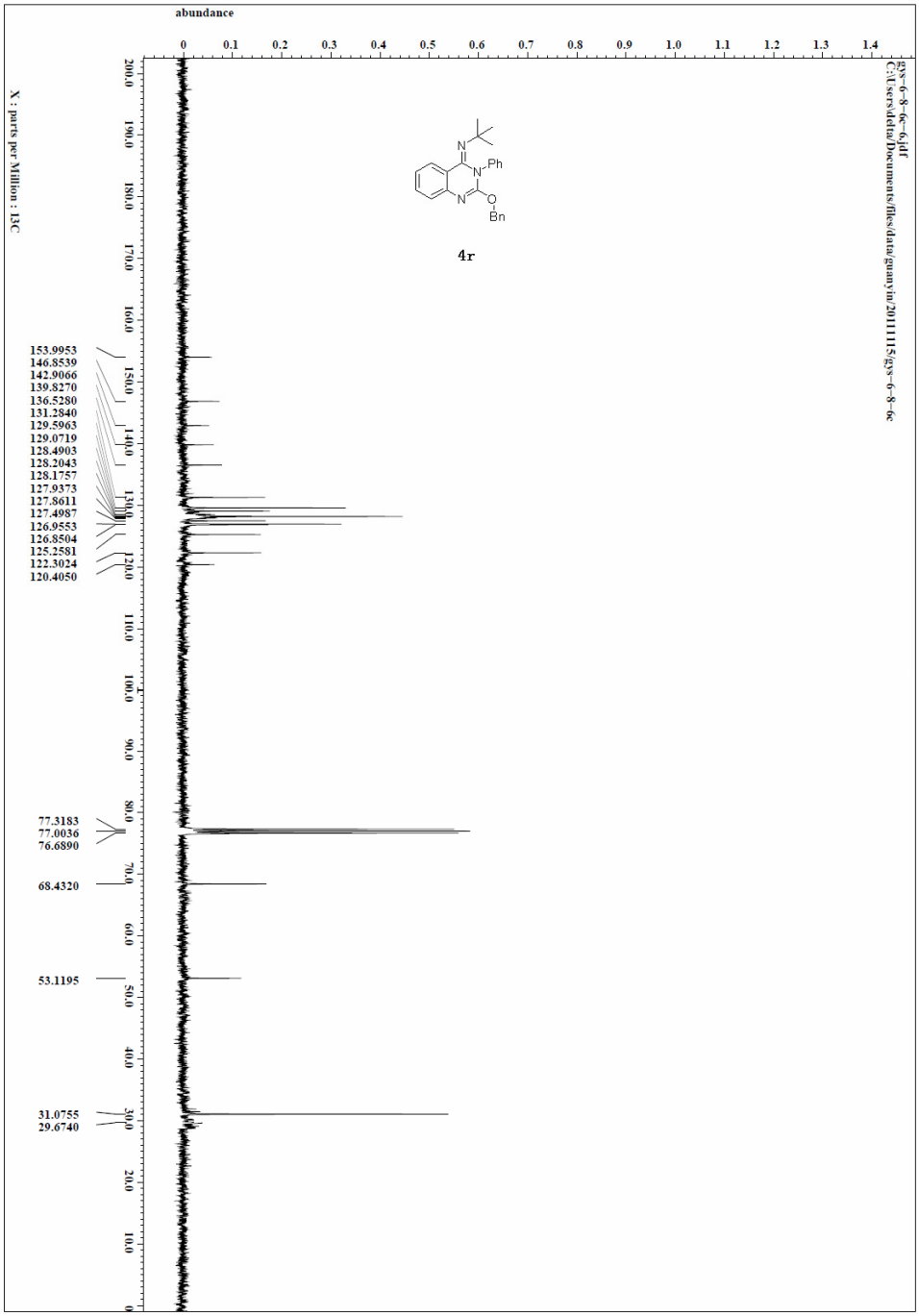

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
gyx-6-14-2c-9.jdf
C:\Users\delta\Documents\files\data\guanyin\20111115\gyx-6-14-2c
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
159.4052
157.0215
154.4663
144.4931
143.2345
142.0713
128.9517
124.4895
124.4133
123.0403
119.0072
117.7867
117.5579
112.5141
112.2757
77.3220
76.9978
76.6832
56.5557
48.5943
30.9935
28.3810
27.6564
F
N
N
Ph
N
N

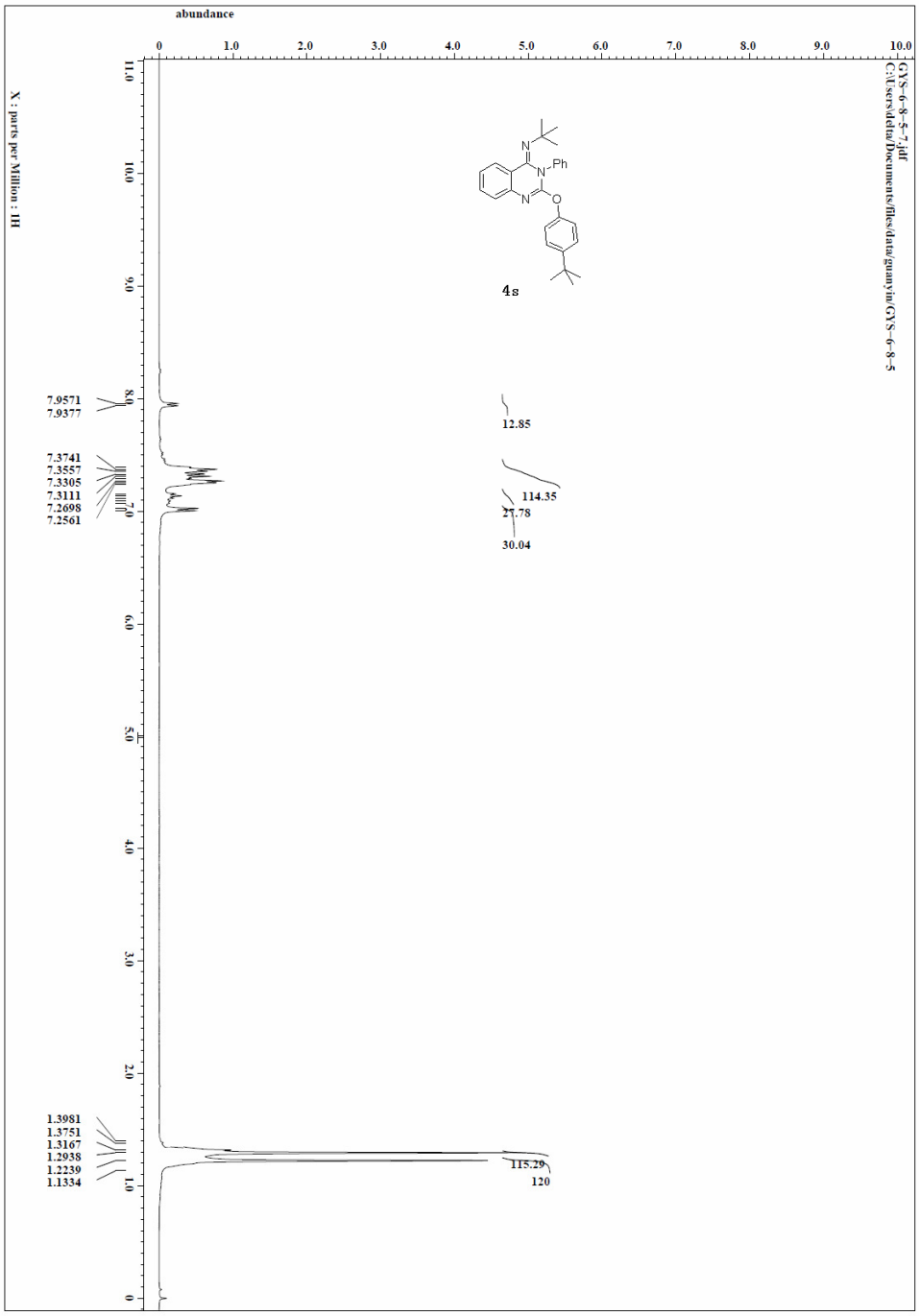
4p

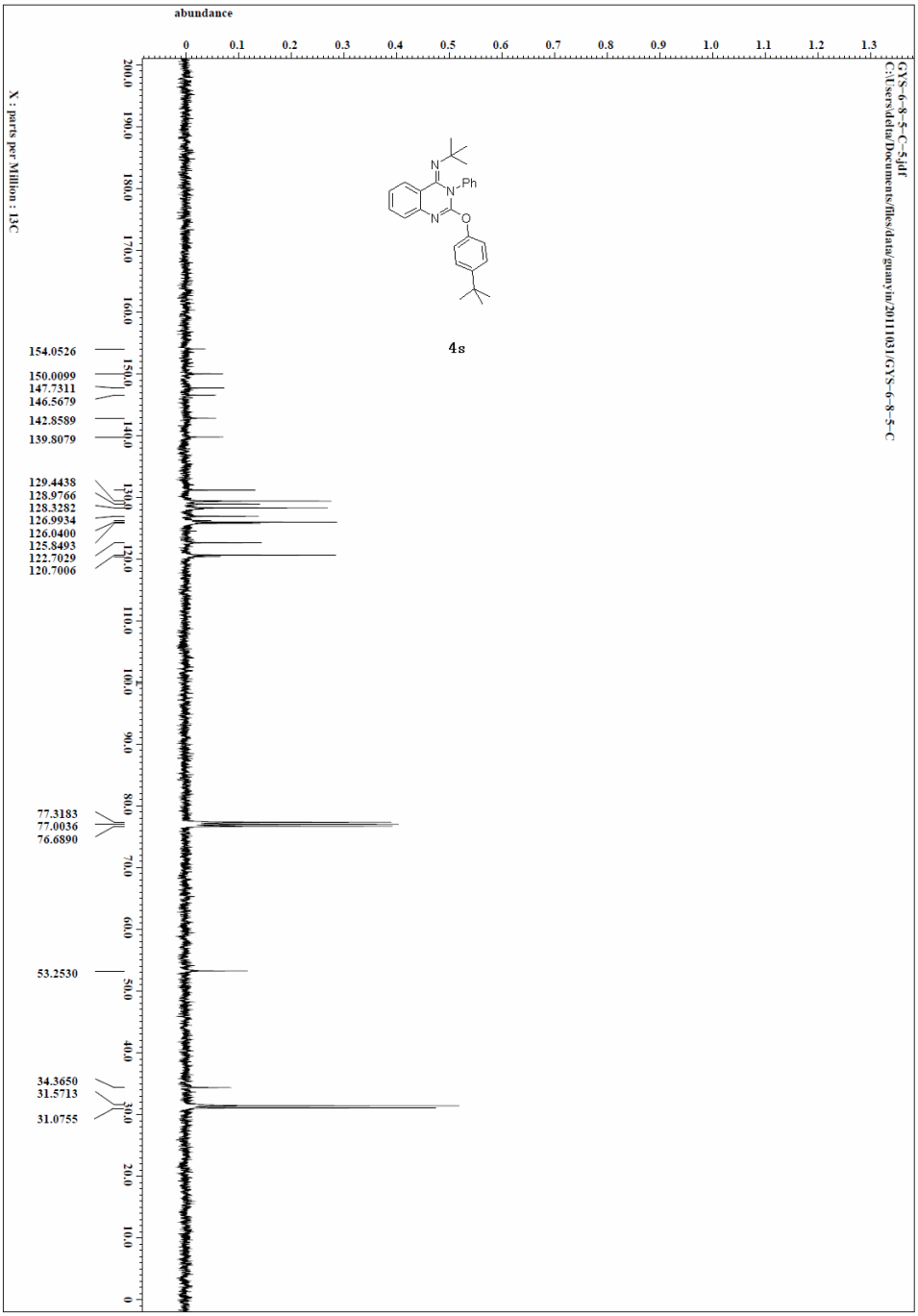

abundance
X : parts per Million : 1H
C:\Users\delta\Documents\files\data\guanyin\20111122\gs-6-14-3
gs-6-14-3-7.jdf
7.4173
7.2260
7.2076
7.1297
7.1103
7.0404
7.0186
3.4619
3.4470
3.4310
2.2832
1.8857
1.8765
1.8674
1.8525
1.4241
0.0002
10
21.03
59.04
38.22
28.65
40.17
94.63
Ph
4q


abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
153.1211
145.8081
145.1788
141.8607
131.6683
130.6672
128.5981
127.0345
123.5734
123.1920
121.5521
77.3116
76.9970
76.6824
55.6109
48.0310
31.2310
25.2624
20.9241
N
Ph
N
N
4q
gys-6-14-3c-5.jdf
C:\Users\delta\Documents\files\data\guanyin\20111122\gys-6-14-3c


abundance
X : parts per Million : 1H
gsx-6-8-6-7.jdf
C:\Users\defu\Documents\files\data\guanyiw\20111115\gsx-6-8-6
7.3648
7.3464
7.3029
7.2846
7.2628
7.2388
7.2227
7.1643
7.1448
7.1299
7.1139
5.3705
1.1883
11.09
14.39
33.85
19.96
30.69
39.13
20
86.49
Ph
Bn
4r


abundance
X : parts per Million : 13C
gsy-6-8-6c-6.jdf
C:\Users\ddfzz\Documents\files\data\guanyiw\20111115\gsy-6-8-6c
Ph
N
O
Bn
4r
153.9953
146.8539
142.9066
139.8270
136.5280
131.2840
129.5963
129.0719
128.4903
128.2043
128.1757
127.9373
127.8611
127.4987
126.9553
126.8504
125.2581
122.3024
120.4050
77.3183
77.0036
76.6890
68.4320
53.1195
31.0755
29.6740


abundance
X : parts per Million : 1H
GYS-6-8-5-7.jdf
C:\Users\data\Documents\files\data\guanyin\GYS-6-8-5
4s
7.9571
7.9377
7.3741
7.3557
7.3305
7.3111
7.2698
7.2561
1.3981
1.3751
1.3167
1.2938
1.2239
1.1334
12.85
114.35
27.78
30.04
115.29
120


abundance
X : parts per Million : 13C
GYS-6-8-5-C-5.jdf
C:\Users\dell\Documents\files\data\guanyin\20111031\GYS-6-8-5-C
4s
154.0526
150.0099
147.7311
146.5679
142.8589
139.8079
129.4438
128.9766
128.3282
126.9934
126.0400
125.8493
122.7029
120.7006
77.3183
77.0036
76.6890
53.2530
34.3650
31.5713
31.0755