Electronic Supplementary Material (ESI) for Chemical Communications

Preparation of quinazolino[3,2-*a*]quinazolines via a palladium-catalyzed three-component reaction of carbodiimide, isocyanide, and amine

Guanyinsheng Qiu,[a] Yaohua He,*[,b] and Jie Wu*[,a,c]

[a] *Department of Chemistry, Fudan University, 220 Handan Road, Shanghai 200433, China*

[b]*Shanghai the 6th People's Hospital, Shanghai Jiaotong University, 600 Yishan Road, Shanghai 200233, China*

[c] *Key Laboratory of Synthetic Organic Chemistry of Natural Substances, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 354 Fenglin Road, Shanghai 200032, China*

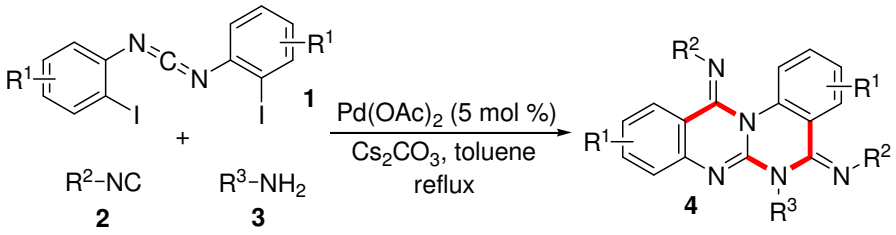
jie_wu@fudan.edu.cn

Supporting Information

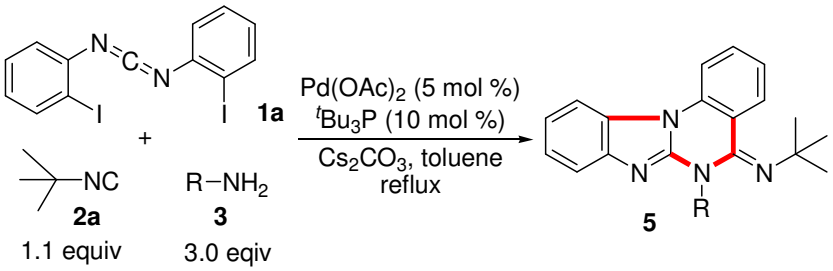
General Materials and Methods:

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 (Zeng, F.; Alper, H. *Org. Lett.* **2010**, *12*, 1188.)

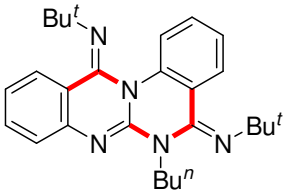
*General procedure of the synthesis of quinazolino[3,2-a]quinazolines and related compounds via a palladium-catalyzed three-component reaction of carbodiimide **1**, isocyanide **2**, and amine **3***



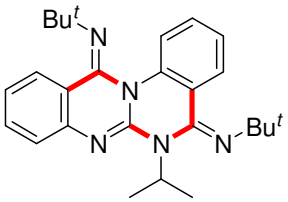
Amine **3** (3.0 equiv) and isocyanide **2** (3.0 equiv) were added to a mixture of carbodiimide **1** (0.2 mmol), $Pd(OAc)_2$ (5 mol %), and Cs_2CO_3 (3.0 equiv) in toluene (3.0 mL). The mixture was stirred at reflux under N_2. After completion of reaction as indicated by TLC (4-12 hrs), the solvent was evaporated and the residue was purified on silica gel to provide the desired product **4**.



Amine **3** (3.0 equiv) and isocyanide **2** (1.1 equiv) were added to a mixture of carbodiimide **1** (0.2 mmol), $Pd(OAc)_2$ (5 mol %), P^tBu_3 (10 mol %), and Cs_2CO_3 (3.0 equiv) in toluene (3.0 mL). The mixture was stirred at reflux under N_2. After completion of reaction as indicated by TLC (4-12 hrs), the solvent was evaporated and the residue was purified on silica gel to provide the desired product **5**.

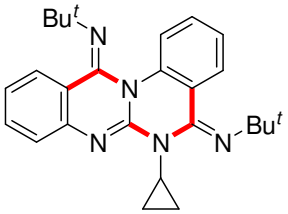


6-Butyl-5,12-bis-*tert*-butylimino-6,12-dihydro-5*H*-quinazolino[3,2-*a*]quinazoline (**4a**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.91 (t, *J* = 7.2 Hz, 3H), 1.20 (s, 9H), 1.28-1.31 (m, 2H), 1.40 (s, 9H), 1.65-1.69 (m, 2H), 4.18-4.21 (m, 2H), 7.04-7.18 (m, 2H), 7.20-7.29 (m, 2H), 7.32-7.36 (m, 2H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.9, 20.2, 29.7, 29.9, 31.9, 43.5, 54.6, 56.3, 118.9, 122.5, 122.7, 124.0, 125.3, 128.3, 129.7, 130.6, 140.4, 142.8, 146.1, 147.4; HRMS Calcd for $C_{27}H_{36}N_5^+$ (ESI, M+H$^+$): 430.2965; found: 430.2956.

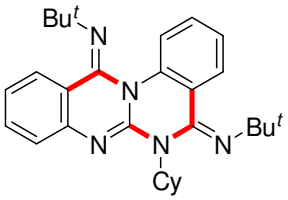


5,12-Bis-*tert*-butylimino-6-isopropyl-6,12-dihydro-5*H*-quinazolino[3,2-*a*]quinazoline (**4b**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.20 (s, 9H), 1.39 (s, 9H), 1.52 (d, *J* = 6.0 Hz, 6H), 5.06-5.09 (m, 1H), 7.05-7.10 (m, 2H), 7.17-7.22 (m, 2H), 7.24-7.30 (m, 2H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.91 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ

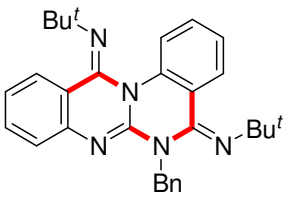
20.4, 29.3, 31.8, 48.5, 55.1, 56.1, 119.0, 122.3, 122.7, 123.9, 125.2, 128.4, 128.6, 129.3, 130.6, 133.6, 133.8, 140.7, 142.8, 146.1, 147.6; HRMS Calcd for $C_{26}H_{34}N_5^+$ (ESI, M+H$^+$): 416.2809; found: 416.2808.



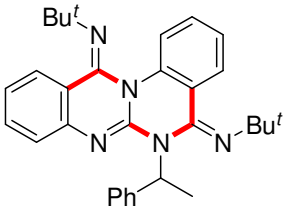
5,12-Bis-*tert*-butylimino-6-cyclopropyl-6,12-dihydro-5*H*-quinazolino[3,2-*a*]quinazoline (**4c**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.55-0.57 (m, 2H), 1.02-1.05 (m, 2H), 1.19 (s, 9H), 1.48 (s, 9H), 3.06-3.07 (m, 1H), 7.08-7.12 (m, 3H), 7.25-7.31 (m, 2H), 7.36-7.39 (m, 1H), 7.53 (d, J = 8.0 Hz, 1H), 7.89 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 10.9, 30.2, 31.5, 55.3, 56.1, 119.05, 122.8, 123.6, 124.4, 125.0, 125.8, 126.3, 129.2, 130.7, 138.8, 139.5, 143.7, 146.2; HRMS Calcd for $C_{26}H_{32}N_5^+$ (ESI, M+H$^+$): 414.2658; found: 414.2647.



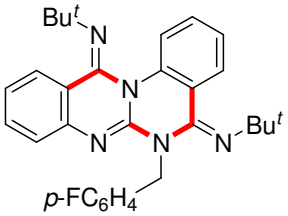
5,12-Bis-*tert*-butylimino-6-cyclohexyl-6,12-dihydro-5*H*-quinazolino[3,2-*a*]quinazoline (**4d**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.19 (s, 9H), 1.39 (s, 9H), 1.66-1.82 (m, 8H), 2.43-2.48 (m, 2H), 4.63-4.68 (m, 1H), 7.02-7.06 (m, 2H), 7.18-7.23 (m, 4H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.91 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.4, 26.1, 26.6, 29.9, 31.8, 48.5, 55.1, 56.1, 57.2, 119.0, 122.3, 122.7, 123.9, 124.8, 125.2, 128.4, 129.3, 130.6, 133.6, 133.8, 140.7, 142.8, 146.1, 147.6; HRMS Calcd for $C_{29}H_{38}N_5^+$ (ESI, M+H$^+$): 456.3122; found: 456.3113.



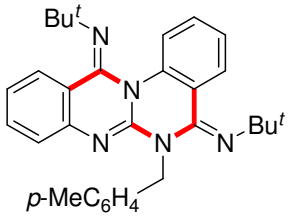
6-Benzyl-5,12-bis-*tert*-butylimino-6,12-dihydro-5*H*-quinazolino[3,2-*a*]quinazoline (**4e**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.20 (s, 9H), 1.39 (s, 9H), 5.45 (s, 2H), 7.05-7.08 (m, 2H), 7.14-7.19 (m, 3H), 7.21-7.35 (m, 6H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.91 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.9, 31.8, 46.4, 54.6, 56.3, 119.1, 122.7, 122.8, 123.0, 124.1, 125.3, 126.3, 127.8, 128.2, 128.5, 129.9, 130.6, 133.6, 133.8, 139.2, 140.3, 142.1, 146.1, 147.3; HRMS Calcd for $C_{30}H_{34}N_5^+$ (ESI, M+H$^+$): 464.2809; found: 464.2826.



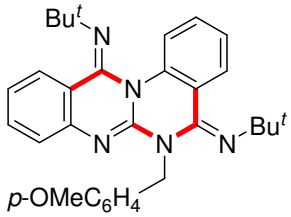
5,12-Bis-*tert*-butylimino-6-(1-phenyl-ethyl)-6,12-dihydro-5*H*-quinazolino[3,2-*a*]quinazoline (**4f**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.09 (s, 9H), 1.21 (s, 9H), 1.96 (d, J = 6.0 Hz, 3H), 6.21-6.26 (m, 1H), 7.03-7.28 (m, 12H), 7.93 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 17.1, 29.9, 31.2, 53.8, 54.5, 56.3, 118.9, 122.8, 124.1, 125.2, 125.8, 127.3, 127.5, 128.4, 128.5, 128.7, 129.5, 130.6, 133.6, 133.8, 139.2, 140.6, 141.4, 146.1, 147.3; HRMS Calcd for $C_{31}H_{36}N_5^+$ (ESI, M+H$^+$): 478.2965; found: 478.2962.



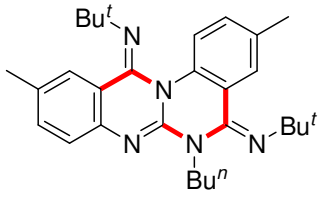
5,12-Bis-*tert*-butylimino-6-(4-fluoro-benzyl)-6,12-dihydro-5*H*-quinazolino[3,2-*a*]quinazoline (**4g**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.22 (s, 9H), 1.34 (s, 9H), 5.39 (s, 2H), 6.88-6.92 (m, 2H), 7.06-7.10 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 1H), 7.25-7.35 (m, 5H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.90 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.9, 31.8, 45.7, 54.7, 56.3, 114.5 (d, $^{2}J_{CF}$ = 21 Hz), 119.0, 122.8, 124.1, 125.4, 128.6, 129.9, 130.0, 130.1, 130.7, 134.9, 139.2, 140.3, 142.1, 145.7, 147.2, 161.5 (d, $^{1}J_{CF}$ = 248 Hz); HRMS Calcd for $C_{30}H_{33}N_5^+$ (ESI, M+H$^+$): 482.2714; found: 482.2693.



5,12-Bis-*tert*-butylimino-6-(4-methyl-benzyl)-6,12-dihydro-5*H*-quinazolino[3,2-*a*]quinazoline (**4h**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.21 (s, 9H), 1.34 (s, 9H), 2.26 (s, 3H), 5.41 (s, 2H), 7.00-7.06 (m, 4H), 7.18-7.32 (m, 6H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.1, 29.9, 31.8, 46.1, 54.6, 56.3, 118.9, 122.6, 122.7, 123.1, 124.1, 125.3, 127.8, 128.3, 128.5, 129.1, 129.8, 135.8, 136.1,140.3, 142.2, 145.8, 147.2; HRMS Calcd for $C_{31}H_{36}N_5^+$ (ESI, M+H$^+$): 478.2965; found: 478.2936.

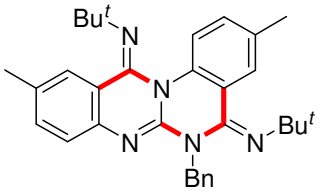


5,12-Bis-*tert*-butylimino-6-(4-methoxy-benzyl)-6,12-dihydro-5*H*-quinazolino[3,2-*a*]quinazoline (**4i**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.21 (s, 9H), 1.36 (s, 9H), 3.74 (s, 3H), 5.38 (s, 2H), 6.75 (d, J = 7.6 Hz, 2H), 7.05-7.08 (m, 2H), 7.20-7.35 (m, 6H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.9, 31.8, 45.7, 54.6, 55.1, 56.3, 113.2, 113.9, 118.9, 122.6, 122.7, 123.1, 124.1, 125.3, 128.5, 129.2, 129.8, 130.6, 131.4, 140.3, 142.3, 145.9, 147.2; HRMS Calcd for $C_{31}H_{36}N_5O^+$ (ESI, M+H$^+$): 494.2914; found: 494.2928.

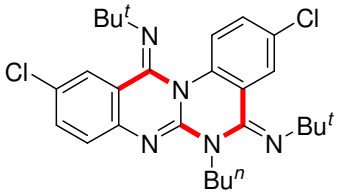


6-Butyl-5,12-bis-*tert*-butylimino-3,10-dimethyl-6,12-dihydro-5*H*-quinazolino[3,2-*a*]quinazoline (**4j**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.91 (t, *J* = 7.2 Hz, 3H), 1.19 (s, 9H), 1.25-1.30 (m, 2H), 1.40 (s, 9H), 1.63-1.67 (m, 2H), 2.34 (s, 3H), 2.37 (s, 3H), 4.17 (t, *J* = 6.8 Hz, 2H), 7.15-7.17 (m, 4H), 7.36 (s, 1H), 7.71 (s, 1H); ^{13}C NMR (100 MHz,

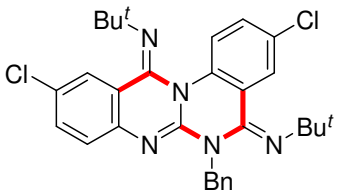
$CDCl_3$) δ 13.9, 20.2, 21.0, 29.9, 31.9, 34.3, 43.4, 50.9, 54.6, 56.2, 118.7, 119.1, 123.8, 125.0, 1257.4, 128.4, 130.3, 131.6, 132.0, 132.2, 133.9, 139.7, 143.1, 143.7, 146.9; HRMS Calcd for $C_{29}H_{40}N_5^+$ (ESI, M+H$^+$): 458.3278; found: 458.3272.



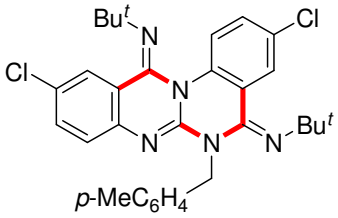
6-Benzyl-5,12-bis-*tert*-butylimino-3,10-dimethyl-6,12-dihydro-5*H*-quinazolino[3,2-*a*] quinazoline (**4k**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.210 (s, 9H), 1.32 (s, 9H), 2.31 (s, 3H), 2.36 (s, 3H), 5.42 (s, 2H), 7.08-7.15 (m, 7H), 7.19-7.22 (m, 2H), 7.32 (s, 1H), 7.71 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.0, 29.9, 31.8, 46.4, 54.5, 56.3, 118.8, 123.1, 124.0, 125.03, 126.3, 127.8, 128.2, 128.5, 128.7, 130.5, 131.6, 132.2, 132.3, 138.1, 139.4, 142.3, 143.5, 147.0; HRMS Calcd for $C_{32}H_{38}N_5^+$ (ESI, M+H$^+$): 492.3122; found: 492.3098.



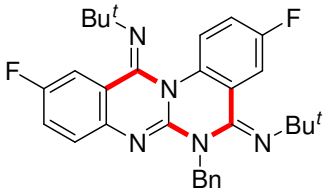
6-Butyl-5,12-bis-*tert*-butylimino-3,10-dichloro-6,12-dihydro-5*H*-quinazolino[3,2-*a*]q uinazoline (**4l**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.92 (t, *J* = 7.6 Hz, 3H), 1.19 (s, 9H), 1.25-1.28 (m, 2H), 1.40 (s, 9H), 1.64-1.697 (m, 2H), 4.14 (t, *J* = 7.2 Hz, 2H), 7.11-7.17 (m, 2H), 7.27-7.32 (m, 2H), 7.55 (s, 1H), 7.86 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.9, 20.1, 29.8, 30.1, 31.8, 43.9, 54.9, 56.6, 120.1, 124.9, 125.6, 125.7, 127.8, 128.3, 129.8, 130.1, 130.8, 138.7, 141.2, 144.5, 146.9; HRMS Calcd for $C_{27}H_{34}Cl_2N_5^+$ (ESI, M+H$^+$): 498.2186; found: 498.2159.



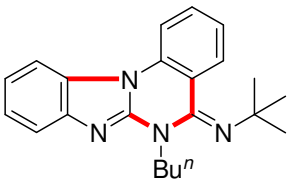
6-Benzyl-5,12-bis-*tert*-butylimino-3,10-dichloro-6,12-dihydro-5*H*-quinazolino[3,2-*a*] quinazoline (**4m**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.21 (s, 9H), 1.38 (s, 9H), 5.39 (s, 2H), 7.11-7.32 (m, 9H), 7.46 (s, 1H), 7.86 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.8, 31.8, 46.7, 54.9, 56.6, 120.2, 125.0, 125.7, 126.6, 127.9, 128.1, 128.2, 128.4, 128.5, 128.7, 129.9, 130.9, 133.6, 133.8, 138.7, 140.5, 144.2, 147.1; HRMS Calcd for $C_{30}H_{32}Cl_2N_5^+$ (ESI, M+H$^+$): 532.2029; found: 532.2027.



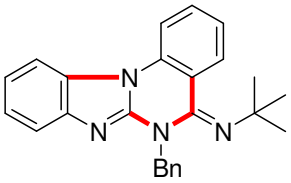
5,12-Bis-*tert*-butylimino-3,10-dichloro-6-(4-methyl-benzyl)-6,12-dihydro-5*H*-quinaz olino[3,2-*a*]quinazoline (**4n**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.21 (s, 9H), 1.35 (s, 9H), 2.28 (s, 3H), 5.35 (s, 2H), 7.04 (d, J = 7.6 Hz, 2H), 7.11-7.18 (m, 6H), 7.46 (s, 1H), 7.85 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.1, 29.8, 31.8, 46.3, 54.9, 56.6, 117.4, 120.2, 121.2, 125.0, 125.7, 127.1, 127.4, 128.3, 128.6, 129.5, 129.9, 130.8, 131.6, 135.6, 136.2, 138.7, 141.2, 147.1; HRMS Calcd for $C_{31}H_{34}Cl_2N_5^+$ (ESI, M+H$^+$): 546.2186; found: 546.2166.



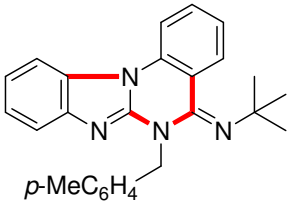
6-Benzyl-5,12-bis-*tert*-butylimino-3,10-difluoro-6,12-dihydro-5*H*-quinazolino[3,2-*a*] quinazoline (**4o**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.20 (s, 9H), 1.33 (s, 9H), 5.39 (s, 2H), 7.03-7.07 (m, 2H), 7.14-7.20 (m, 5H), 7.29-7.33 (m, 3H),7.58-7.61 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.8, 31.7, 46.7, 54.8, 56.5, 111.1 (d, $^{2}J_{CF}$ = 23 Hz), 115.0 (d, $^{2}J_{CF}$ = 25 Hz), 117.1 (d, $^{2}J_{CF}$ = 23 Hz), 118.2 (d, $^{2}J_{CF}$ = 23 Hz), 120.5 (d, $^{3}J_{CF}$ = 8 Hz), 125.7, 126.6, 128.1, 128.5, 128.7, 133.6, 133.8, 136.5, 137.1, 138.9, 140.8, 146.7, 157.8 (d, $^{1}J_{CF}$ = 243 Hz), 159.1 (d, $^{1}J_{CF}$ = 242 Hz); HRMS Calcd for $C_{30}H_{32}F_2N_5^+$ (ESI, M+H$^+$): 500.2626; found: 500.2594.



tert-Butyl-(6-butyl-6*H*-6,7,11b-triaza-benzo[c]fluoren-5-ylidene)-amine (**5a**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.98 (t, *J* = 7.2 Hz, 3H), 1.41-1.45 (m, 2H), 1.64 (s, 9H), 1.81-1.85 (m, 2H), 2.38-2.41 (s, 1H), 4.15-4.18 (m, 1H), 7.08-7.19 (m, 3H), 7.25-7.30 (m, 1H), 7.41-7.48 (m, 2H), 8.17 (d, *J* = 8.0 Hz, 1H), 8.83 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.8, 20.1, 30.1, 31.7, 41.3, 53.6, 107.0, 116.1, 116.7, 119.9, 120.7, 123.7, 125.5, 127.9, 130.3, 131.4, 132.0, 140.9, 148.2, 150.1; HRMS Calcd for $C_{22}H_{27}N_4^+$ (ESI, M+H$^+$): 347.2230; found: 347.2213.

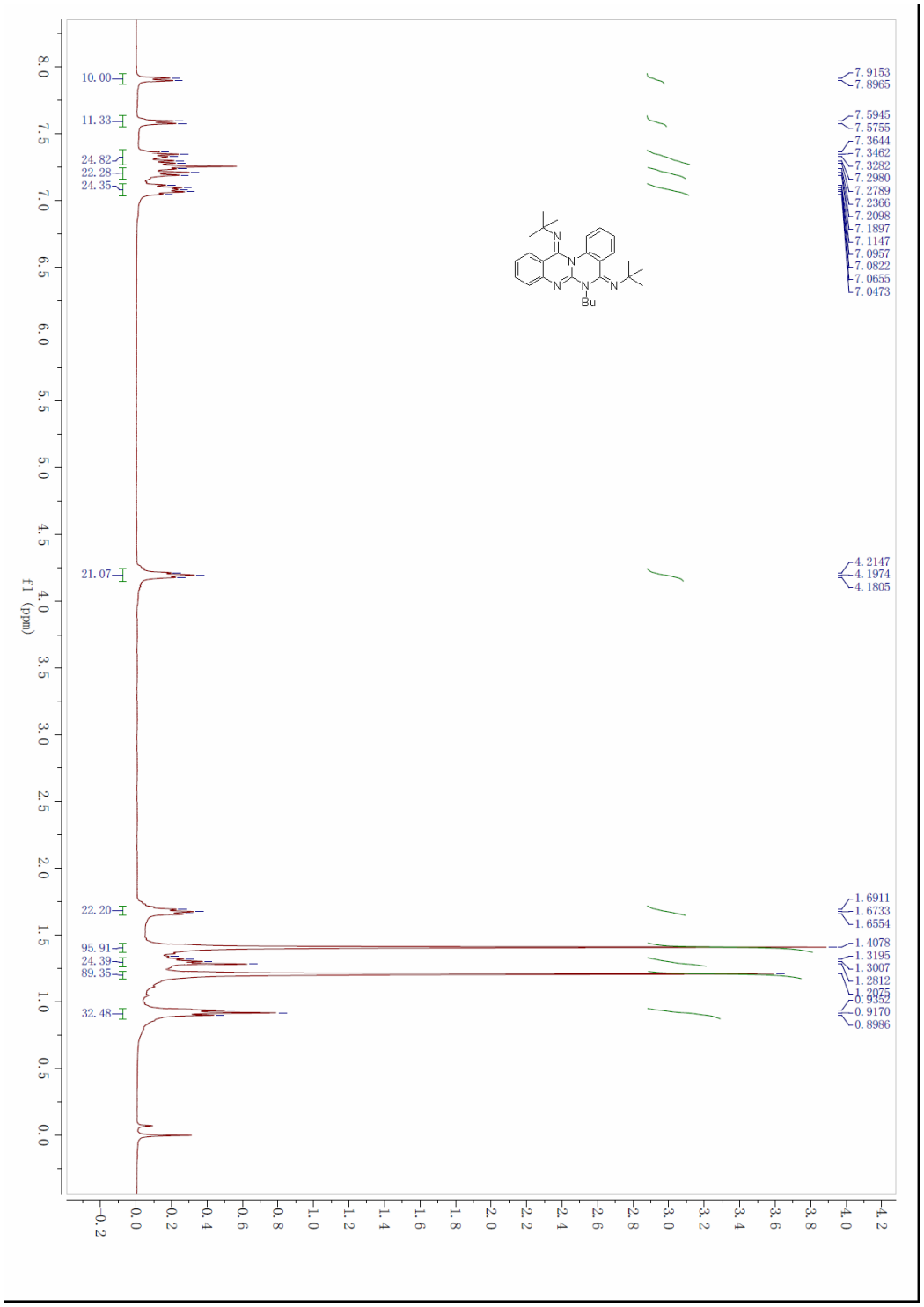


(6-Benzyl-6*H*-6,7,11b-triaza-benzo[c]fluoren-5-ylidene)-*tert*-butyl-amine (**5b**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.65 (s, 9H), 5.39 (s, 2H), 7.00 (d, *J* = 7.6 Hz, 1H), 7.11-7.21 (m, 3H), 7.25-7.31 (m, 3H), 7.36-7.37 (m, 2H), 7.41-7.48 (m, 2H), 8.19 (d, *J* = 8.0 Hz, 1H), 8.83 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.7, 45.1, 53.7, 107.7, 116.0, 116.7, 120.2, 121.1, 123.9, 125.6, 127.4, 127.7, 128.1, 128.7, 130.4, 131.5, 131.8, 135.9, 141.6, 148.6; HRMS Calcd for $C_{25}H_{25}N_4^+$ (ESI, M+H$^+$): 381.2074; found: 381.2086.



tert-Butyl-[6-(4-methyl-benzyl)-6*H*-6,7,11b-triaza-benzo[c]fluoren-5-ylidene]-amine (**5c**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.65 (s, 9H), 2.34 (s, 3H), 5.35 (s, 2H), 7.00-7.25 (m, 8H), 7.41-7.48 (m, 2H), 8.19 (d, *J* = 7.2 Hz, 1H), 8.83 (d, *J* = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.1, 31.7, 44.8, 53.5, 107.7, 116.7, 120.2, 121.0, 123.8,

125.6, 127.4, 129.4, 130.4, 131.5, 131.8, 132.9, 137.4, 141.6, 148.9; HRMS Calcd for $C_{26}H_{27}N_4^+$ (ESI, $M+H^+$): 395.2230; found: 395.2221.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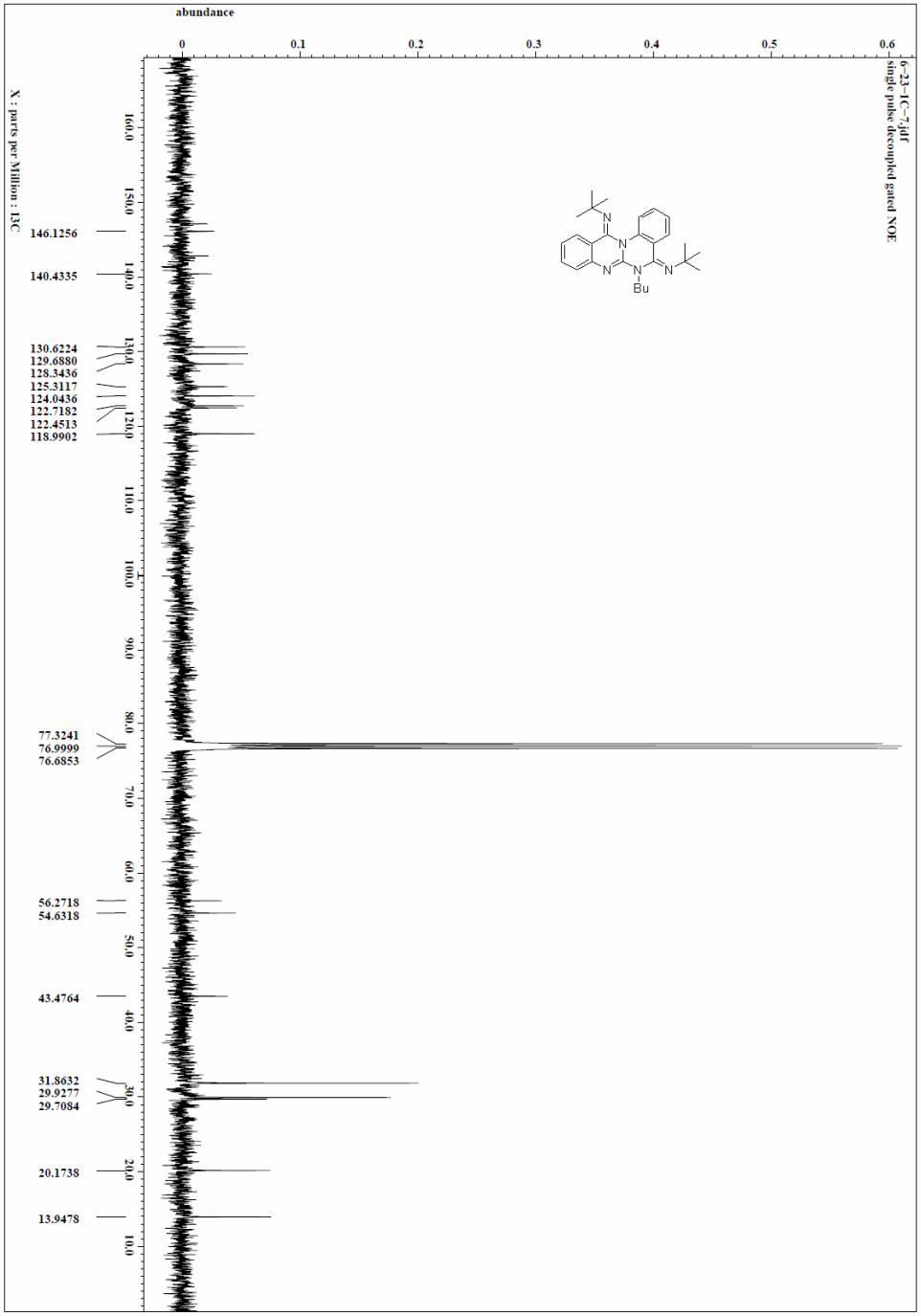
11.33
24.82
22.28
24.35
21.07
22.20
95.91
24.39
89.35
32.48
7.9153
7.8965
7.5945
7.5755
7.3644
7.3462
7.3282
7.2980
7.2789
7.2366
7.2098
7.1897
7.1147
7.0957
7.0822
7.0655
7.0473
4.2147
4.1974
4.1805
1.6911
1.6733
1.6554
1.4078
1.3195
1.3007
1.2812
1.2075
0.9352
0.9170
0.8986
Bu
f1 (ppm)


abundance
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0.1
0.2
0.3
0.4
0.5
0.6
6-23-1C-7.jdf
single pulse decoupled gated NOE
X : parts per Million : 13C
146.1256
140.4335
130.6224
129.6880
128.3436
125.3117
124.0436
122.7182
122.4513
118.9902
77.3241
76.9999
76.6853
56.2718
54.6318
43.4764
31.8632
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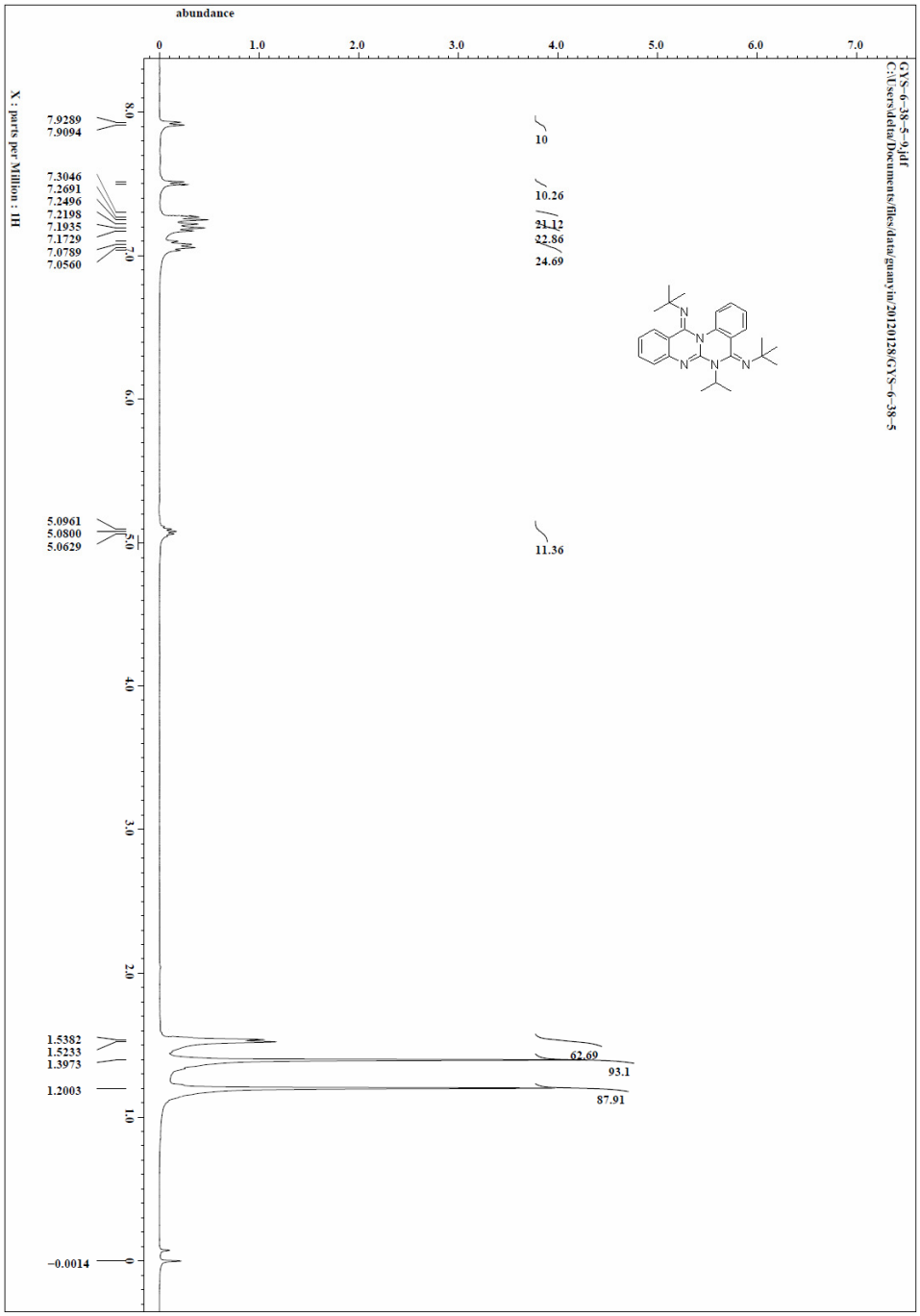
29.7084
20.1738
13.9478
Bu


abundance
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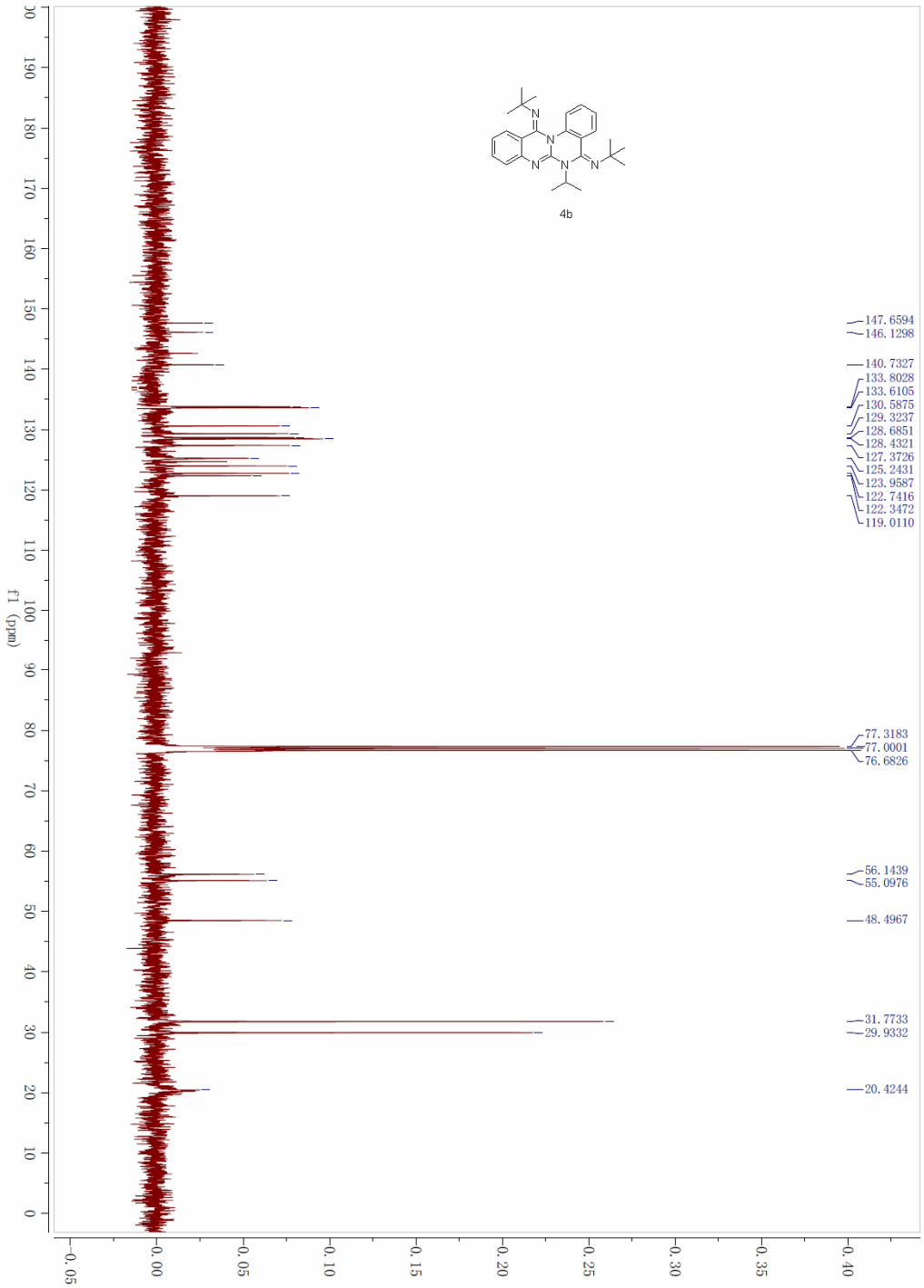
1.0
2.0
3.0
4.0
5.0
6.0
7.0
X : parts per Million : 1H
GYS-6-38-5-9.jdf
C:\Users\delta\Documents\files\data\guanyin\20120128\GYS-6-38-5
7.9289
7.9094
7.3046
7.2691
7.2496
7.2198
7.1935
7.1729
7.0789
7.0560
5.0961
5.0800
5.0629
1.5382
1.5233
1.3973
1.2003
-0.0014
10
10.26
21.12
22.86
24.69
11.36
62.69
93.1
87.91


4b
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146.1298
140.7327
133.8028
133.6105
130.5875
129.3237
128.6851
128.4321
127.3726
125.2431
123.9587
122.7416
122.3472
119.0110
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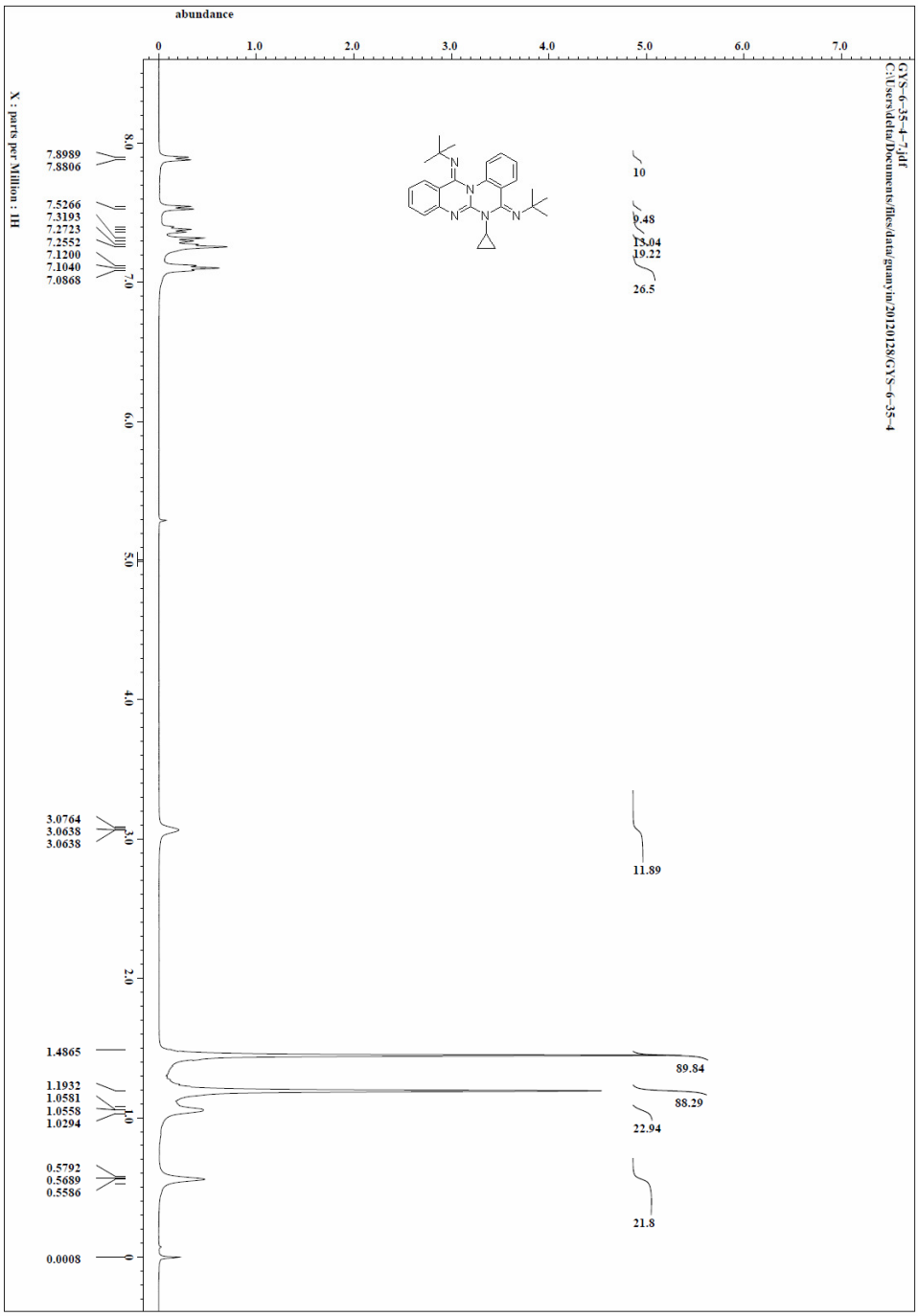
77.0001
76.6826
56.1439
55.0976
48.4967
31.7733
29.9332
20.4244
f1 (ppm)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2.0
3.0
4.0
5.0
6.0
7.0
X : parts per Million : 1H
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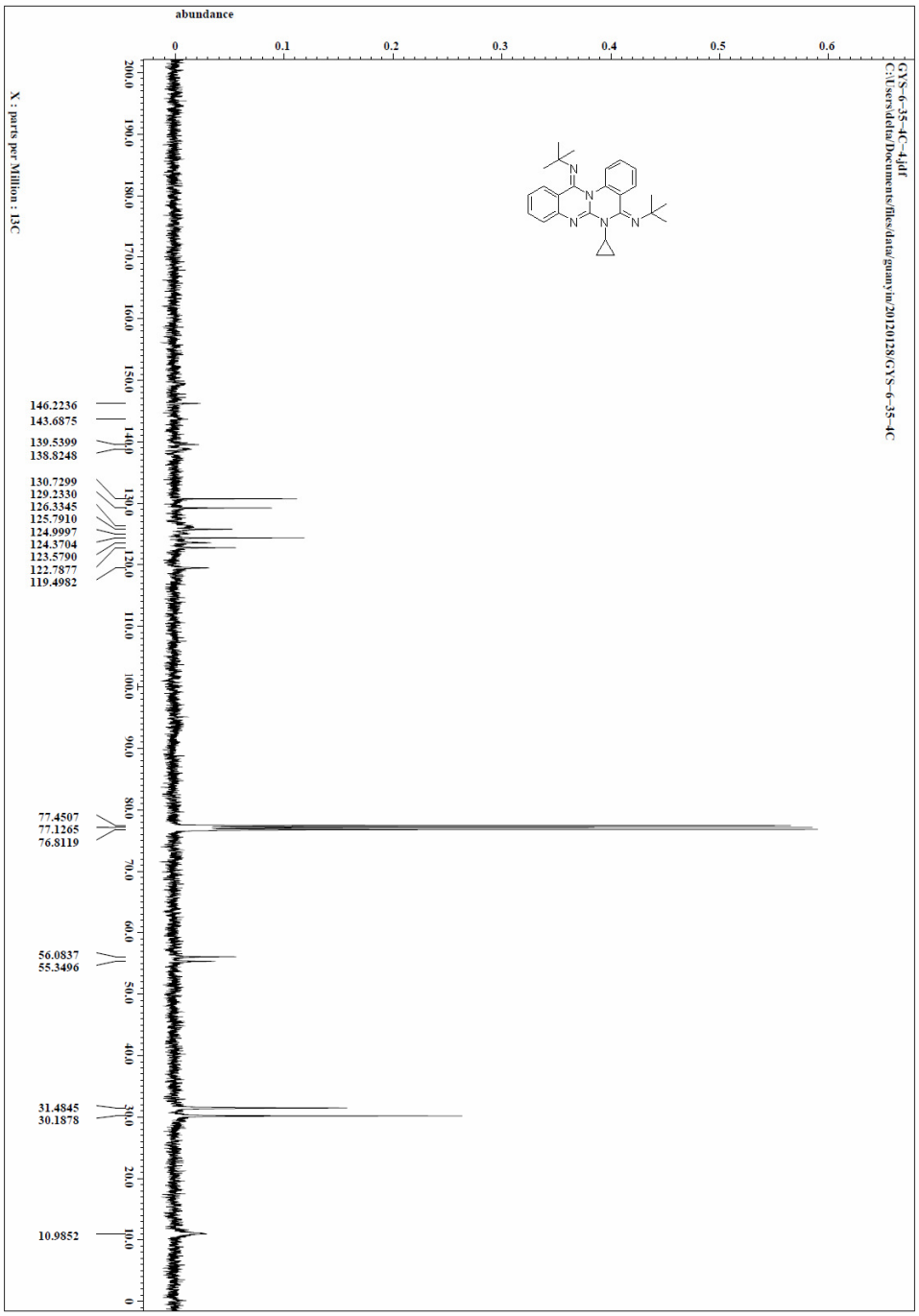
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8989
7.8806
7.5266
7.3193
7.2723
7.2552
7.1200
7.1040
7.0868
3.0764
3.0638
3.0638
1.4865
1.1932
1.0581
1.0558
1.0294
0.5792
0.5689
0.5586
0.0008
10
9.48
13.04
19.22
26.5
11.89
89.84
88.29
22.94
21.8
GYS-6-35-4-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20120128\GYS-6-35-4


abundance
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0.2
0.3
0.4
0.5
0.6
X : parts per Million : 13C
GYS-6-35-4C-4.jdf
C:\Users\delta\Documents\files\data\guanyin\20120128\GYS-6-35-4C
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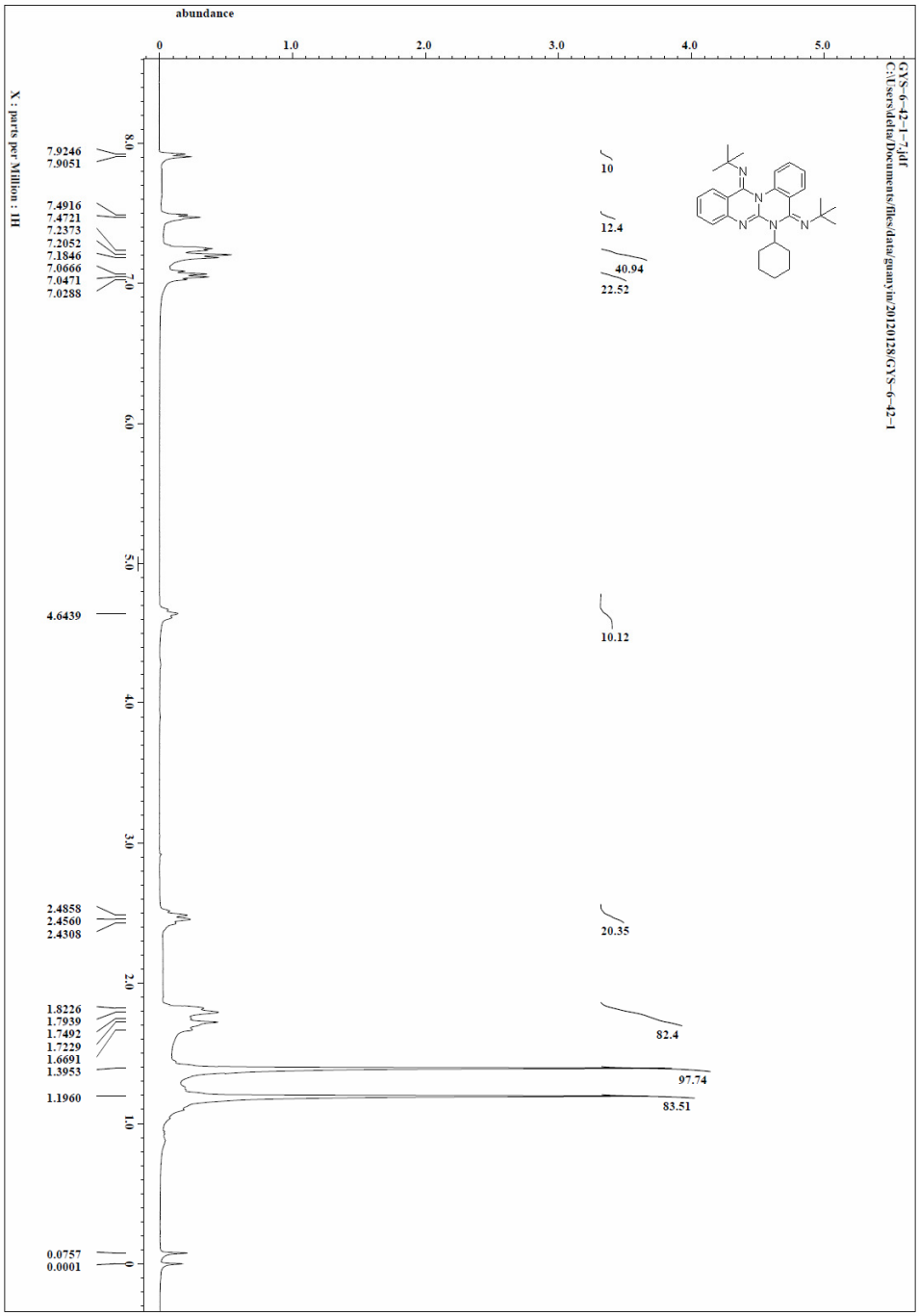
139.5399
138.8248
130.7299
129.2330
126.3345
125.7910
124.9997
124.3704
123.5790
122.7877
119.4982
77.4507
77.1265
76.8119
56.0837
55.3496
31.4845
30.1878
10.9852


abundance
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1.0
2.0
3.0
4.0
5.0
X : parts per Million : 1H
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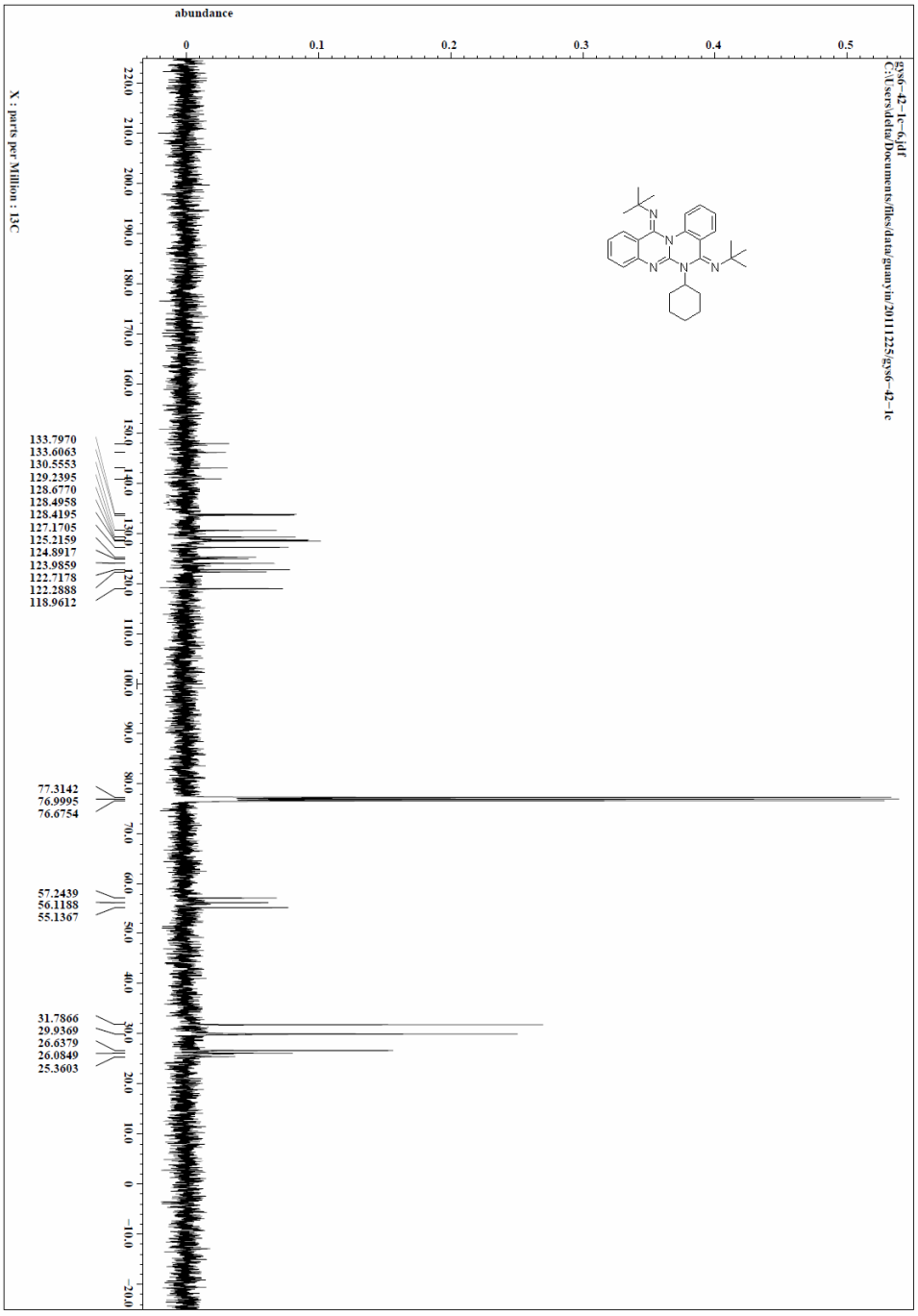
7.4721
7.2373
7.2052
7.1846
7.0666
7.0471
7.0288
4.6439
2.4858
2.4560
2.4308
1.8226
1.7939
1.7492
1.7229
1.6691
1.3953
1.1960
0.0757
0.0001
10
12.4
40.94
22.52
10.12
20.35
82.4
97.74
83.51
GYS-6-42-1-7.jdf
C:\Users\delta\Documents\flies\data\guanyin\20120128\GYS-6-42-1


abundance
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0.1
0.2
0.3
0.4
0.5
X : parts per Million : 13C
gxs6-42-1c-6.jdf
C:\Users\data\Documents\files\data\guanyin\20111225\gxs6-42-1c
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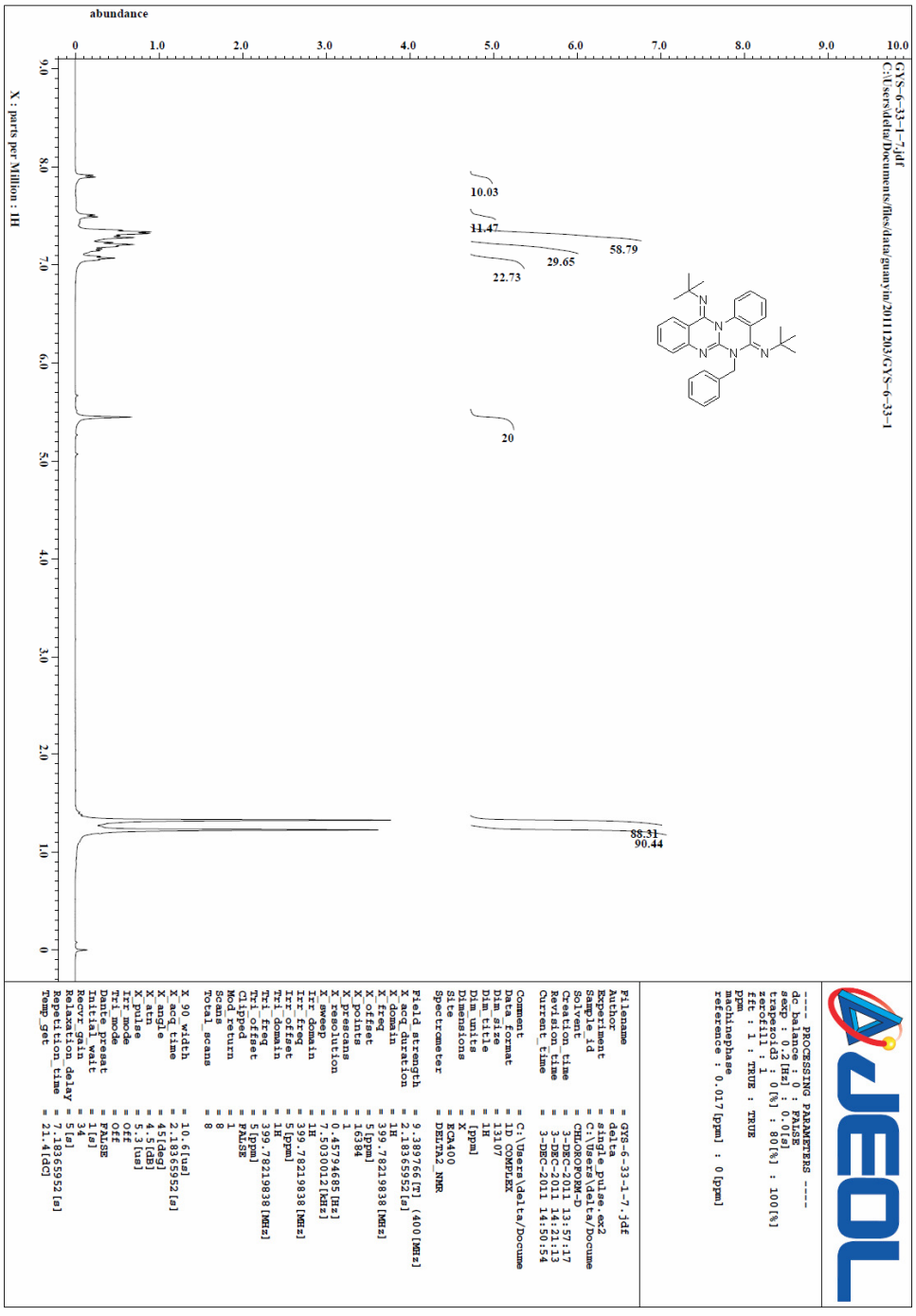
133.6063
130.5553
129.2395
128.6770
128.4958
128.4195
127.1705
125.2159
124.8917
123.9859
122.7178
122.2888
118.9612
77.3142
76.9995
76.6754
57.2439
56.1188
55.1367
31.7866
29.9369
26.6379
26.0849
25.3603


GYS-6-33-1-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20111203\GYS-6-33-1
abundance
X : parts per Million : 1H
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11.47
58.79
29.65
22.73
20
88.31
90.44
--- PROCESSING PARAMETERS ---
gb : 0 [Hz] : 0 [%]
lb : 0.2 [Hz] : 0 [%]
sscp : 0 [Hz] : 0 [%]
trapezoid3 : 0 [%] : 80 [%] : 100 [%]
zerofill : 1
fft : 1 : TRUE : TRUE
ppm
machinephase
reference : 0.017 [ppm] : 0 [ppm]
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Author = delta
Experiment = single_pulse.ex2
Sample_id = C:\Users\delta\Docume
Solvent = CHLOROFORM-D
Creation_time = 3-DEC-2011 13:57:17
Revision_time = 3-DEC-2011 14:21:13
Current_time = 3-DEC-2011 14:50:154
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Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA400
Spectrometer = DELTA2_NMR
Field_strength = 9.389766 [T] (400 [MHz]
X_acq_duration = 2.18355952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
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 = 2.18355952 [s]
X_angle = 45 [deg]
X_atn = 5.3 [us]
X_pulse = off
Irr_mode = off
Tri_mode = off
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Relaxation_delay = 5 [s]
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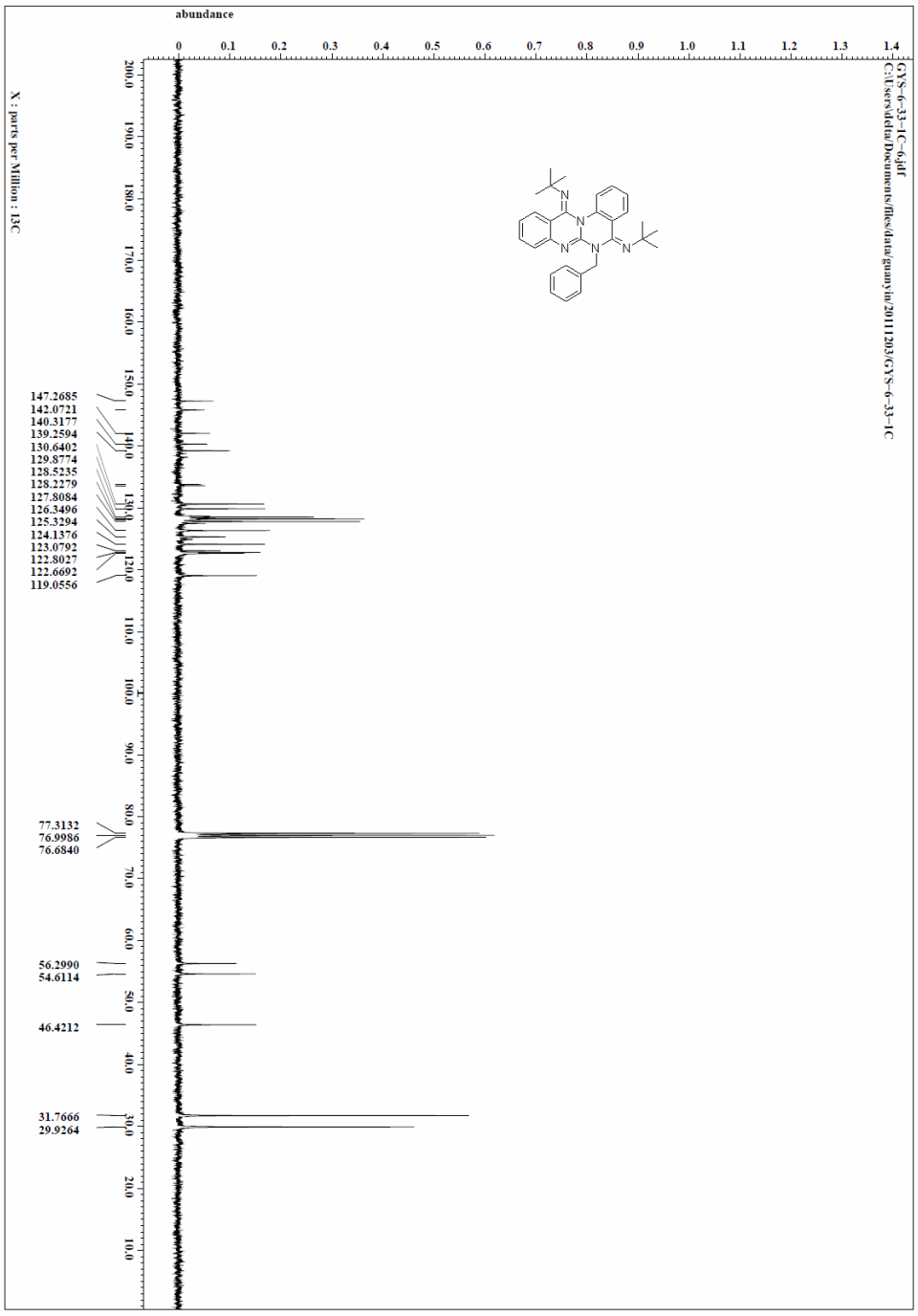
Temp_get = 21.4 [dC]


abundance
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0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
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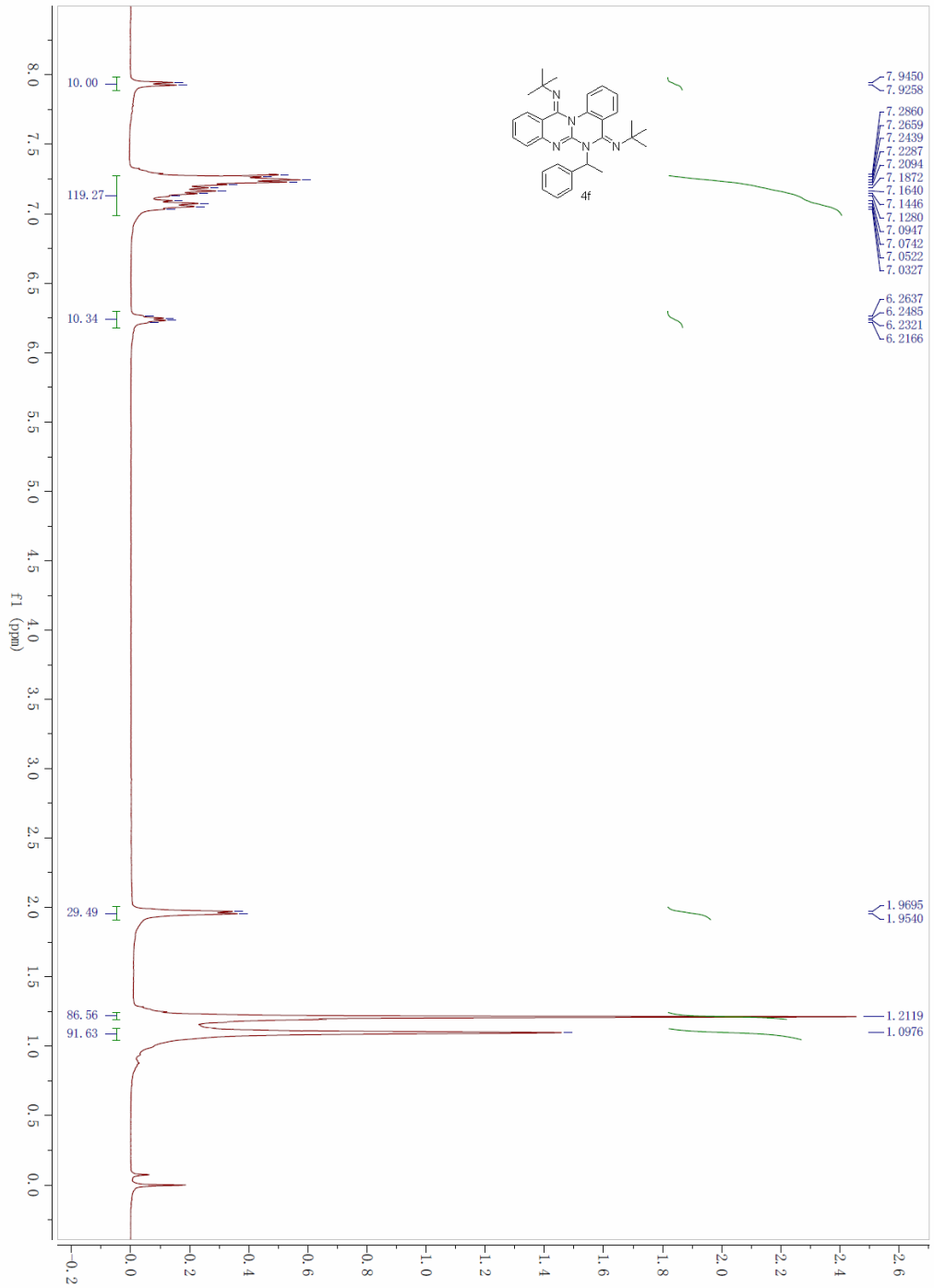
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
147.2685
142.0721
140.3177
139.2594
130.6402
129.8774
128.5235
128.2279
127.8084
126.3496
125.3294
124.1376
123.0792
122.8027
122.6692
119.0556
77.3132
76.9986
76.6840
56.2990
54.6114
46.4212
31.7666
29.9264
GYS-6-33-1C-6.jdf
C:\Users\dell\Documents\files\data\guanyin\20111203\GYS-6-33-1C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10.34
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86.56
91.63
4f
7.9450
7.9258
7.2860
7.2659
7.2439
7.2287
7.2094
7.1872
7.1640
7.1446
7.1280
7.0947
7.0742
7.0522
7.0327
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6.2485
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1.9540
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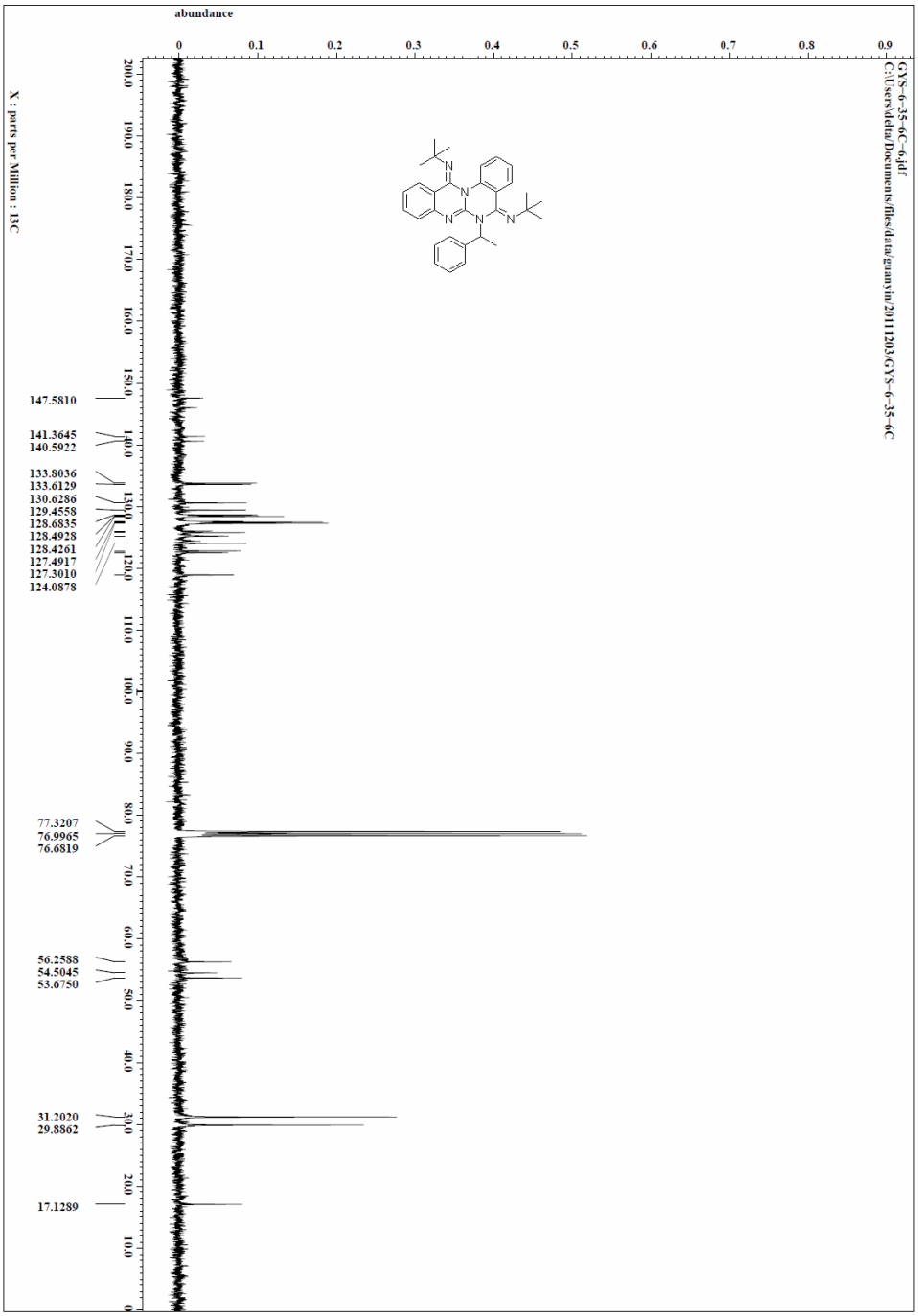
1.0976
f1 (ppm)


abundance
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0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
X : parts per Million : 13C
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141.3645
140.5922
133.8036
133.6129
130.6286
129.4558
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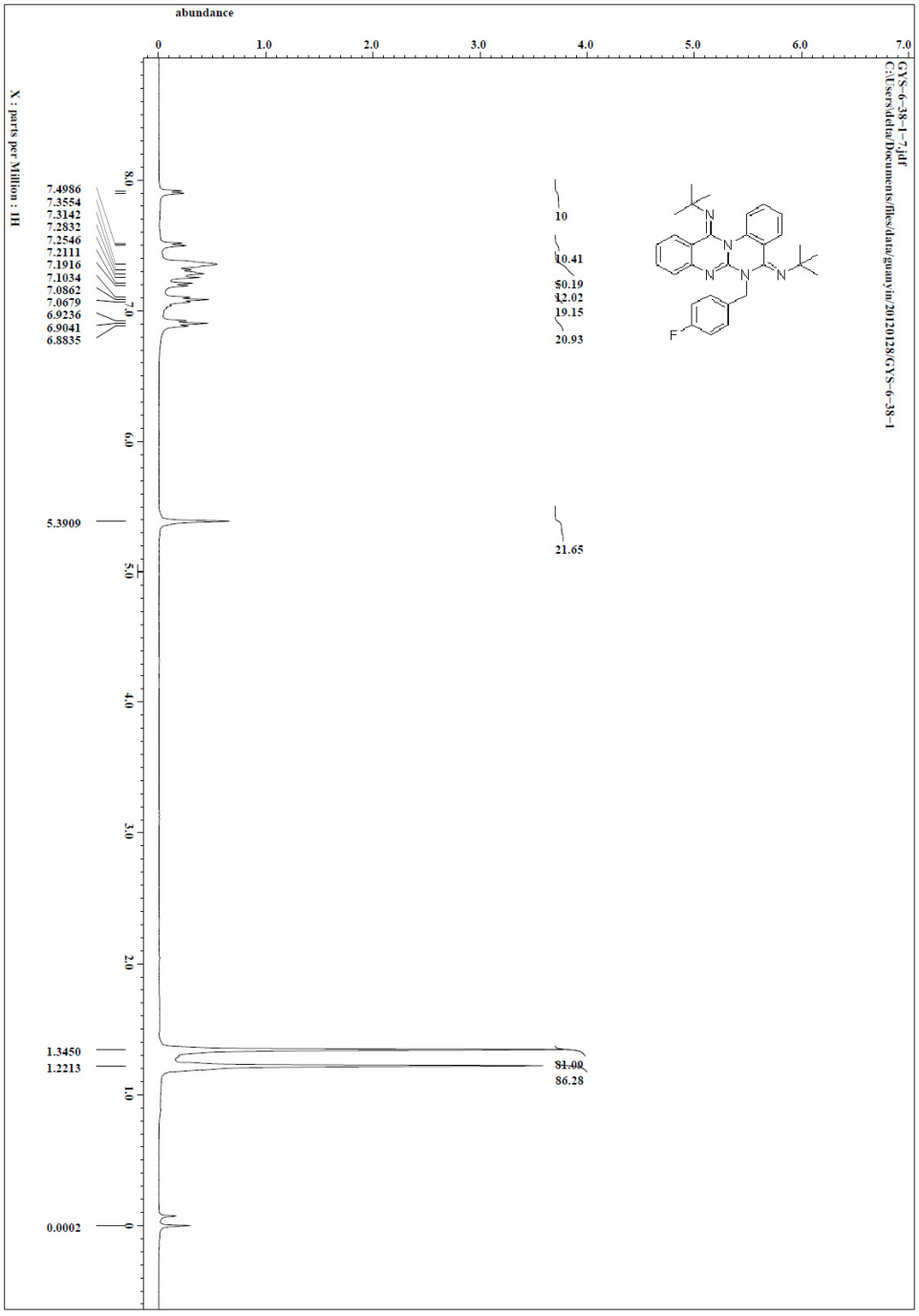
128.4928
128.4261
127.4917
127.3010
124.0878
77.3207
76.9965
76.6819
56.2588
54.5045
53.6750
31.2020
29.8862
17.1289
GYS-6-35-6C-6.jdf
C:\Users\dell\Documents\files\data\guanyin\20111203\GYS-6-35-6C


abundance
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2.0
3.0
4.0
5.0
6.0
7.0
X : parts per Million : 1H
GYS-6-38-1-7.jdf
C:\Users\ddfa\Documents\files\data\guanyin\20120128\GYS-6-38-1
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7.3554
7.3142
7.2832
7.2546
7.2111
7.1916
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7.0862
7.0679
6.9236
6.9041
6.8835
5.3909
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10
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10.19
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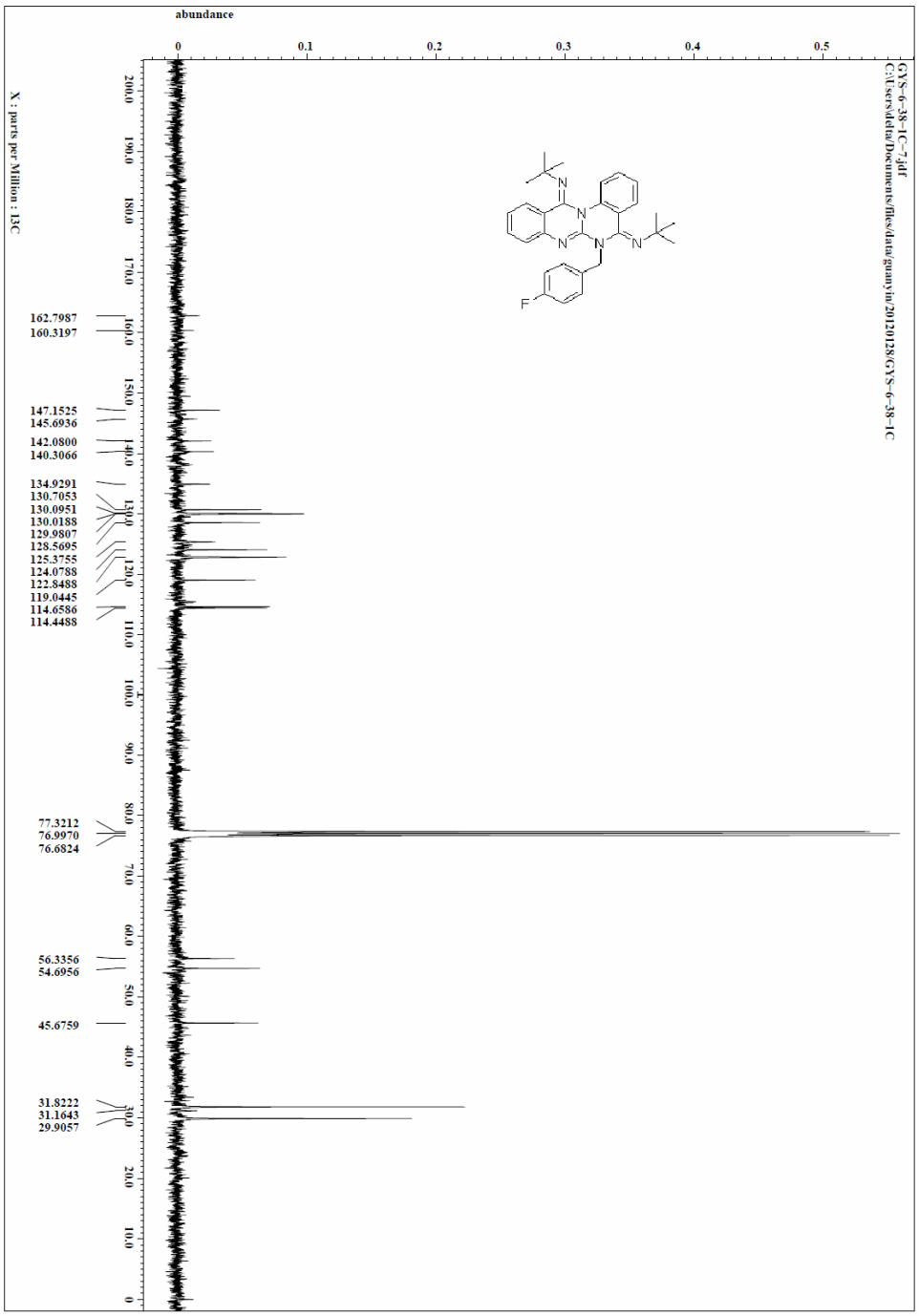
20.93
21.65
81.09
86.28
F


abundance
0
0.1
0.2
0.3
0.4
0.5
X : parts per Million : 13C
GYS-6-38-1C-7.jdf
C:\Users\ldd\a\Documents\files\data\guanyin\20120128\GYS-6-38-1C
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145.6936
142.0800
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134.9291
130.7053
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130.0188
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125.3755
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122.8488
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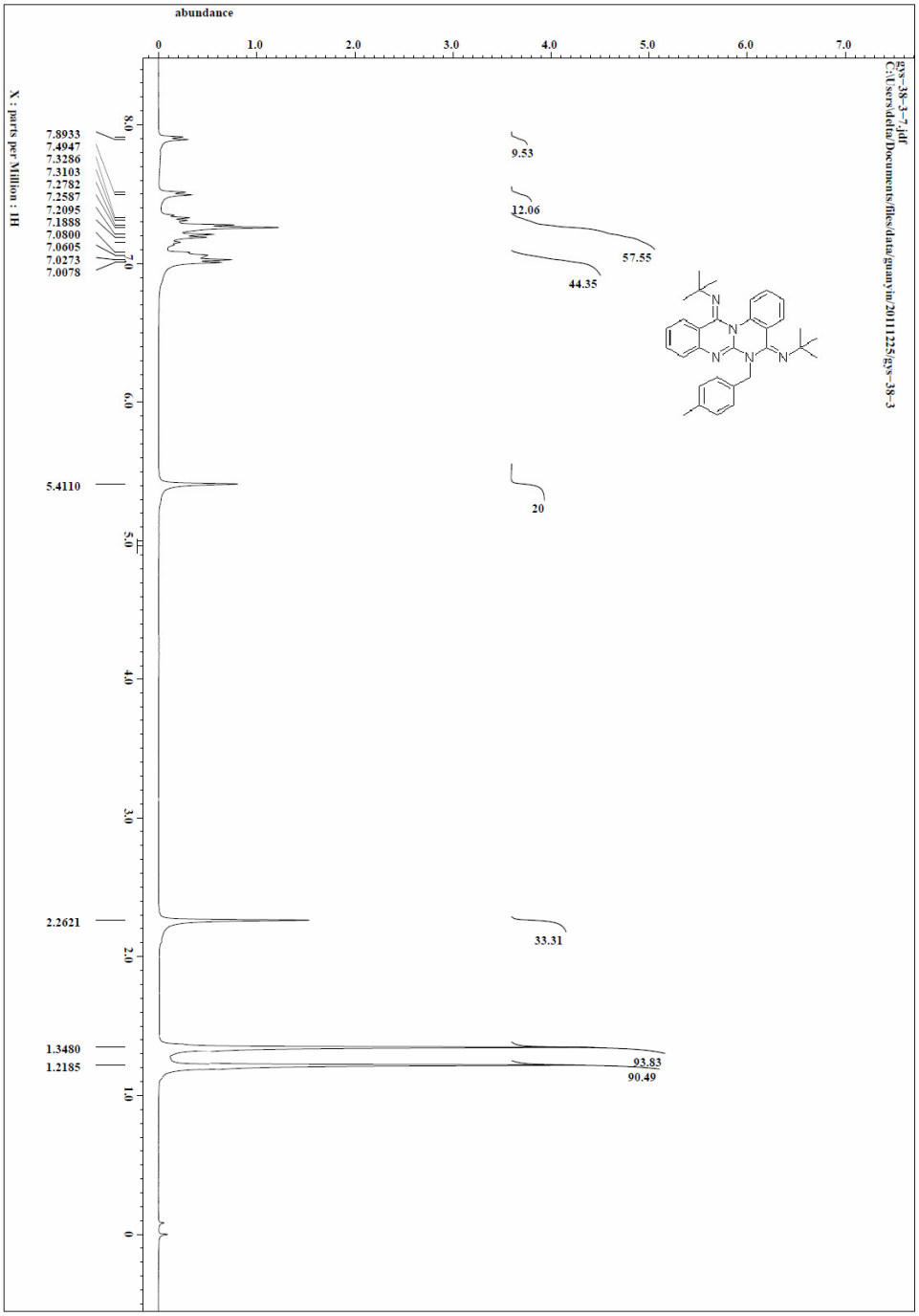
29.9057
F


abundance
X : parts per Million : 1H
gzs-38-3-7.jdf
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7.2587
7.2095
7.1888
7.0800
7.0605
7.0273
7.0078
5.4110
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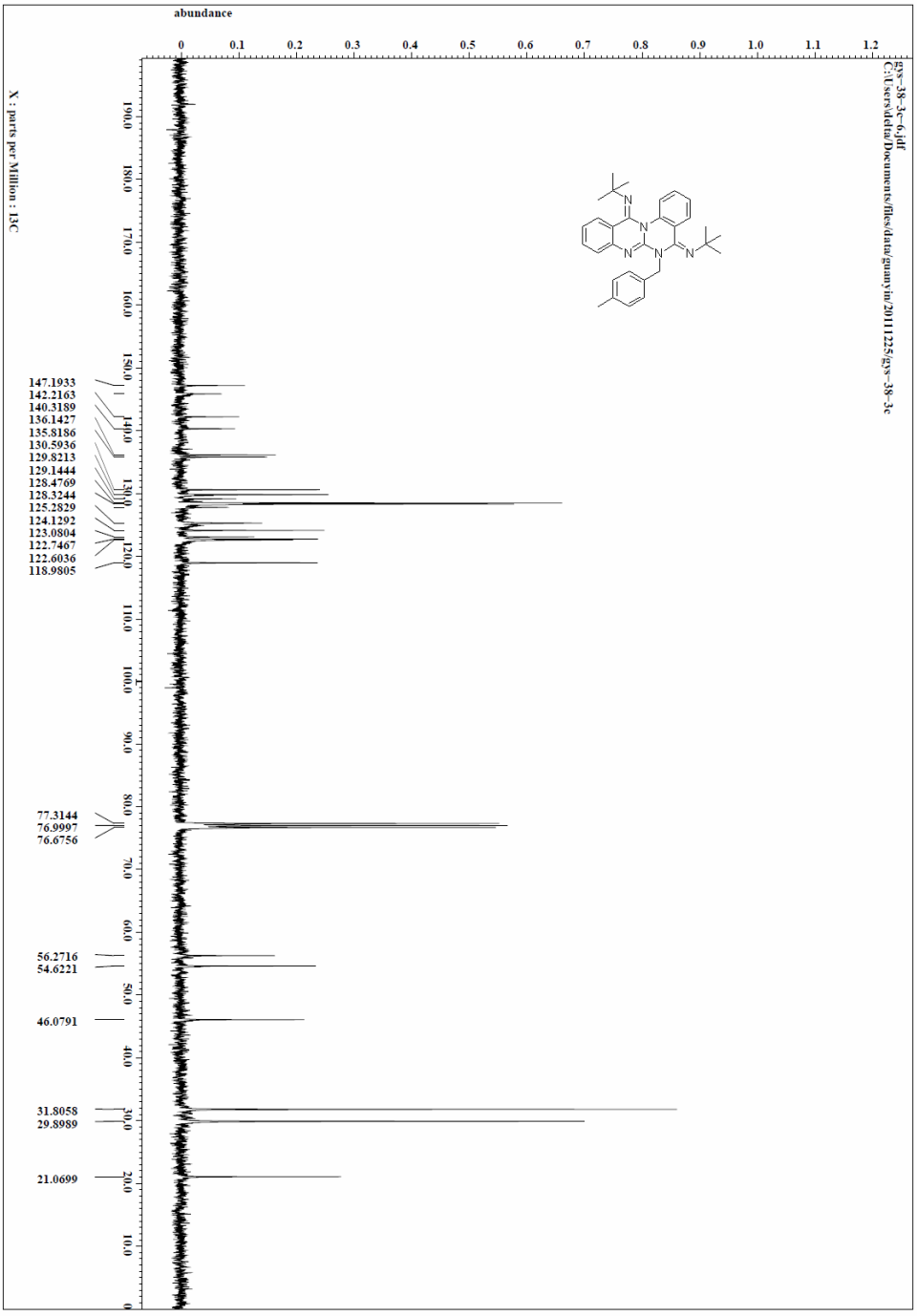
1.3480
1.2185
9.53
12.06
57.55
44.35
20
33.31
93.83
90.49


abundance
X : parts per Million : 13C
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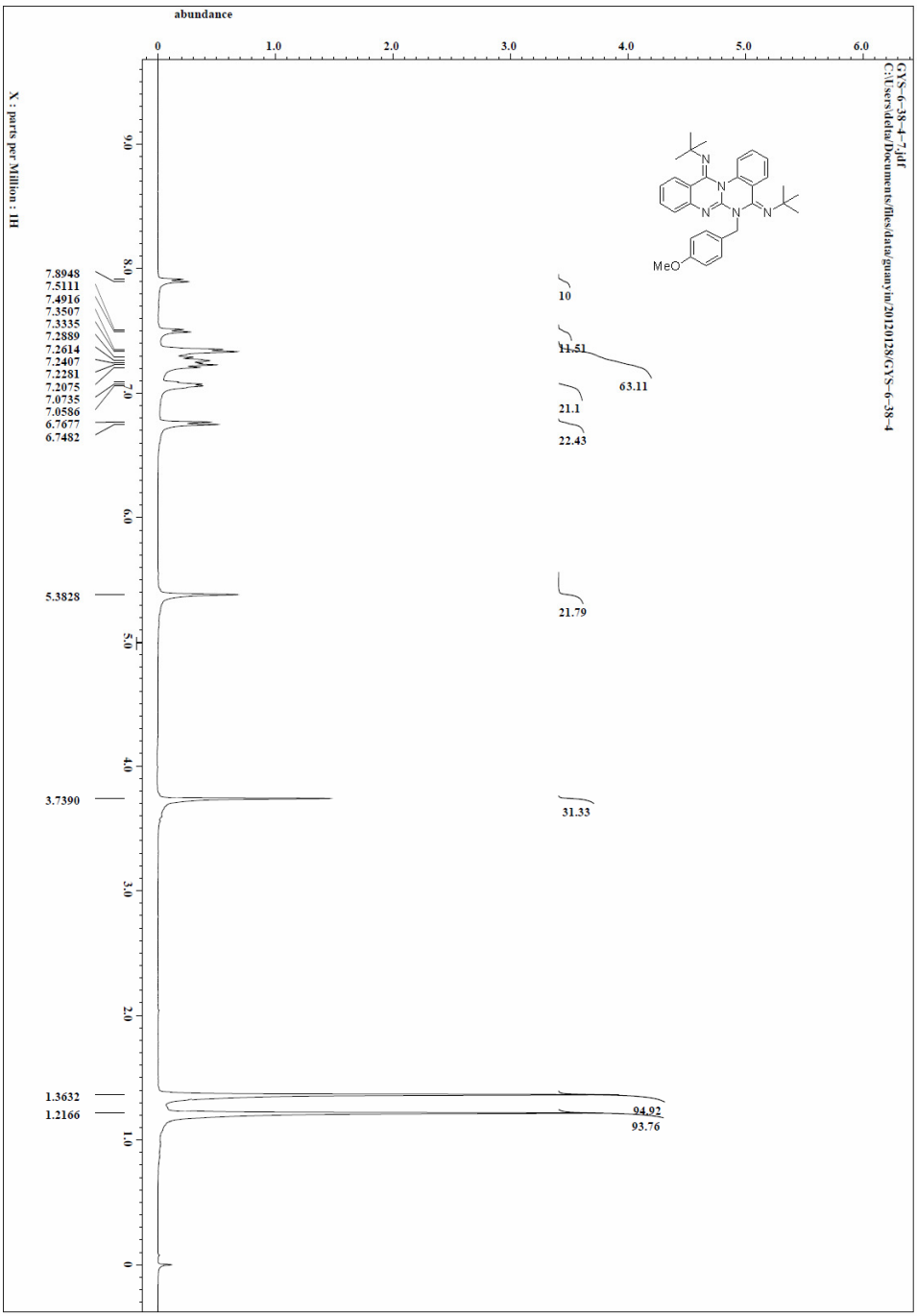
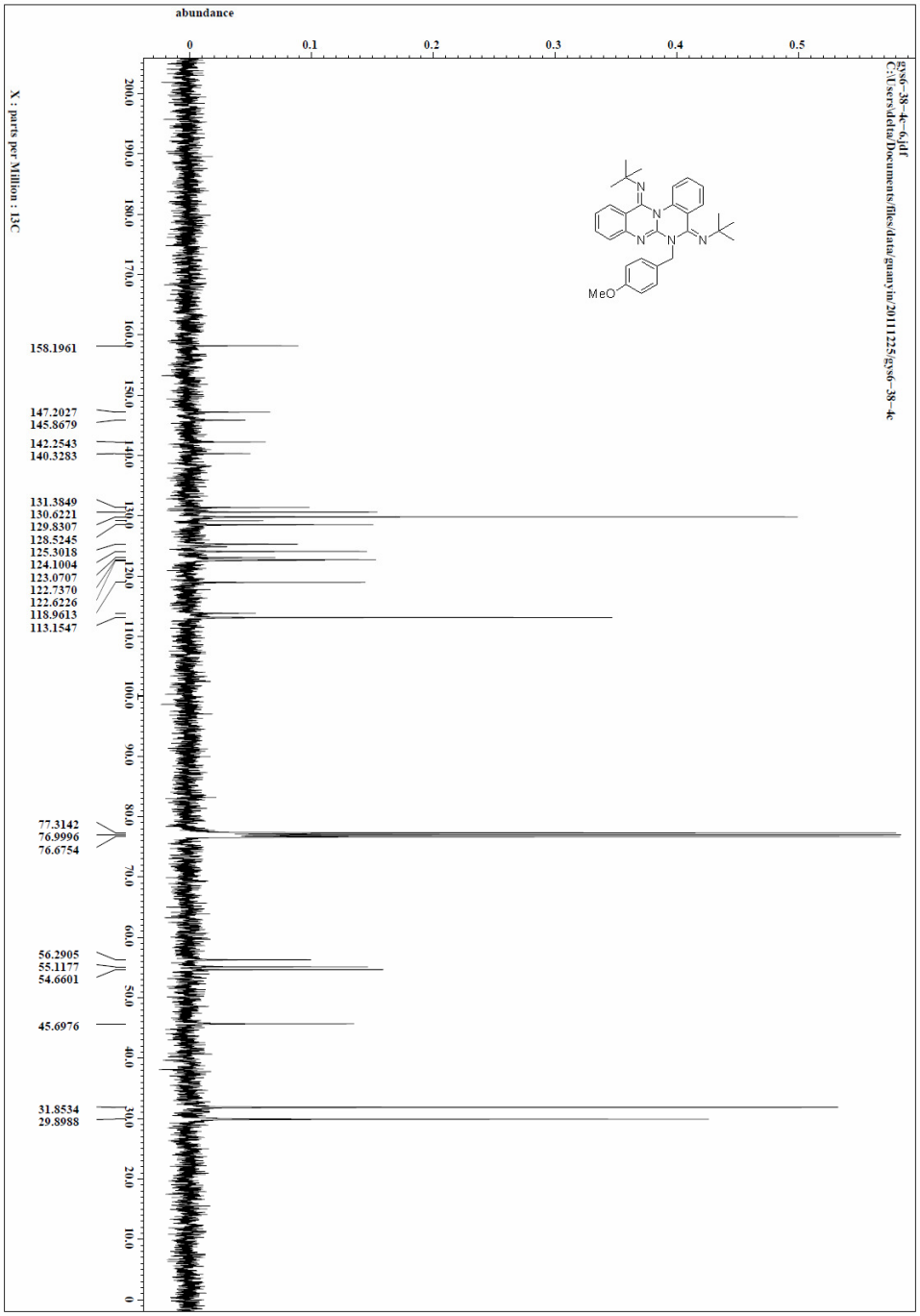
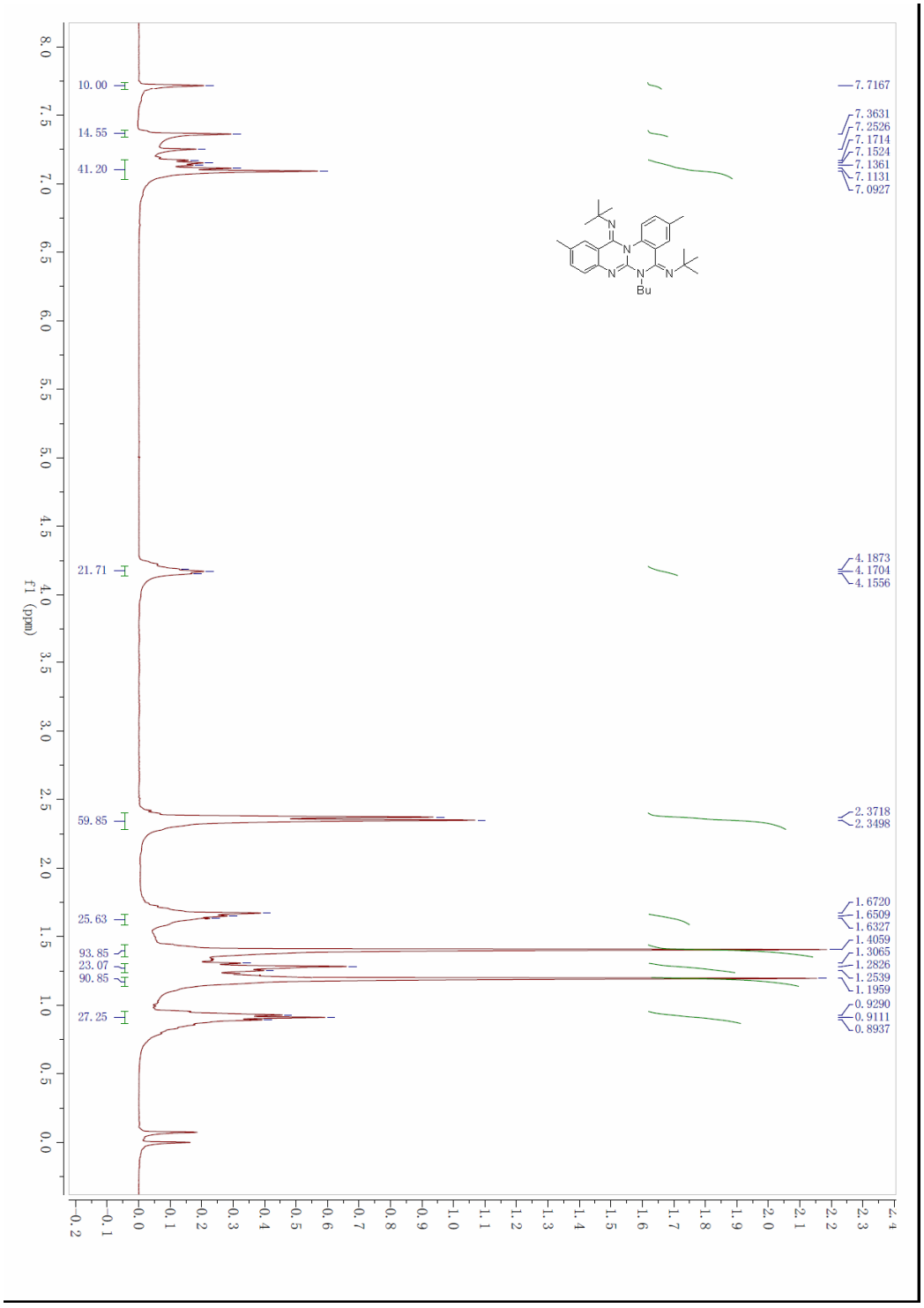
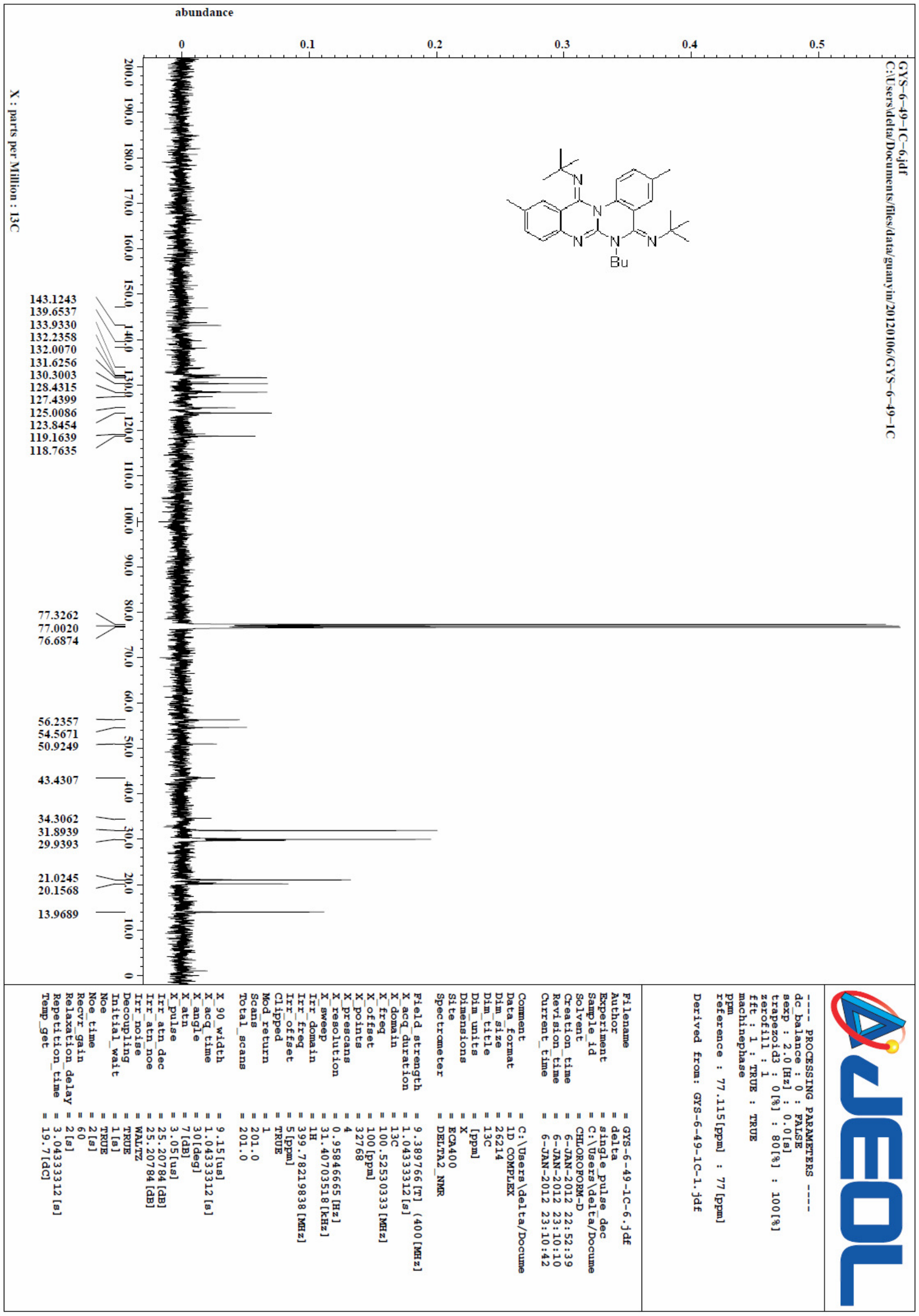
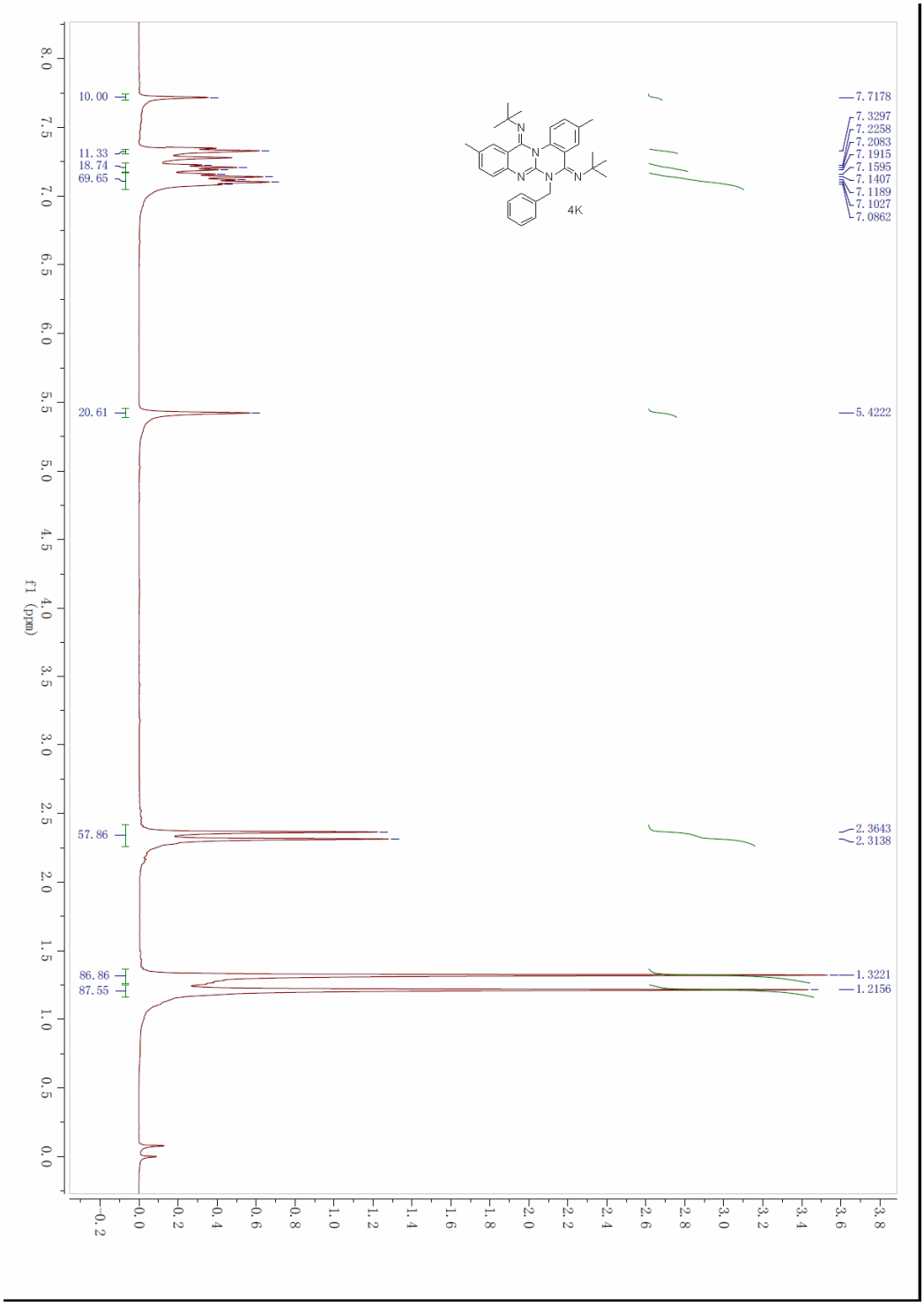
128.4769
128.3244
125.2829
124.1292
123.0804
122.7467
122.6036
118.9805
77.3144
76.9997
76.6756
56.2716
54.6221
46.0791
31.8058
29.8989
21.0699
gsy-38-3c-6.jdf
C:\Users\dell\Documents\files\data\guanyin\20111225\gsy-38-3c

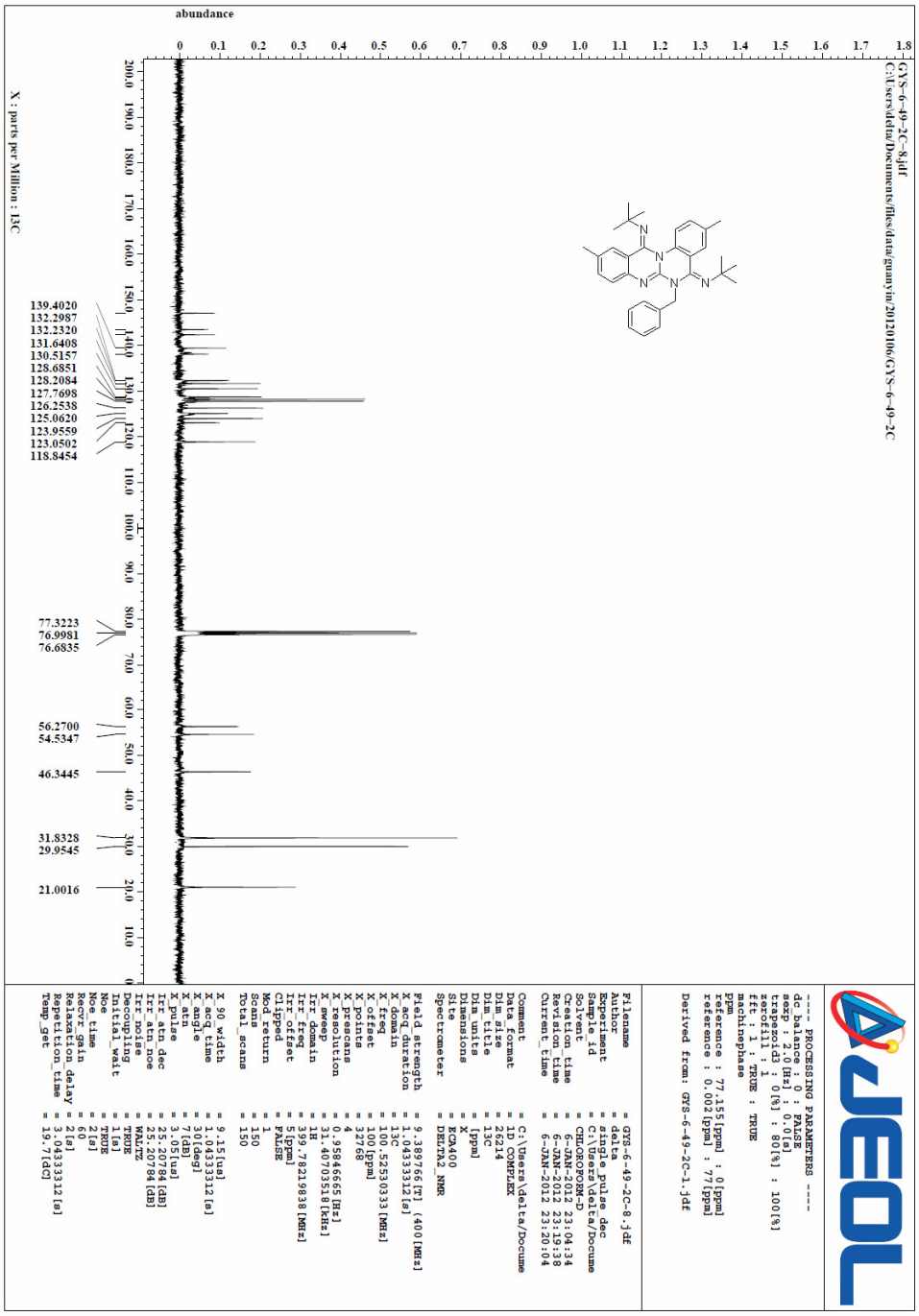

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
X : parts per Million : 1H
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8948
7.5111
7.4916
7.3507
7.3335
7.2889
7.2614
7.2407
7.2281
7.2075
7.0735
7.0586
6.7677
6.7482
5.3828
3.7390
1.3632
1.2166
10
11.51
63.11
21.1
22.43
21.79
31.33
94.92
93.76
MeO
GYS-6-38-4-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20120128\GYS-6-38-4

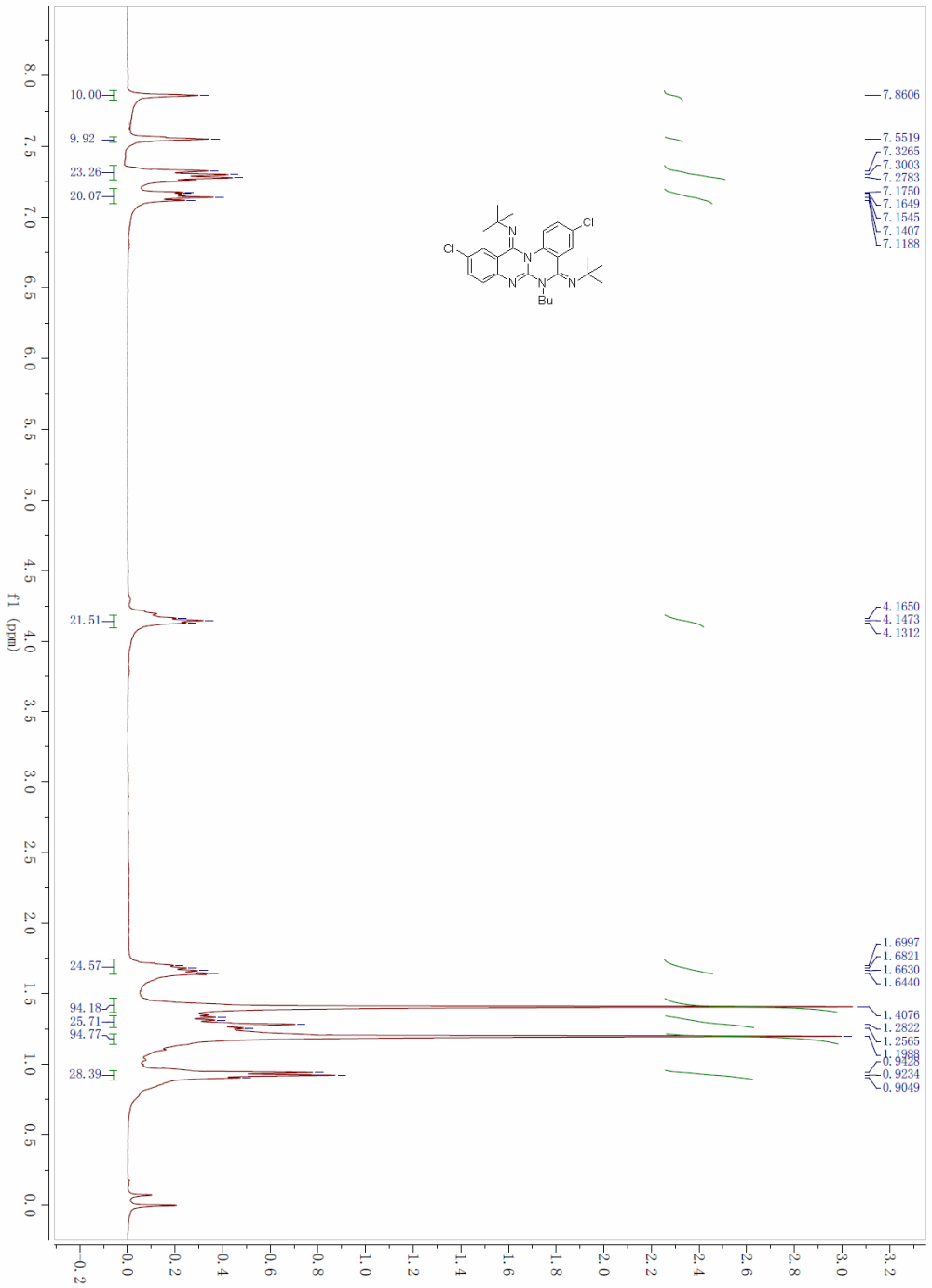

abundance
0
0.1
0.2
0.3
0.4
0.5
X : parts per Million : 13C
gss6-38-4c-6.jdf
C:\Users\ddta\Documents\files\data\guanyin\20111225\gss6-38-4c
158.1961
147.2027
145.8679
142.2543
140.3283
131.3849
130.6221
129.8307
128.5245
125.3018
124.1004
123.0707
122.7370
122.6226
118.9613
113.1547
77.3142
76.9996
76.6754
56.2905
55.1177
54.6601
45.6976
31.8534
29.8988
MeO

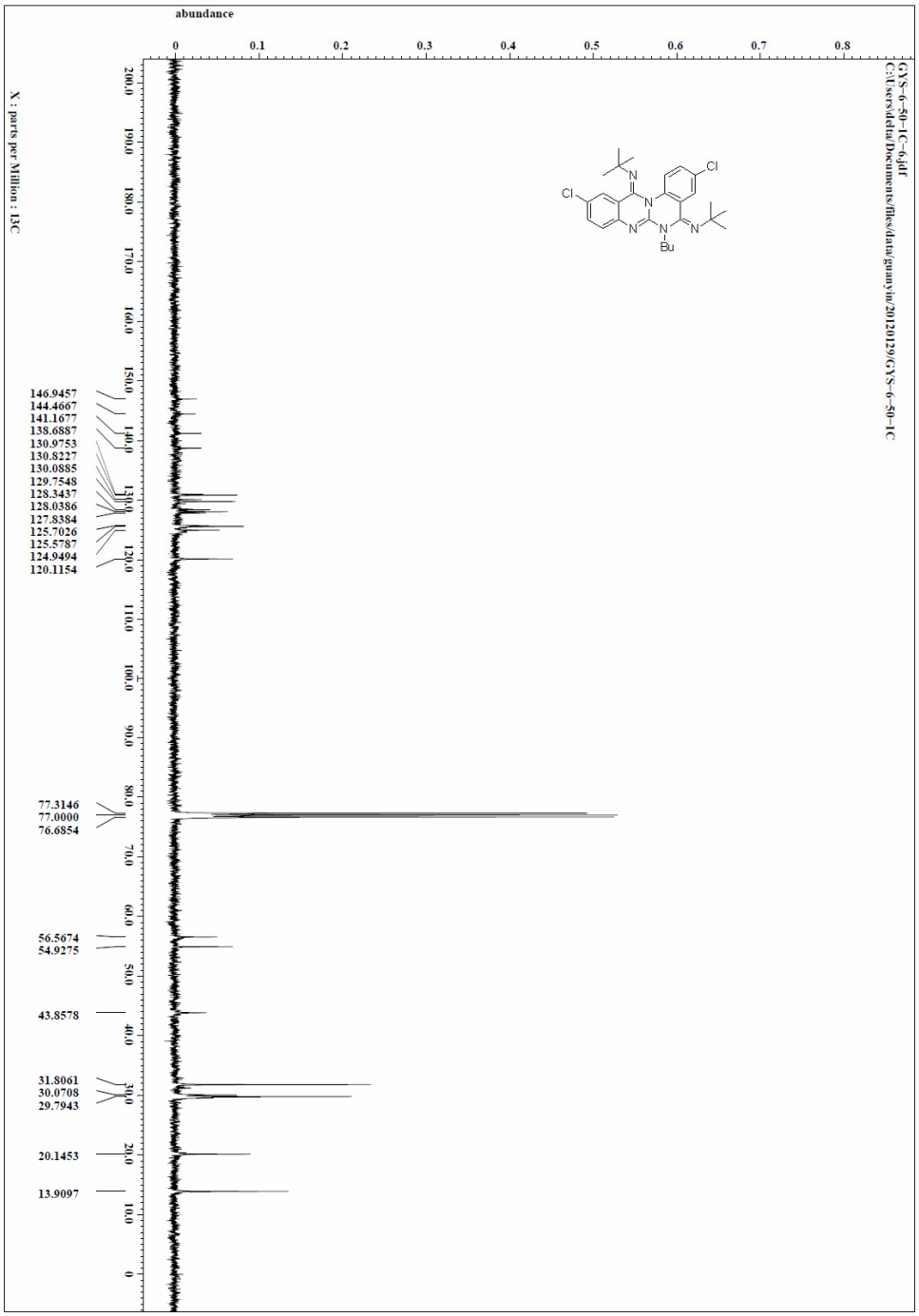

10.00
14.55
41.20
21.71
59.85
25.63
93.85
23.07
90.85
27.25
7.7167
7.3631
7.2526
7.1714
7.1524
7.1361
7.1131
7.0927
4.1873
4.1704
4.1556
2.3718
2.3498
1.6720
1.6509
1.6327
1.4059
1.3065
1.2826
1.2539
1.1959
0.9290
0.9111
0.8937
Bu
f1 (ppm)

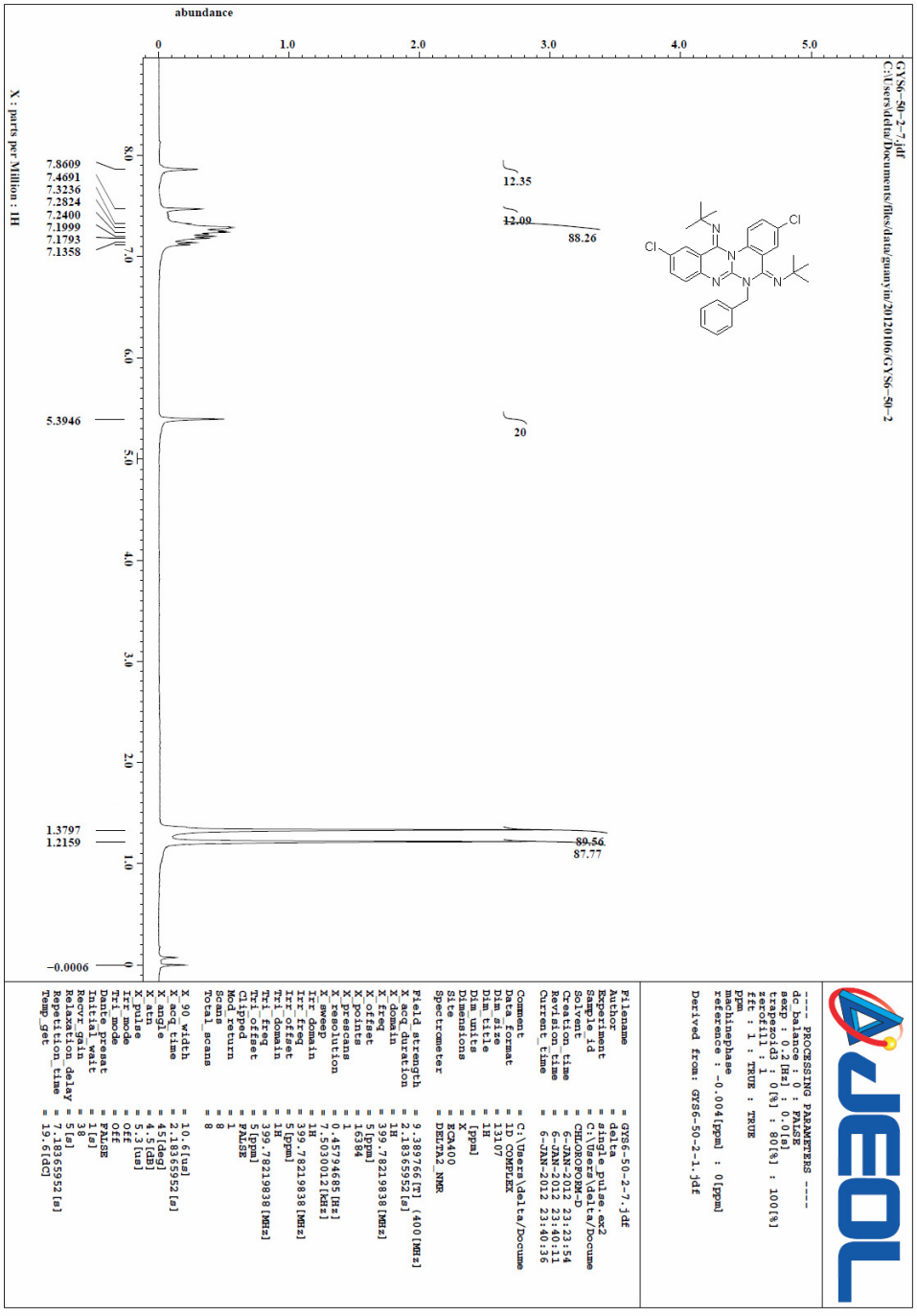

abundance
X : parts per Million : 13C
GYS-6-49-1C-6.jdf
143.1243
139.6537
133.9330
132.2358
132.0070
131.6256
130.3003
128.4315
127.4399
125.0086
123.8454
119.1639
118.7635
77.3262
77.0020
76.6874
56.2357
54.5671
50.9249
43.4307
34.3062
31.8939
29.9393
21.0245
20.1568
13.9689

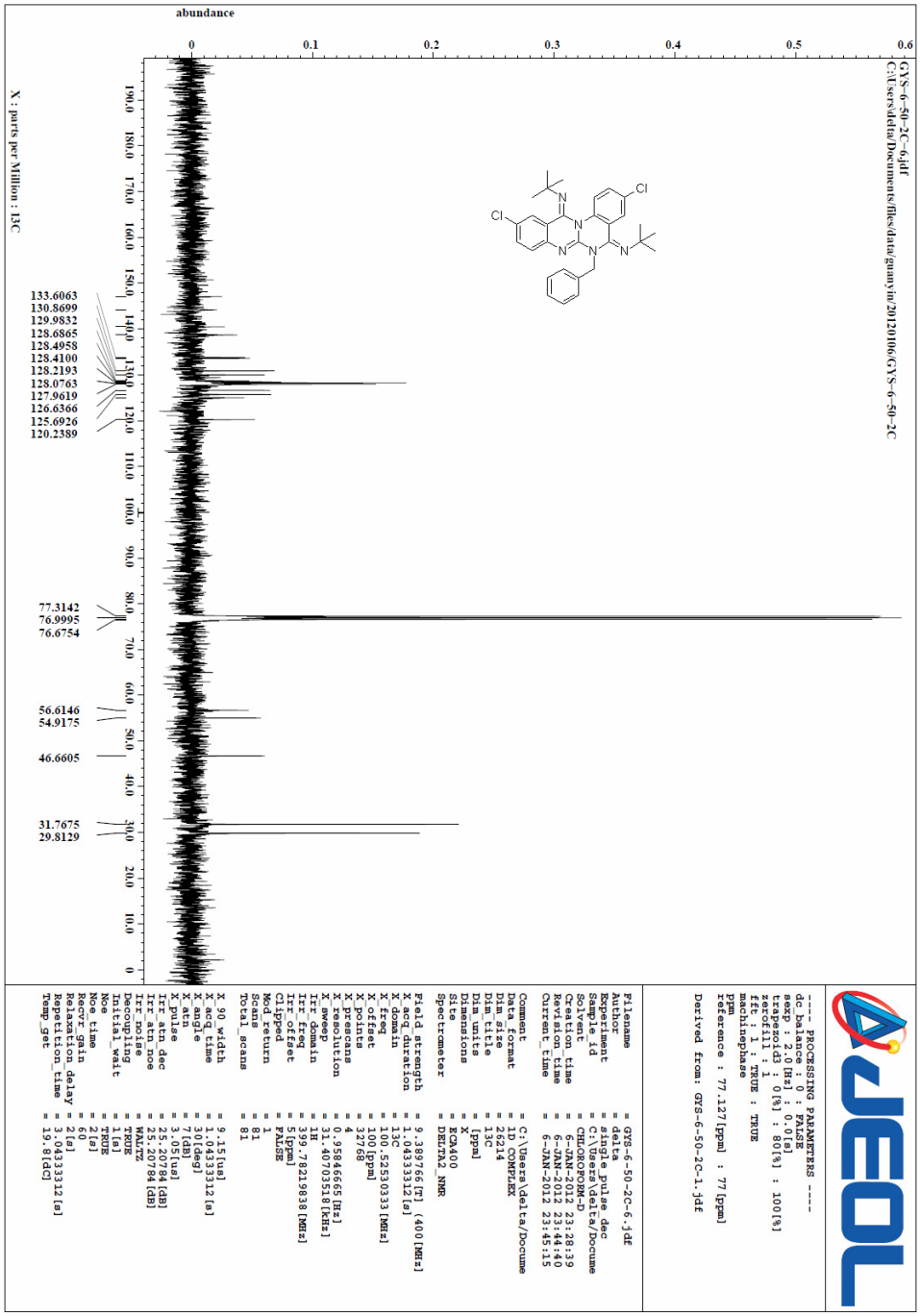

10.00
11.33
18.74
69.65
20.61
57.86
86.86
87.55
7.7178
7.3297
7.2258
7.2083
7.1915
7.1595
7.1407
7.1189
7.1027
7.0862
5.4222
2.3643
2.3138
1.3221
1.2156
4K
f1 (ppm)

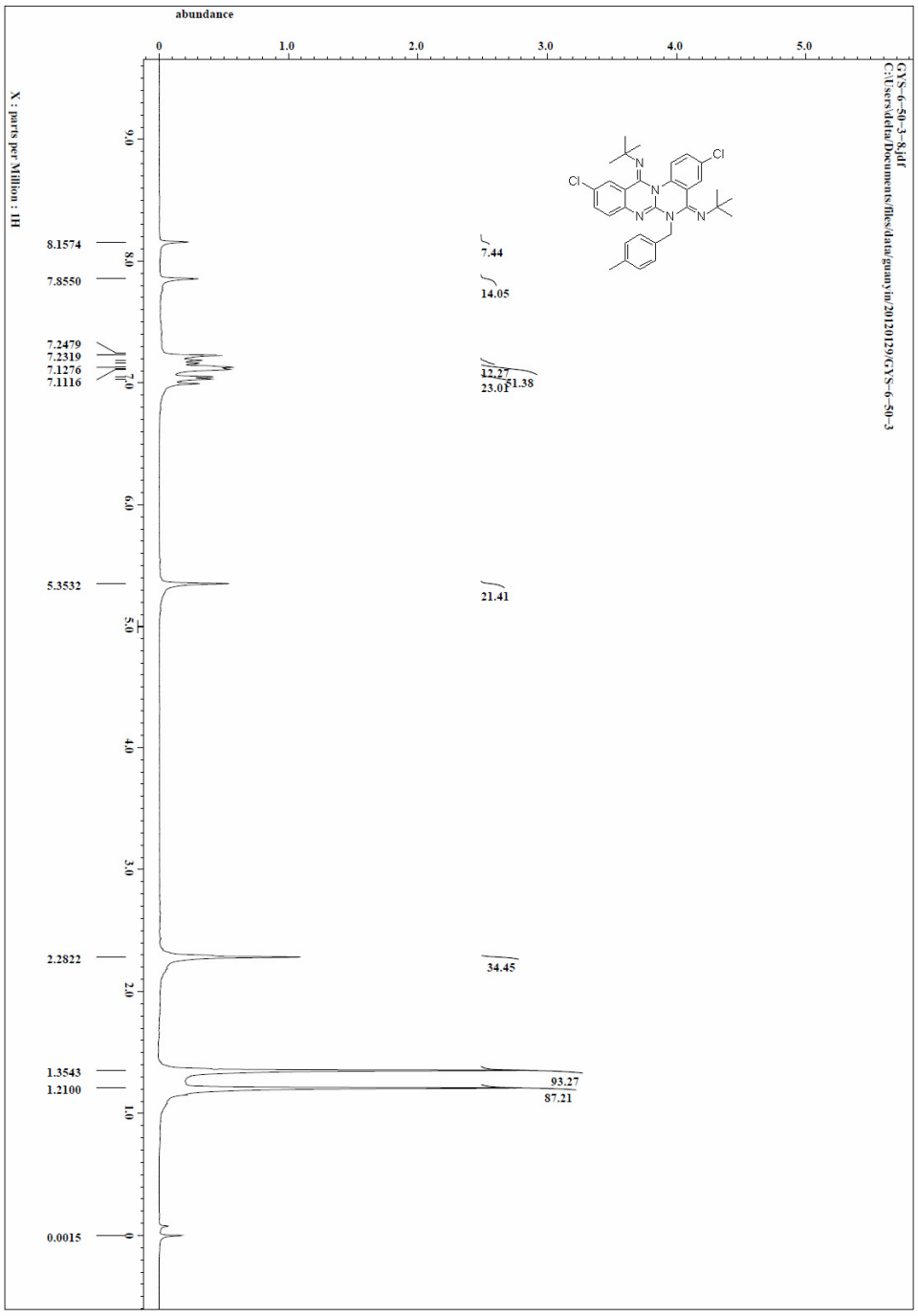

abundance
X : parts per Million : 13C
GYS-6-49-2C-8.jdf
C:\Users\delta\Documents\files\data\guanyin\20120106\GYS-6-49-2C
139.4020
132.2987
132.2320
131.6408
130.5157
128.6851
128.2084
127.7698
126.2538
125.0620
123.9559
123.0502
118.8454
77.3223
76.9981
76.6835
56.2700
54.5347
46.3445
31.8328
29.9545
21.0016
JEOL
---- PROCESSING PARAMETERS ----
dc balance : 0 : FALSE
exsp : 2.0 [Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
ft_mode : magnitudephase
ppm : 77.155[ppm] : 0[ppm]
reference : 0.002[ppm] : 77[ppm]
Derived from: GYS-6-49-2C-1.jdf
Filename = GYS-6-49-2C-8.jdf
Author =
Experiment = delta
Sample_id = single_pulse_dec
Solvent = C:\Users\delta\Docume
Sample_comment = CHLOROFORM-D
Revision_time = 6-JAN-2012 23:04:34
Current_time = 6-JAN-2012 23:19:38
Comment = 6-JAN-2012 23:20:04
Data_format = C:\Users\delta\Docume
Dim_count = 1D COMPLEX
Dim_title = 128.214
Dim_units = [ppm]
Dimensions = X
Site = ECA400
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_resolution = 13C 4.883312[s]
X_domain = 100.525303333[MHz]
X_freq = 100[ppm]
X_offset = 32768
X_points = 4
X_prescans = 0.958466665[Hz]
X_resolution = 18.407035518[kHz]
X_window = 399.78219838[MHz]
Irr_domain = 5[ppm]
Irr_freq = FALSE
Irr_offset = 1
Clipped = 150
Mod_return = 1
Scans = 150
Total_scans
X_90_width = 9.15[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 7[dB]
X_pulse = 3.05[us]
Irr_atn_dec = 25.20784[dB]
Irr_atn_hse = 25.20784[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2.0[s]
Repetition_time = 3.043333312[s]
Temp_get = 19.7[dC]

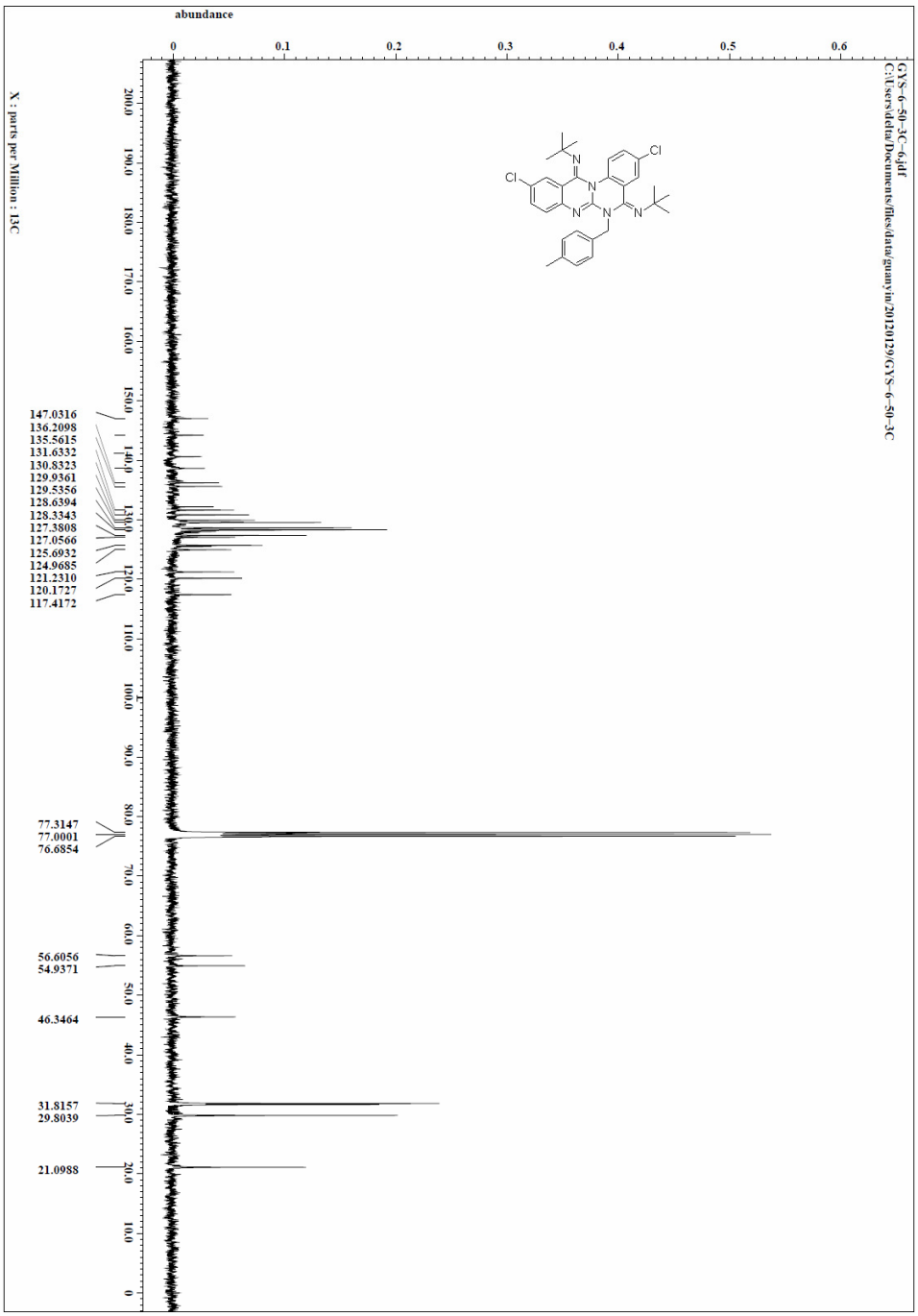

10.00
9.92
23.26
20.07
21.51
24.57
94.18
25.71
94.77
28.39
7.8606
7.5519
7.3265
7.3003
7.2783
7.1750
7.1649
7.1545
7.1407
7.1188
4.1650
4.1473
4.1312
1.6997
1.6821
1.6630
1.6440
1.4076
1.2822
1.2565
1.1988
0.9428
0.9234
0.9049
Cl
Cl
N
N
N
N
Bu
f1 (ppm)

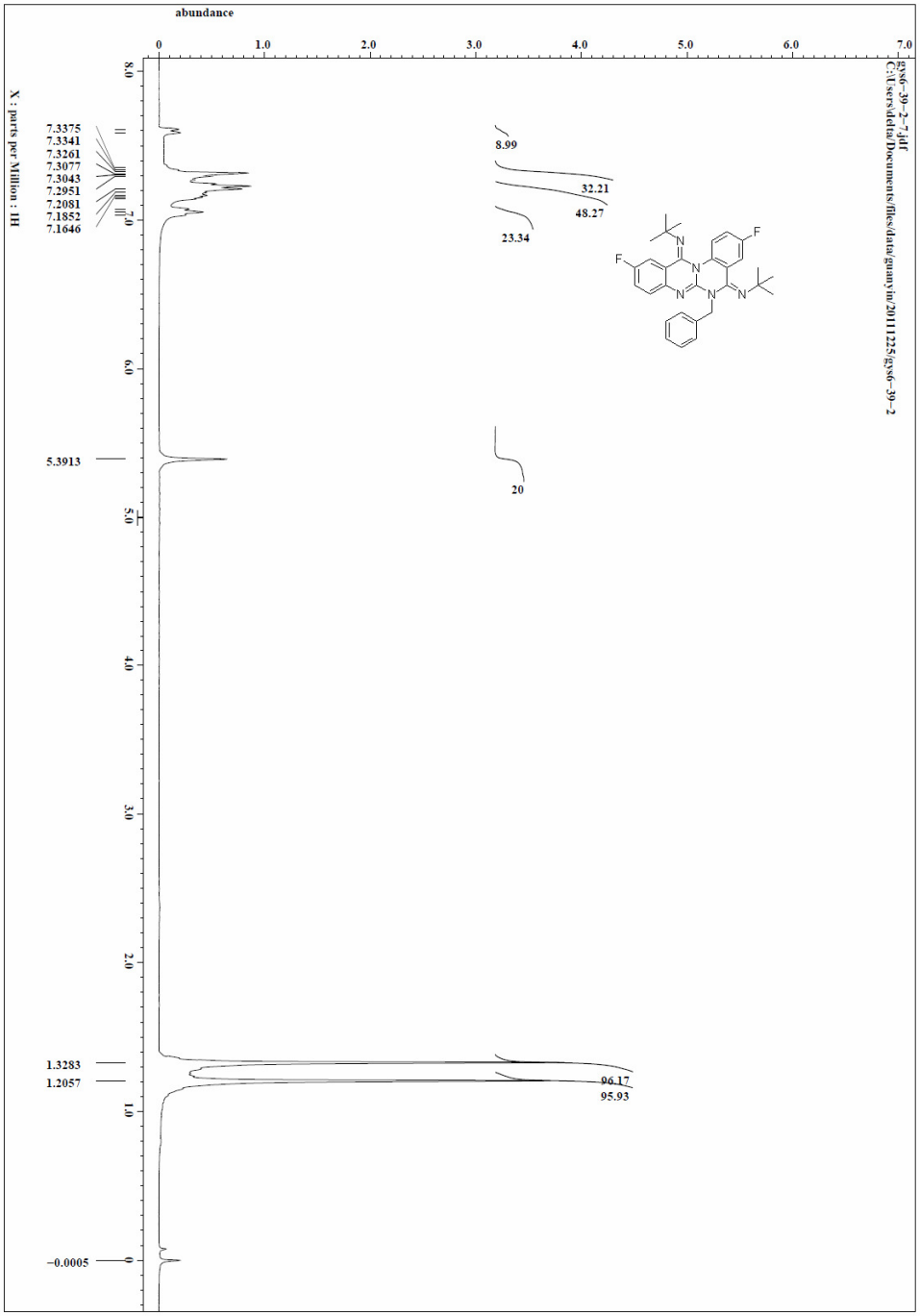

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
X : parts per Million : 13C
GYS-6-50-1C-6.jdf
C:\Users\delta\Documents\files\data\guanyin\20120129\GYS-6-50-1C
146.9457
144.4667
141.1677
138.6887
130.9753
130.8227
130.0885
129.7548
128.3437
128.0386
127.8384
125.7026
125.5787
124.9494
120.1154
77.3146
77.0000
76.6854
56.5674
54.9275
43.8578
31.8061
30.0708
29.7943
20.1453
13.9097
Cl
Cl
N
N
N
N
Bu

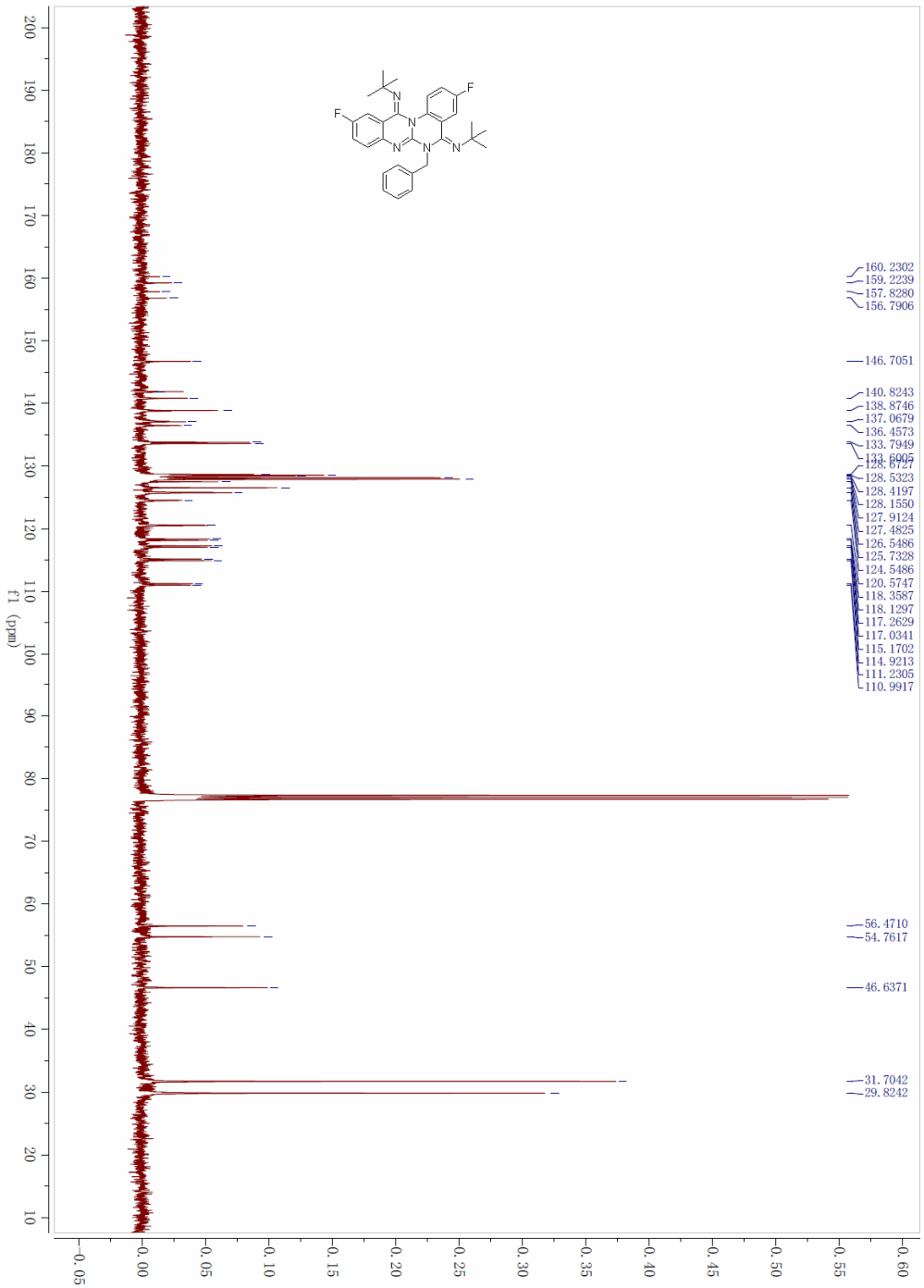

abundance
GYS6-50-2-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20120106\GYS6-50-2
X : parts per Million : 1H
7.8609
7.4691
7.3236
7.2824
7.2400
7.1999
7.1793
7.1358
5.3946
1.3797
1.2159
-0.0006
12.35
12.09
88.26
20
89.56
87.77
Cl
Cl
N
N
N
N
N
Filename = GYS6-50-2-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = C:\Users\delta\Docume
Solvent = CHLOROFORM-d1
Creation_time = 6-JAN-2012 23:23:54
Revision_time = 6-JAN-2012 23:40:11
Current_time = 6-JAN-2012 23:40:36
Comment = C:\Users\delta\Docume
Data_format = 1D COMPLEX
Dim_size = 131072
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECA400
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.457946[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]
Mod_freturn = FALSE
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]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
Temp_get = 19.6[dC]
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
flatten : 1 : TRUE : TRUE
ppm : 1 : 0[ppm]
machinephase
reference : -0.004[ppm] : 0[ppm]
Derived from: GYS6-50-2-1.jdf

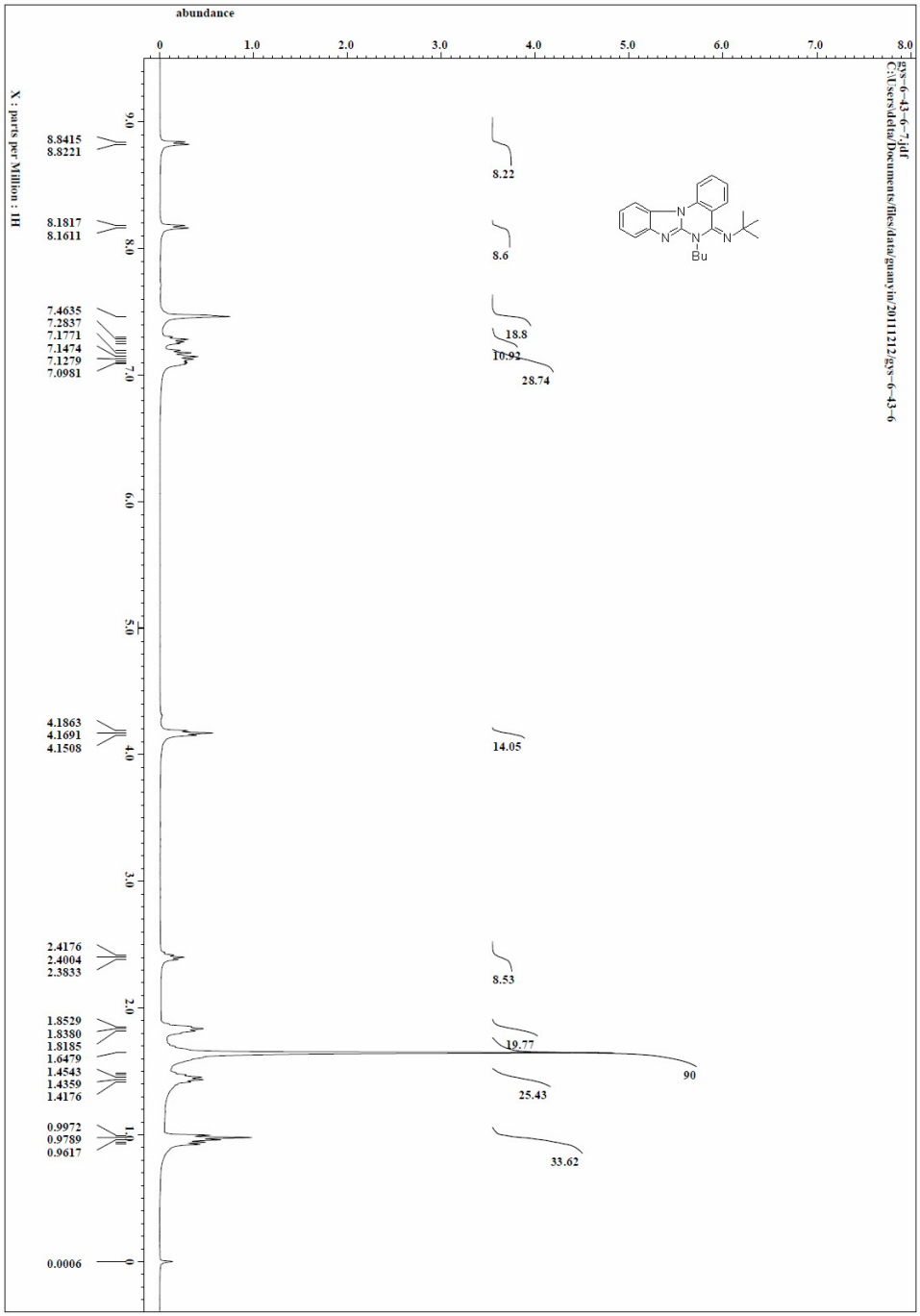

GYS-6-50-2C-6.jdf
C:\Users\delta\Documents\files\data\guanyin\20120106\GYS-6-50-2C
abundance
X : parts per Million : 13C
133.6063
130.8699
129.9832
128.6865
128.4958
128.4100
128.2193
128.0763
127.9619
126.6366
125.6926
120.2389
77.3142
76.9995
76.6754
56.6146
54.9175
46.6605
31.7675
29.8129
Cl
Cl
N
N
N
N
N
Filename = GYS-6-50-2C-6.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = C:\Users\delta\Docume
Solvent = CHLOROFORM-D
Creation_time = 6-JAN-2012 23:28:39
Revision_time = 6-JAN-2012 23:44:40
Current_time = 6-JAN-2012 23:45:15
Comment = C:\Users\delta\Docume
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = PPM
Dimensions = X
Site = RCA400
Spectrometer = DELTA2_NMR
Field_strength = 9.389766 [T] (400 [MHz]
X_acq_duration = 1.043333 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 31.407035 [Hz]
X_sweep = 32810.78 [Hz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 81
Total_scans = 81
X_90_width = 9.15 [us]
X_acq_time = 1.043333 [s]
X_angle = 30 [deg]
X_atn = 7 [dB]
X_pulse = 3.05 [us]
Irr_atn_dec = 25.2078 [dB]
Irr_atn_noe = 25.2078 [dB]
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 2 [s]
Recyc_gain = 60
Relaxation_delay = 2 [s]
Repetition_time = 3.043333 [s]
Temp_set = 19.8 [dC]
---- PROCESSING PARAMETERS ----
dc_balance : FALSE
expp : 2.0 [Hz] : 0.0 [s]
trapezoid3 : 0 [%] : 80 [%] : 100 [%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm : 1 : 1
reference : 77.127 [ppm] : 77 [ppm]
Derived from: GYS-6-50-2C-1.jdf

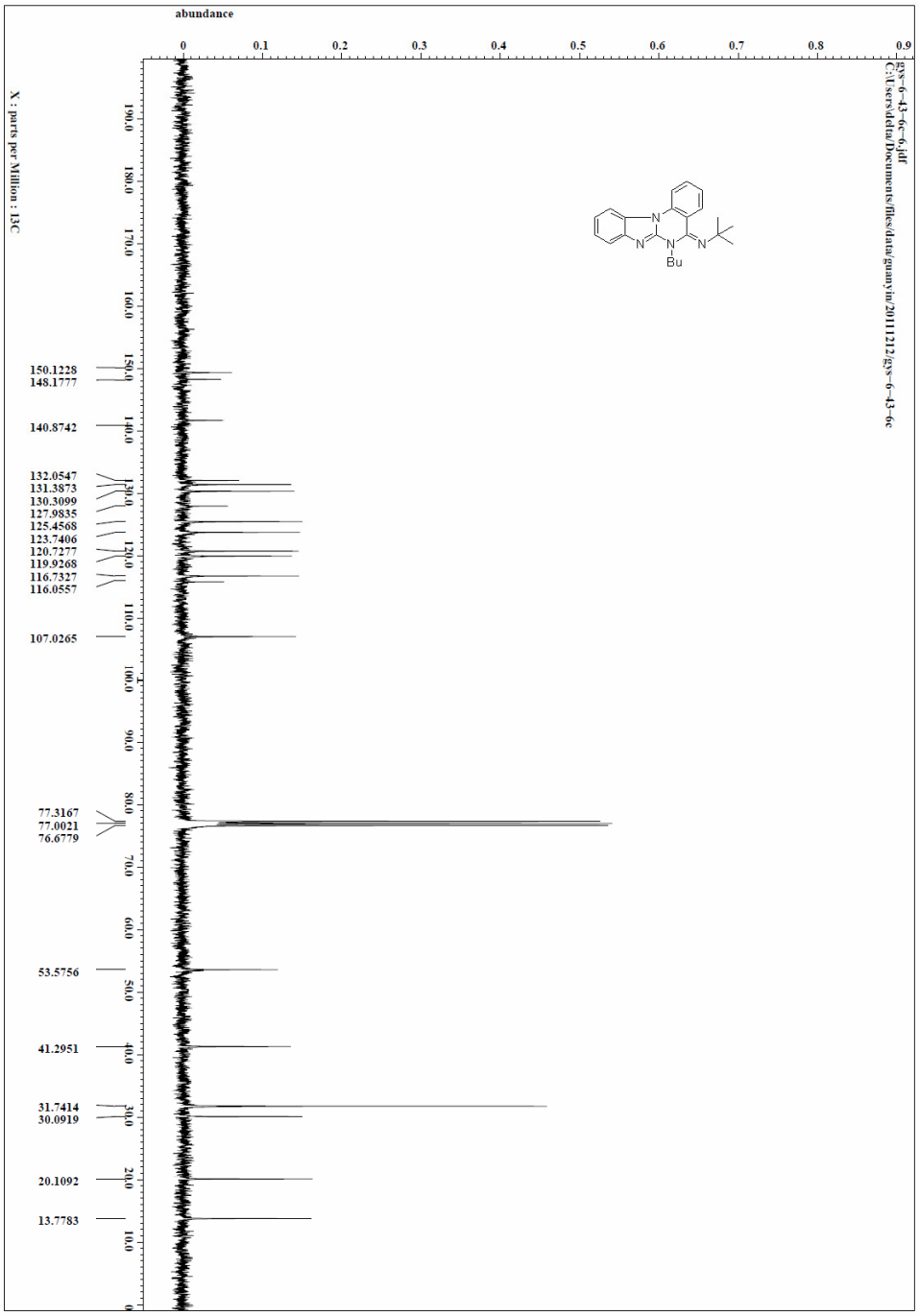

abundance
X : parts per Million : 1H
GYS-6-50-3-8.jdf
C:\Users\delta\Documents\files\data\guanyin\20120129\GYS-6-50-3
8.1574
7.8550
7.2479
7.2319
7.1276
7.1116
5.3532
2.2822
1.3543
1.2100
0.0015
7.44
14.05
12.27
23.01
51.38
21.41
34.45
93.27
87.21
Cl
Cl
N

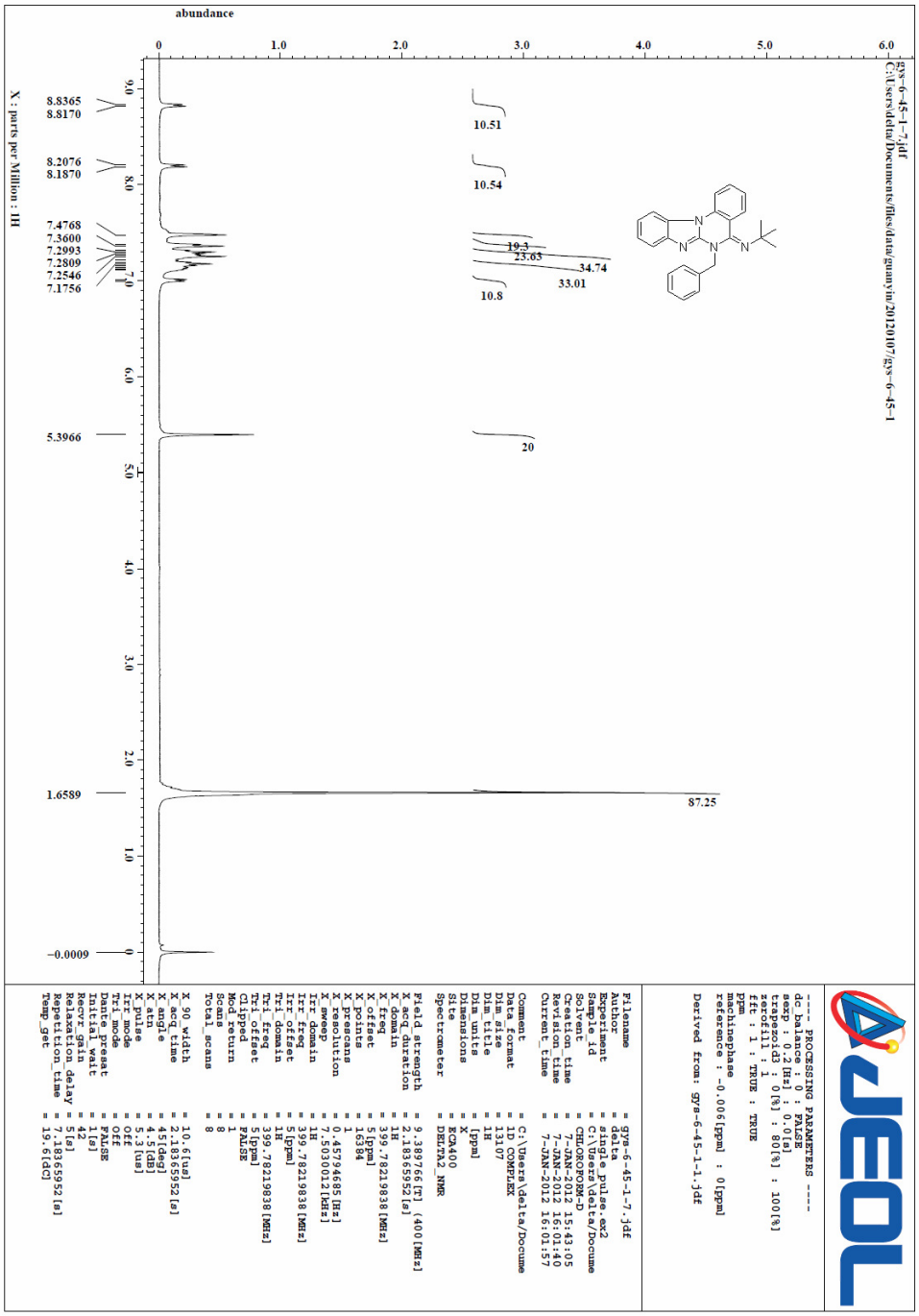

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
X : parts per Million : 13C
GYS-6-50-3C-6.jdf
C:\Users\delta\Documents\flies\data\guanyin\20120129\GYS-6-50-3C
147.0316
136.2098
135.5615
131.6332
130.8323
129.9361
129.5356
128.6394
128.3343
127.3808
127.0566
125.6932
124.9685
121.2310
120.1727
117.4172
77.3147
77.0001
76.6854
56.6056
54.9371
46.3464
31.8157
29.8039
21.0988
Cl
Cl
N
N
N
N

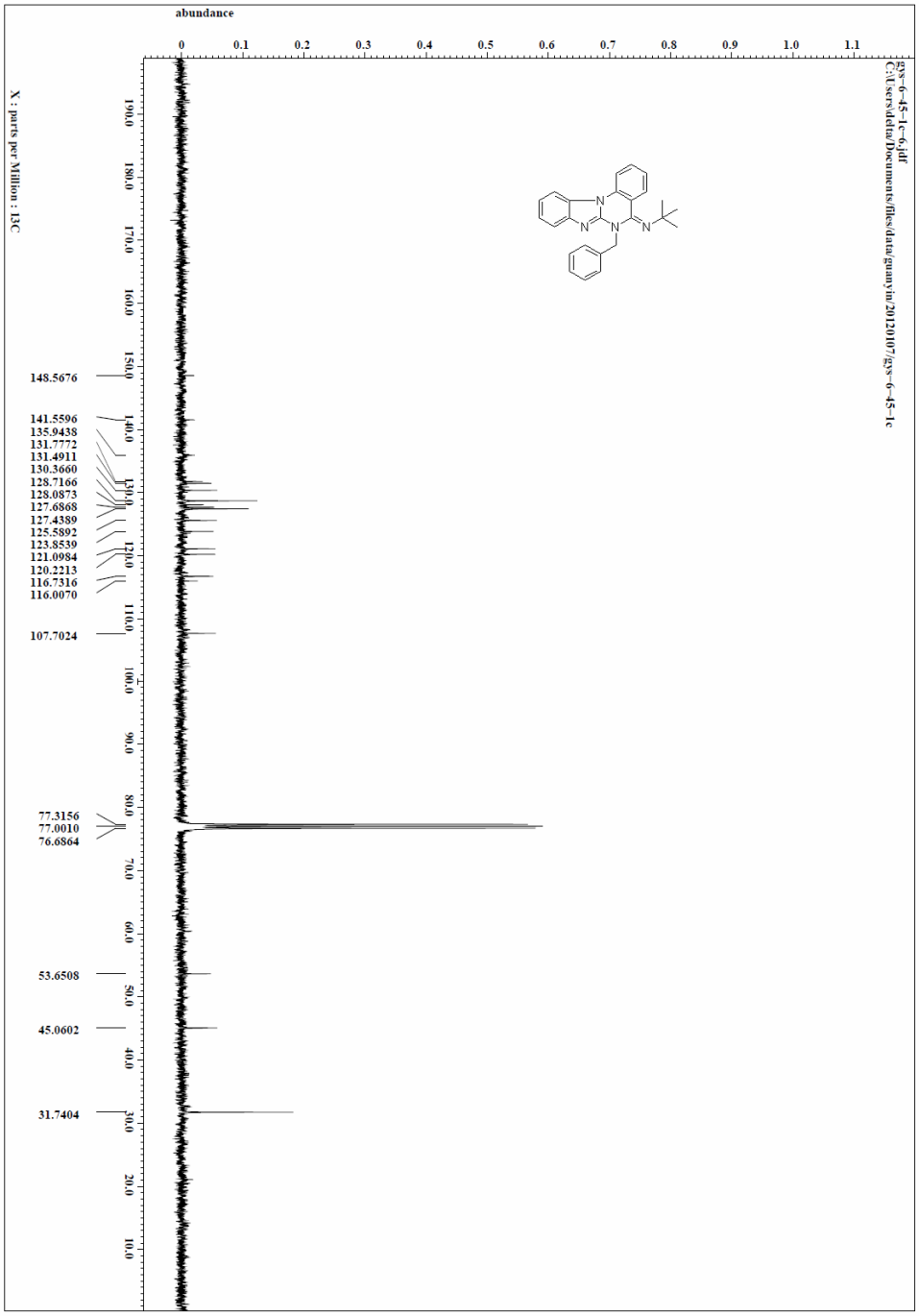

abundance
X : parts per Million : 1H
7.3375
7.3341
7.3261
7.3077
7.3043
7.2951
7.2081
7.1852
7.1646
5.3913
1.3283
1.2057
−0.0005
8.99
32.21
48.27
23.34
20
96.17
95.93
F
F
N
N
N
N
N
gs6−39−2−7.jdf
C:\Users\dd\a Documents\files\data\guany in\20111225\gs6−39−2

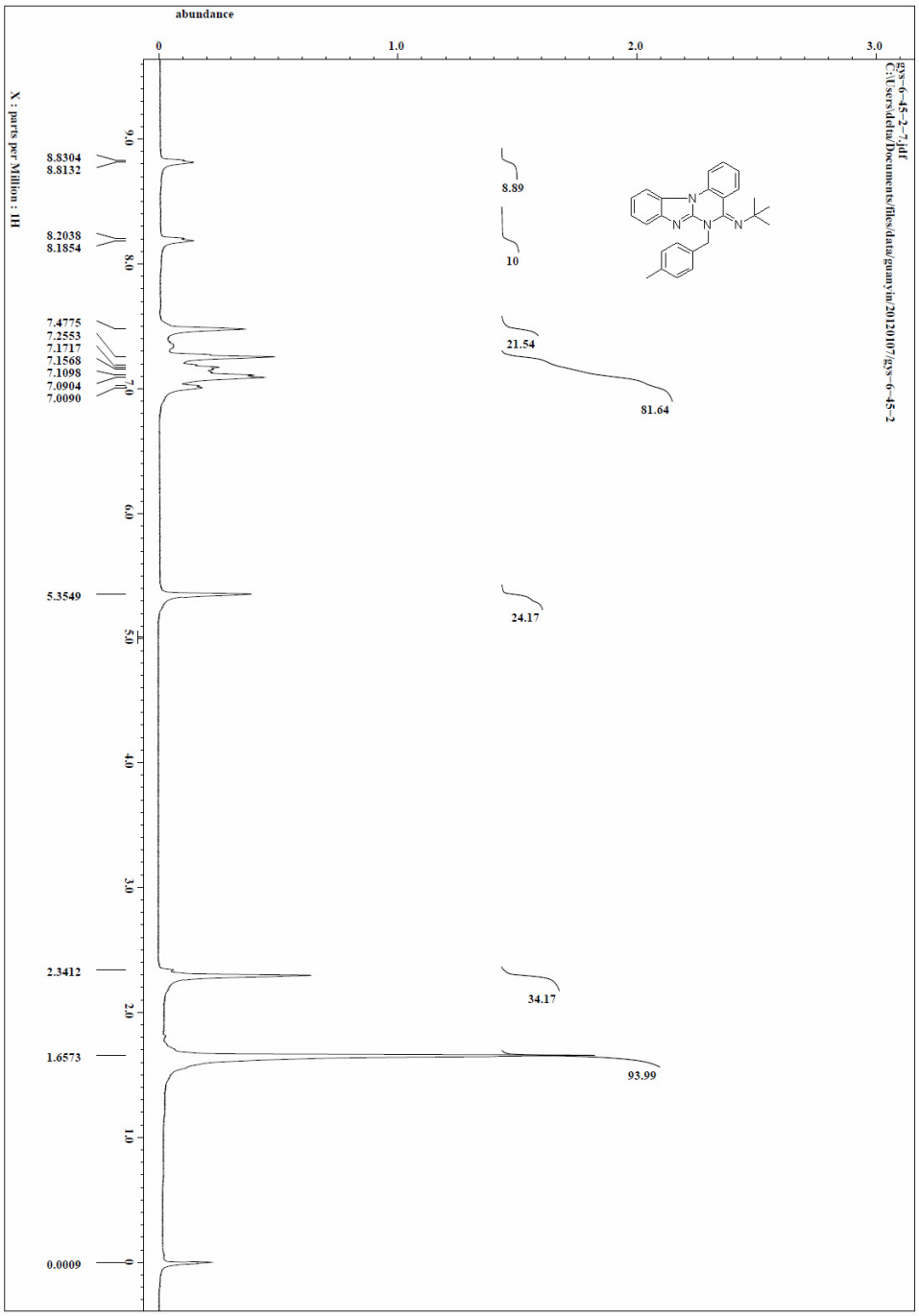

160.2302
159.2239
157.8280
156.7906
146.7051
140.8243
138.8746
137.0679
136.4573
133.7949
133.6005
128.6727
128.5323
128.4197
128.1550
127.9124
127.4825
126.5486
125.7328
124.5486
120.5747
118.3587
118.1297
117.2629
117.0341
115.1702
114.9213
111.2305
110.9917
56.4710
54.7617
46.6371
31.7042
29.8242
f1 (ppm)

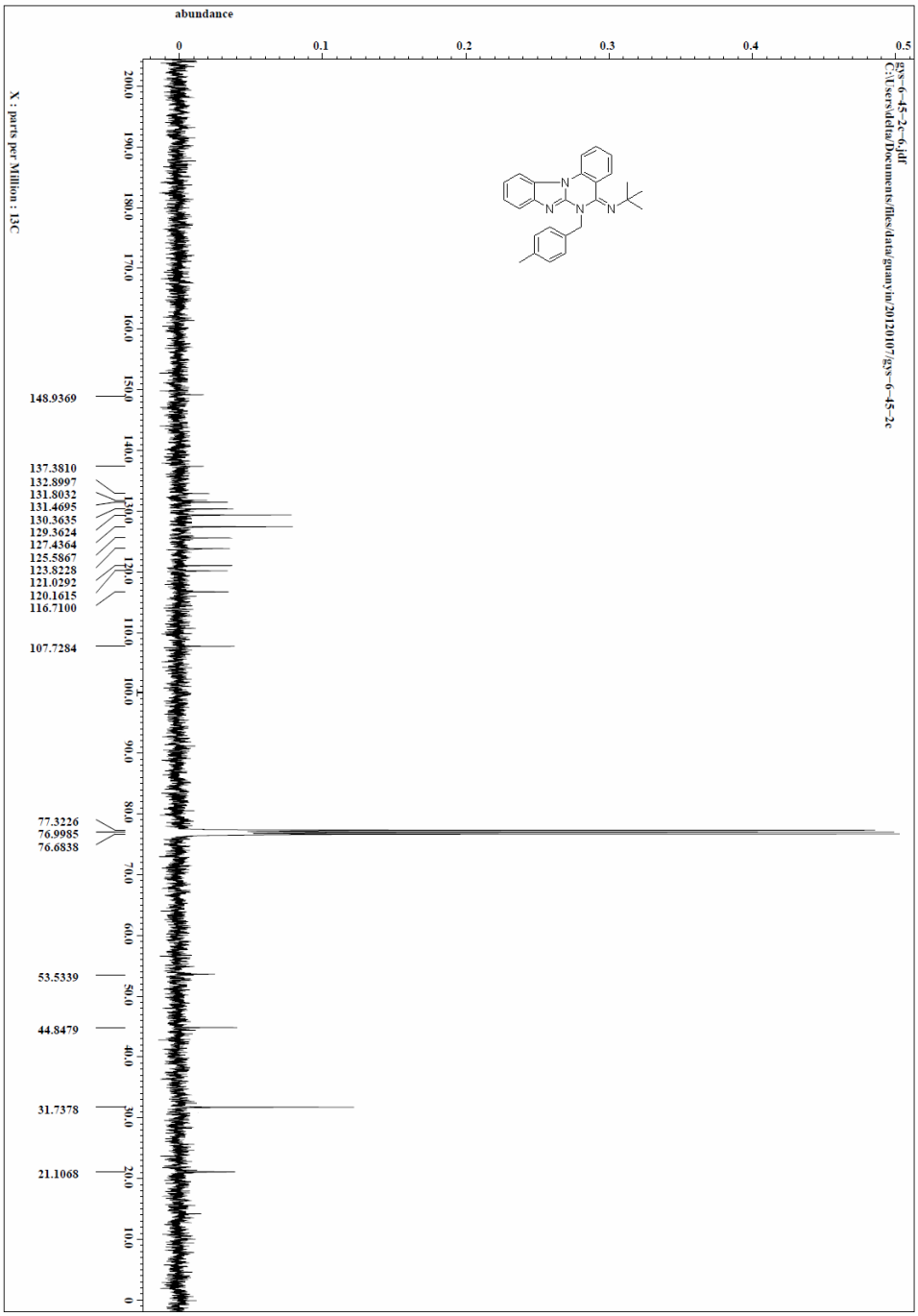

abundance
X : parts per Million : 1H
gss-6-43-6-7.jdf
C:\Users\delta\Documents\flks\data\guanyin\20111212\gss-6-43-6
8.8415
8.8221
8.1817
8.1611
7.4635
7.2837
7.1771
7.1474
7.1279
7.0981
4.1863
4.1691
4.1508
2.4176
2.4004
2.3833
1.8529
1.8380
1.8185
1.6479
1.4543
1.4359
1.4176
0.9972
0.9789
0.9617
0.0006
8.22
8.6
18.8
10.92
28.74
14.05
8.53
19.77
90
25.43
33.62
N
N
N
N
Bu


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
150.1228
148.1777
140.8742
132.0547
131.3873
130.3099
127.9835
125.4568
123.7406
120.7277
119.9268
116.7327
116.0557
107.0265
77.3167
77.0021
76.6779
53.5756
41.2951
31.7414
30.0919
20.1092
13.7783
N
N
N
N
Bu
gys-6-43-6c-6.jdf
C:\Users\delta\Documents\files\data\guanyin\20111212\gys-6-43-6c


gys-6-45-1-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20120107\gys-6-45-1
abundance
X : parts per Million : 1H
8.8365
8.8170
8.2076
8.1870
7.4768
7.3600
7.2993
7.2809
7.2546
7.1756
5.3966
1.6589
-0.0009
10.51
10.54
19.3
23.65
34.74
33.01
10.8
20
87.25
JEOL
Filename = gys-6-45-1-7.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = C:\Users\delta\Docume
Solvent = CHLOROFORM-D
Creation_time = 7-JAN-2012 15:43:05
Revision_time = 7-JAN-2012 16:01:40
Current_time = 7-JAN-2012 16:01:57
Comment = C:\Users\delta\Docume
Data_format = 1D COMPLEX
Dim_size = 15107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = RQA400
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
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
Max_index = 2
Scans = 8
Total_scans = 8
X_90_width = 10.6[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 5.3[dB]
X_pulse = 5.3[dB]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recyc_grain = 42
Recyc_wait = 5[s]
Relaxation_delay = 7.1836595[s]
Repetition_time = 19.6[dC]
---- PROCESSING PARAMETERS ----
dc- balance : 0 : FALSE
exp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
ph
mach
reference : -0.006[ppm] : 0[ppm]
Derived from: gys-6-45-1-1.jdf


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
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
148.5676
141.5596
135.9438
131.7772
131.4911
130.3660
128.7166
128.0873
127.6868
127.4389
125.5892
123.8539
121.0984
120.2213
116.7316
116.0070
107.7024
77.3156
77.0010
76.6864
53.6508
45.0602
31.7404
zys-6-45-1c-6.jdf
C:\Users\delta\Documents\files\data\guanyin\20120107\zys-6-45-1c
N
N
N
N


abundance
0
1.0
2.0
3.0
X : parts per Million : 1H
8.8304
8.8132
8.2038
8.1854
7.4775
7.2553
7.1717
7.1568
7.1098
7.0904
7.0090
5.3549
2.3412
1.6573
0.0009
8.89
10
21.54
81.64
24.17
34.17
93.99
gzs-6-45-2-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20120107\gzs-6-45-2


abundance
0
0.1
0.2
0.3
0.4
0.5
X : parts per Million : 13C
gsx-6-45-2c-6.jdf
C:\Users\delta\Documents\flks\data\guanyin\20120107\gsx-6-45-2c
148.9369
137.3810
132.8997
131.8032
131.4695
130.3635
129.3624
127.4364
125.5867
123.8228
121.0292
120.1615
116.7100
107.7284
77.3226
76.9985
76.6838
53.5339
44.8479
31.7378
21.1068