Supplementary Material (ESI) for Chemical Communications

Synthesis of fluorinated allenes via palladium-catalyzed monofluoromethylation using FBSM

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Electronic Supplementary Information

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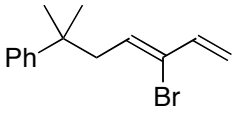
Experimental Section.

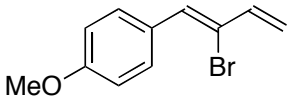
General. All anaerobic and/or moisture sensitive manipulations were carried out with standard Schlenk techniques under predried nitrogen or with glovebox techniques under prepurified argon. ^{1}H NMR (at 400 MHz) and ^{13}C NMR (at 100 MHz) chemical shifts are reported in ppm downfield of internal tetramethylsilane. Tetrahydrofuran (from benzophenone-ketyl) and dichloromethane (from CaH_2) were distilled under nitrogen prior to use. FBSM,[1] bromodienes (**2a**,[2] **2c**,[2] **2d**,[3] **2h**,[4] **2j**,[5] **2l**,[6] **2m**[6]), dienyl triflate **2k**,[7] [PdCl(π-allyl)]$_2$,[8] and dpbp[9] were prepared according to the reported methods. All the other chemicals were obtained from commercial sources and used as received unless otherwise noted.

Bromodienes (2). The following bromodienes were prepared from the commercially available corresponding aldehydes by a two-step sequence described in a previous report,[3] in which the preparation of **2d** was described in detail. The characterization data of previously unknown bromodienes were described below.

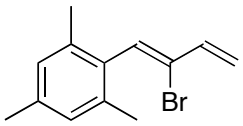
(*Z*)-3-Bromo-6-methyl-6-phenyl-1,3-heptadiene (2b). ^{1}H NMR ($CDCl_3$): δ 1.35 (s, 6H), 2.69 (d, J = 7.0 Hz, 2H), 5.11 (d, J = 10.6 Hz, 1H), 5.50 (d, J = 16.3 Hz, 1H), 5.70 (t, J = 7.0 Hz, 1H), 6.19 (dd, J = 16.3 and 10.6 Hz, 1H), 7.17-7.22 (m, 1H), 7.29-7.37 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 29.0, 38.3, 45.9, 117.4, 125.8, 125.9, 127.2, 128.3, 132.3, 135.9, 148.6. EI-HRMS Calcd for $C_{14}H_{17}Br$: 264.0514. Found: 264.0512.



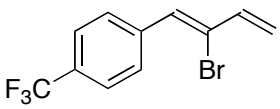
(*Z*)-2-Bromo-1-(4-methoxyphenyl)-1,3-butadiene (2e). ^{1}H NMR ($CDCl_3$): δ 3.83 (s, 3H), 5.28 (d, J = 10.4 Hz, 1H), 5.67 (d, J = 16.3 Hz, 1H), 6.48 (dd, J = 16.3 and 10.4 Hz, 1H), 6.90 (d, J = 8.6 Hz, 2H), 6.92 (s, 1H), 7.70 (d, J = 8.6 Hz, 2H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 55.3, 113.6, 118.0, 122.0, 128.0, 131.2, 131.9, 137.3, 159.6. EI-HRMS Calcd for $C_{11}H_{11}BrO$: 237.9993. Found: 238.0001.



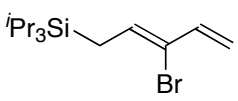
(*Z*)-2-Bromo-1-(2,4,6-trimethylphenyl)-1,3-butadiene (2f). ^{1}H NMR ($CDCl_3$): δ 2.17 (s, 6H), 2.28 (s, 3H), 5.32 (d, J = 10.4 Hz, 1H), 5.73 (d, J = 16.3 Hz, 1H), 6.54 (dd, J = 16.3 and 10.4 Hz, 1H), 6.88 (s, 2H), 6.93 (s, 1H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 20.1, 21.2, 118.9, 128.0, 128.9, 132.6, 133.1, 135.5, 135.7, 137.3. EI-HRMS Calcd for $C_{13}H_{15}Br$: 250.0357. Found: 250.0352.



(*Z*)-2-Bromo-1-[4-(trifluoromethyl)phenyl]-1,3-butadiene (2g). ^{1}H NMR ($CDCl_3$): δ 5.42 (d, J = 10.3 Hz, 1H), 5.80 (d, J = 16.3 Hz, 1H), 6.51 (dd, J = 16.3 and 10.3 Hz, 1H), 7.00 (s, 1H), 7.62 (d, J = 8.3 Hz, 2H), 7.77 (d, J = 8.3 Hz, 2H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 120.6, 124.1 (q, J_{CF} = 272.1 Hz), 125.1 (q, J_{CF} = 4.0 Hz), 126.1, 129.7, 130.1, 130.8, 136.7, 139.1. ^{19}F NMR ($CDCl_3$): δ –62.6. EI-HRMS Calcd for $C_{11}H_8BrF_3$: 275.9761. Found: 275.9769.

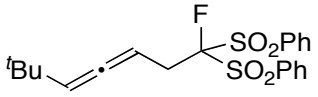


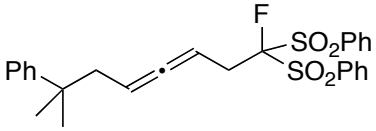
(*Z*)-3-Bromo-5-triisopropylsilyl-1,3-pentadiene (2i). ^{1}H NMR ($CDCl_3$): δ 1.02-1.11 (m, 21H), 1.92 (d, J = 8.2 Hz, 2H), 5.06 (d, J = 10.5 Hz, 1H), 5.42 (d, J = 16.5 Hz, 1H), 6.08 (t, J = 8.2 Hz, 1H), 6.31 (dd, J = 10.5 and 16.5 Hz, 1H). ^{13}C NMR ($CDCl_3$): δ 11.4, 16.4, 18.7, 115.3, 123.9, 133.4, 136.2. EI-HRMS Calcd for $C_{14}H_{27}BrSi$: 302.1065. Found: 302.1074.

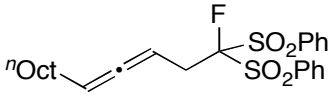


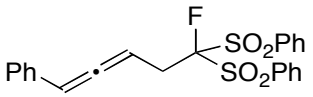
Palladium-Catalyzed Reaction of 2a-l with FBSM. A general procedure is given below. To a mixture of [PdCl(π-allyl)]$_2$ (1.8 mg, 5.0 μmol), dpbp (5.7 mg, 11 μmol), FBSM (70 mg, 0.22 mmol), and KO^{t}Bu (27 mg, 0.24 mmol) in dichloromethane (2.0 mL) was added the bromodiene **2** (0.20 mmol) by means of syringe under nitrogen. After stirring the mixture for 12 h at 40 °C, the mixture was diluted with ether and filtered through a short pad of silica gel to remove precipitated inorganic salts. The silica gel pad was washed with a small amount of Et_2O three times and the combined solution was evaporated under

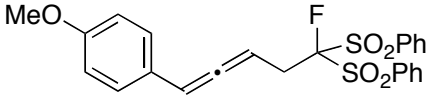
reduced pressure. The residue was purified by chromatography on silica gel to give the FBSM-allene **3**. The characterization data of **3** are given below.

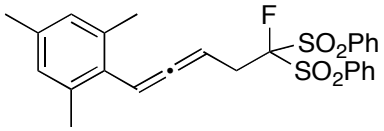
1-Fluoro-6,6-dimethyl-1,1-bis(phenylsulfonyl)-3,4-heptadiene (3a). 
^{1}H NMR ($CDCl_3$): δ 0.94 (s, 3H), 3.06-3.22 (m, 2H), 5.09-5.17 (m, 2H), 7.54-7.58 (m, 4H), 7.70-7.74 (m, 2H), 7.91-7.95 (m, 4H). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 29.9, 31.4 (d, J_{CF} = 18.7 Hz), 31.8, 82.9 (d, J_{CF} = 7.6 Hz), 104.3 114.3 (d, J_{CF} = 267.9 Hz), 128.98, 129.03, 130.90 (d, J_{CF} = 1.0 Hz), 130.91 (d, J_{CF} = 1.4 Hz), 135.0, 135.24, 135.26, 135.4, 204.1. ^{19}F NMR ($CDCl_3$): δ –142.3 (dd, J_{HF} = 18.5 and 15.6 Hz). Anal. Calcd for $C_{21}H_{23}FO_4S_2$: C, 59.69; H, 5.49. Found: C, 59.39; H, 5.56. EI-HRMS Calcd for $C_{21}H_{23}FO_4S_2$: 422.1022. Found: 422.101.

1-Fluoro-7-methyl-7-phenyl-1,1-bis(phenylsulfonyl)-3,4-octadiene (3b). 
^{1}H NMR ($CDCl_3$): δ 1.26 (s, 3H), 1.28 (s, 3H), 2.21-2.31 (m, 2H), 2.81-3.12 (m, 2H), 4.77-4.83 (m, 1H), 4.98-5.04 (m, 1H), 7.16-7.21 (m, 1H), 7.28-7.33 (m, 4H), 7.52-7.58 (m, 4H), 7.68-7.74 (m, 2H), 7.89-7.93 (m, 4H). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 28.4, 28.5, 30.9 (d, J_{CF} = 18.7 Hz), 38.1, 43.4, 80.1 (d, J_{CF} = 8.2 Hz), 88.9, 114.4 (d, J_{CF} = 267.9 Hz), 125.8, 125.9, 128.1, 129.01, 129.02, 130.93, 130.94, 135.22, 135.23, 135.28, 135.4, 148.4, 207.8. ^{19}F NMR ($CDCl_3$): δ –142.0 (dd, J_{HF} = 16.0 and 17.9 Hz). Anal. Calcd for $C_{27}H_{27}FO_4S_2$: C, 65.04; H, 5.46. Found: C, 64.94; H, 5.63. EI-HRMS Calcd for $C_{27}H_{27}FO_4S_2$: 498.1335. Found: 498.1326.

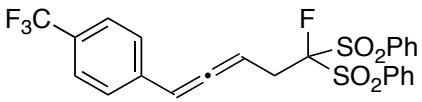
1-Fluoro-1,1-bis(phenylsulfonyl)-3,4-tridecadiene (3c). 
^{1}H NMR ($CDCl_3$): δ 0.88 (t, J = 6.9 Hz, 3H), 1.25-1.32 (m, 12H), 1.89-1.95 (m, 2H), 3.02-3.21 (m, 2H), 5.04-5.14 (m, 2H), 7.51-7.58 (m, 4H), 7.69-7.74 (m, 2H), 7.91-7.95 (m, 4H). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 14.1, 22.7, 28.2, 29.0, 29.1, 29.3, 29.4, 31.1 (d, J_{CF} = 18.7 Hz), 31.9, 81.0 (d, J_{CF} = 8.1 Hz), 92.5, 114.4 (d, J_{CF} = 267.9 Hz), 129.0, 130.92, 130,93, 130.94, 130.95, 135.2, 135.3, 135.4, 206.6. ^{19}F NMR ($CDCl_3$): δ –141.9 (t, J_{HF} = 17.1 Hz). Anal. Calcd for $C_{25}H_{31}FO_4S_2$: C, 62.73; H, 6.53. Found: C, 62.88; H, 6.56. EI-HRMS Calcd for $C_{25}H_{31}FO_4S_2$: 478.1648. Found: 478.1643.

5-Fluoro-1-phenyl-5,5-bis(phenylsulfonyl)-1,2-pentadiene (3d). 
^{1}H NMR ($CDCl_3$): δ 3.16-3.31 (m, 2H), 5.66 (td, J = 7.4 and 6.4 Hz, 1H), 6.16 (dt, J = 6.4 and 2.4 Hz, 1H), 7.18-7.30 (m, 5H), 7.50-7.57 (m, 4H), 7.66-7.74 (m, 2H), 7.93-7.95 (m, 4H). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 30.9 (d, J_{CF} = 19.2 Hz), 85.4 (d, J_{CF} = 8.1 Hz), 95.9, 114.1 (d, J_{CF} = 267.8 Hz), 127.1, 127.3, 128.6, 129.07, 129.09, 130.91 (d, J_{CF} = 1.4 Hz), 130.93 (d, J_{CF} = 1.4 Hz), 133.3, 135.0, 135.2, 135.35, 135.37, 207.8. ^{19}F NMR ($CDCl_3$): δ –141.4 (t, J_{HF} = 17.1 Hz). Anal. Calcd for $C_{23}H_{19}FO_4S_2$: C, 62.43; H, 4.33. Found: C, 62.48; H, 4.75. EI-HRMS Calcd for $C_{23}H_{19}FO_4S_2$: 442.0709. Found: 442.0709.

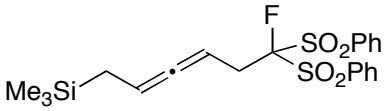
5-Fluoro-1-(4-methoxyphenyl)-5,5-bis(phenylsulfonyl)-1,2-pentadiene (3e). 
^{1}H NMR ($CDCl_3$): δ 3.14-3.29 (m, 2H), 3.79 (s, 3H), 5.62 (td, J = 7.3 and 6.4 Hz, 1H), 6.12 (dt, J = 6.4 and 2.4 Hz, 1H), 6.81-6.84 (m, 2H), 7.14-7.18 (m, 2H), 7.51-7.57 (m, 4H), 7.67-7.74 (m, 2H), 7.93-7.96 (m, 4H). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 31.1 (d, J_{CF} = 18.7 Hz), 55.3, 85.3 (d, J_{CF} = 8.1 Hz), 95.4, 114.1, 114.2 (d, J_{CF} = 267.9 Hz), 125.5, 128.3, 129.06, 129.09, 130.93, 130.94, 135.0, 135.2, 135.34, 135.35, 159.0, 207.4. ^{19}F NMR ($CDCl_3$): δ –141.4 (t, J_{HF} = 17.1 Hz). Anal. Calcd for $C_{24}H_{21}FO_5S_2$: C, 61.00; H, 4.48. Found: C, 60.87; H, 4.61. EI-HRMS Calcd for $C_{24}H_{21}FO_5S_2$: 472.0814. Found: 472.0815.

5-Fluoro-5,5-bis(phenylsulfonyl)-1-(2,4,6-trimethylphenyl)-1,2-pentadiene (3f). 
^{1}H NMR ($CDCl_3$): δ 2.23 (s, 6H), 2.26 (s, 3H), 3.10-3.27 (m, 2H), 5.42 (dt, J = 7.1 and 6.7 Hz, 1H), 6.24 (dt, J = 6.7 and 3.2 Hz, 1H), 6.85 (s, 2H), 7.51-7.55 (m, 4H), 7.68-7.74 (m, 2H), 7.91-7.96 (m, 4H). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 20.9, 21.1, 31.0 (d, J_{CF} = 18.6 Hz), 82.2 (d, J_{CF} = 8.6 Hz), 91.2, 114.2 (d, J_{CF} = 267.9 Hz), 127.6, 128.98, 129.03, 129.1, 130.92 (d, J_{CF} = 0.9 Hz), 130.94 (d, J_{CF} = 1.5 Hz), 135.1,

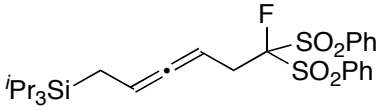
135.2, 135.31, 135.32, 136.4, 136.7, 208.2. ^{19}F NMR ($CDCl_3$): δ –141.8 (t, J_{HF} = 16.0 Hz). Anal. Calcd for $C_{26}H_{25}FO_4S_2$: C, 64.44; H, 5.20. Found: C, 64.46; H, 5.33. EI-HRMS Calcd for $C_{26}H_{25}FO_4S_2$: 484.1178. Found: 484.1172.

5-Fluoro-5,5-bis(phenylsulfonyl)-1-(4-trifluoromethylphenyl)-1,2-pentadiene (3g). 

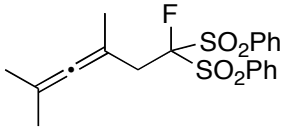
^{1}H NMR ($CDCl_3$): δ 3.17-3.33 (m, 2H), 5.78 (td, J = 7.3 and 6.4 Hz, 1H), 6.21 (dt, J = 6.4 and 2.5 Hz, 1H), 7.35 (d, J = 8.2 Hz, 2H), 7.51-7.58 (m, 6H), 7.67-7.75 (m, 2H), 7.91-7.94 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 30.8 (d, J_{CF} = 19.1 Hz), 86.2 (d, J_{CF} = 8.2 Hz), 95.1, 114.0 (d, J_{CF} = 267.4 Hz), 121.5 (d, J_{CF} = 271.8 Hz), 125.6 (q, J_{CF} = 4.0 Hz), 127.3, 129.13, 129.15, 130.90 (d, J_{CF} = 1.5 Hz), 130.93 (d, J_{CF} = 1.4 Hz), 134.9, 135.1, 135.43, 135.45, 137.30, 137.31, 208.5. ^{19}F NMR ($CDCl_3$): δ –62.3, –141.2 (dd, J_{HF} = 17.2 and 13.7 Hz). Anal. Calcd for $C_{24}H_{18}F_4O_4S_2$: C, 56.46; H, 3.55. Found: C, 56.68; H, 3.60. EI-HRMS Calcd for $C_{24}H_{18}F_4O_4S_2$: 510.0583. Found: 510.0571.

6-Fluoro-6,6-bis(phenylsulfonyl)-1-trimethylsilyl-2,3-hexadiene (3h). 

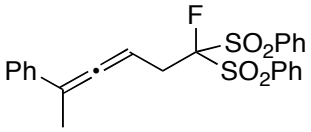
^{1}H NMR ($CDCl_3$): δ –0.02 (s, 9H), 1.23-1.27 (m, 2H), 2.96-3.20 (m, 2H), 5.06-5.12 (m, 2H), 7.53-7.58 (m, 4H), 7.69-7.74 (m, 2H), 7.91-7.95 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ –2.0, 17.4, 31.5 (d, J_{CF} = 18.6 Hz), 80.4 (d, J_{CF} = 7.7 Hz), 89.0, 114.5 (d, J_{CF} = 267.9 Hz), 129.01, 129.02, 130.90 (d, J_{CF} = 1.5 Hz), 130.94 (d, J_{CF} = 1.4 Hz), 135.22, 135.23, 135.3, 135.4, 207.0. ^{19}F NMR ($CDCl_3$): δ –142.1 (dd, J_{HF} = 19.9 and 17.1 Hz). Anal. Calcd for $C_{21}H_{25}FO_4S_2Si$: C, 55.72; H, 5.57. Found: C, 55.85; H, 5.54. EI-HRMS Calcd for $C_{21}H_{25}FO_4S_2Si$: 452.0948. Found: 452.0953.

6-Fluoro-6,6-bis(phenylsulfonyl)-1-triisopropylsilyl-2,3-hexadiene (3i). 

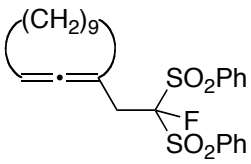
^{1}H NMR ($CDCl_3$): δ 1.02 (br, 21H), 1.37-1.40 (m, 2H), 2.99-3.06 (m, 1H), 3.12-3.18 (m, 1H), 5.02-5.09 (m, 1H), 5.13-5.17 (m, 1H), 7.53-7.58 (m, 4H), 7.69-7.74 (m, 2H), 7.91-7.96 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 10.0, 10.9, 18.7, 31.1 (d, J_{CF} = 18.7 Hz), 80.5 (d, J_{CF} = 8.1 Hz), 89.9, 114.6 (d, J_{CF} = 267.9 Hz), 128.98, 129.00, 130.87 (d, J_{CF} = 1.4 Hz), 130.93 (d, J_{CF} = 1.4 Hz), 135.19, 135.20, 135.38, 135.43, 206.8. ^{19}F NMR ($CDCl_3$): δ –142.2 (t, J_{HF} = 17.1 Hz). Anal. Calcd for $C_{27}H_{37}FO_4S_2Si$: C, 60.41; H, 6.95. Found: C, 60.47; H, 6.88. EI-HRMS Calcd for $C_{27}H_{37}FO_4S_2Si$: 536.1887. Found: 536.1887.

6-Fluoro-2,4-dimethyl-6,6-bis(phenylsulfonyl)-2,3-hexadiene (3j). 

^{1}H NMR ($CDCl_3$): δ 1.58 (d, J = 1.6 Hz, 3H), 1.60 (s, 6H), 3.07 (d, J = 21.3 Hz, 2H), 7.53-7.57 (m, 4H), 7.69-7.73 (m, 2H), 7.90-7.93 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 20.0 (d, J_{CF} = 2.2 Hz), 20.2, 35.3 (d, J_{CF} = 17.2 Hz), 88.0 (d, J_{CF} = 2.4 Hz), 94.9, 116.1 (d, J_{CF} = 271.0 Hz), 128.9, 130.8 (d, J_{CF} = 1.2 Hz), 135.1, 135.5, 203.2. ^{19}F NMR ($CDCl_3$): δ –144.0 (t, J_{HF} = 21.4 Hz). Anal. Calcd for $C_{20}H_{21}FO_4S_2$: C, 58.80; H, 5.18. Found: C, 58.53; H, 5.23. EI-HRMS Calcd for $C_{20}H_{21}FO_4S_2$: 408.0865. Found: 408.0870.

6-Fluoro-2-phenyl-6,6-bis(phenylsulfonyl)-2,3-hexadiene (3k). 

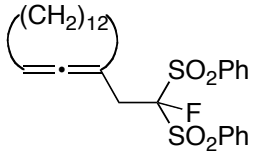
^{1}H NMR ($CDCl_3$): δ 2.04 (d, J = 2.8 Hz, 3H), 3.13-3.30 (m, 2H), 5.66 (tq, J = 7.5 and 2.8 Hz, 1H), 7.18-7.22 (m, 1H), 7.27-7.33 (m, 4H), 7.49-7.55 (m, 4H), 7.65-7.73 (m, 2H), 7.91-7.95 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 16.6, 31.1 (d, J_{CF} = 18.9 Hz), 83.2 (d, J_{CF} = 7.9 Hz), 102.2, 114.3 (d, J_{CF} = 267.6 Hz), 126.0, 127.0, 128.3, 129.02, 129.04, 130.86 (d, J_{CF} = 1.4 Hz), 130.90 (d, J_{CF} = 1.4 Hz), 135.0, 135.2, 135.27, 135.30, 136.1, 207.0. ^{19}F NMR ($CDCl_3$): δ –141.1 (t, J_{HF} = 17.1 Hz). Anal. Calcd for $C_{24}H_{21}FO_4S_2$: C, 63.14; H, 4.64. Found: C, 62.45; H, 4.89. EI-HRMS Calcd for $C_{24}H_{21}FO_4S_2$: 456.0865. Found: 456.0866.

1-[2-Fluoro-2,2-bis(phenylsulfonyl)ethyl]-1,2-cyclododecadiene (3l). 

^{1}H NMR ($CDCl_3$): δ 0.99-1.21 (m, 5H), 1.28-1.44 (m, 9H), 1.80-1.85 (m, 1H), 1.92-2.03 (m, 3H), 3.06-3.27 (m, 2H), 4.61-4.64 (m, 1H), 7.51-7.57 (m, 4H), 7.67-7.73 (m, 2H), 7.89-7.95 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 21.69, 21.72, 22.5, 23.4, 24.8, 25.7, 26.62, 26.65, 30.8 (d, J_{CF} = 1.9 Hz), 31.4 (d, J_{CF} = 17.3 Hz), 90.0, 92.2 (d, J_{CF} = 2.0 Hz), 116.1 (d, J_{CF}

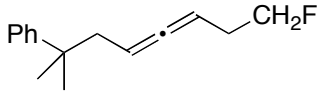
= 271.7 Hz), 128.8, 128.9, 130.9 (d, J_{CF} = 1.5 Hz), 131.0 (d, J_{CF} = 1.4 Hz), 135.0, 135.1, 135.6, 135.7, 207.0. ^{19}F NMR ($CDCl_3$): δ –144.2 (dd, J_{HF} = 25.6 and 17.1 Hz). Anal. Calcd for $C_{26}H_{31}FO_4S_2$: C, 63.65; H, 6.37. Found: C, 63.69; H, 6.46. EI-HRMS Calcd for $C_{26}H_{31}FO_4S_2$: 490.1648. Found: 490.1648.

1-[2-Fluoro-2,2-bis(phenylsulfonyl)ethyl]-1,2-cyclopentadecadiene (3m). ^{1}H NMR ($CDCl_3$): δ 1.19-1.44 (m, 20H), 1.72-1.77 (m, 2H), 1.85-2.01 (m, 2H), 3.10-3.25 (m, 2H), 4.88-4.94 (m, 1H), 7.51-7.57 (m, 4H), 7.67-7.73 (m, 2H), 7.88-7.95 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 26.3, 26.5, 26.8, 26.9, 27.0, 27.1, 27.3, 27.7, 28.0, 28.1, 28.4, 32.6 (d, J_{CF} = 2.4 Hz), 33.6 (d, J_{CF} = 17.3 Hz), 92.6, 95.1 (d, J_{CF} = 1.90 Hz), 116.0 (d, J_{CF} = 271.2 Hz), 128.8, 128.9, 130.93 (d, J_{CF} = 1.0 Hz), 130.94 (d, J_{CF} = 1.4 Hz), 135.02, 135.05, 135.6, 135.7, 204.9. ^{19}F NMR ($CDCl_3$): δ –143.7 (dd, J_{HF} = 22.8 and 19.9 Hz). Anal. Calcd for $C_{29}H_{37}FO_4S_2$: C, 65.38; H, 7.00. Found: C, 65.44; H, 7.02. EI-HRMS Calcd for $C_{29}H_{37}FO_4S_2$: 532.2117. Found: 532.2117.

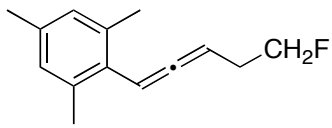


Desulfonylation of 2. A general procedure is given below. Magnesium turnings (250 mg, 10.3 mmol) and THF (2 mL) were placed in a Schlenk flask under nitrogen, and 1,2-dibromoethane (50 μL, 0.58 mmol) was added via syringe. The mixture was gently stirred at room temperature until the evolution of ethylene ceased. To the flask was added a solution of **2** (0.30 mmol) in a mixture of THF (1 mL) and MeOH (1 mL) at 0 °C. The mixtrure was stirred at 0 °C for 3 h. The reaction mixture was quenched with water and extracted with pentane three times and the combined organic solution was evaporated under reduced pressure. The residue was purified by chromatography on silica gel to give the monofluoromethylated allene **1**. The characterization data of **1** are given below.

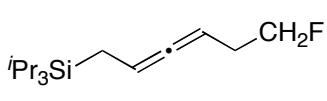
1-Fluoro-7-methyl-7-phenyl-3,4-octadiene (1b). ^{1}H NMR ($CDCl_3$): δ 1.34 (s, 6H), 2.18-2.29 (m, 2H), 2.32 (dd, J = 7.8 and 2.4 Hz, 2H), 4.35 (dt, J = 47.1 and 6.5 Hz, 2H), 4.83-5.00 (m, 2H), 7.15-7.20 (m, 1H), 7.28-7.35 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 28.2, 28.8, 30.0 (d, J_{CF} = 20.6 Hz), 38.2, 44.2, 80.1 (d, J_{CF} = 8.2 Hz), 83.2 (d, J_{CF} = 166.8 Hz), 84.6 (d, J_{CF} = 8.6 Hz), 88.1, 125.6, 126.0, 128.1, 148.7, 206.1. ^{19}F NMR ($CDCl_3$): δ –217.5 (dd, J_{HF} = 47.0 and 22.8 Hz). Anal. Calcd for $C_{15}H_{19}F$: C, 82.53; H, 8.77. Found: C, 82.26; H, 8.99. EI-HRMS Calcd for $C_{15}H_{19}F$: 218.1471. Found: 218.1481.



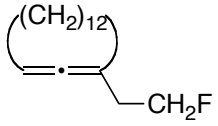
5-Fluoro-1-(2,4,6-trimethylphenyl)-1,2-pentadiene (1f). ^{1}H NMR ($CDCl_3$): δ 2.26 (s, 3H), 2.32 (s, 6H), 2.44-2.56 (m, 2H), 4.43-4.63 (m, 2H), 5.30 (td, J = 7.0 and 6.6 Hz, 1H), 6.28 (dt, J = 6.6 and 3.2 Hz, 1H), 6.86 (s, 2H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 20.9, 21.2, 31.3 (d, J_{CF} = 20.6 Hz), 83.0 (d, J_{CF} = 167.7 Hz), 86.6 (d, J_{CF} = 8.2 Hz), 90.5, 128.4, 129.1, 136.3, 136.4, 207.1. ^{19}F NMR ($CDCl_3$): δ –217.4 (tt, J_{HF} = 46.7 and 23.9 Hz Hz). Anal. Calcd for $C_{14}H_{17}F$: C, 82.31; H, 8.39. Found: C, 82.15; H, 8.68. EI-HRMS Calcd for $C_{14}H_{17}F$: 204.1314. Found: 204.1315.



6-Fluoro-1-triisopropylsilyl-2,3-hexadiene (1i). ^{1}H NMR ($CDCl_3$): δ 1.04-1.08 (m, 21H), 1.45 (dd, J = 8.6 and 2.5 Hz, 2H), 2.32-2.44 (m, 2H), 4.47 (dt, J = 47.2 and 6.4 Hz, 2H), 5.00-5.06 (m, 1H), 5.15-5.22 (m, 1H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 10.6, 11.0, 18.7, 30.5 (d, J_{CF} = 20.6 Hz), 83.4 (d, J_{CF} = 167.3 Hz), 85.1 (d, J_{CF} = 9.1 Hz), 88.9, 205.1. ^{19}F NMR ($CDCl_3$): δ –217.3 (tt, J_{HF} = 46.9 and 22.8 Hz Hz). Anal. Calcd for $C_{15}H_{29}FSi$: C, 70.24; H, 11.40. Found: C, 70.04; H, 11.60. A molecular ion peak was not detected in a HRMS spectrum for this compound.



1-(2-Fluoroethyl)-1,2-cyclopentadecadiene (1m). ^{1}H NMR ($CDCl_3$): δ 1.26-1.54 (m, 20H), 1.87-2.09 (m, 4H), 2.24-2.43 (m, 2H), 4.51 (dt, J = 47.2 and 6.7 Hz, 2H), 5.09-5.16 (m, 1H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 26.4, 26.5, 26.98, 27.00, 27.10, 27.13, 27.4, 27.7, 28.1, 28.4, 28.8, 32.9, 33.6 (d, J_{CF} = 20.6 Hz), 82.6 (d, J_{CF} = 165.8 Hz), 93.1, 99.5 (d, J_{CF} = 7.6 Hz), 201.2. ^{19}F NMR ($CDCl_3$): δ –216.8 (tt, J_{HF} = 47.0 and 19.9 Hz Hz). Anal.



Calcd for $C_{17}H_{29}F$: C, 80.89; H, 11.58. Found: C, 80.48; H, 11.84. EI-HRMS Calcd for $C_{17}H_{29}F$: 252.2253. Found: 252.2251.

References.

(1) Fukuzumi, T.; Shibata, N.; Sugiura, M.; Yasui, H.; Nakamura, S.; Toru, T. *Angew. Chem. Int. Ed.* **2006**, *45*, 4973.
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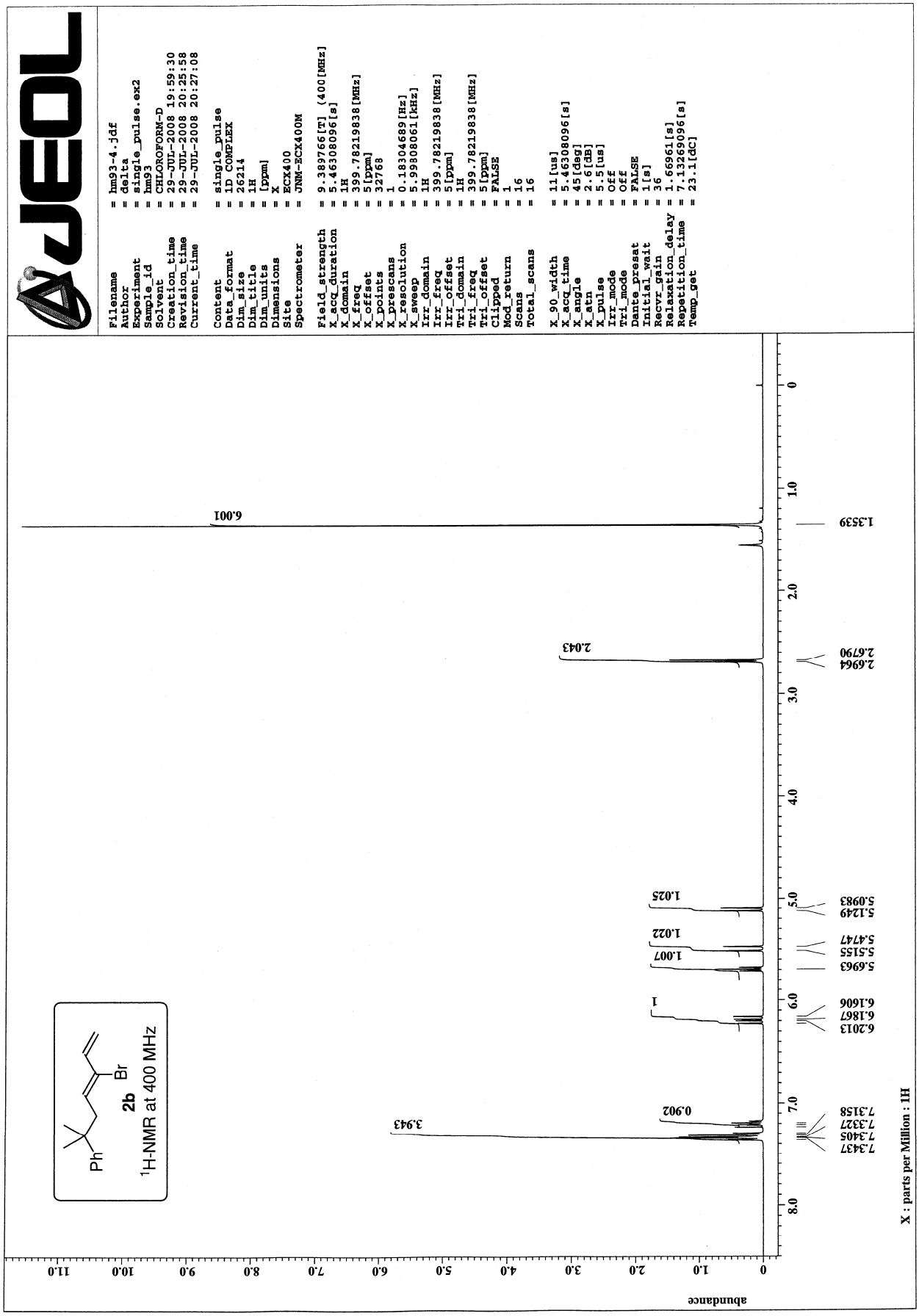
(9) Ogasawara, M.; Yoshida, K.; Hayashi, T. *Organometallics* **2000**, *19*, 1567.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Ph
Br
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abundance
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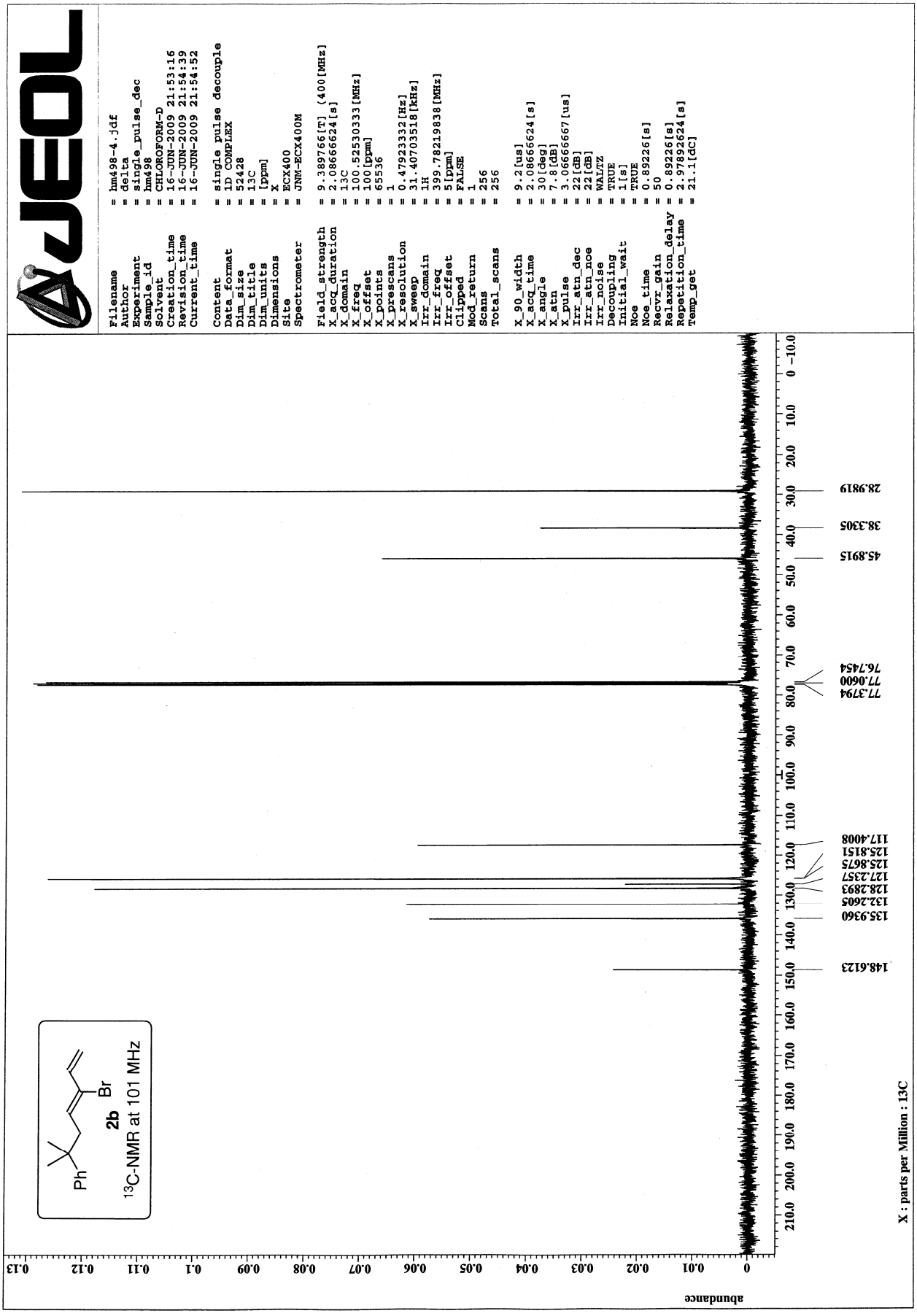
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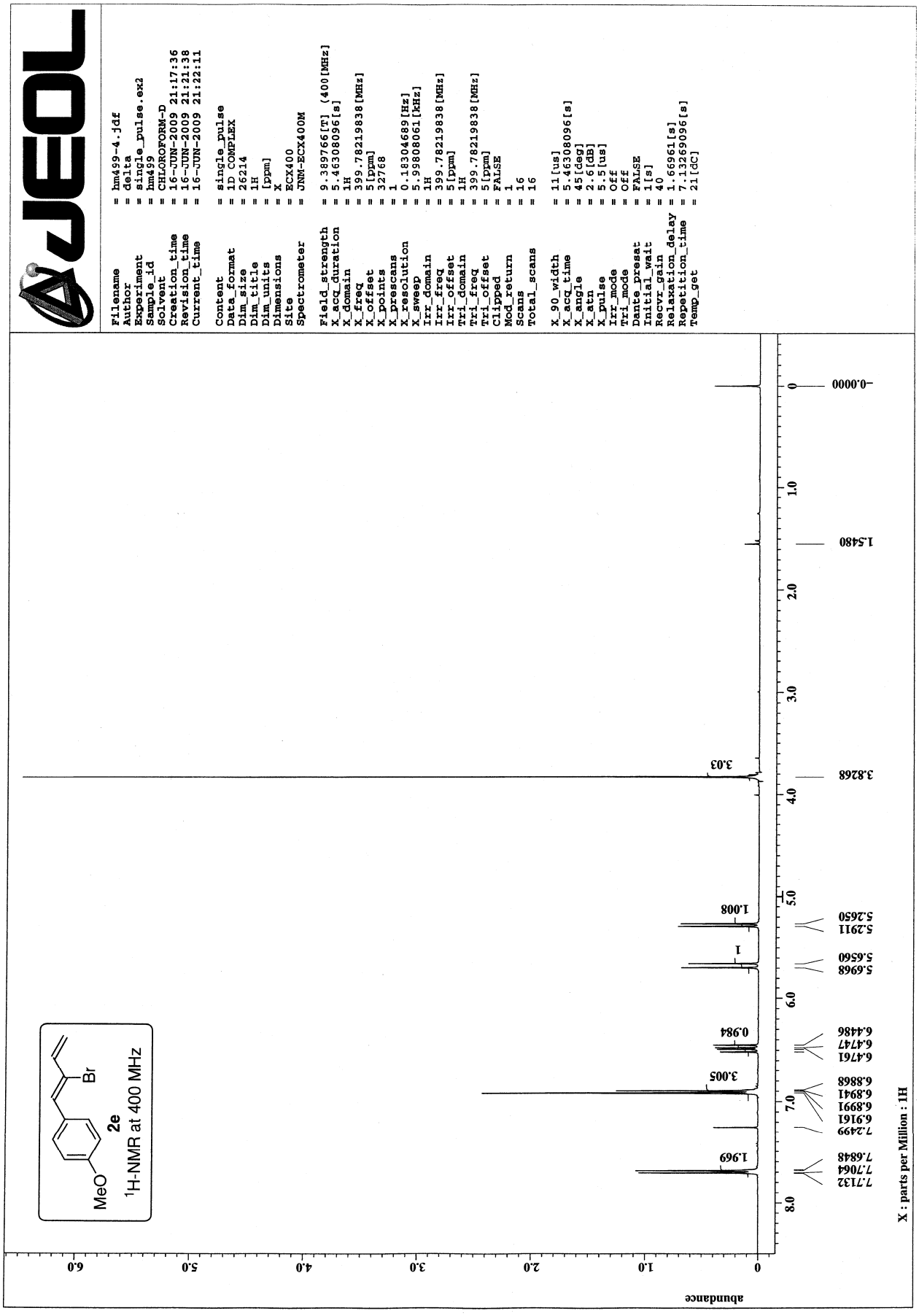
abundance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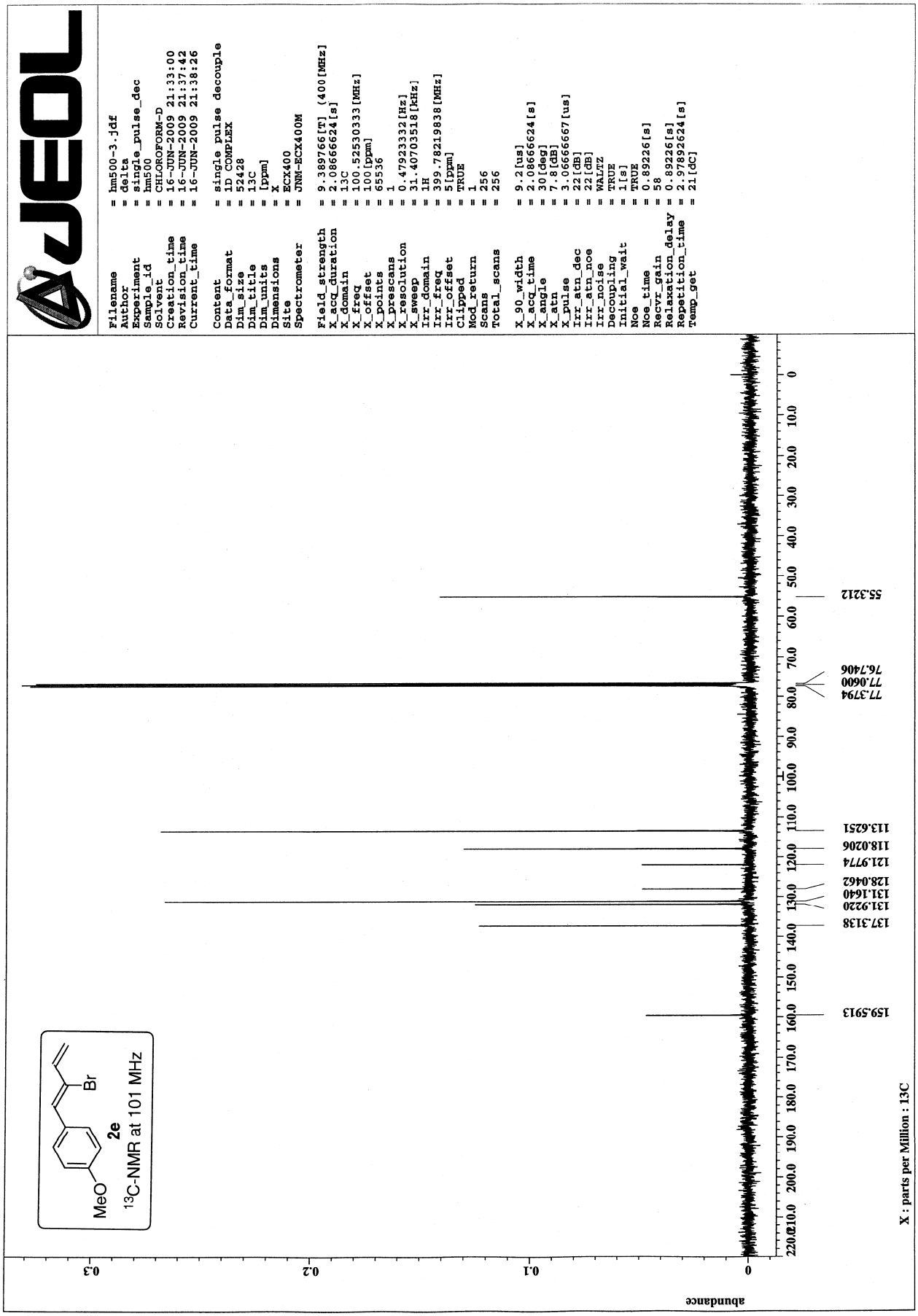
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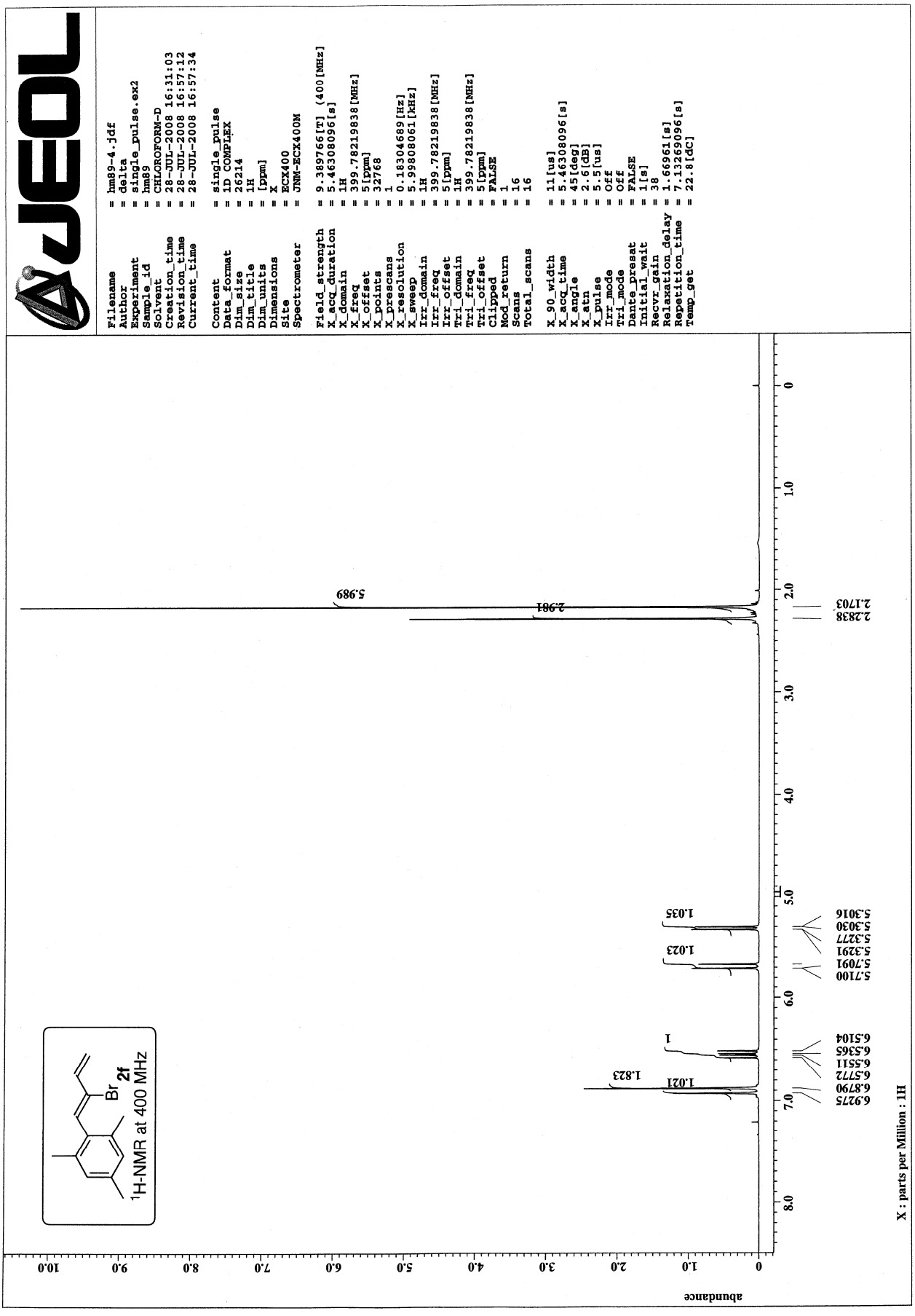
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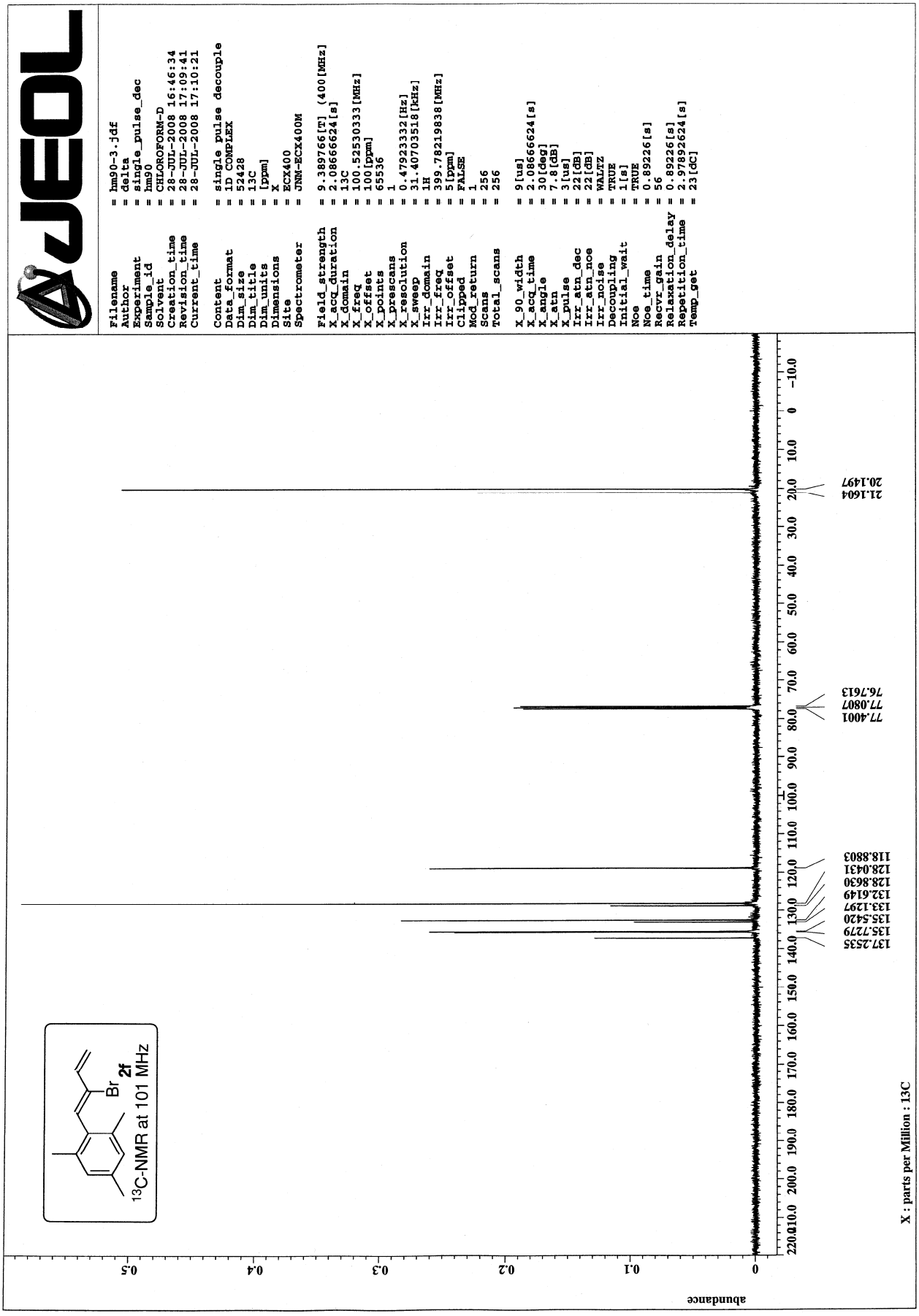
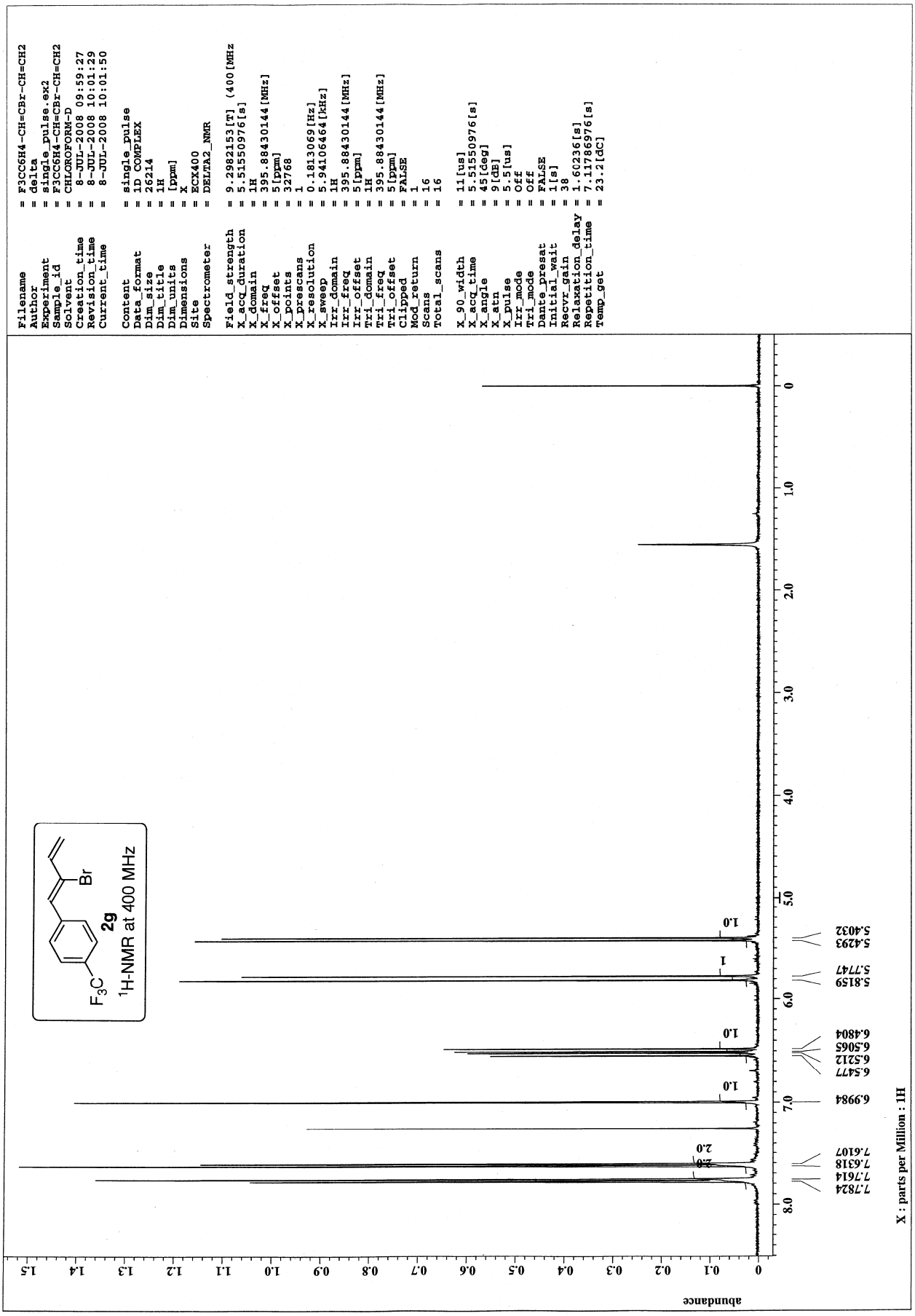
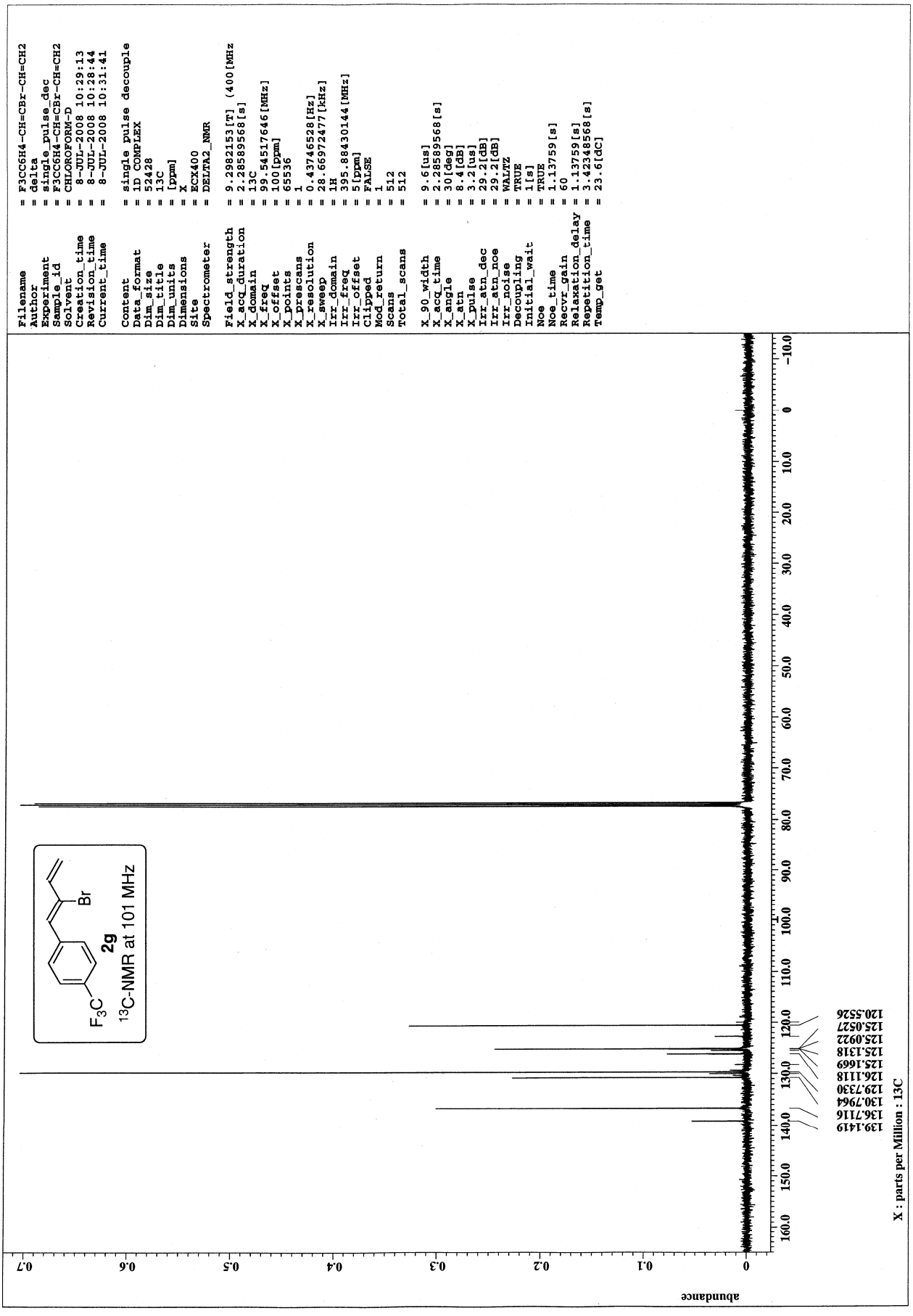
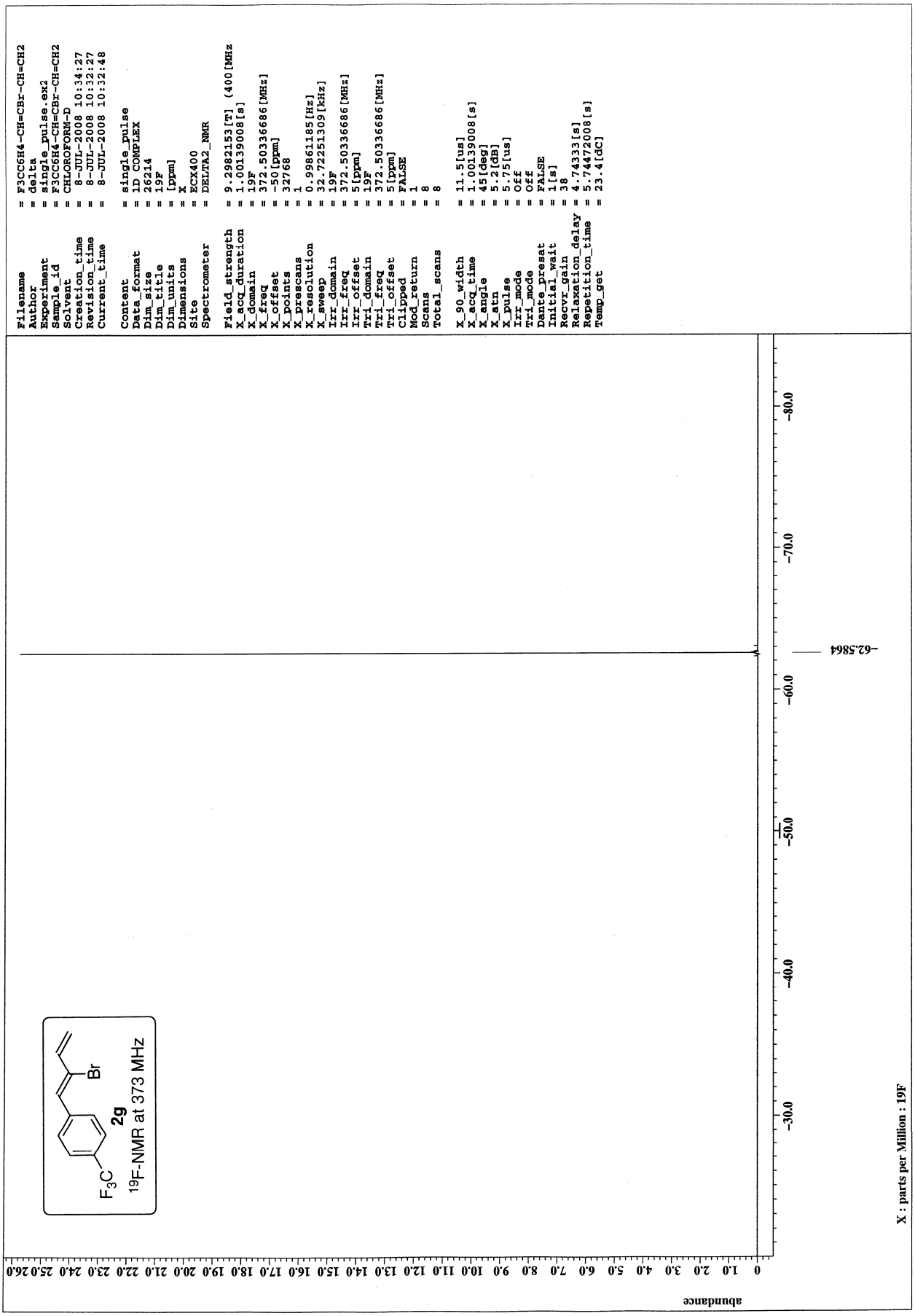
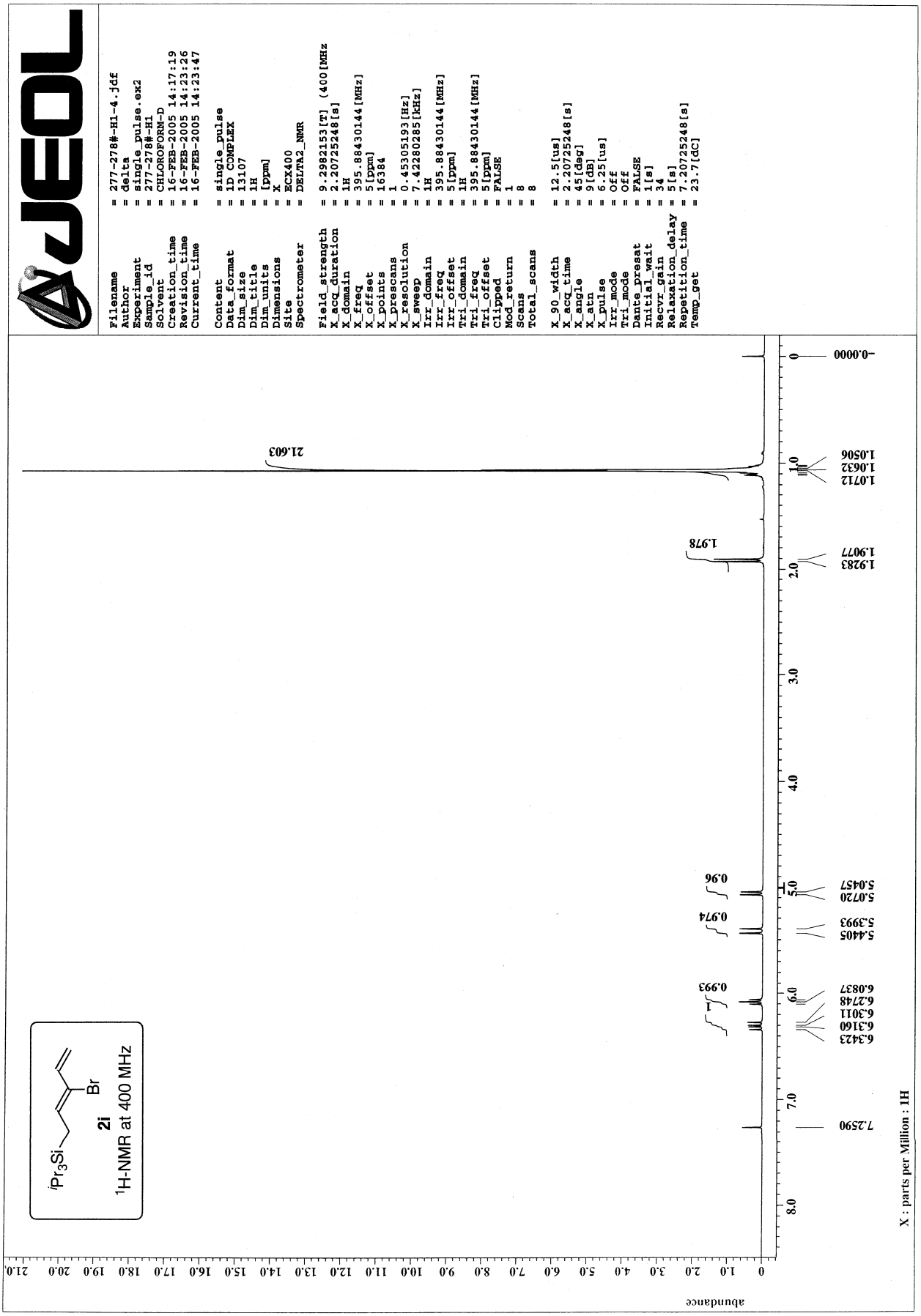
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 5.463080960[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.183046891[Hz]
X_sweep = 5.998080610[kHz]
Irr_domain = 1H
Irr_freq = 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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.463080960[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 1.669611[s]
Repetition_time = 7.132690960[s]
Temp_get = 22.8[dC]
Br
2f
1H-NMR at 400 MHz
5.989
2.981
2.838
2.170
1.035
1.023
1.021
1.823
1
6.927
6.879
6.577
6.551
6.536
6.510
5.710
5.709
5.329
5.327
5.303
5.301
abundance
X : parts per Million : 1H

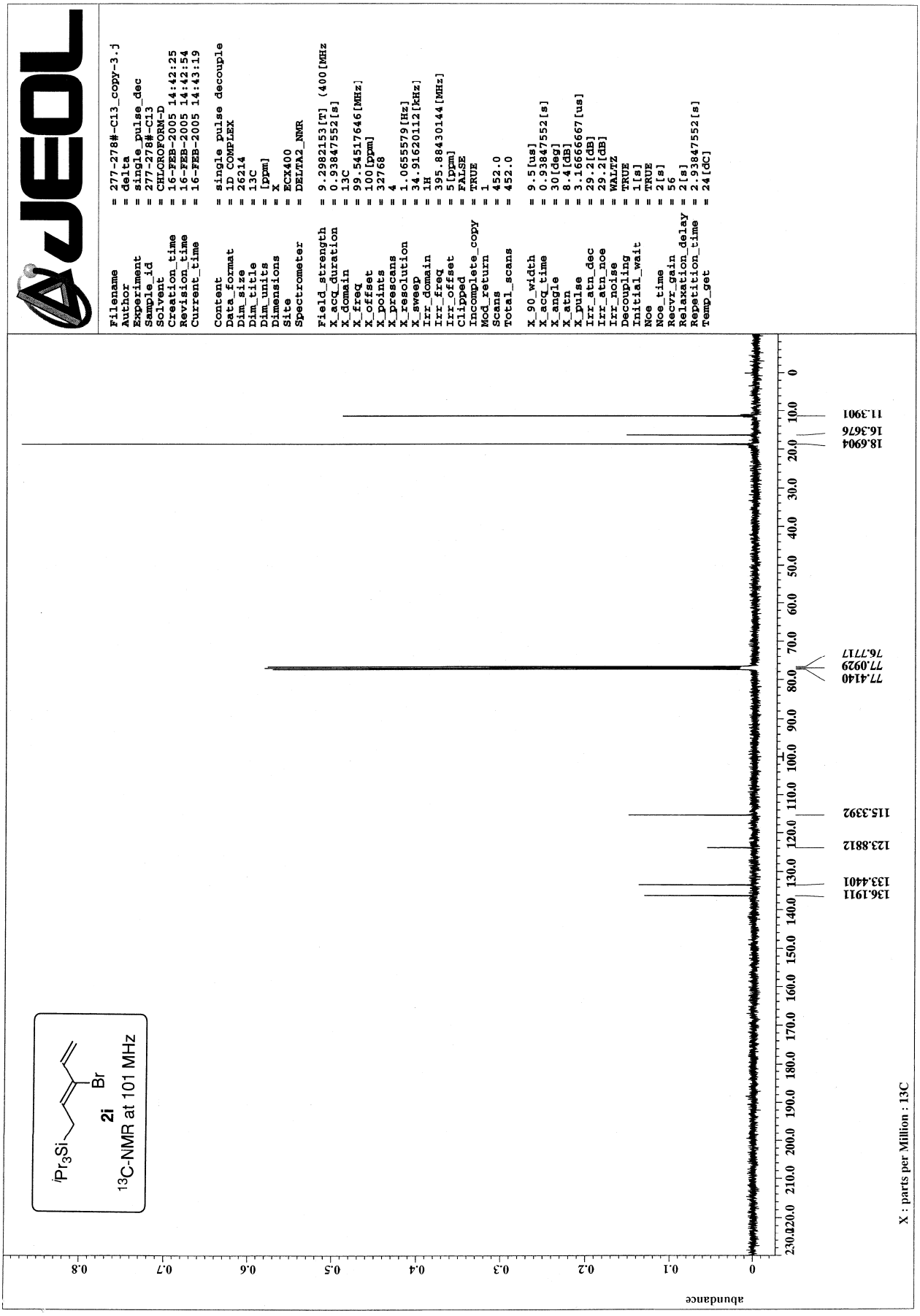

JEOL
Filename = hm90-3.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm90
Solvent = CHLOROFORM-D
Creation_time = 28-JUL-2008 16:46:34
Revision_time = 28-JUL-2008 17:09:41
Current_time = 28-JUL-2008 17:10:21
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.525303333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.479233332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 56
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 23[dC]
Br
2f
13C-NMR at 101 MHz
abundance
X : parts per Million : 13C
137.2535
135.7279
135.5420
133.1297
132.6149
128.8630
128.0431
118.8803
77.4001
77.0807
76.7613
21.1604
20.1497

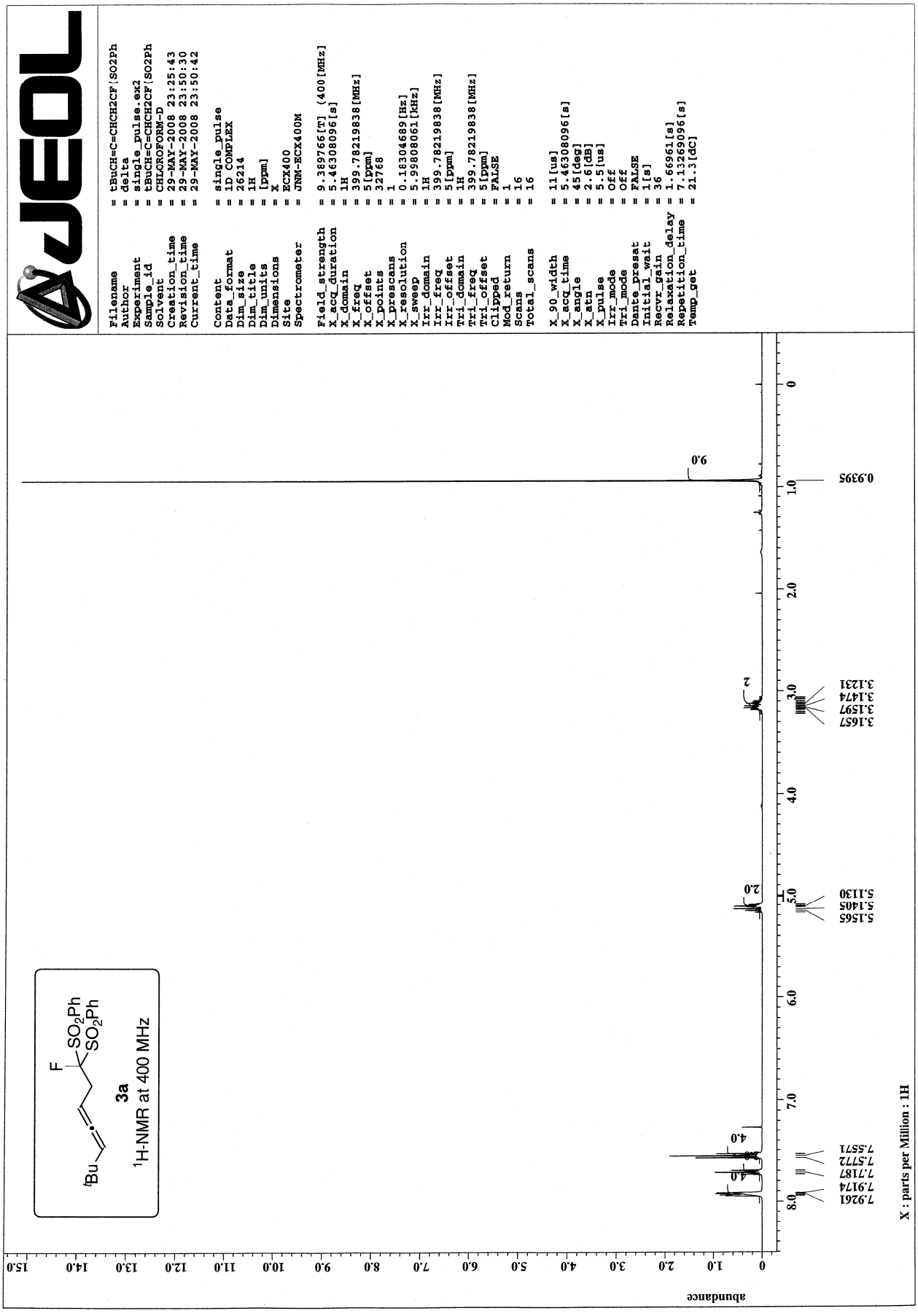

Filename = F3CC6H4-CH=CBr-CH=CH2
Author = delta
Experiment = single_pulse.ex2
Sample_id = F3CC6H4-CH=CBr-CH=CH2
Solvent = CHLOROFORM-D
Creation_time = 8-JUL-2008 09:59:27
Revision_time = 8-JUL-2008 10:01:29
Current_time = 8-JUL-2008 10:01:50
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 5.51550976[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18130691[Hz]
X_sweep = 5.94106464[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.51550976[s]
X_angle = 45[deg]
X_atn = 9[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 1.60236[s]
Repetition_time = 7.11786976[s]
Temp_get = 23.2[dC]
Br
2g
F3C
1H-NMR at 400 MHz
abundance
X : parts per Million : 1H
7.7824
7.7614
7.6318
7.6107
6.9984
6.5477
6.5212
6.5065
6.4804
5.8159
5.7747
5.4293
5.4032
2.0
1.0
1
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

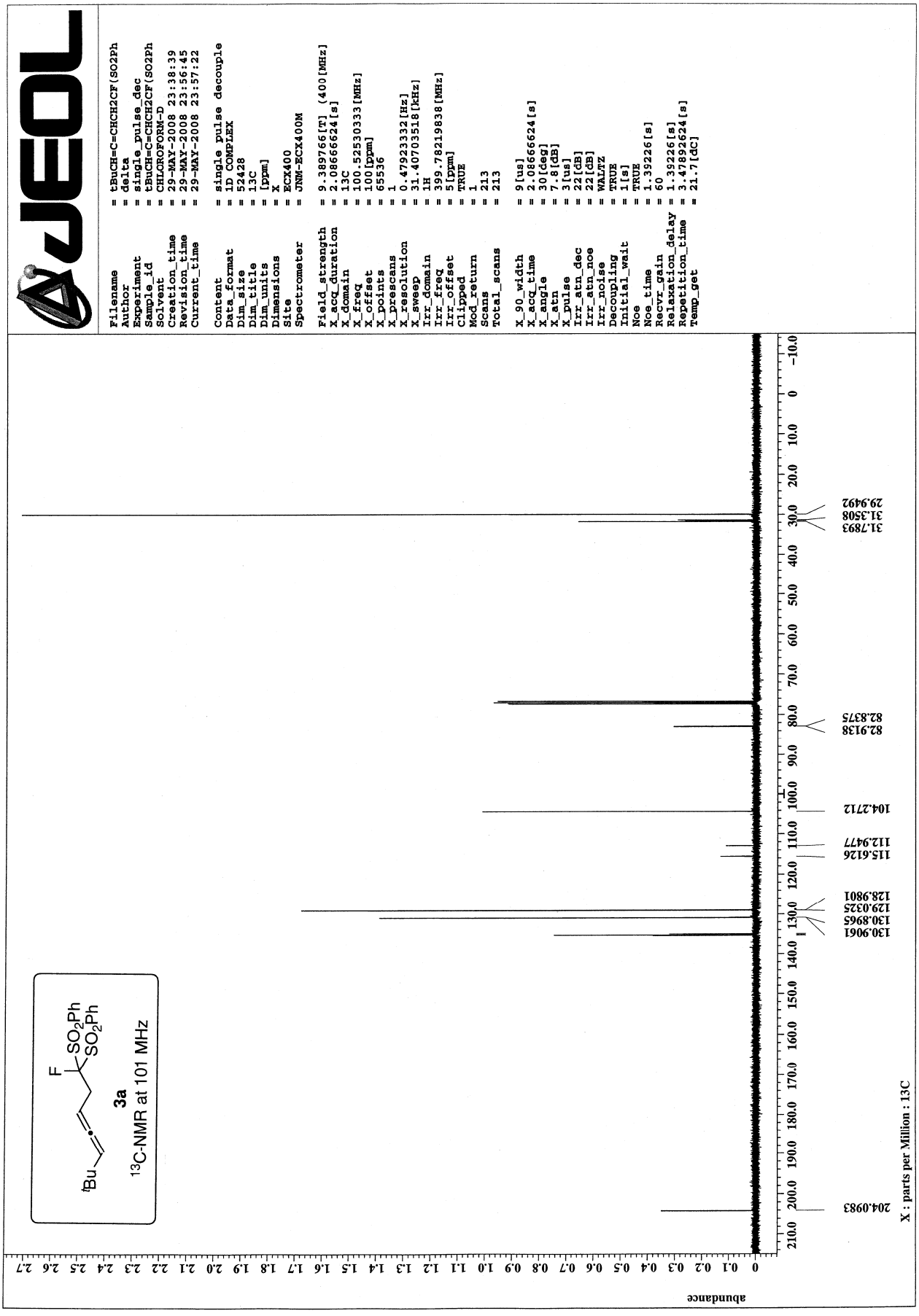

Filename = F3CC6H4-CH=CBr-CH=CH2
Author = delta
Experiment = single_pulse_dec
Sample_id = F3CC6H4-CH=CBr-CH=CH2
Solvent = CHLOROFORM-D
Creation_time = 8-JUL-2008 10:29:13
Revision_time = 8-JUL-2008 10:28:44
Current_time = 8-JUL-2008 10:31:41
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.28589568[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.43746528[Hz]
X_sweep = 28.66972477[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 512
Total_scans = 512
X_90_width = 9.6[us]
X_acq_time = 2.28589568[s]
X_angle = 30[deg]
X_atn = 8.4[dB]
X_pulse = 3.2[us]
Irr_atn_dec = 29.2[dB]
Irr_atn_noe = 29.2[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 1.13759[s]
Recvr_gain = 60
Relaxation_delay = 1.13759[s]
Repetition_time = 3.42348568[s]
Temp_get = 23.6[dC]
F3C
Br
2g
13C-NMR at 101 MHz
abundance
X : parts per Million : 13C
139.1419
136.7116
130.7964
129.7330
126.1118
125.1669
125.1318
125.0922
125.0527
120.5526

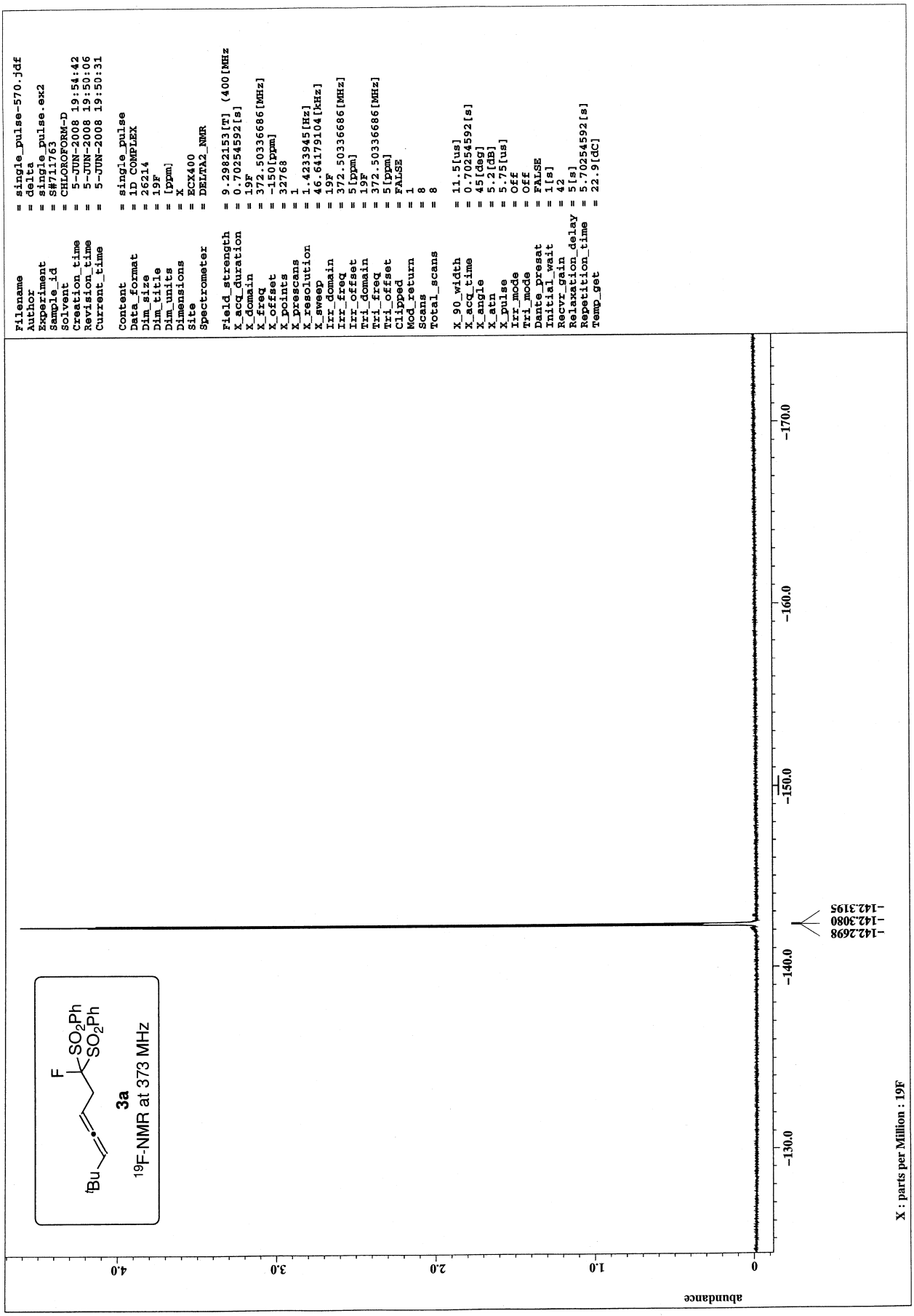

Filename = F3CC6H4-CH=CBr-CH=CH2
Author = delta
Experiment = single_pulse.ex2
Sample_id = F3CC6H4-CH=CBr-CH=CH2
Solvent = CHLOROFORM-D
Creation_time = 8-JUL-2008 10:34:27
Revision_time = 8-JUL-2008 10:32:27
Current_time = 8-JUL-2008 10:32:48
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.00139008[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -50[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.99861185[Hz]
X_sweep = 32.72251309[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 1.00139008[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 4.74333[s]
Repetition_time = 5.74472008[s]
Temp_get = 23.4[dC]
Br
2g
F3C
19F-NMR at 373 MHz
-62.5864
abundance
X : parts per Million : 19F

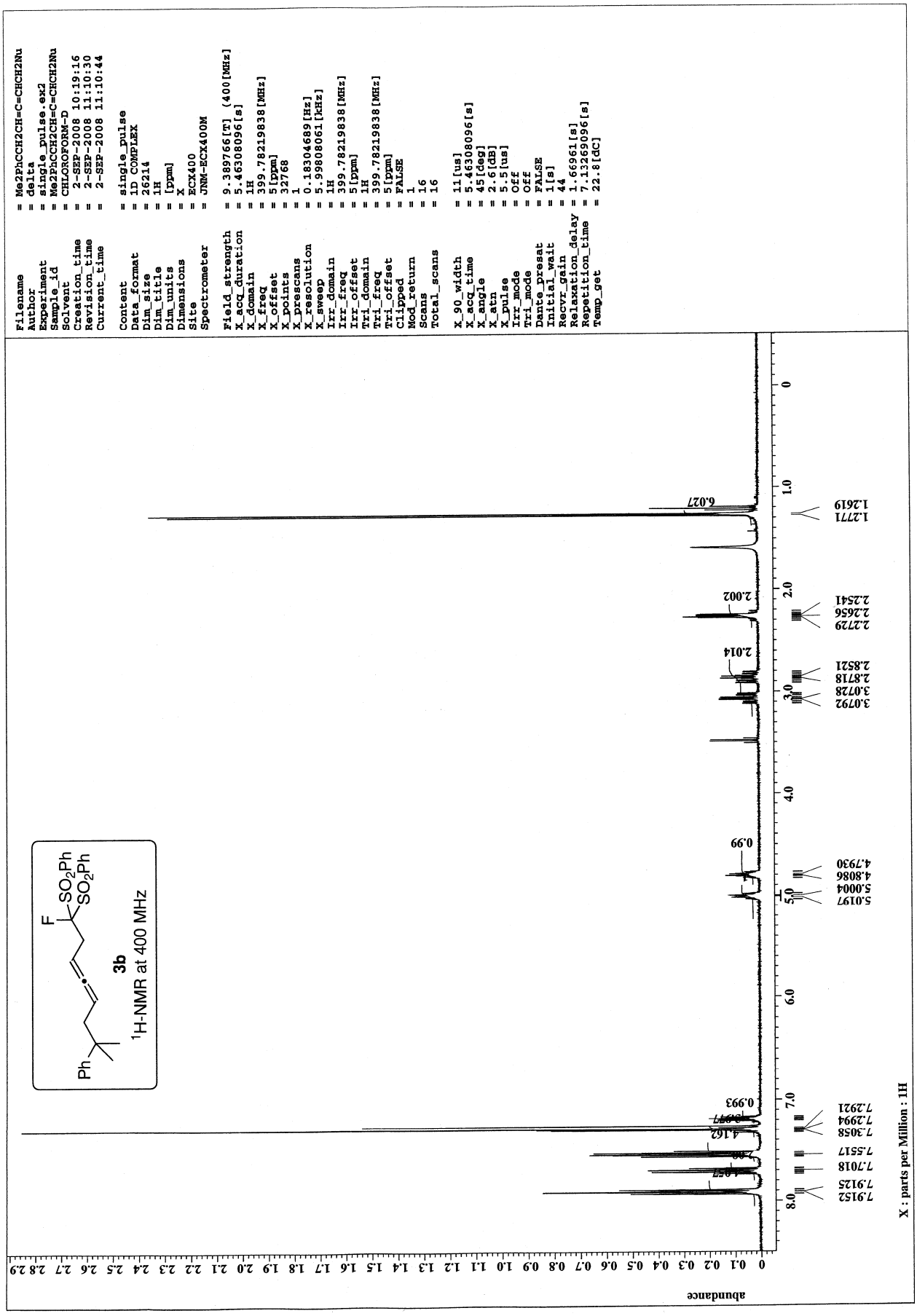

JEOL
Filename = 277-278#-H1-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 277-278#-H1
Solvent = CHLOROFORM-D
Creation_time = 16-FEB-2005 14:17:19
Revision_time = 16-FEB-2005 14:23:26
Current_time = 16-FEB-2005 14:23:47
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 12.5[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 9[dB]
X_pulse = 6.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 23.7[dC]
iPr3Si
Br
2i
1H-NMR at 400 MHz
21.603
1.978
0.96
0.974
0.993
1
7.2590
6.3423
6.3160
6.3011
6.2748
6.0837
5.4405
5.3993
5.0720
5.0457
1.9283
1.9077
1.0712
1.0632
1.0506
-0.0000
abundance
X : parts per Million : 1H

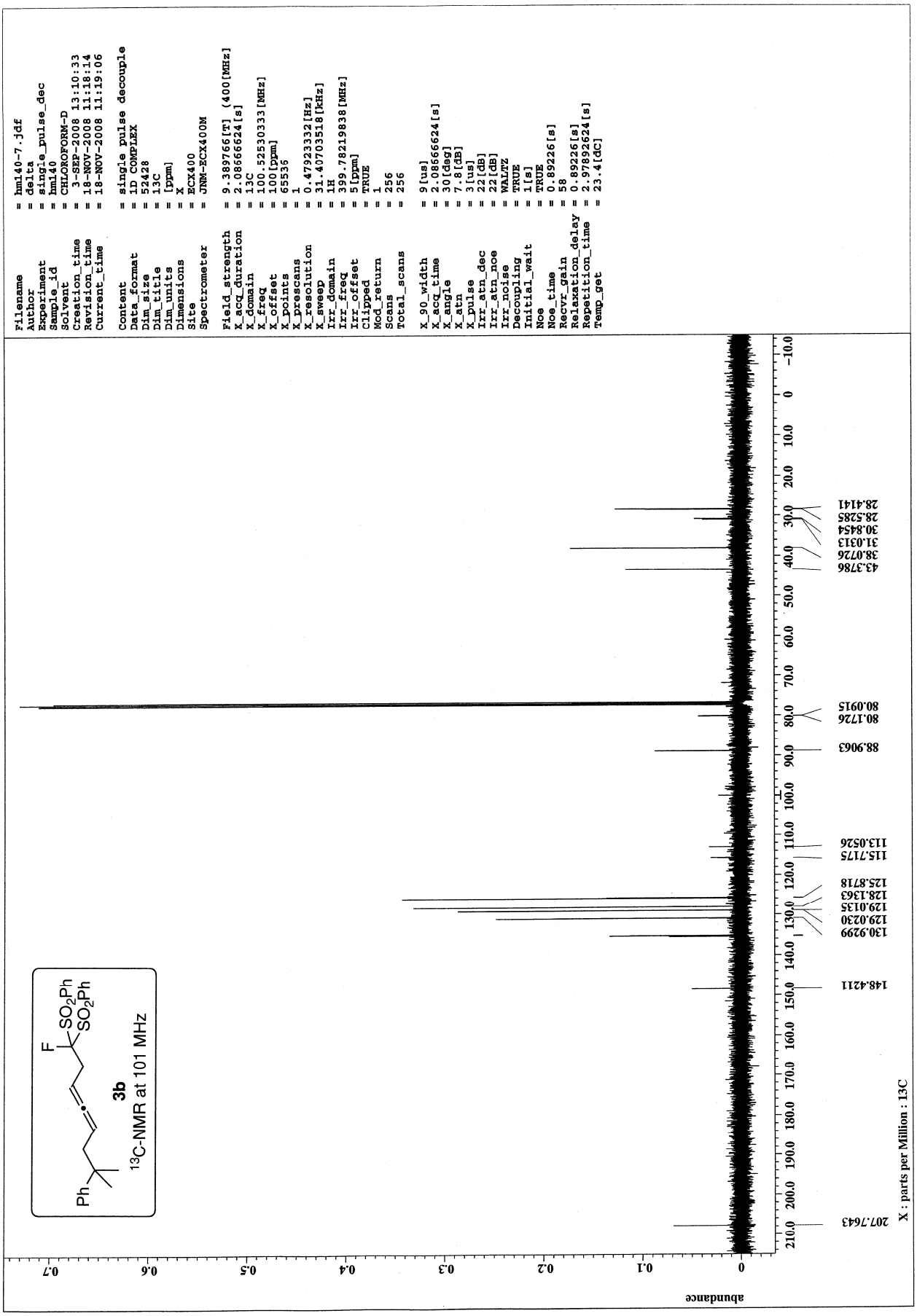

JEOL
Filename = 277-278#-C13_copy-3.j
Author = delta
Experiment = single_pulse_dec
Sample_id = 277-278#-C13
Solvent = CHLOROFORM-D
Creation_time = 16-FEB-2005 14:42:25
Revision_time = 16-FEB-2005 14:42:54
Current_time = 16-FEB-2005 14:43:19
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.93847552[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.0655579[Hz]
X_sweep = 34.91620112[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Incomplete_copy = TRUE
Mod_return = 1
Scans = 452.0
Total_scans = 452.0
X_90_width = 9.5[us]
X_acq_time = 0.93847552[s]
X_angle = 30[deg]
X_atn = 8.4[dB]
X_pulse = 3.16666667[us]
Irr_atn_dec = 29.2[dB]
Irr_atn_noe = 29.2[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 56
Relaxation_delay = 2[s]
Repetition_time = 2.93847552[s]
Temp_get = 24[dC]
iPr3Si
Br
2i
13C-NMR at 101 MHz
11.3901
16.3676
18.6904
76.7717
77.0929
77.4140
115.3392
123.8812
133.4401
136.1911
abundance
X : parts per Million : 13C

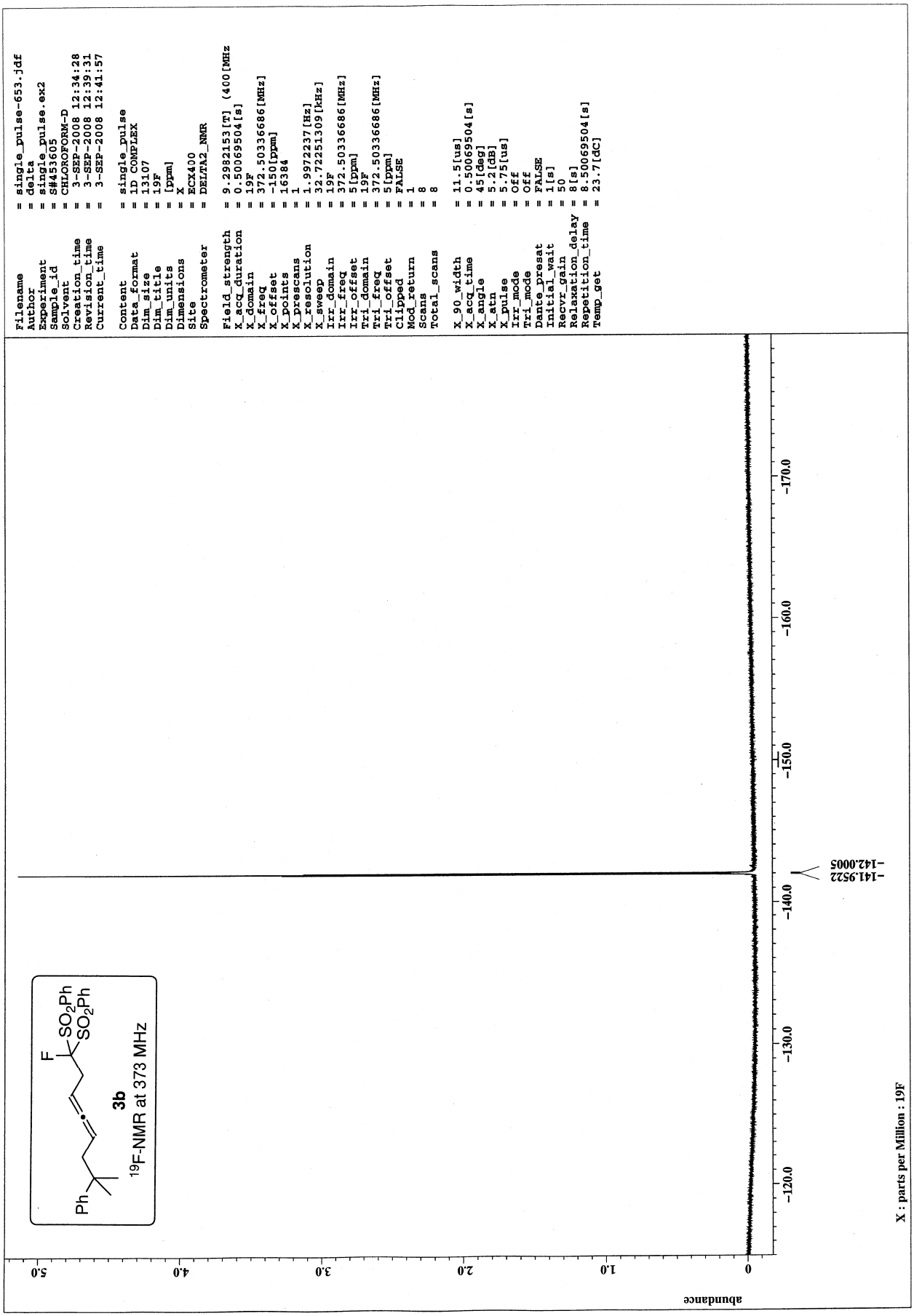

JEOL
Filename = tBuCH=C=CHCH2CF(SO2Ph
Author = delta
Experiment = single_pulse.ex2
Sample_id = tBuCH=C=CHCH2CF(SO2Ph
Solvent = CHLOROFORM-D
Creation_time = 29-MAY-2008 23:25:43
Revision_time = 29-MAY-2008 23:50:30
Current_time = 29-MAY-2008 23:50:42
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 21.3[dC]
F
SO2Ph
SO2Ph
tBu
3a
1H-NMR at 400 MHz
9.0
2
2.0
4.0
4.0
0.9395
3.1657
3.1597
3.1474
3.1231
5.1565
5.1405
5.1130
7.9261
7.9174
7.7187
7.5772
7.5571
abundance
X : parts per Million : 1H

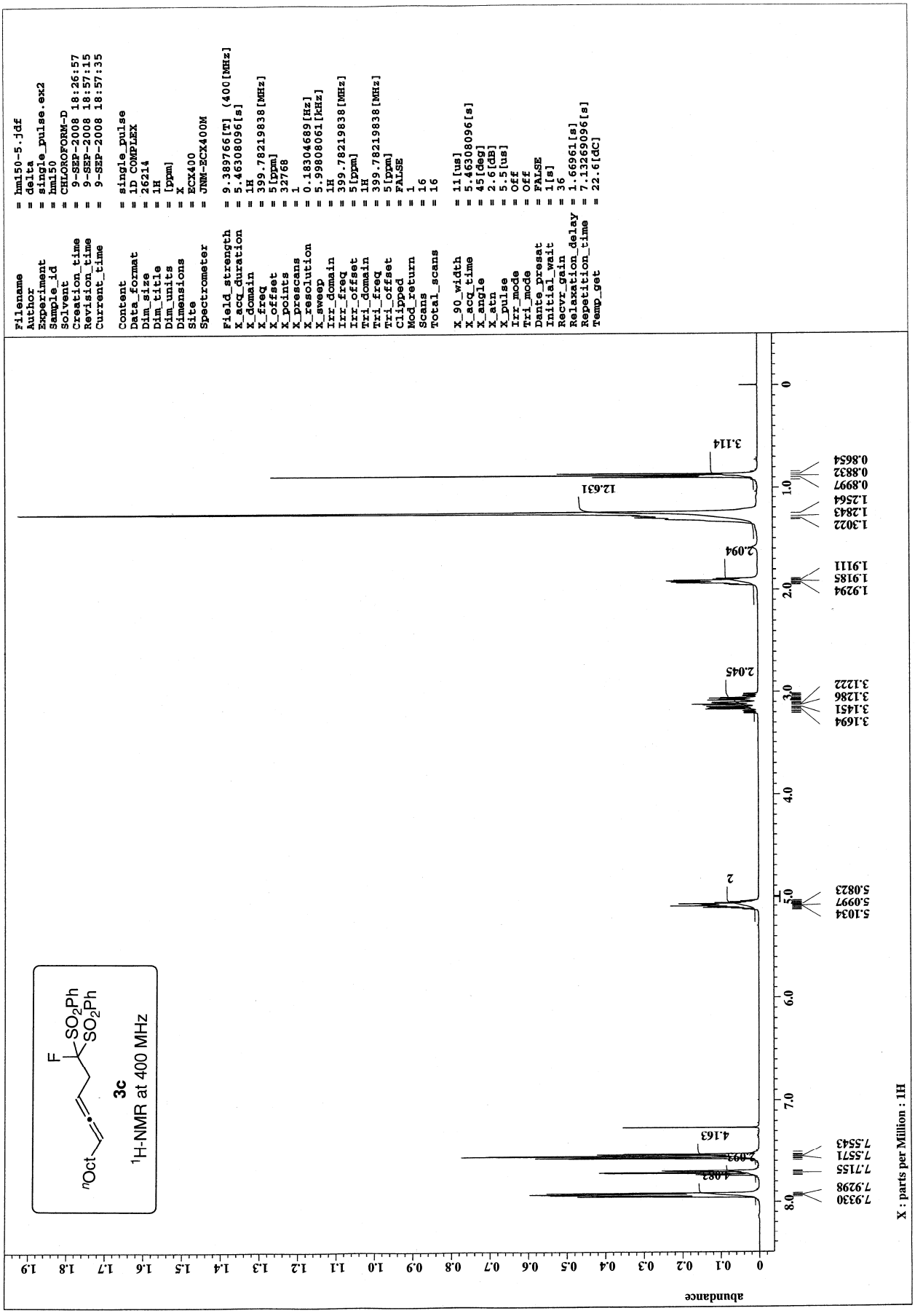

JEOL
Filename = tBuCH=C=CHCH2CF(SO2Ph
Author = delta
Experiment = single_pulse_dec
Sample_id = tBuCH=C=CHCH2CF(SO2Ph
Solvent = CHLOROFORM-D
Creation_time = 29-MAY-2008 23:38:39
Revision_time = 29-MAY-2008 23:56:45
Current_time = 29-MAY-2008 23:57:22
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 213
Total_scans = 213
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 1.39226[s]
Recvr_gain = 60
Relaxation_delay = 1.39226[s]
Repetition_time = 3.47892624[s]
Temp_get = 21.7[dC]
F
SO2Ph
SO2Ph
tBu
3a
13C-NMR at 101 MHz
31.7893
31.3508
29.9492
82.9138
82.8375
104.2712
115.6126
112.9477
130.9061
130.8965
129.0325
128.9801
204.0983
X : parts per Million : 13C
abundance

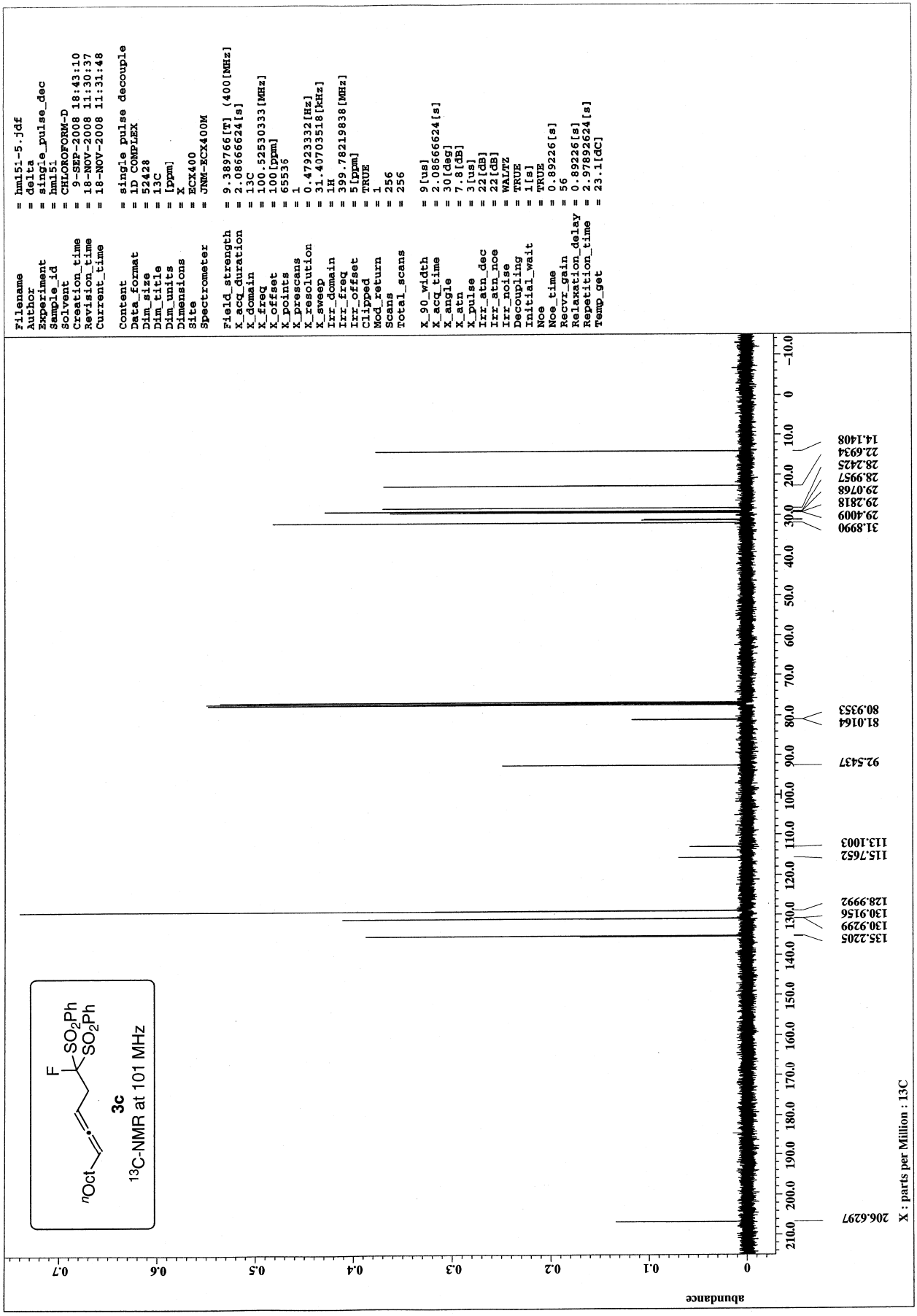

Filename = single_pulse-570.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#711763
Solvent = CHLOROFORM-D
Creation_time = 5-JUN-2008 19:54:42
Revision_time = 5-JUN-2008 19:50:06
Current_time = 5-JUN-2008 19:50:31
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.70254592[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -150[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 1.42339945[Hz]
X_sweep = 46.64179104[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.70254592[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 5.70254592[s]
Temp_get = 22.9[dC]
F
SO2Ph
SO2Ph
tBu
3a
19F-NMR at 373 MHz
abundance
4.0
3.0
2.0
1.0
0
-130.0
-140.0
-150.0
-160.0
-170.0
-142.2698
-142.3080
-142.3195
X : parts per Million : 19F

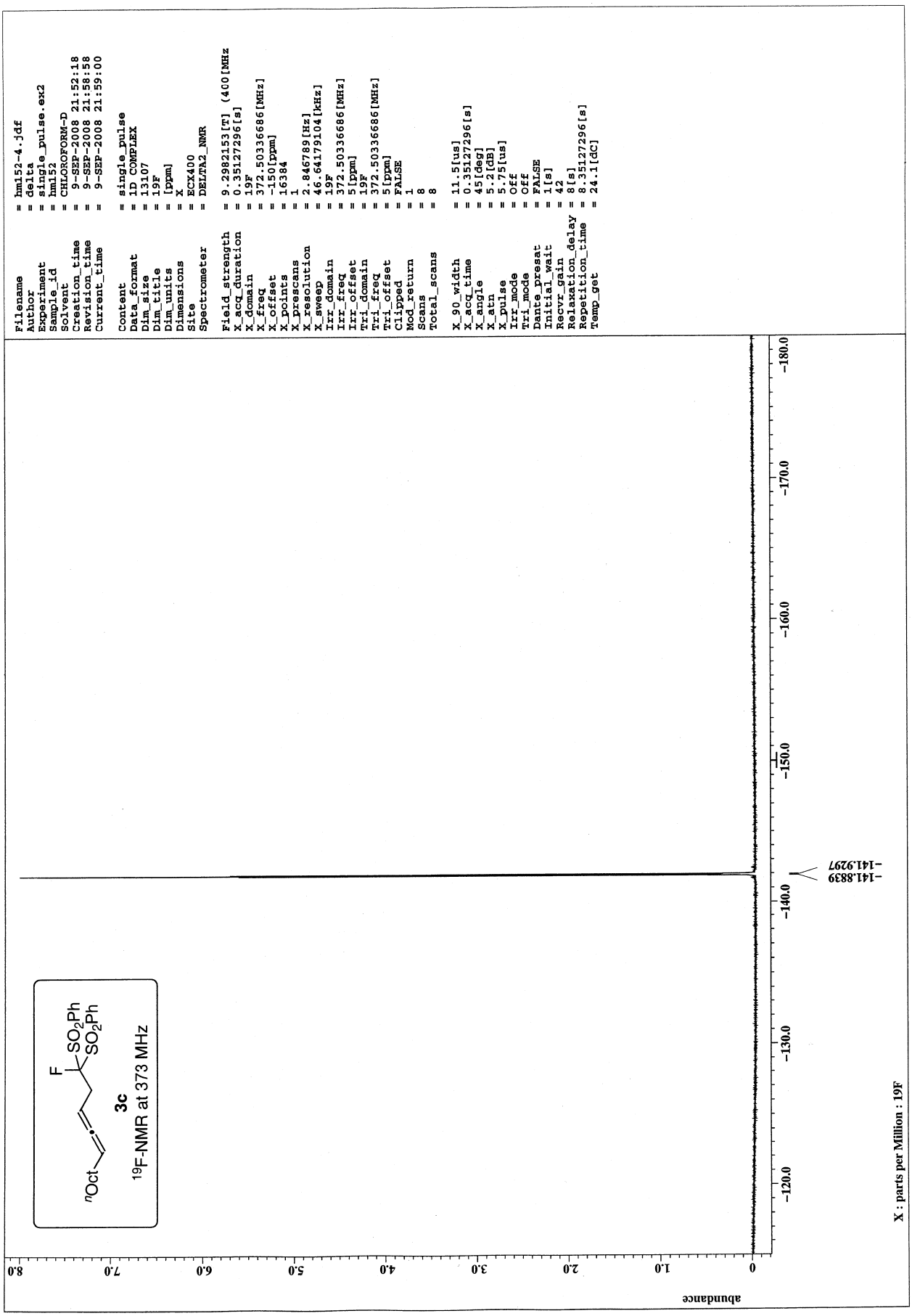

Filename = Me2PhCCH2CH=C=CHCH2Nu
Author = delta
Experiment = single_pulse.ex2
Sample_id = Me2PhCCH2CH=C=CHCH2Nu
Solvent = CHLOROFORM-D
Creation_time = 2-SEP-2008 10:19:16
Revision_time = 2-SEP-2008 11:10:30
Current_time = 2-SEP-2008 11:10:44
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Date_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 22.8[dC]
F
SO2Ph
SO2Ph
Ph
3b
1H-NMR at 400 MHz
abundance
X : parts per Million : 1H
6.027
2.002
2.014
0.99
0.993
1.2771
1.2619
2.2729
2.2656
2.2541
3.0792
3.0728
2.8718
2.8521
5.0197
5.0004
4.8086
4.7930
7.9152
7.9125
7.7018
7.5517
7.3058
7.2994
7.2921
4.162

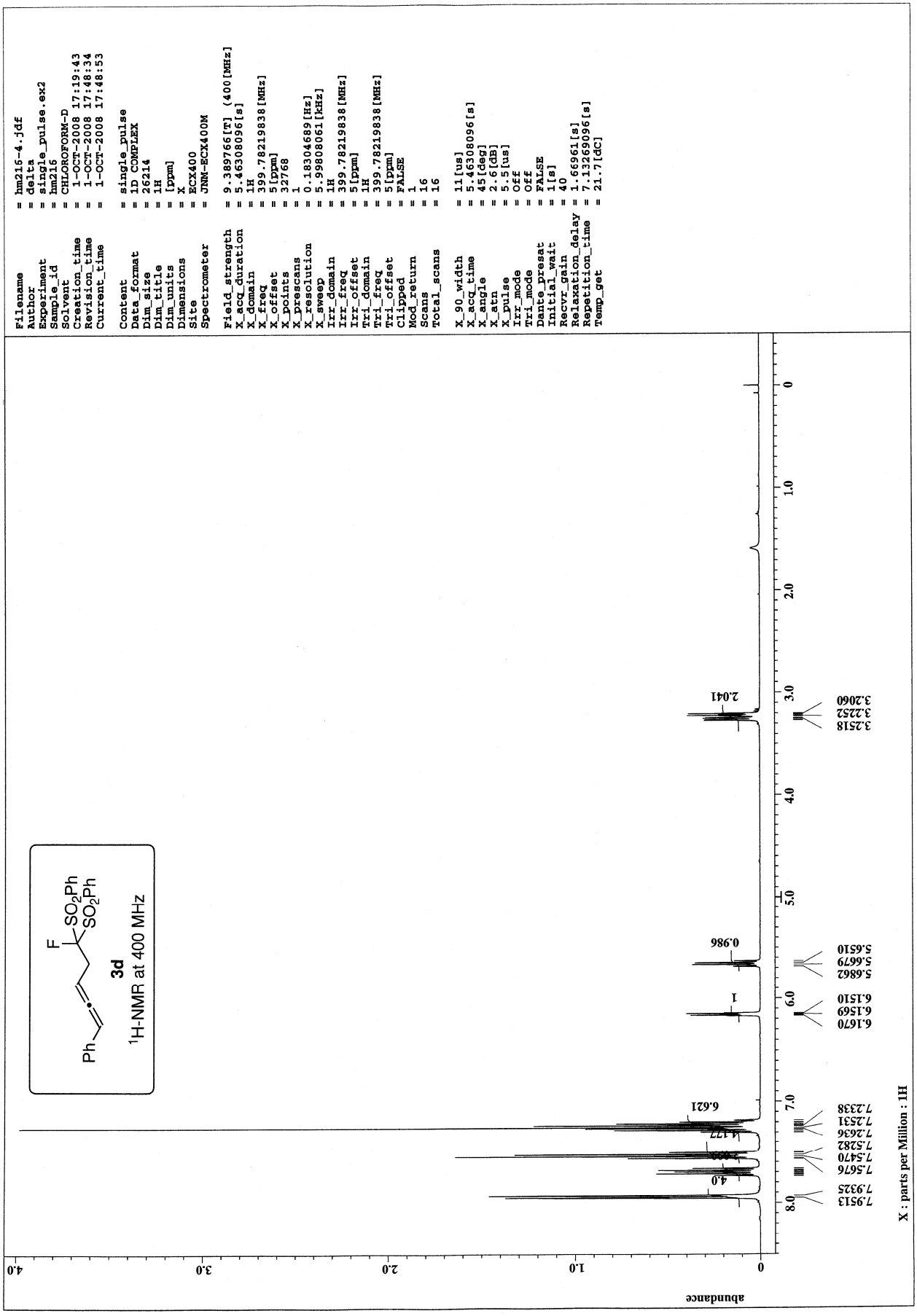

Filename = hm140-7.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm140
Solvent = CHLOROFORM-D
Creation_time = 3-SEP-2008 13:10:33
Revision_time = 18-NOV-2008 11:18:14
Current_time = 18-NOV-2008 11:19:06
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 58
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 23.4[dC]
F
SO2Ph
SO2Ph
Ph
3b
13C-NMR at 101 MHz
abundance
X : parts per Million : 13C
207.7643
148.4211
130.9299
129.0230
129.0135
128.1363
125.8718
115.7175
113.0526
88.9063
80.1726
80.0915
43.3786
38.0726
31.0313
30.8454
28.5285
28.4141

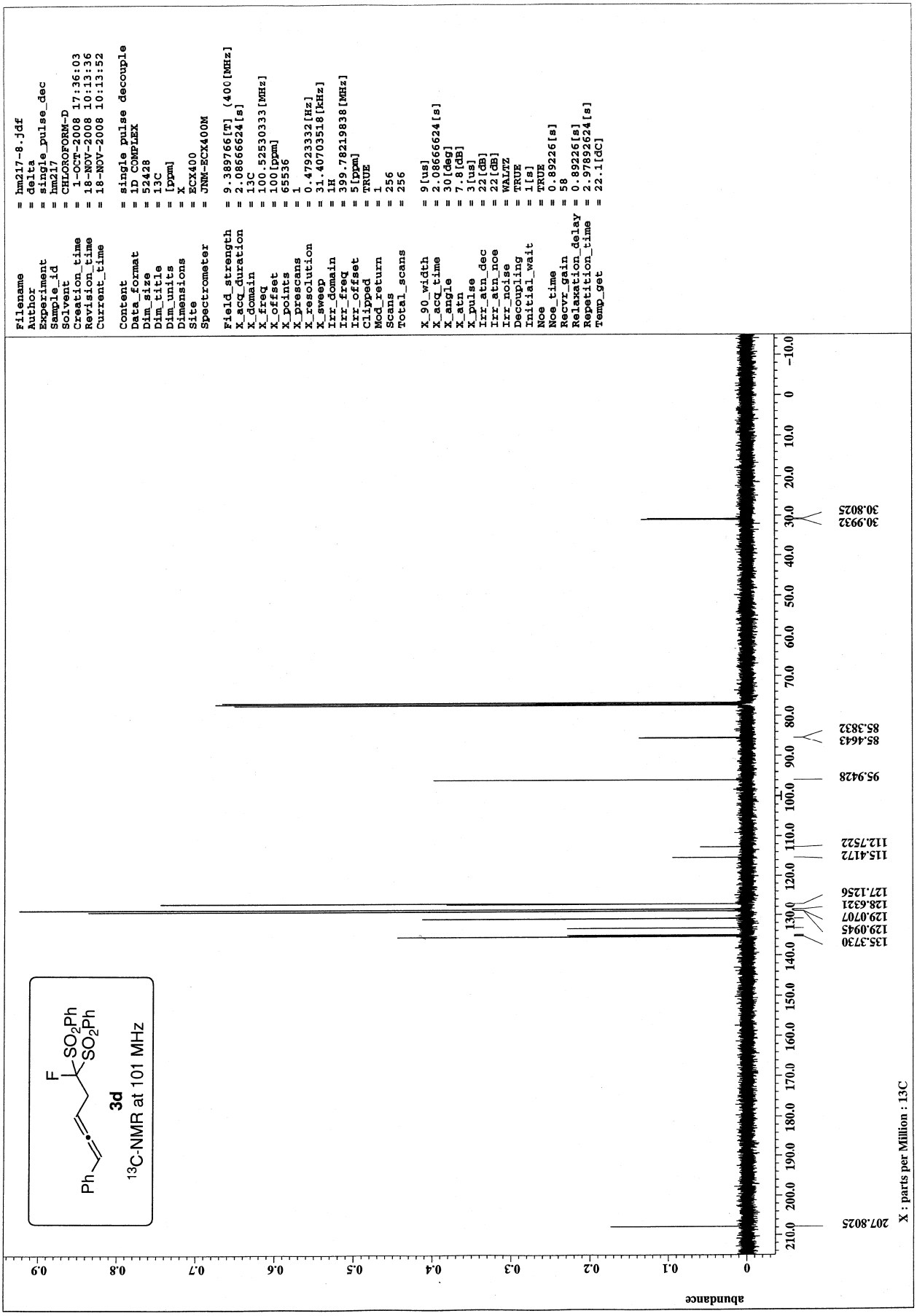

Filename = single_pulse-653.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = SM453605
Solvent = CHLOROFORM-D
Creation_time = 3-SEP-2008 12:34:28
Revision_time = 3-SEP-2008 12:39:31
Current_time = 3-SEP-2008 12:41:57
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.50069504[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -150[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 1.99722371[Hz]
X_sweep = 32.72251309[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.50069504[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 50
Relaxation_delay = 8[s]
Repetition_time = 8.50069504[s]
Temp_get = 23.7[dC]
F
SO2Ph
SO2Ph
Ph
3b
19F-NMR at 373 MHz
abundance
5.0
4.0
3.0
2.0
1.0
0
-120.0
-130.0
-140.0
-150.0
-160.0
-170.0
-141.9522
-142.0005
X : parts per Million : 19F

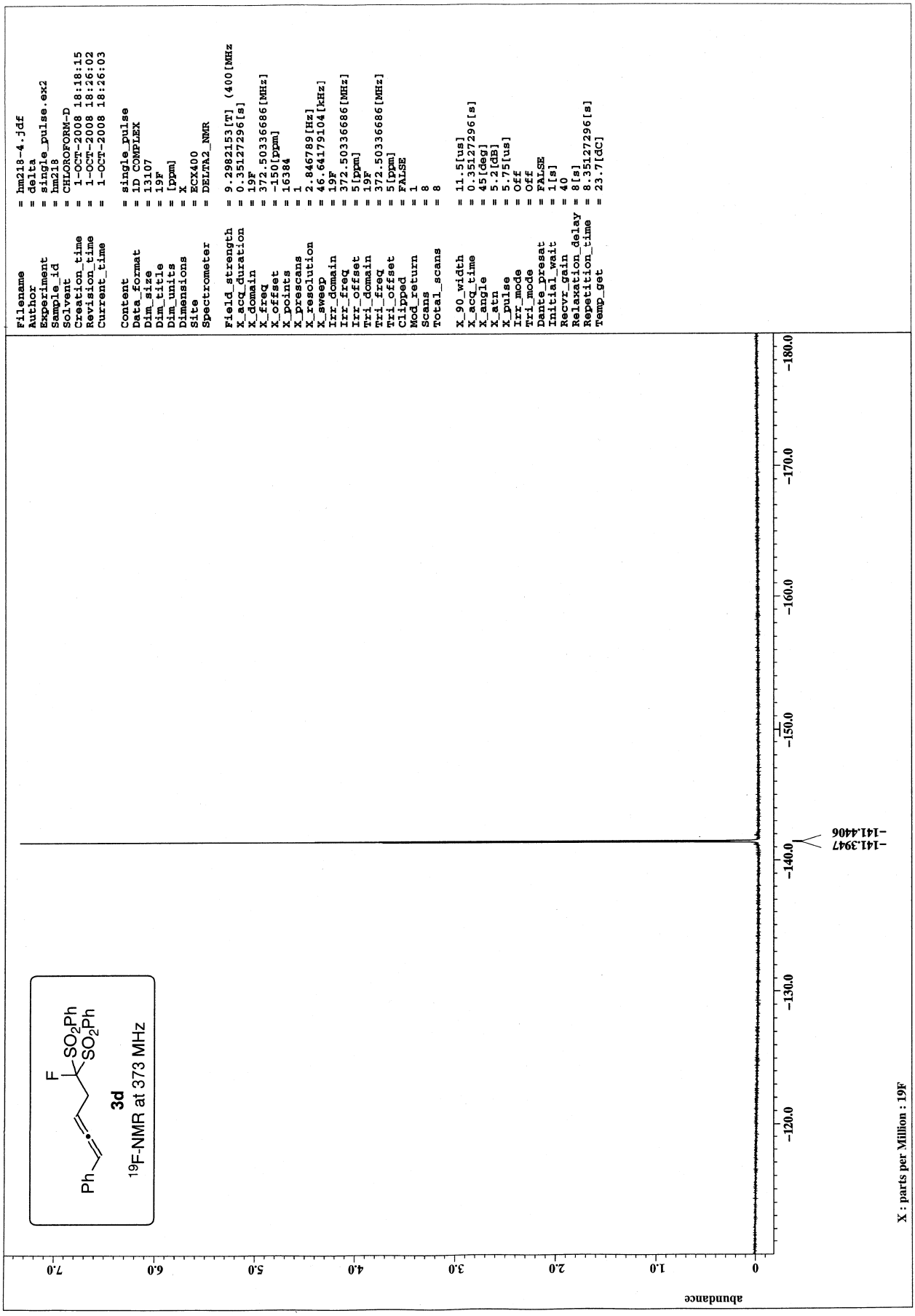

Filename = hm150-5.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm150
Solvent = CHLOROFORM-D
Creation_time = 9-SEP-2008 18:26:57
Revision_time = 9-SEP-2008 18:57:15
Current_time = 9-SEP-2008 18:57:35
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 22.6[dC]
F
SO2Ph
SO2Ph
nOct
3c
1H-NMR at 400 MHz
abundance
X : parts per Million : 1H
12.631
4.163
2.094
2.045
2
3.114
7.9330
7.9298
7.7155
7.5571
7.5543
5.1034
5.0997
5.0823
3.1694
3.1451
3.1286
3.1222
1.9294
1.9185
1.9111
1.3022
1.2843
1.2564
0.8997
0.8832
0.8654

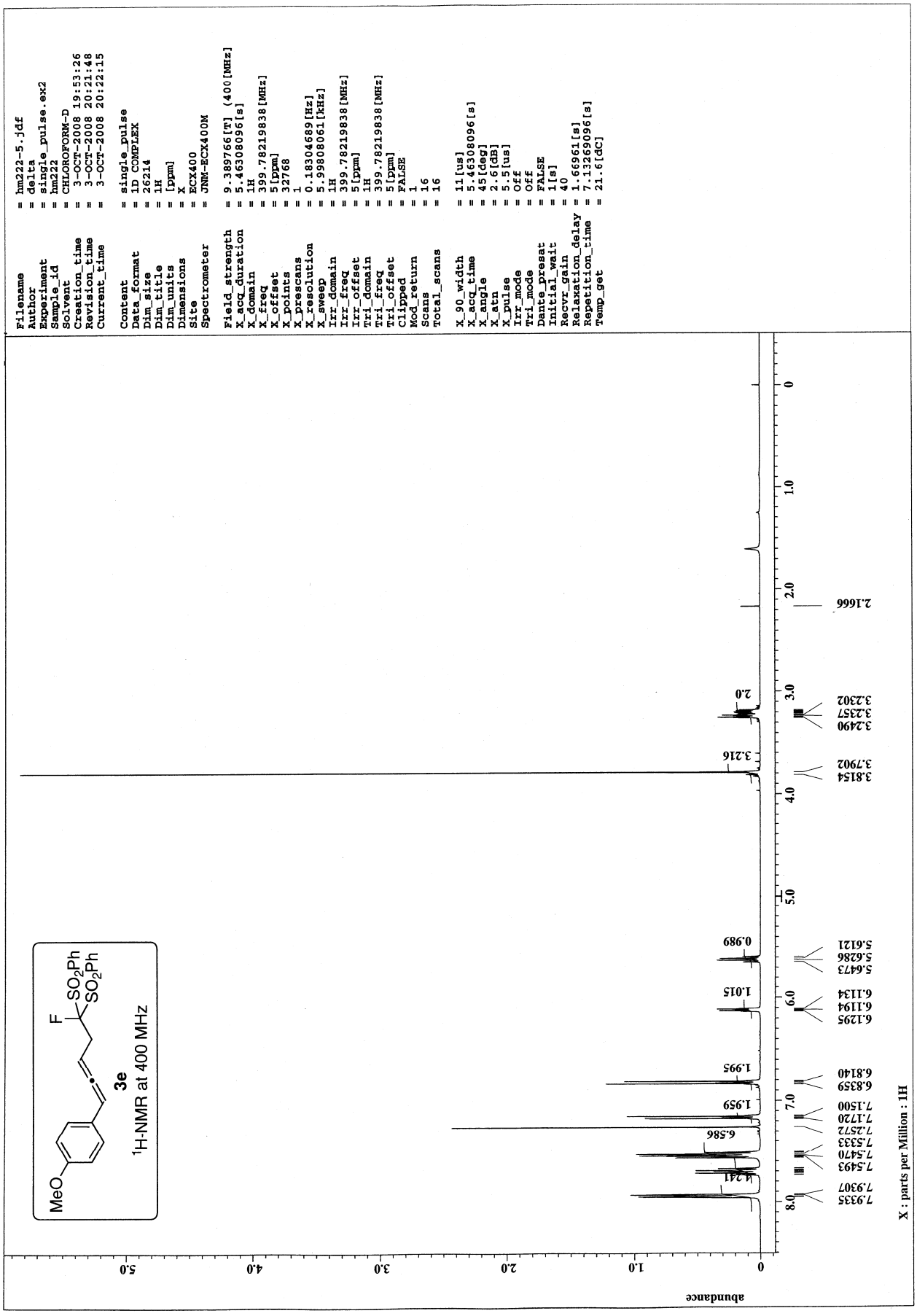

Filename = hm151-5.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm151
Solvent = CHLOROFORM-D
Creation_time = 9-SEP-2008 18:43:10
Revision_time = 18-NOV-2008 11:30:37
Current_time = 18-NOV-2008 11:31:48
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 56
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 23.1[dC]
F
SO2Ph
SO2Ph
nOct
3c
13C-NMR at 101 MHz
206.6297
135.2205
130.9299
130.9156
128.9992
115.7652
113.1003
92.5437
81.0164
80.9353
31.8990
29.4009
29.2818
29.0768
28.9957
28.2425
22.6934
14.1408
abundance
X : parts per Million : 13C

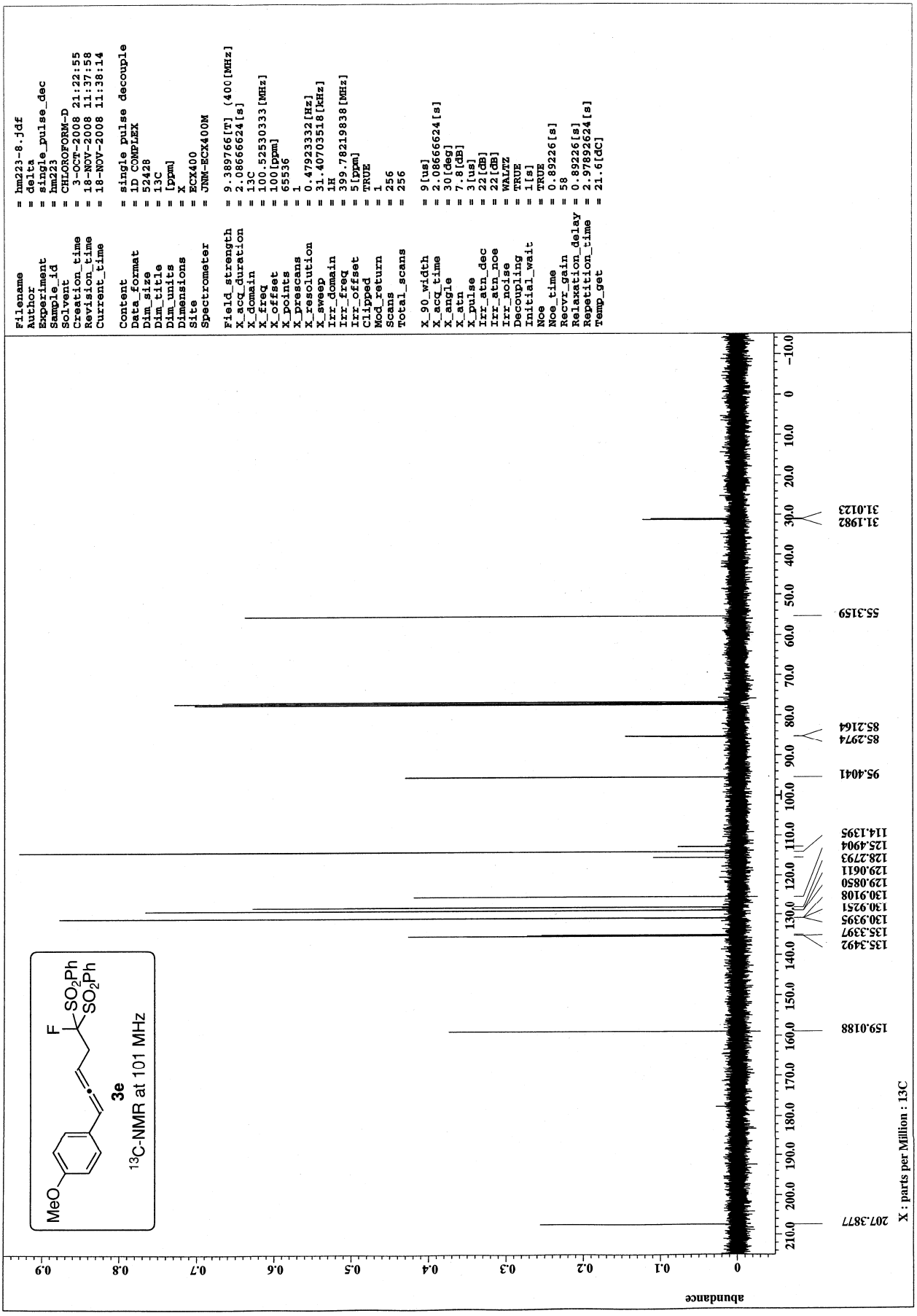

Filename = hm152-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm152
Solvent = CHLOROFORM-D
Creation_time = 9-SEP-2008 21:52:18
Revision_time = 9-SEP-2008 21:58:58
Current_time = 9-SEP-2008 21:59:00
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.35127296[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -150[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 2.846789[Hz]
X_sweep = 46.64179104[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.35127296[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 8[s]
Repetition_time = 8.35127296[s]
Temp_get = 24.1[dC]
F
SO2Ph
SO2Ph
nOct
3c
19F-NMR at 373 MHz
abundance
-141.8839
-141.9297
X : parts per Million : 19F

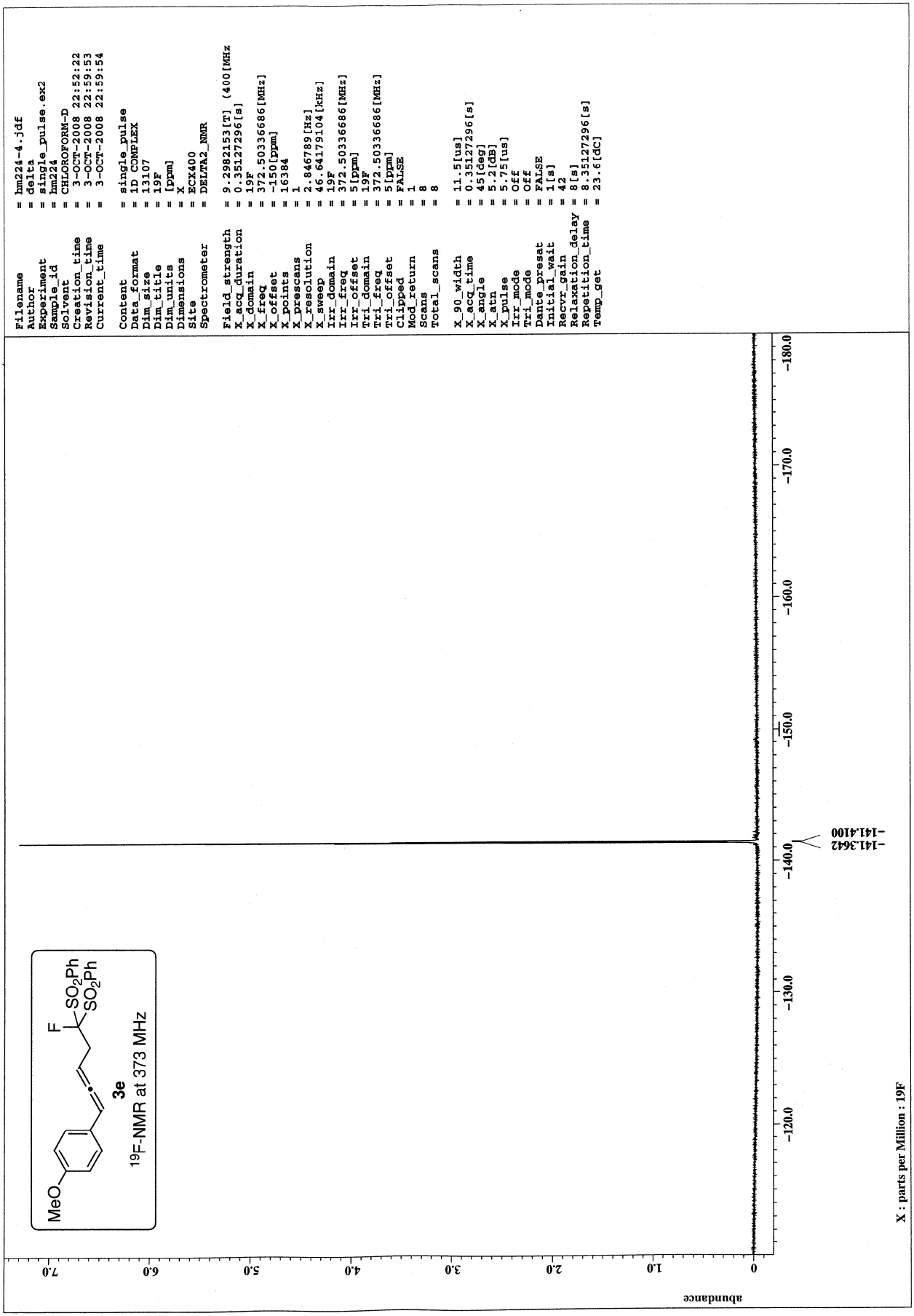

Filename = hm216-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm216
Solvent = CHLOROFORM-D
Creation_time = 1-OCT-2008 17:19:43
Revision_time = 1-OCT-2008 17:48:34
Current_time = 1-OCT-2008 17:48:53
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 21.7[dC]
F
SO2Ph
SO2Ph
Ph
3d
1H-NMR at 400 MHz
abundance
X : parts per Million : 1H
7.9513
7.9325
7.5676
7.5470
7.5282
7.2636
7.2531
7.2338
6.1670
6.1569
6.1510
5.6862
5.6679
5.6510
3.2518
3.2252
3.2060
4.0
4.177
6.621
1
0.986
2.041

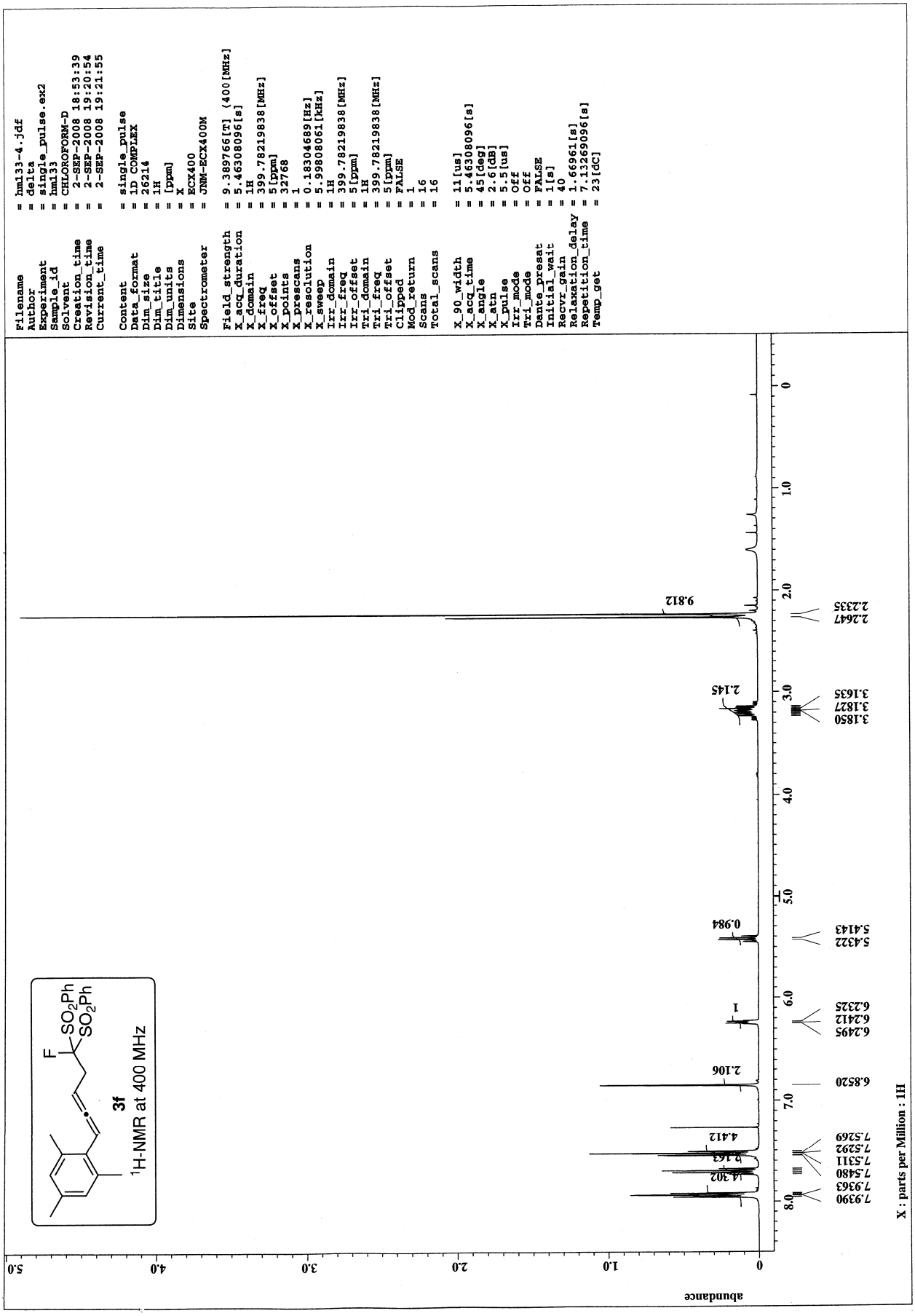

Filename = hm217-8.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm217
Solvent = CHLOROFORM-D
Creation_time = 1-OCT-2008 17:36:03
Revision_time = 18-NOV-2008 10:13:36
Current_time = 18-NOV-2008 10:13:52
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 58
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 22.1[dC]
F
SO2Ph
SO2Ph
Ph
3d
13C-NMR at 101 MHz
abundance
X : parts per Million : 13C
207.8025
135.3730
129.0945
129.0707
128.6321
127.1256
115.4172
112.7522
95.9428
85.4643
85.3832
30.9932
30.8025

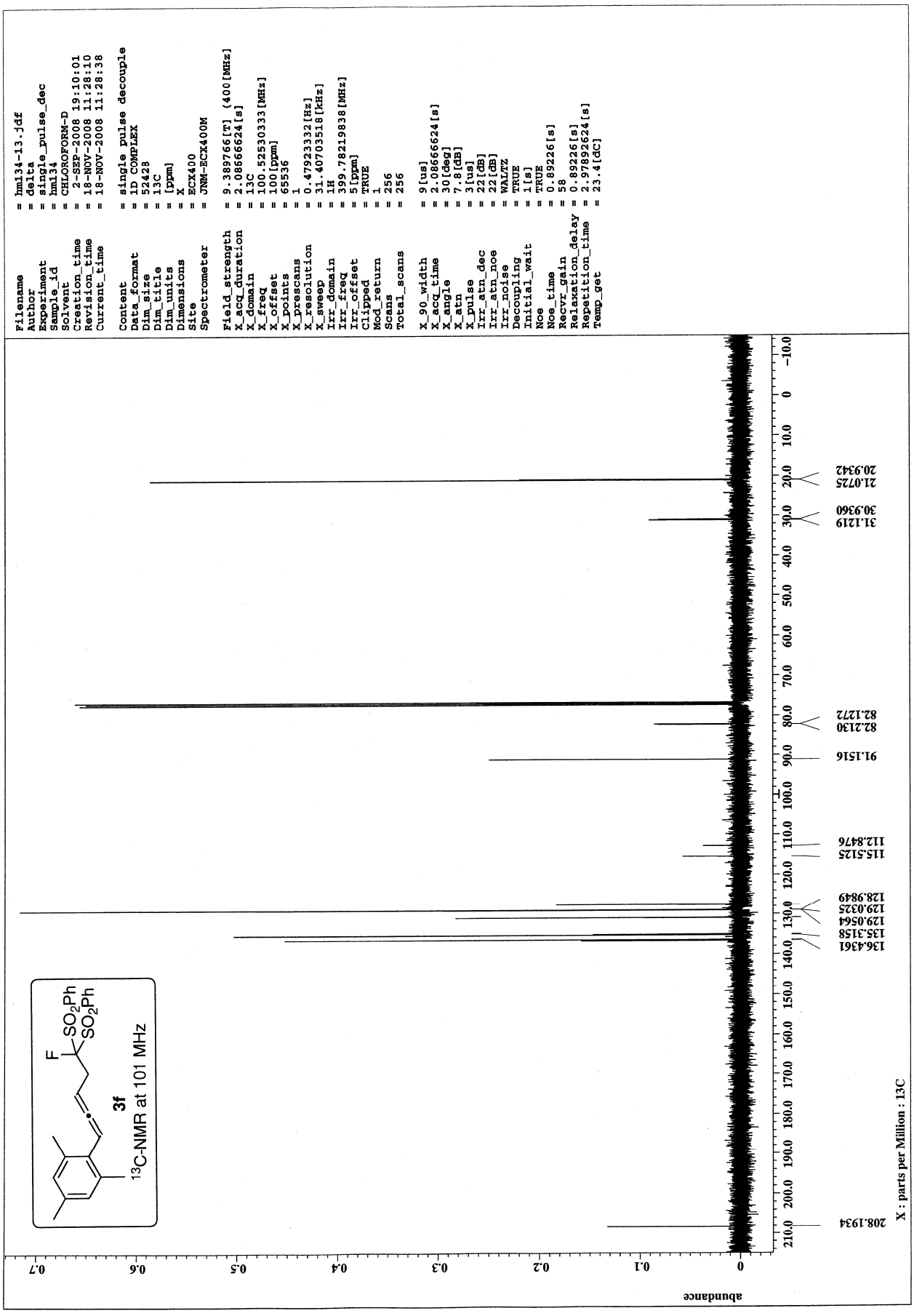

Filename = hm218-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm218
Solvent = CHLOROFORM-D
Creation_time = 1-OCT-2008 18:18:15
Revision_time = 1-OCT-2008 18:26:02
Current_time = 1-OCT-2008 18:26:03
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.35127296[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -150[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 2.846789[Hz]
X_sweep = 46.64179104[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.35127296[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 8[s]
Repetition_time = 8.35127296[s]
Temp_get = 23.7[dC]
F
SO2Ph
SO2Ph
Ph
3d
19F-NMR at 373 MHz
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-120.0
-130.0
-140.0
-150.0
-160.0
-170.0
-180.0
-141.3947
-141.4406
X : parts per Million : 19F

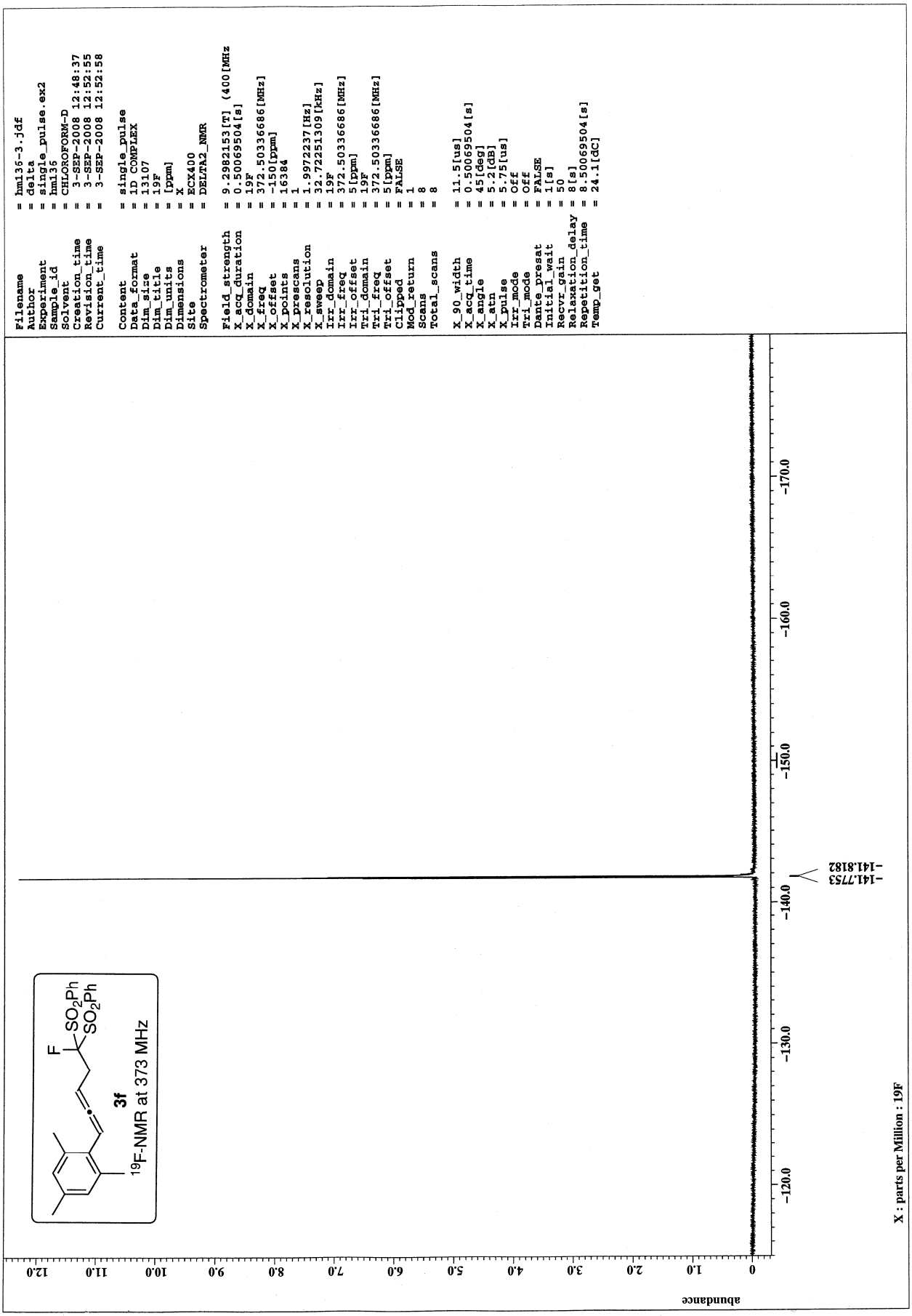

Filename = hm222-5.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm222
Solvent = CHLOROFORM-D
Creation_time = 3-OCT-2008 19:53:26
Revision_time = 3-OCT-2008 20:21:48
Current_time = 3-OCT-2008 20:22:15
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 21.6[dC]
MeO
F
SO2Ph
SO2Ph
3e
1H-NMR at 400 MHz
abundance
X : parts per Million : 1H
7.9335
7.9307
7.5493
7.5470
7.5333
7.2572
7.1720
7.1500
6.8359
6.8140
6.1295
6.1194
6.1134
5.6473
5.6286
5.6121
3.8154
3.7902
3.2490
3.2357
3.2302
2.1666
6.586
3.241
3.216
1.995
1.959
1.015
0.989
2.0

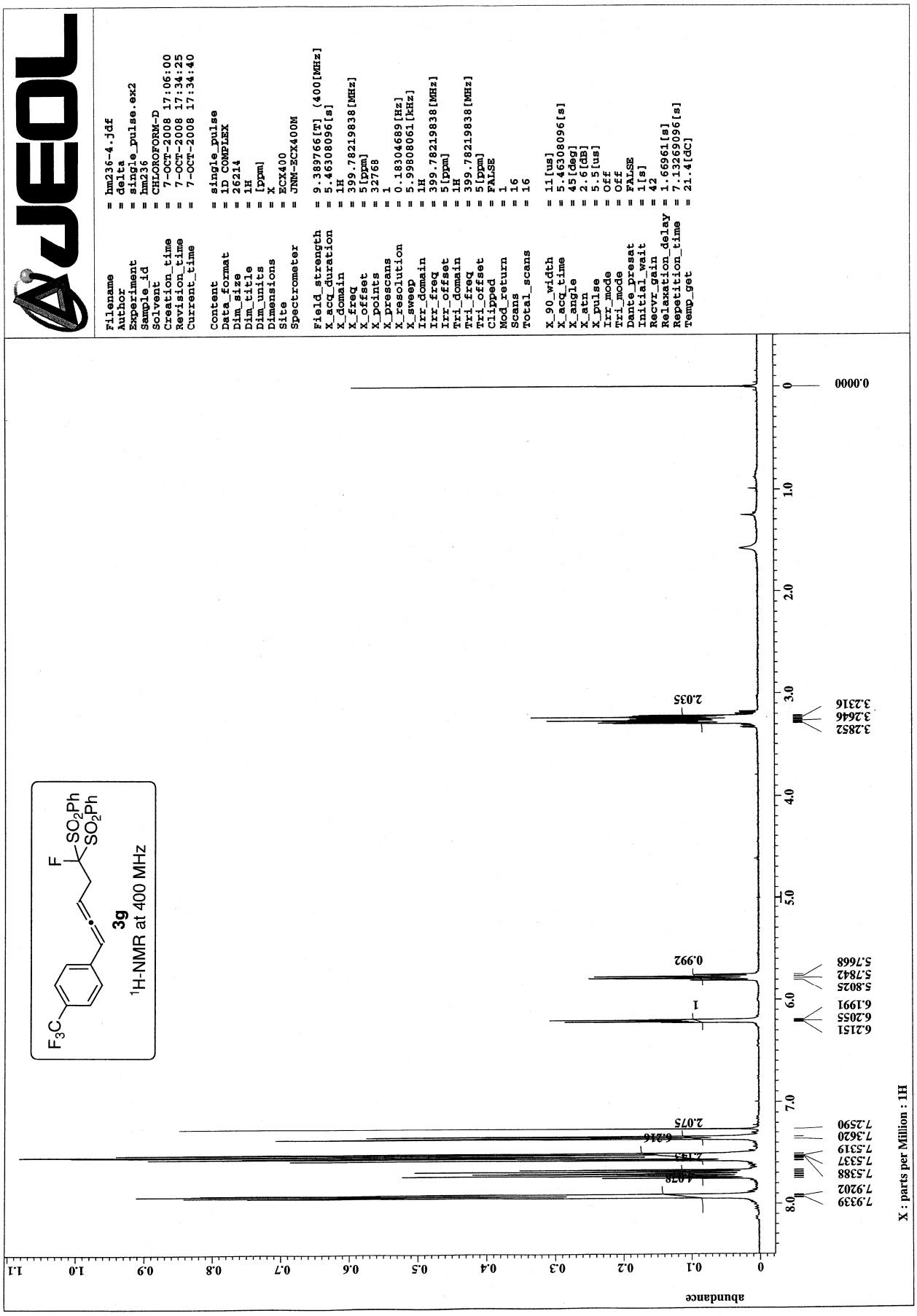

Filename = hm223-8.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm223
Solvent = CHLOROFORM-D
Creation_time = 3-OCT-2008 21:22:55
Revision_time = 18-NOV-2008 11:37:58
Current_time = 18-NOV-2008 11:38:14
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.525303333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 58
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 21.6[dC]
MeO
F
SO2Ph
SO2Ph
3e
13C-NMR at 101 MHz
abundance
X : parts per Million : 13C
207.3877
159.0188
135.3492
135.3397
130.9395
130.9251
130.9108
129.0850
129.0611
128.2793
125.4904
114.1395
95.4041
85.2974
85.2164
55.3159
31.1982
31.0123

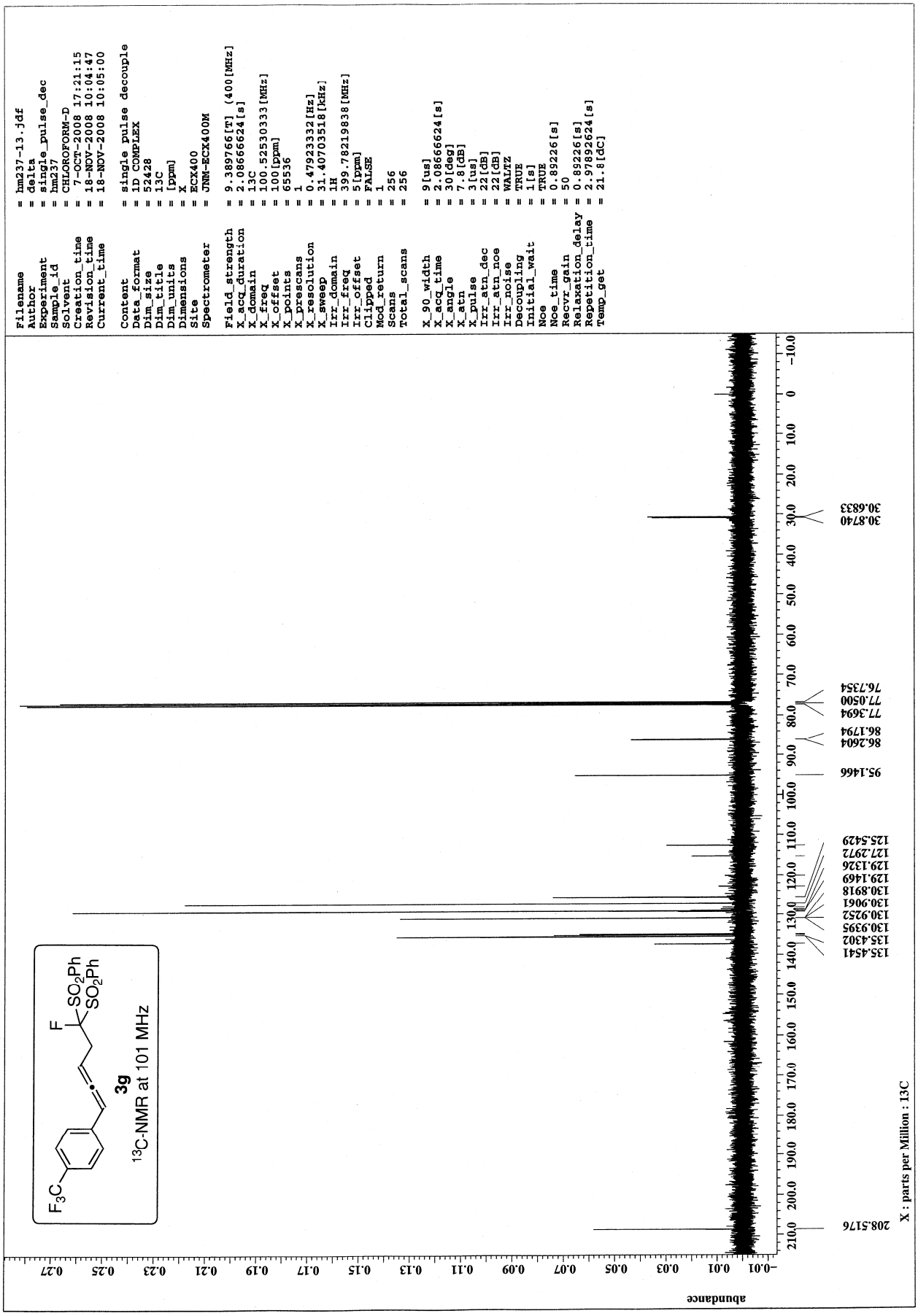

Filename = hm224-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm224
Solvent = CHLOROFORM-D
Creation_time = 3-OCT-2008 22:52:22
Revision_time = 3-OCT-2008 22:59:53
Current_time = 3-OCT-2008 22:59:54
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.35127296[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -150[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 2.846789[Hz]
X_sweep = 46.64179104[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.35127296[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 8[s]
Repetition_time = 8.35127296[s]
Temp_get = 23.6[dC]
MeO
F
SO2Ph
SO2Ph
3e
19F-NMR at 373 MHz
-141.3642
-141.4100
abundance
X : parts per Million : 19F

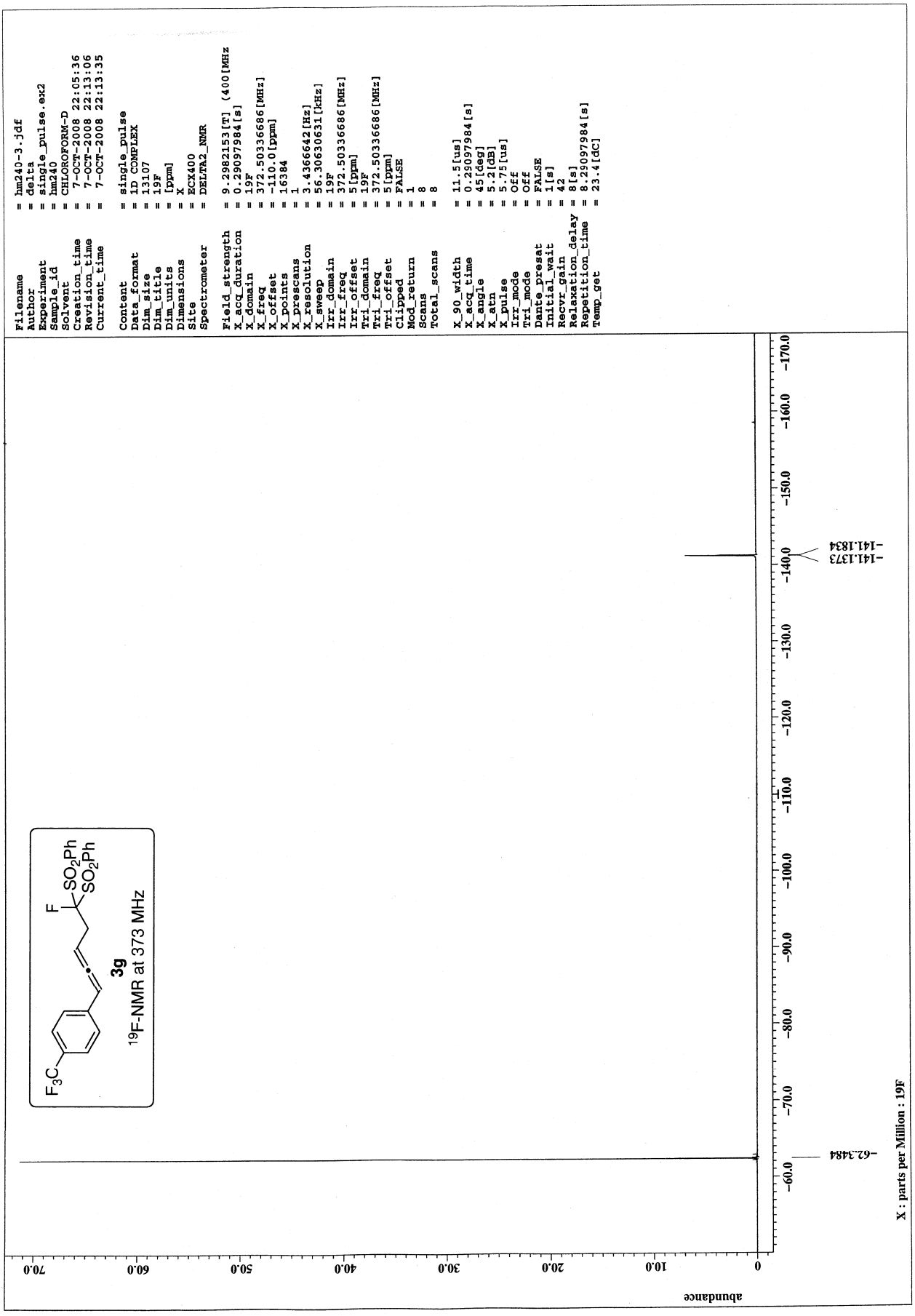

Filename = hm133-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm133
Solvent = CHLOROFORM-D
Creation_time = 2-SEP-2008 18:53:39
Revision_time = 2-SEP-2008 19:20:54
Current_time = 2-SEP-2008 19:21:55
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 23[dC]
F
SO2Ph
SO2Ph
3f
1H-NMR at 400 MHz
abundance
X : parts per Million : 1H
9.812
2.145
2.106
1
0.984
4.412
4.302
2.2647
2.2335
3.1850
3.1827
3.1635
5.4322
5.4143
6.2495
6.2412
6.2325
6.8520
7.9390
7.9363
7.5480
7.5311
7.5292
7.5269

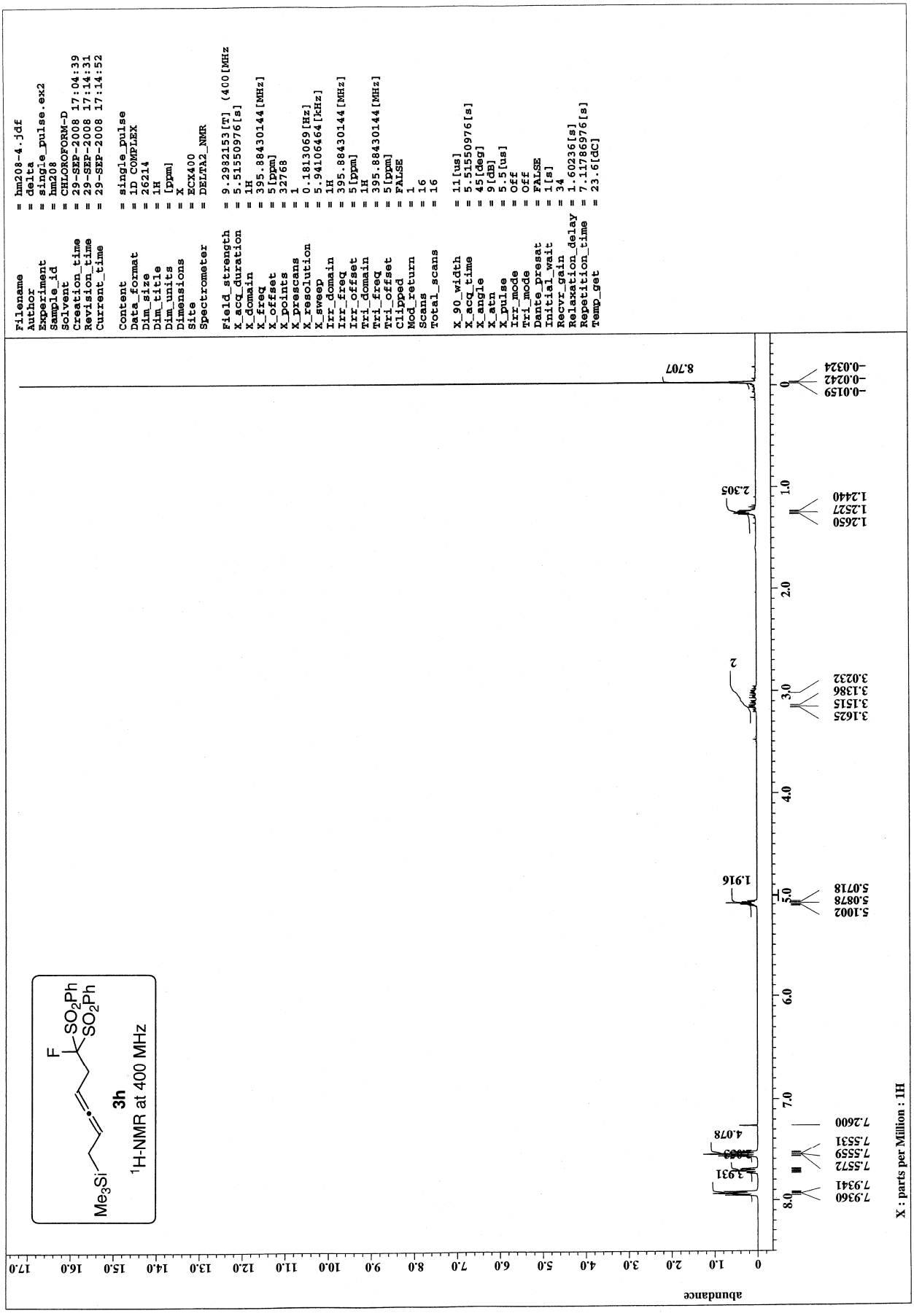

Filename = hm134-13.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm134
Solvent = CHLOROFORM-D
Creation_time = 2-SEP-2008 19:10:01
Revision_time = 18-NOV-2008 11:28:10
Current_time = 18-NOV-2008 11:28:38
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 58
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 23.4[dC]
F
SO2Ph
SO2Ph
3f
13C-NMR at 101 MHz
abundance
X : parts per Million : 13C
208.1934
136.4361
135.3158
129.0564
129.0325
128.9849
115.5125
112.8476
91.1516
82.2130
82.1272
31.1219
30.9360
21.0725
20.9342

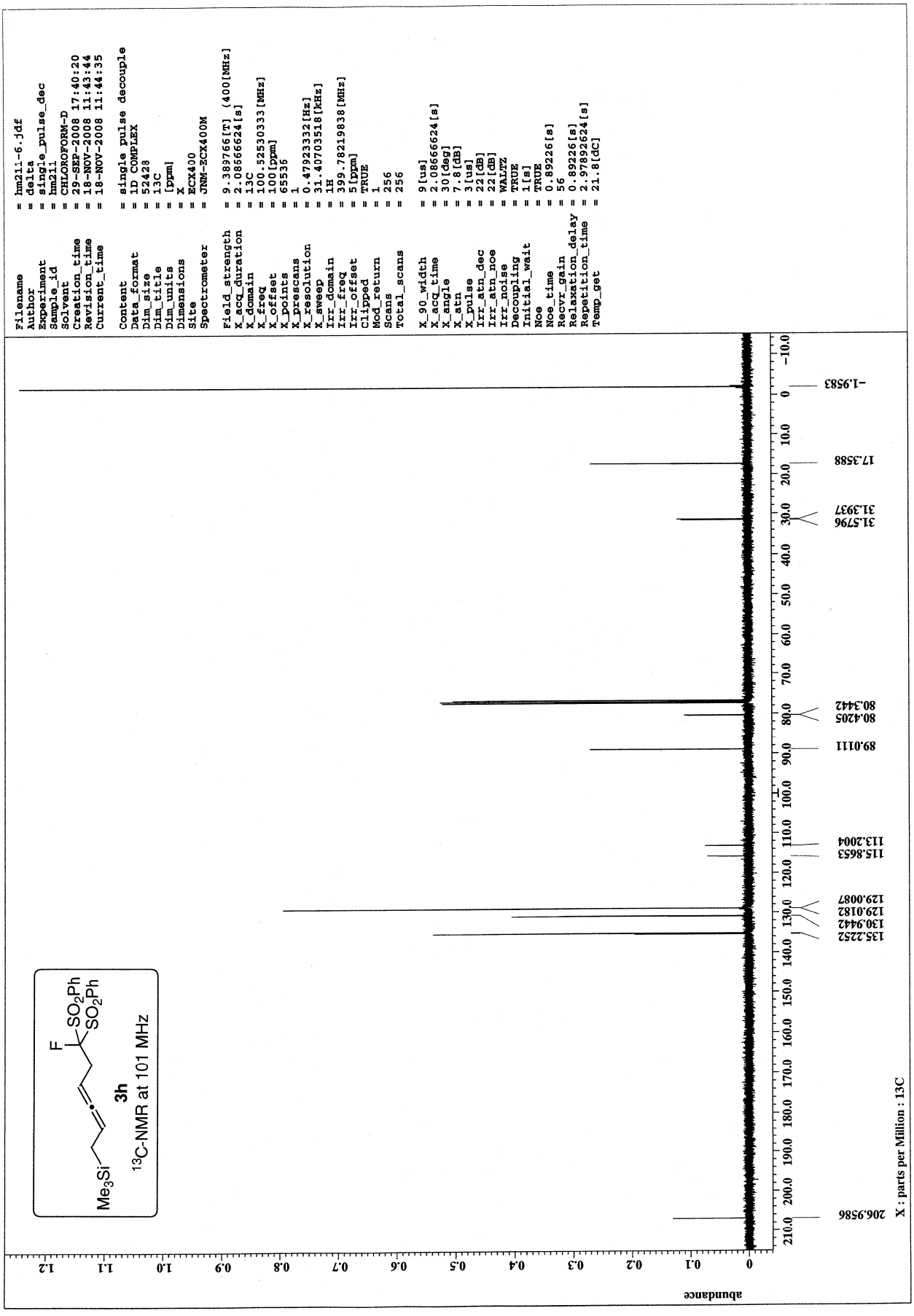

Filename = hm136-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm136
Solvent = CHLOROFORM-D
Creation_time = 3-SEP-2008 12:48:37
Revision_time = 3-SEP-2008 12:52:55
Current_time = 3-SEP-2008 12:52:58
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.50069504[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -150[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 1.99722237[Hz]
X_sweep = 32.72251309[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.50069504[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 50
Relaxation_delay = 8[s]
Repetition_time = 8.50069504[s]
Temp_get = 24.1[dC]
F
SO2Ph
SO2Ph
3f
19F-NMR at 373 MHz
abundance
X : parts per Million : 19F
-141.7753
-141.8182

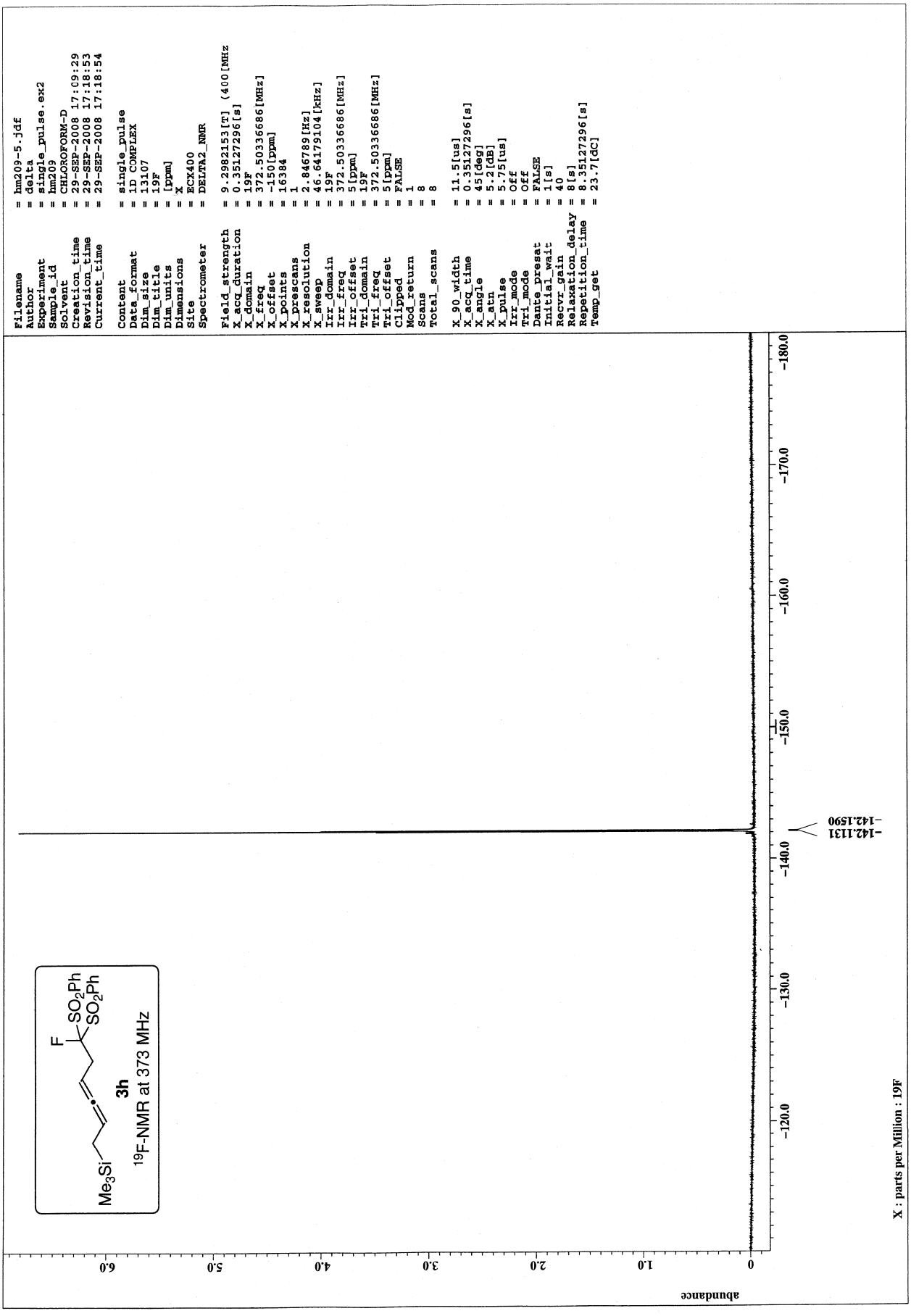

JEOL
Filename = hm236-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm236
Solvent = CHLOROFORM-D
Creation_time = 7-OCT-2008 17:06:00
Revision_time = 7-OCT-2008 17:34:25
Current_time = 7-OCT-2008 17:34:40
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 21.4[dC]
F
SO2Ph
SO2Ph
F3C
3g
1H-NMR at 400 MHz
abundance
X : parts per Million : 1H
0.0000
3.2852
3.2646
3.2316
2.035
0.992
1
6.2151
6.2055
6.1991
5.8025
5.7842
5.7668
2.075
6.216
7.153
4.078
7.9339
7.9202
7.5388
7.5337
7.5319
7.3620
7.2590

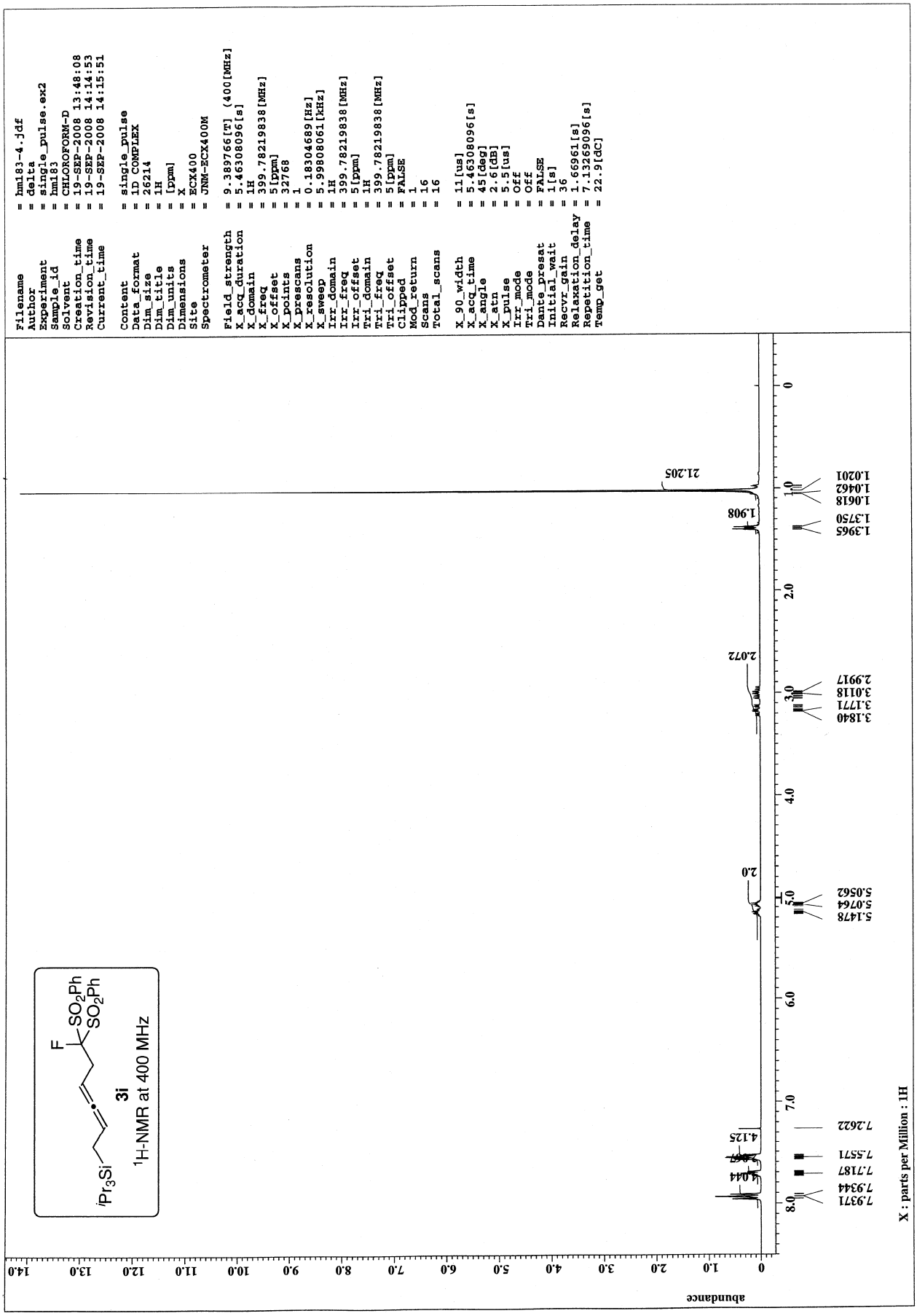

Filename = hm237-13.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm237
Solvent = CHLOROFORM-D
Creation_time = 7-OCT-2008 17:21:15
Revision_time = 18-NOV-2008 10:04:47
Current_time = 18-NOV-2008 10:05:00
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 50
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 21.8[dC]
F
SO2Ph
SO2Ph
F3C
3g
13C-NMR at 101 MHz
208.5176
135.4541
135.4302
130.9395
130.9252
130.9061
130.8918
129.1469
129.1326
127.2972
125.5429
95.1466
86.2604
86.1794
77.3694
77.0500
76.7354
30.8740
30.6833
X : parts per Million : 13C
abundance

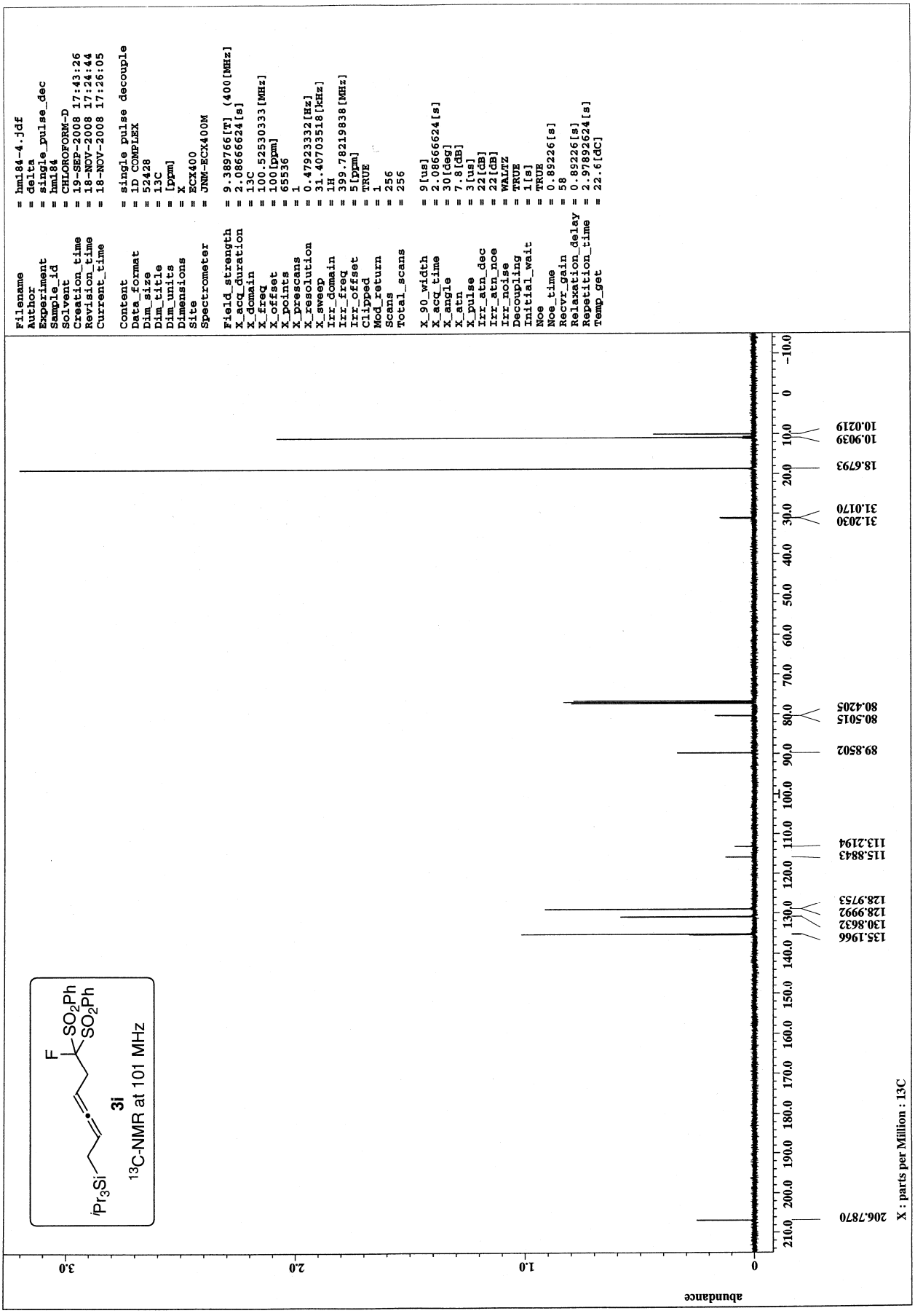

Filename = hm240-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm240
Solvent = CHLOROFORM-D
Creation_time = 7-OCT-2008 22:05:36
Revision_time = 7-OCT-2008 22:13:06
Current_time = 7-OCT-2008 22:13:35
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.29097984[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -110.0[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 3.4366642[Hz]
X_sweep = 56.30630631[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.29097984[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Date_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 8[s]
Repetition_time = 8.29097984[s]
Temp_get = 23.4[dC]
F
SO2Ph
SO2Ph
F3C
3g
19F-NMR at 373 MHz
abundance
X : parts per Million : 19F
-62.3484
-141.1373
-141.1834

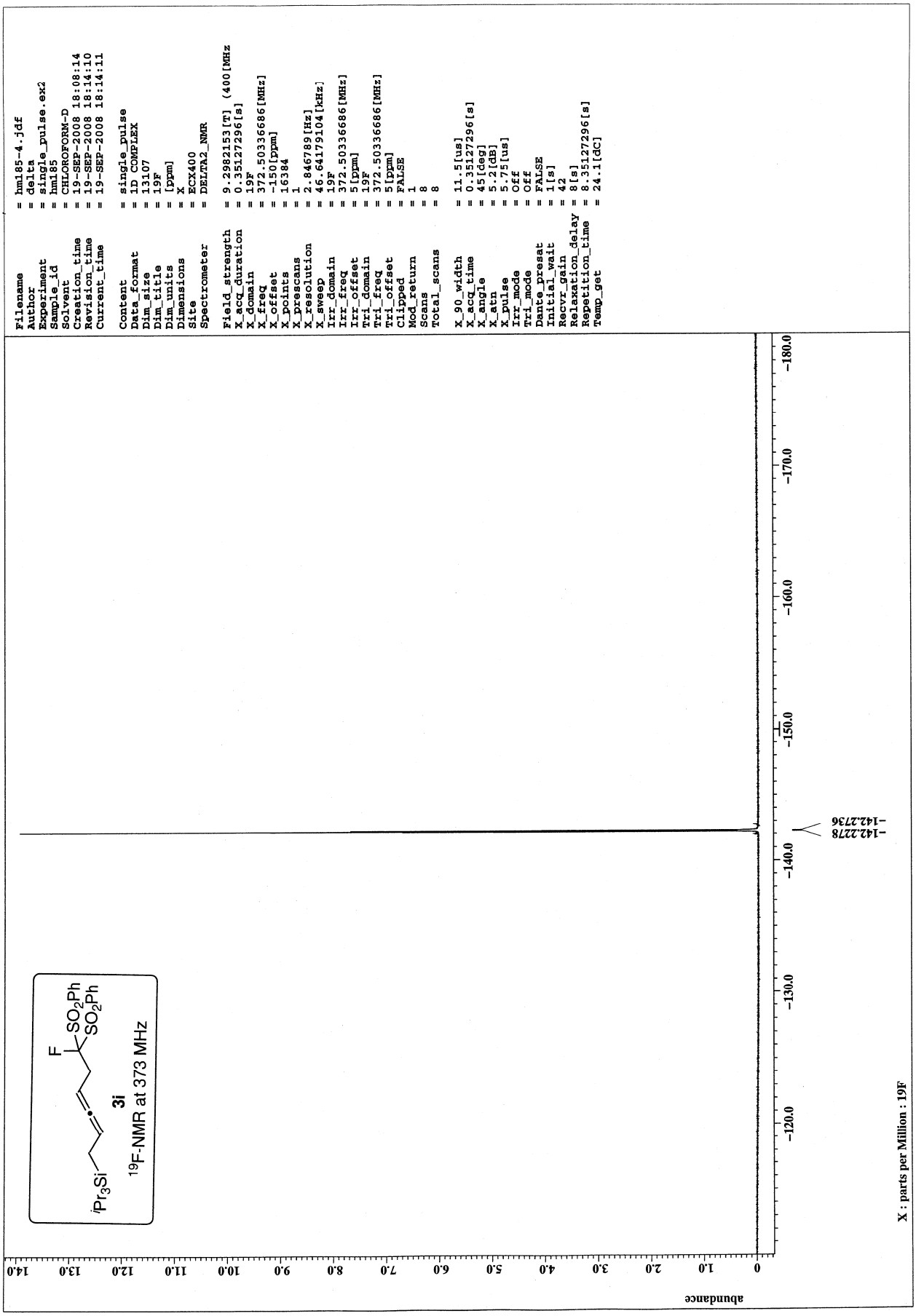

Filename = hm208-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm208
Solvent = CHLOROFORM-D
Creation_time = 29-SEP-2008 17:04:39
Revision_time = 29-SEP-2008 17:14:31
Current_time = 29-SEP-2008 17:14:52
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2932153[T] (400[MHz
X_acq_duration = 5.51550976[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.1813069[Hz]
X_sweep = 5.94106464[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.51550976[s]
X_angle = 45[deg]
X_atn = 9[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 1.60236[s]
Repetition_time = 7.11786976[s]
Temp_get = 23.6[dC]
F
SO2Ph
SO2Ph
Me3Si
3h
1H-NMR at 400 MHz
8.707
2.305
1.916
4.078
3.931
2
abundance
X : parts per Million : 1H

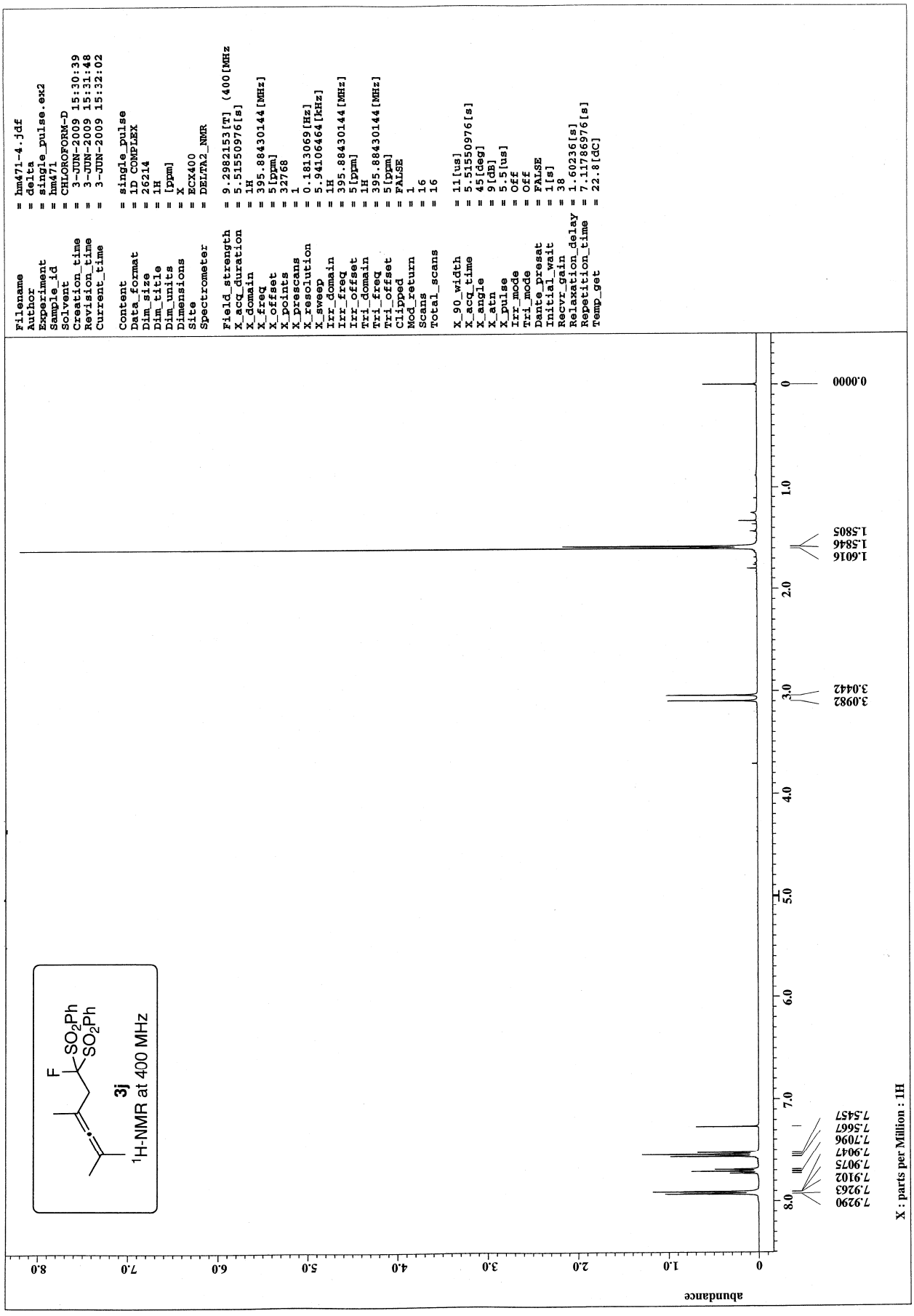

Filename = hm211-6.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm211
Solvent = CHLOROFORM-D
Creation_time = 29-SEP-2008 17:40:20
Revision_time = 18-NOV-2008 11:43:44
Current_time = 18-NOV-2008 11:44:35
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 56
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 21.8[dC]
F
SO2Ph
SO2Ph
Me3Si
3h
13C-NMR at 101 MHz
-1.9583
17.3588
31.5796
31.3937
80.4205
80.3442
89.0111
113.2004
115.8653
129.0087
129.0182
130.9442
135.2252
206.9586
X : parts per Million : 13C
abundance

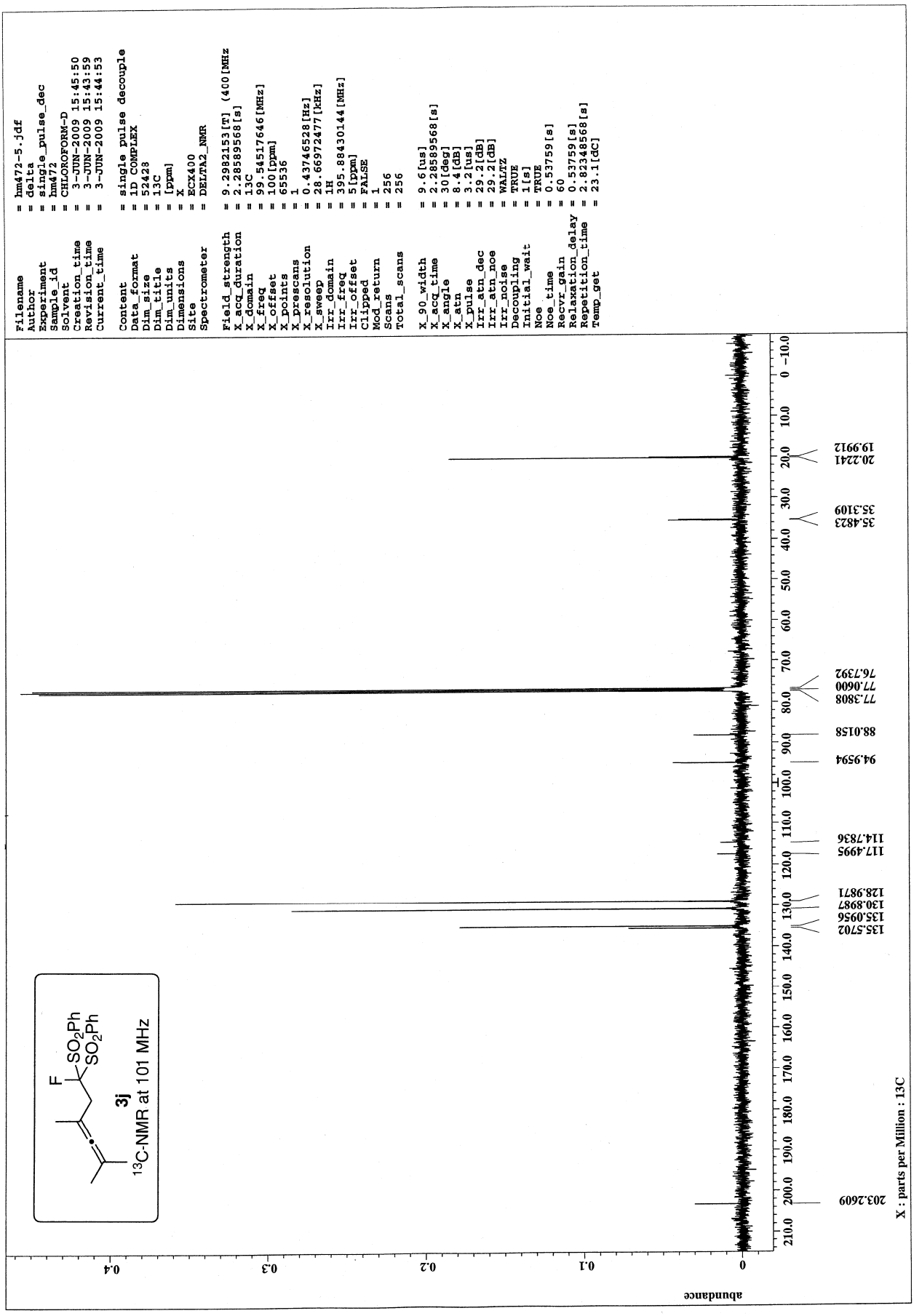

Filename = hm209-5.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm209
Solvent = CHLOROFORM-D
Creation_time = 29-SEP-2008 17:09:29
Revision_time = 29-SEP-2008 17:18:53
Current_time = 29-SEP-2008 17:18:54
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.35127296[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -150[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 2.846789[Hz]
X_sweep = 46.64179104[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.35127296[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 8[s]
Repetition_time = 8.35127296[s]
Temp_get = 23.7[dC]
F
SO2Ph
SO2Ph
Me3Si
3h
19F-NMR at 373 MHz
abundance
-142.1131
-142.1590
X : parts per Million : 19F

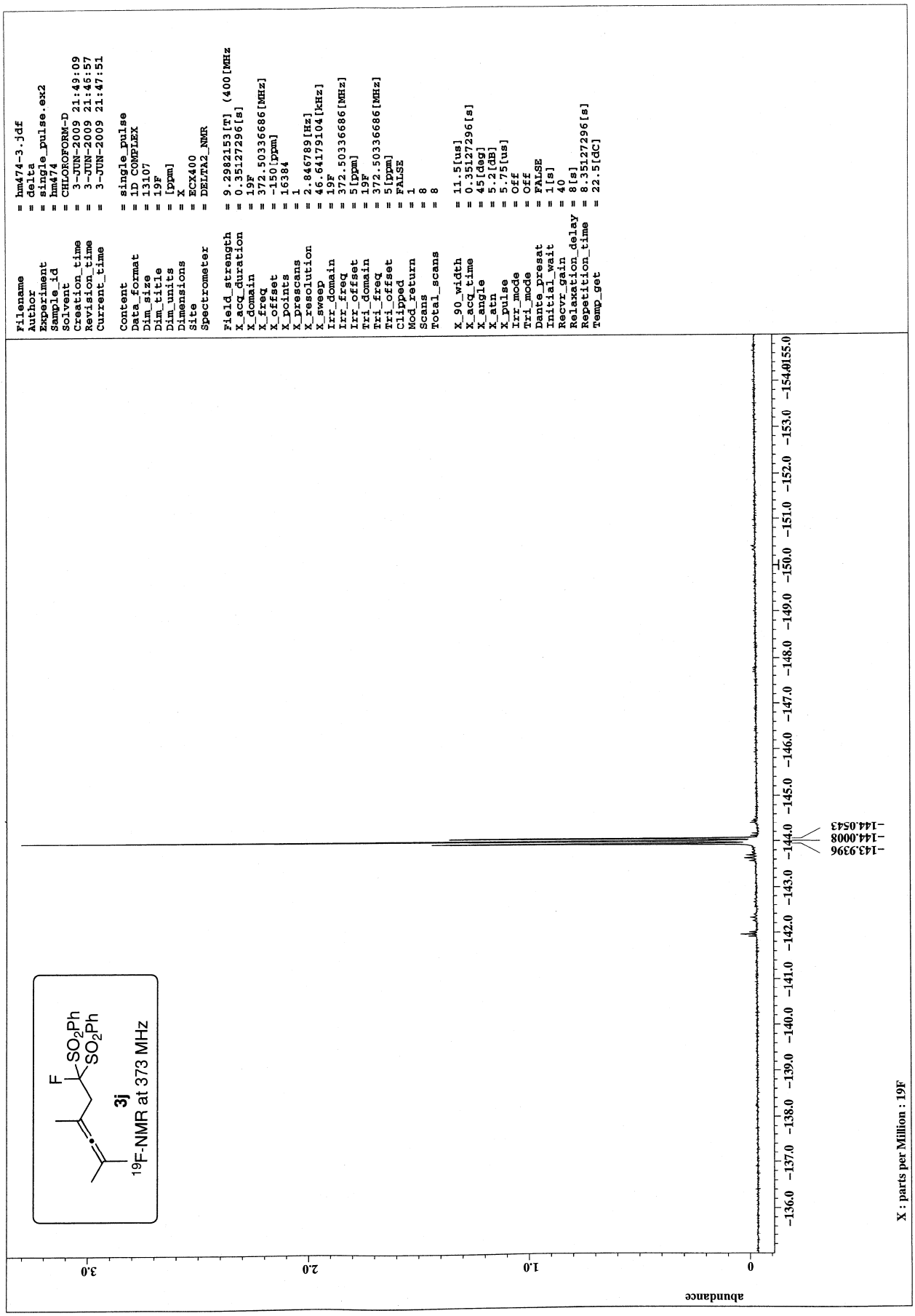

Filename = hm183-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm183
Solvent = CHLOROFORM-D
Creation_time = 19-SEP-2008 13:48:08
Revision_time = 19-SEP-2008 14:14:53
Current_time = 19-SEP-2008 14:15:51
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 22.9[dC]
F
SO2Ph
SO2Ph
iPr3Si
3i
1H-NMR at 400 MHz
21.205
1.908
2.072
2.0
4.125
4.044
4.067
7.9371
7.9344
7.7187
7.5571
7.2622
5.1478
5.0764
5.0562
1.3965
1.3750
1.0618
1.0462
1.0201
3.1840
3.1771
3.0118
2.9917
abundance
X : parts per Million : 1H

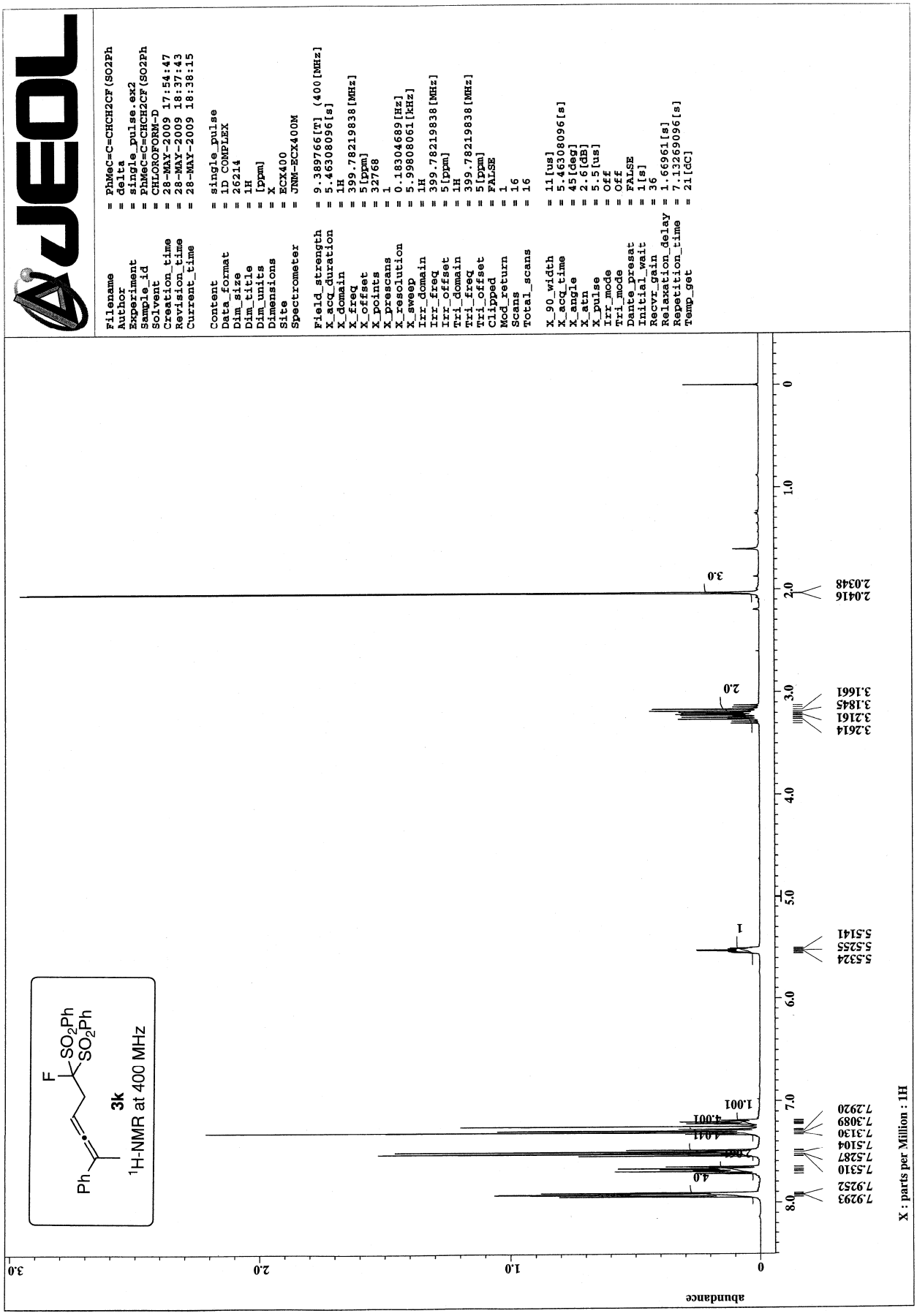

Filename = hm184-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm184
Solvent = CHLOROFORM-D
Creation_time = 19-SEP-2008 17:43:26
Revision_time = 18-NOV-2008 17:24:44
Current_time = 18-NOV-2008 17:26:05
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 58
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 22.6[dC]
F
SO2Ph
SO2Ph
iPr3Si
3i
13C-NMR at 101 MHz
206.7870
135.1966
130.8632
128.9992
128.9753
115.8843
113.2194
89.8502
80.5015
80.4205
31.2030
31.0170
18.6793
10.9039
10.0219
X : parts per Million : 13C
abundance

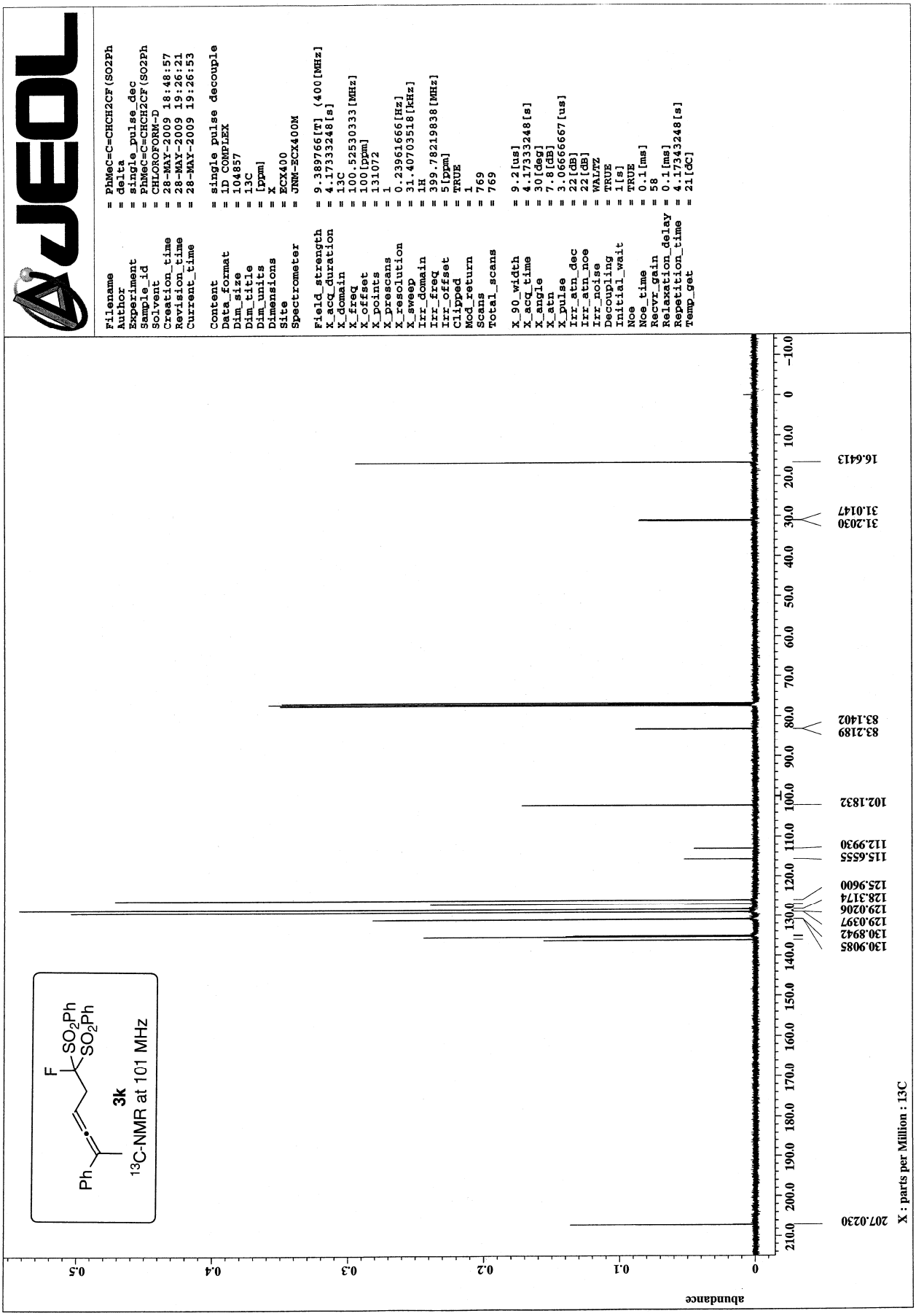

Filename = hm185-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm185
Solvent = CHLOROFORM-D
Creation_time = 19-SEP-2008 18:08:14
Revision_time = 19-SEP-2008 18:14:10
Current_time = 19-SEP-2008 18:14:11
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.35127296[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -150[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 2.846789[Hz]
X_sweep = 46.64179104[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.35127296[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 8[s]
Repetition_time = 8.35127296[s]
Temp_get = 24.1[dC]
F
SO2Ph
SO2Ph
iPr3Si
3i
19F-NMR at 373 MHz
abundance
-142.2278
-142.2736
X : parts per Million : 19F

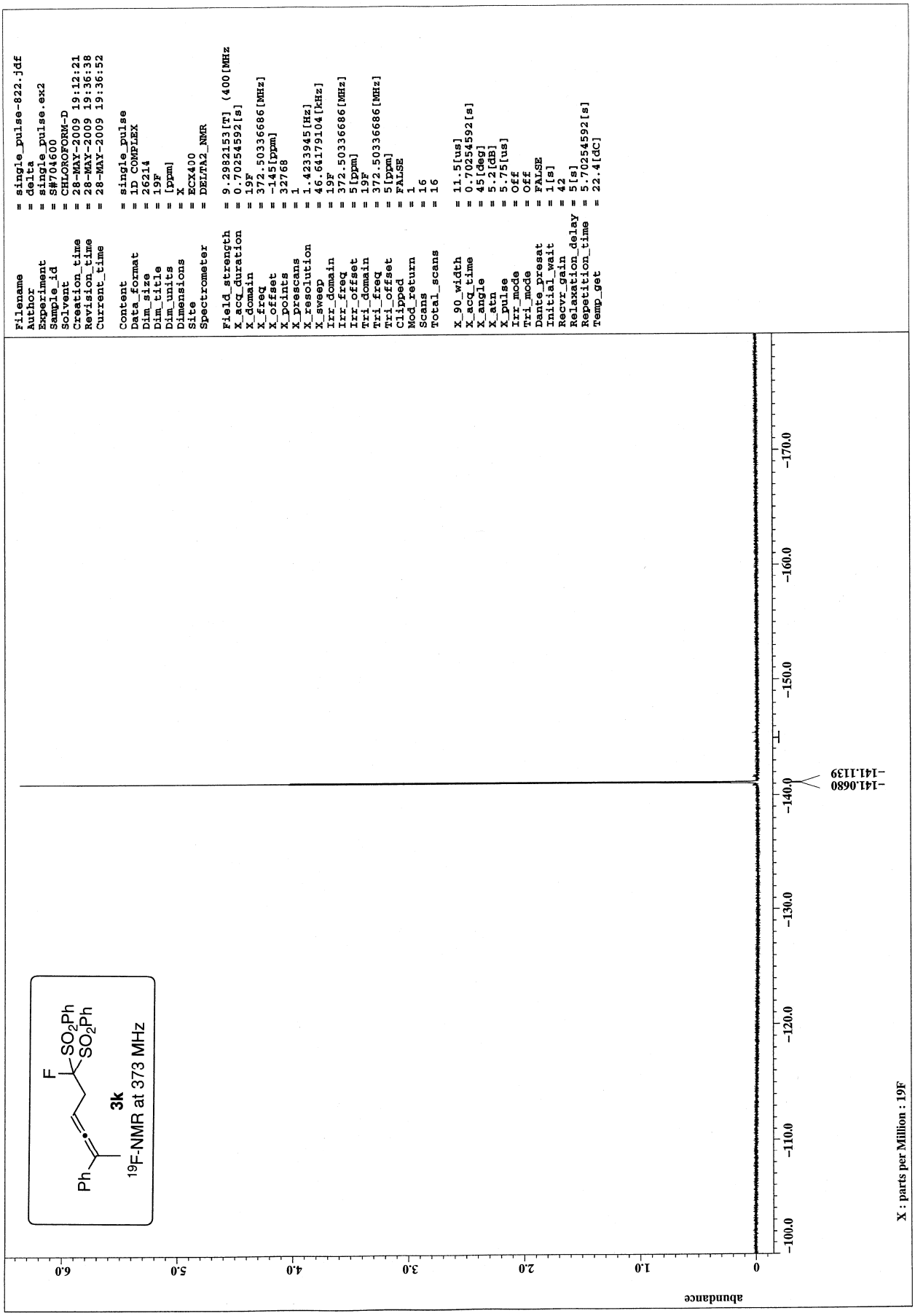

Filename = hm471-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm471
Solvent = CHLOROFORM-D
Creation_time = 3-JUN-2009 15:30:39
Revision_time = 3-JUN-2009 15:31:48
Current_time = 3-JUN-2009 15:32:02
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 5.51550976[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.1813069[Hz]
X_sweep = 5.94106464[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.51550976[s]
X_angle = 45[deg]
X_atn = 9[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 1.60236[s]
Repetition_time = 7.11786976[s]
Temp_get = 22.8[dC]
F
SO2Ph
SO2Ph
3j
1H-NMR at 400 MHz
abundance
X : parts per Million : 1H
7.9290
7.9263
7.9102
7.9075
7.9047
7.7096
7.5667
7.5457
3.0982
3.0442
1.6016
1.5846
1.5805
0.0000

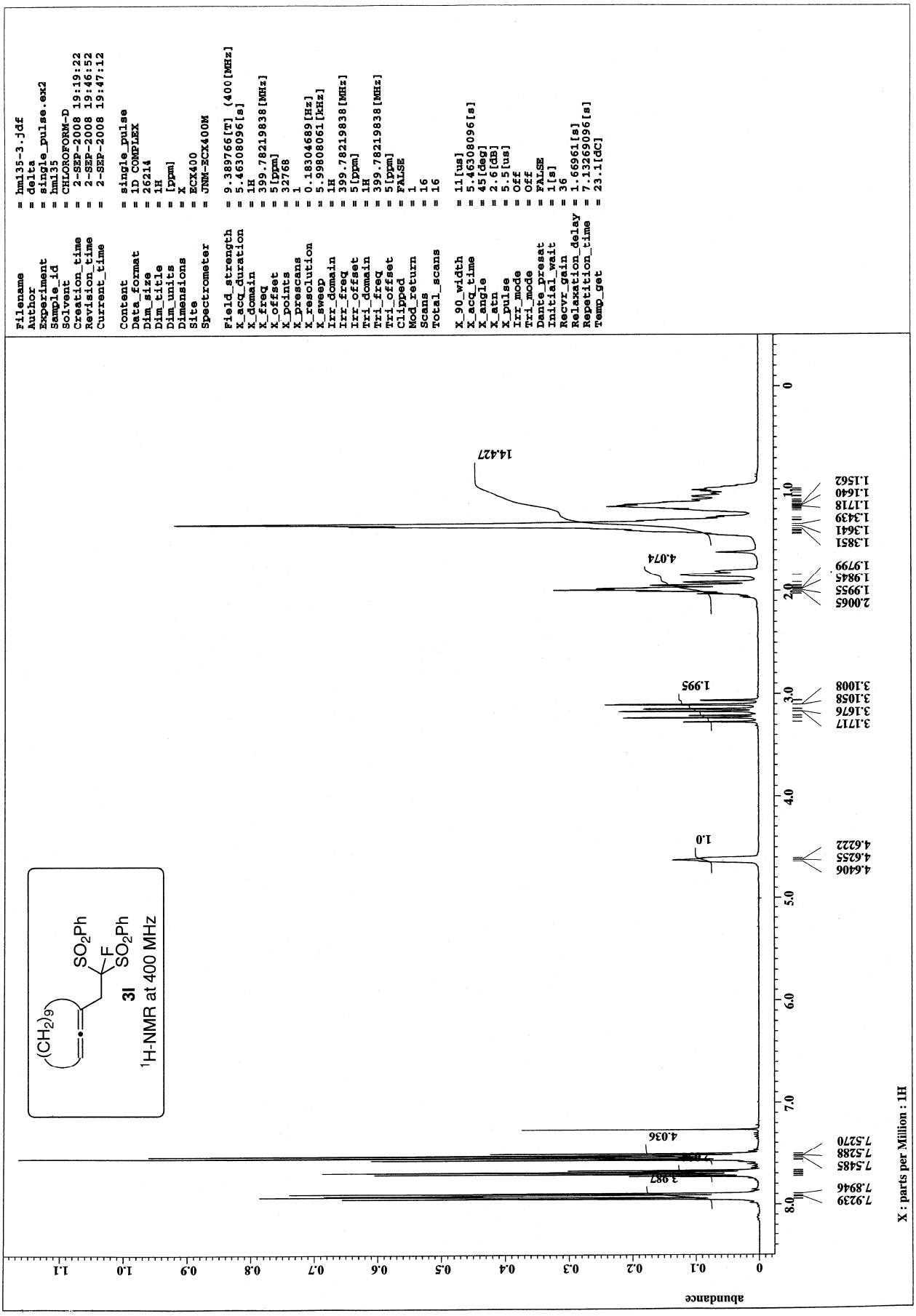

Filename = hm472-5.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm472
Solvent = CHLOROFORM-D
Creation_time = 3-JUN-2009 15:45:50
Revision_time = 3-JUN-2009 15:43:59
Current_time = 3-JUN-2009 15:44:53
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2932153[T] (400[MHz
X_acq_duration = 2.28589568[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.43746528[Hz]
X_sweep = 28.66972477[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9.6[us]
X_acq_time = 2.28589568[s]
X_angle = 30[deg]
X_atn = 8.4[dB]
X_pulse = 3.2[us]
Irr_atn_dec = 29.2[dB]
Irr_atn_noe = 29.2[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.53759[s]
Recvr_gain = 60
Relaxation_delay = 0.53759[s]
Repetition_time = 2.82348568[s]
Temp_get = 23.1[dC]
F
SO2Ph
SO2Ph
3j
13C-NMR at 101 MHz
abundance
X : parts per Million : 13C
203.2609
135.5702
135.0956
130.8987
128.9871
117.4995
114.7836
94.9594
88.0158
77.3808
77.0600
76.7392
35.4823
35.3109
20.2241
19.9912

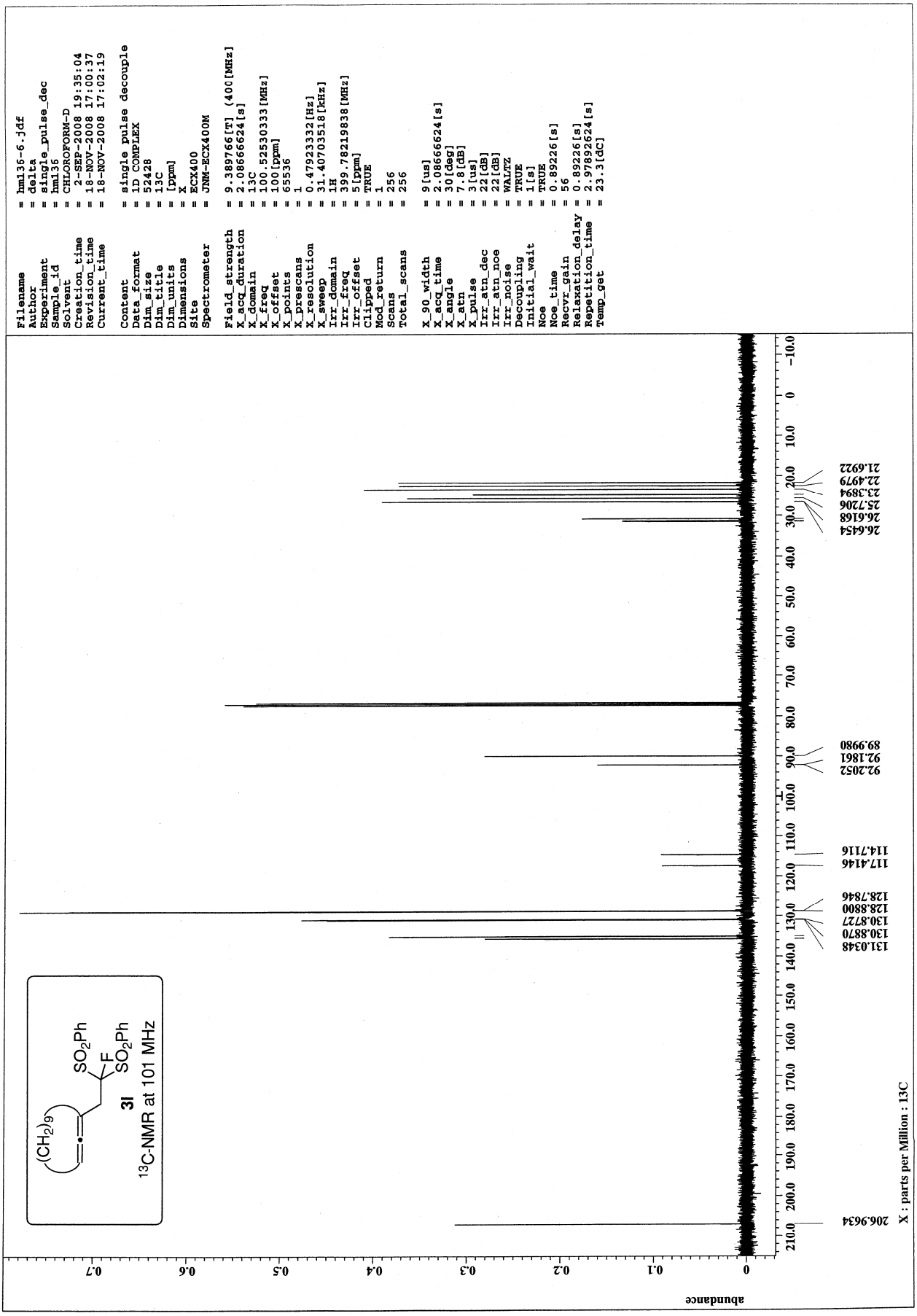

Filename = hm474-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm474
Solvent = CHLOROFORM-D
Creation_time = 3-JUN-2009 21:49:09
Revision_time = 3-JUN-2009 21:46:57
Current_time = 3-JUN-2009 21:47:51
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.35127296[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -150[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 2.846789[Hz]
X_sweep = 46.64179104[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.35127296[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recyc_gain = 40
Relaxation_delay = 8[s]
Repetition_time = 8.35127296[s]
Temp_get = 22.5[dC]
F
SO2Ph
SO2Ph
3j
19F-NMR at 373 MHz
abundance
3.0
2.0
1.0
0
-136.0 -137.0 -138.0 -139.0 -140.0 -141.0 -142.0 -143.0 -144.0 -145.0 -146.0 -147.0 -148.0 -149.0 -150.0 -151.0 -152.0 -153.0 -154.0 -155.0
-143.9396
-144.0008
-144.0543
X : parts per Million : 19F

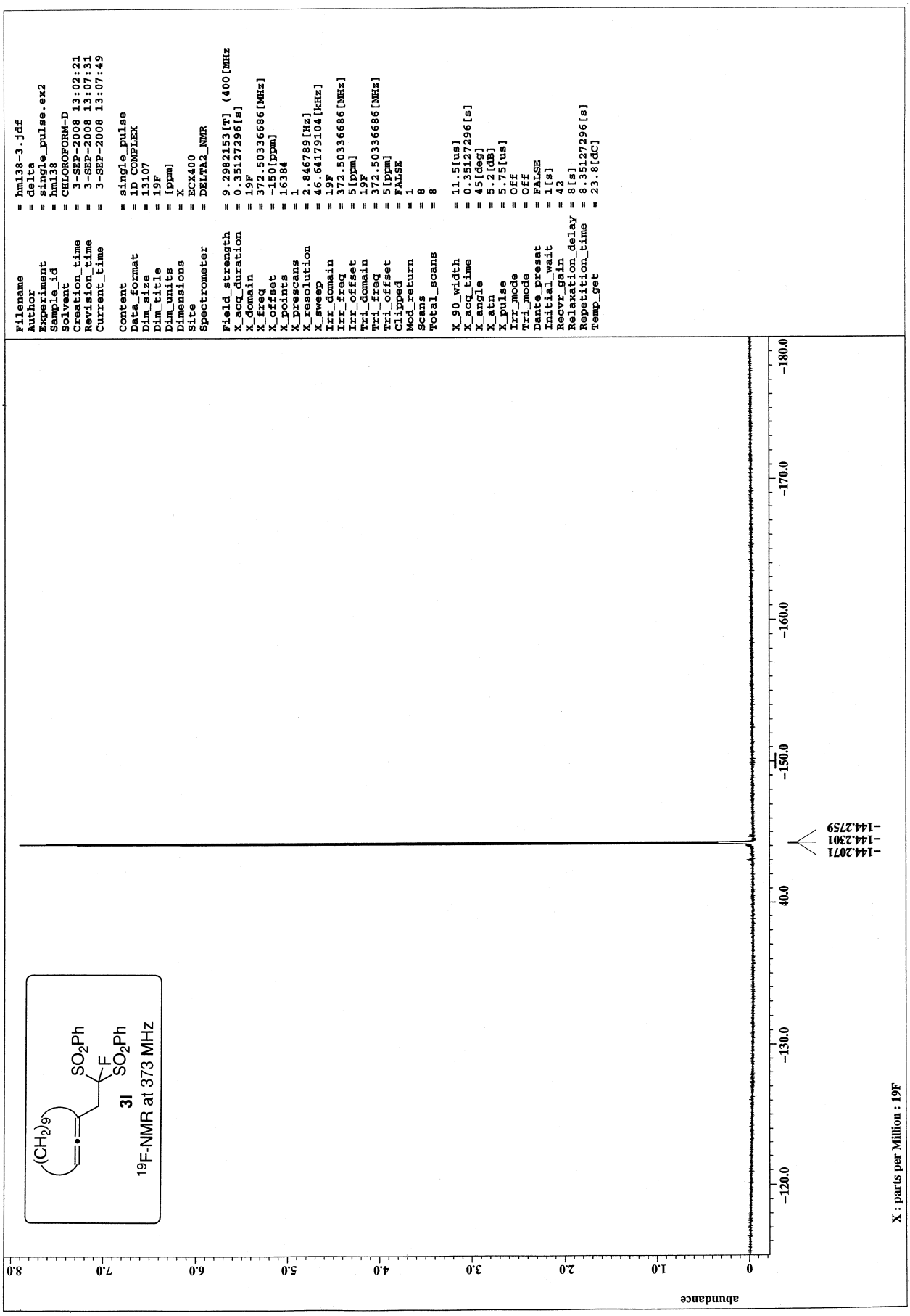

JEOL
Filename = PhMeC=C=CHCH2CF(SO2Ph
Author = delta
Experiment = single_pulse.ex2
Sample_id = PhMeC=C=CHCH2CF(SO2Ph
Solvent = CHLOROFORM-D
Creation_time = 28-MAY-2009 17:54:47
Revision_time = 28-MAY-2009 18:37:43
Current_time = 28-MAY-2009 18:38:15
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 21[dC]
F
SO2Ph
SO2Ph
Ph
3k
1H-NMR at 400 MHz
abundance
X : parts per Million : 1H
7.9293
7.9252
7.5310
7.5287
7.5104
7.3130
7.3089
7.2920
5.5324
5.5255
5.5141
3.2614
3.2161
3.1845
3.1661
2.0416
2.0348
4.0
4.041
4.001
1.001
3.0
2.0
1
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0

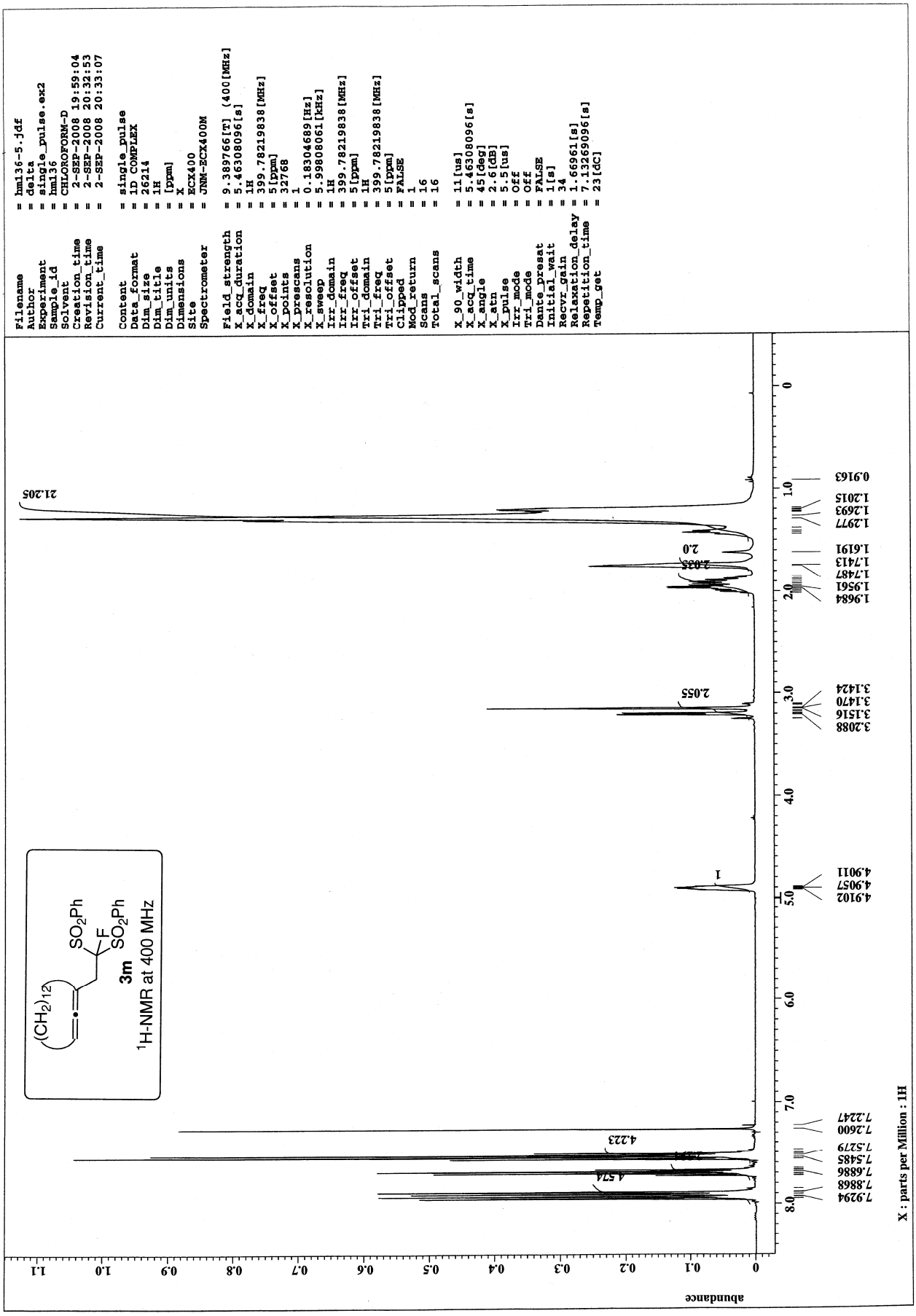

JEOL
Filename = PhMeC=C=CHCH2CF(SO2Ph
Author = delta
Experiment = single_pulse_dec
Sample_id = PhMeC=C=CHCH2CF(SO2Ph
Solvent = CHLOROFORM-D
Creation_time = 28-MAY-2009 18:48:57
Revision_time = 28-MAY-2009 19:26:21
Current_time = 28-MAY-2009 19:26:53
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 104857
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 4.17333248[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 131072
X_prescans = 1
X_resolution = 0.23961666[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 769
Total_scans = 769
X_90_width = 9.2[us]
X_acq_time = 4.17333248[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3.06666667[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.1[ms]
Recvr_gain = 58
Relaxation_delay = 0.1[ms]
Repetition_time = 4.17343248[s]
Temp_get = 21[dC]
F
SO2Ph
SO2Ph
Ph
3k
13C-NMR at 101 MHz
16.6413
31.2030
31.0147
83.2189
83.1402
102.1832
115.6555
112.9930
125.9600
128.3174
129.0206
129.0397
130.8942
130.9085
207.0230
X : parts per Million : 13C
abundance

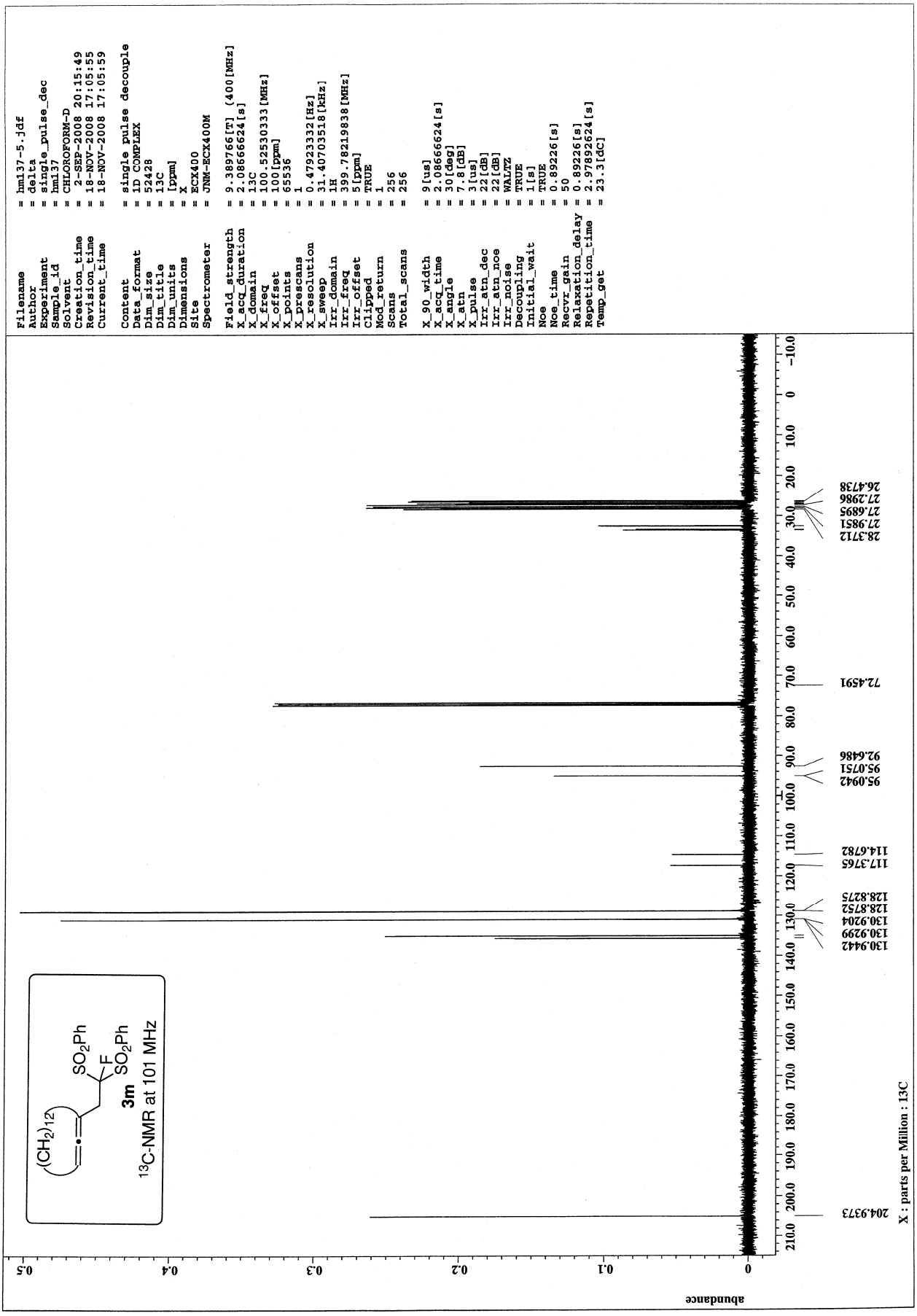

Filename = single_pulse-822.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = S#704600
Solvent = CHLOROFORM-D
Creation_time = 28-MAY-2009 19:12:21
Revision_time = 28-MAY-2009 19:36:38
Current_time = 28-MAY-2009 19:36:52
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2932153[T] (400[MHz
X_acq_duration = 0.70254592[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -145[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 1.4233945[Hz]
X_sweep = 46.64179104[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11.5[us]
X_acq_time = 0.70254592[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 5.70254592[s]
Temp_get = 22.4[dC]
F
SO2Ph
SO2Ph
Ph
3k
19F-NMR at 373 MHz
abundance
-141.0680
-141.1139
X : parts per Million : 19F

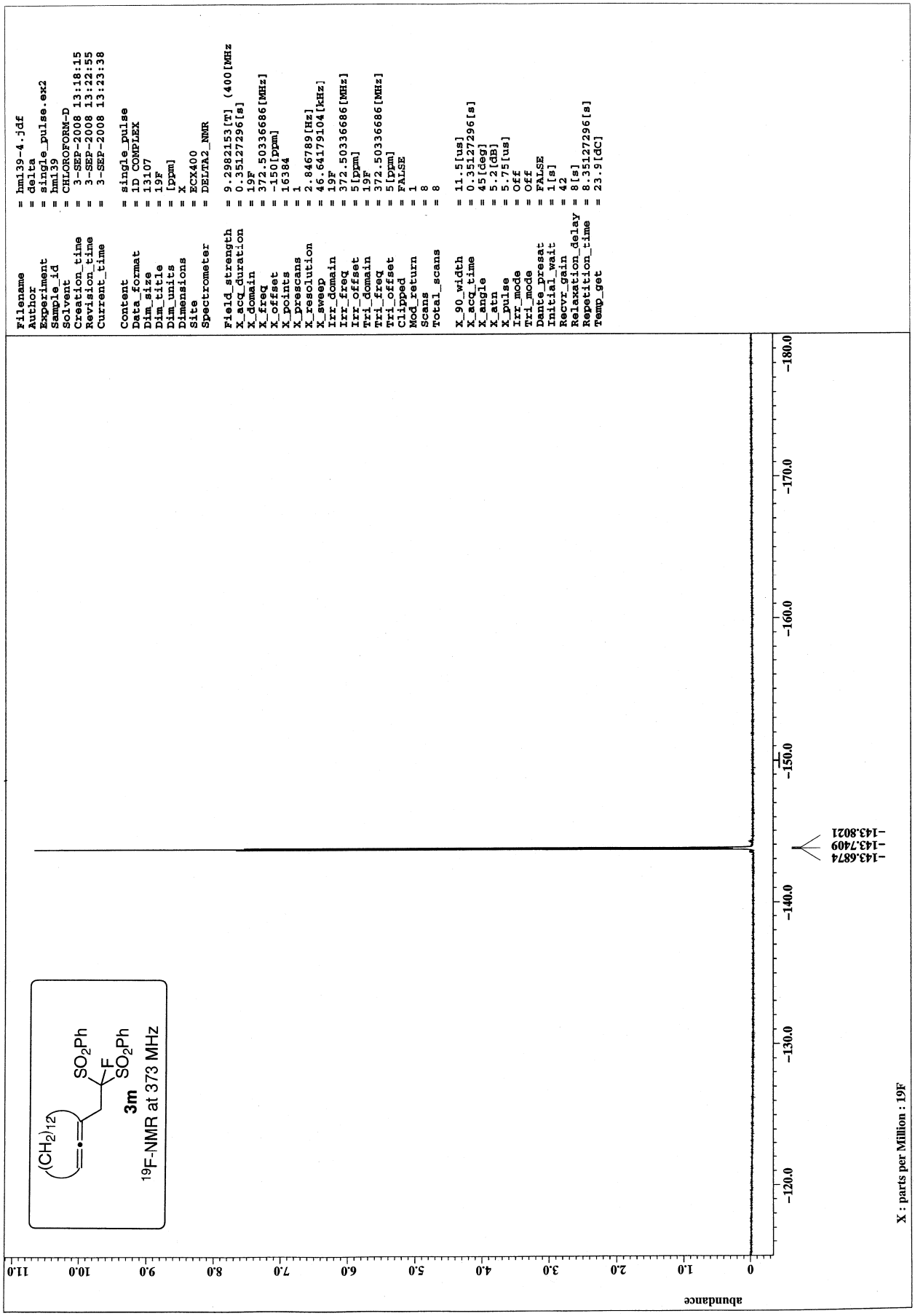

Filename = hm135-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm135
Solvent = CHLOROFORM-D
Creation_time = 2-SEP-2008 19:19:22
Revision_time = 2-SEP-2008 19:46:52
Current_time = 2-SEP-2008 19:47:12
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 23.1[dC]
(CH2)9
SO2Ph
F
SO2Ph
3l
1H-NMR at 400 MHz
abundance
X : parts per Million : 1H
14.427
4.074
1.995
4.036
1.0
3.987
7.9239
7.8946
7.5485
7.5288
7.5270
4.6406
4.6255
4.6222
3.1717
3.1676
3.1058
3.1008
2.0065
1.9955
1.9845
1.9799
1.3851
1.3641
1.3439
1.1718
1.1640
1.1562

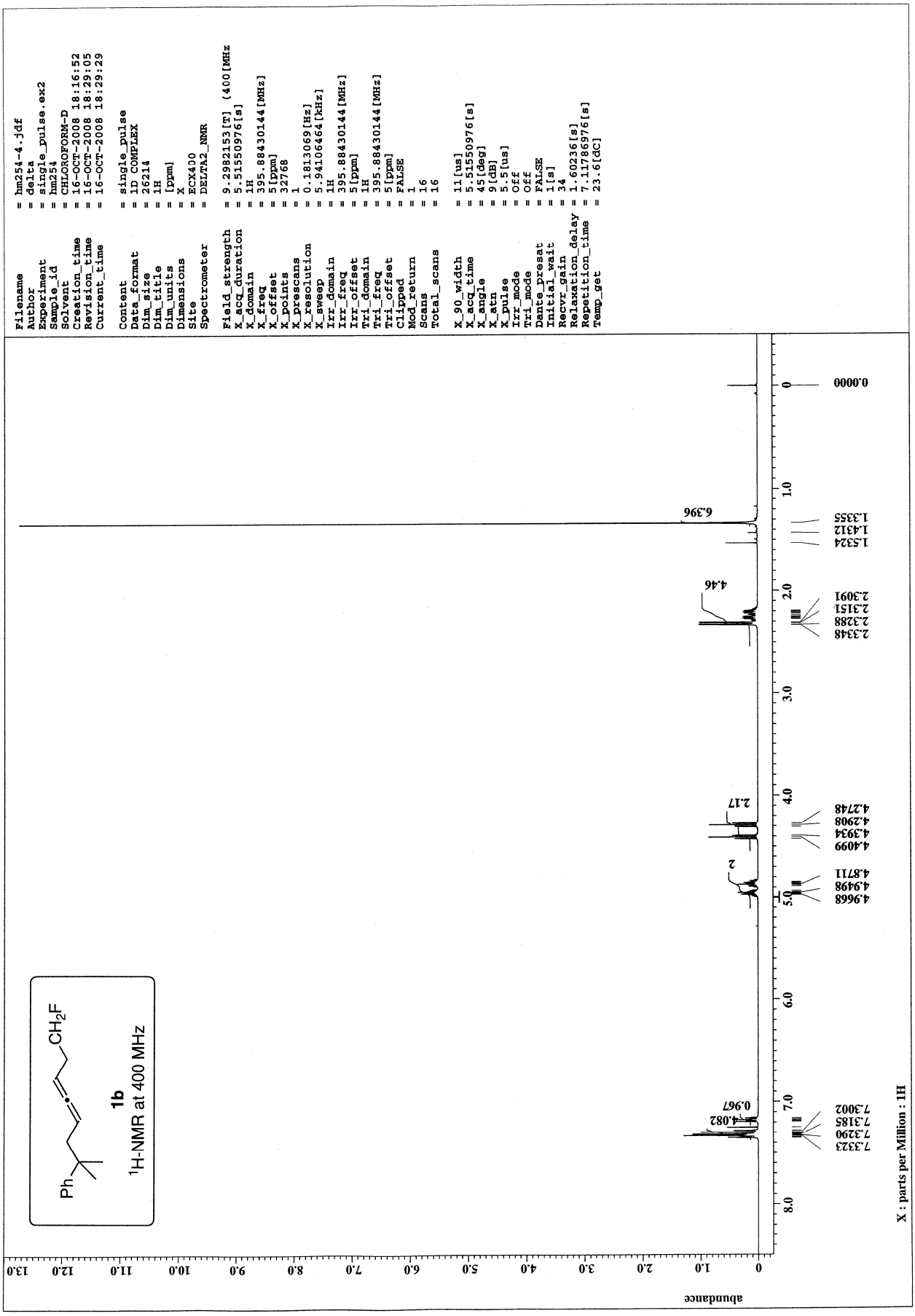

Filename = hm136-6.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm136
Solvent = CHLOROFORM-D
Creation_time = 2-SEP-2008 19:35:04
Revision_time = 18-NOV-2008 17:00:37
Current_time = 18-NOV-2008 17:02:19
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.525303333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 56
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 23.3[dC]
(CH2)9
SO2Ph
F
SO2Ph
3l
13C-NMR at 101 MHz
206.9634
131.0348
130.8870
130.8727
128.8800
128.7846
117.4146
114.7116
92.2052
92.1861
89.9980
26.6454
26.6168
25.7206
23.3894
22.4979
21.6922
X : parts per Million : 13C
abundance

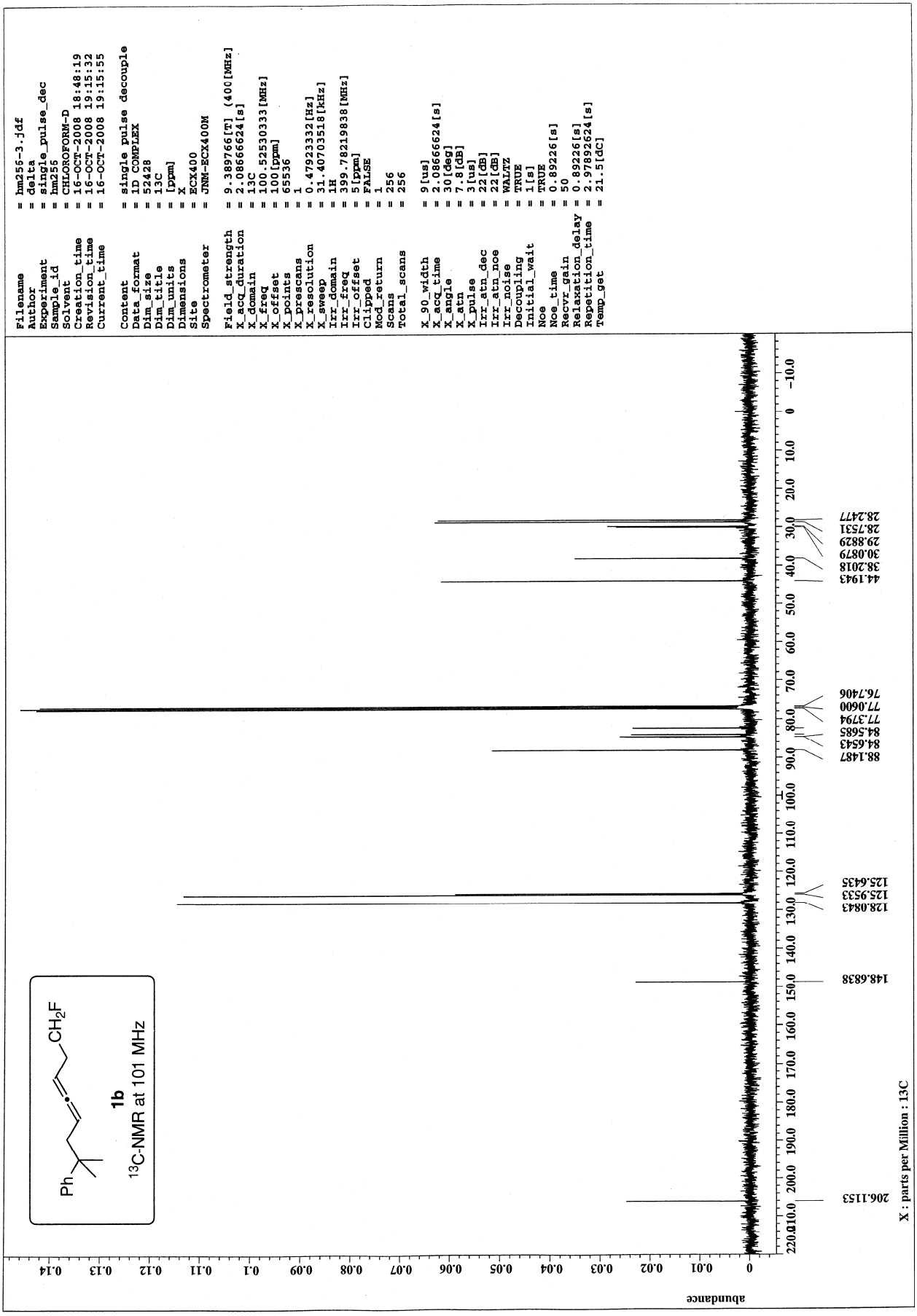

Filename = hm138-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm138
Solvent = CHLOROFORM-D
Creation_time = 3-SEP-2008 13:02:21
Revision_time = 3-SEP-2008 13:07:31
Current_time = 3-SEP-2008 13:07:49
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.35127296[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -150[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 2.846789[Hz]
X_sweep = 46.64179104[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.35127296[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 8[s]
Repetition_time = 8.35127296[s]
Temp_get = 23.8[dC]
(CH2)9
SO2Ph
F
SO2Ph
3l
19F-NMR at 373 MHz
abundance
X : parts per Million : 19F
-144.2071
-144.2301
-144.2759

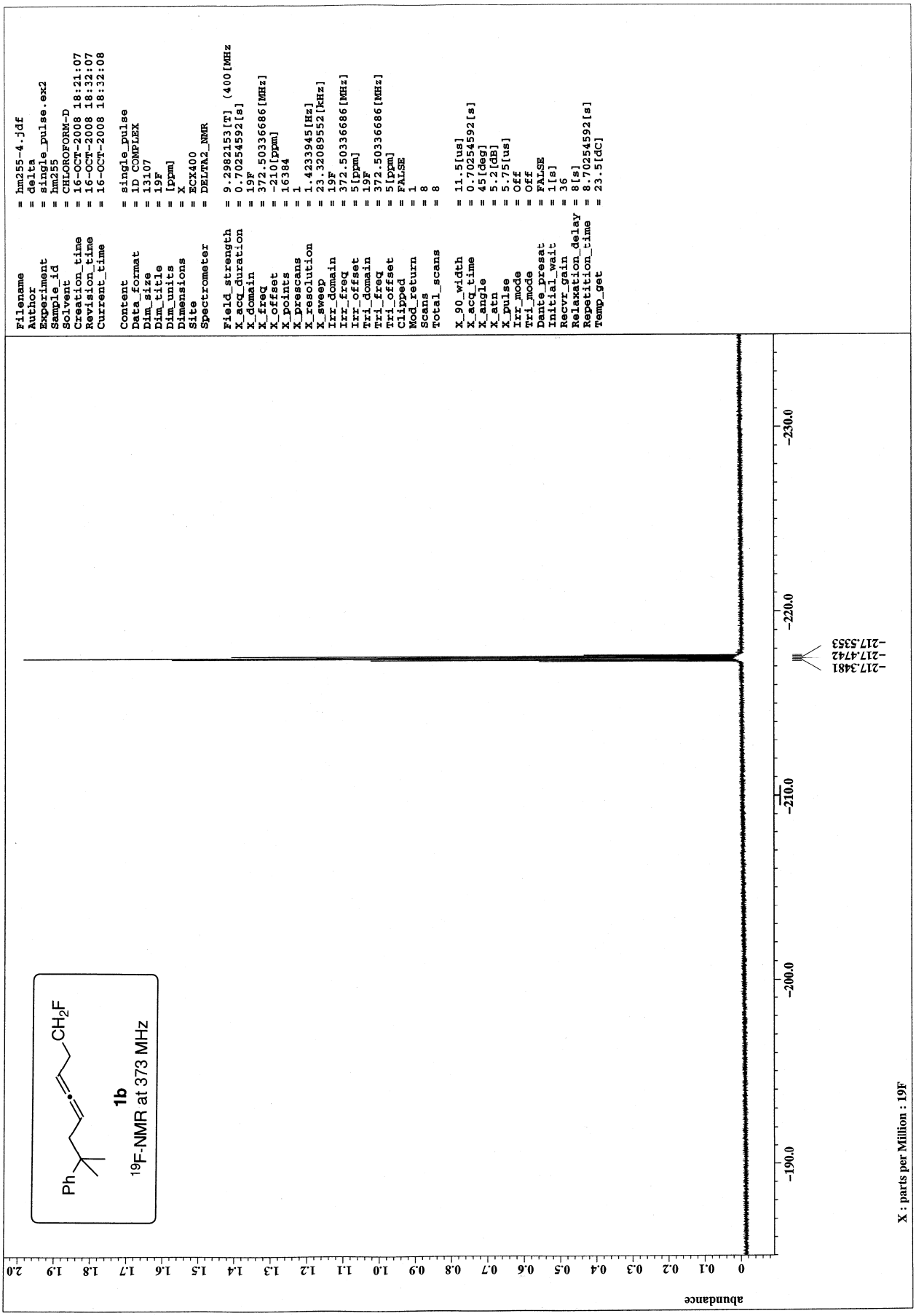

Filename = hm136-5.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm136
Solvent = CHLOROFORM-D
Creation_time = 2-SEP-2008 19:59:04
Revision_time = 2-SEP-2008 20:32:53
Current_time = 2-SEP-2008 20:33:07
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 23[dC]
(CH2)12
SO2Ph
F
SO2Ph
3m
1H-NMR at 400 MHz
21.205
2.035
2.0
2.055
1
4.223
4.574
abundance
X : parts per Million : 1H
7.9294
7.8868
7.6886
7.5485
7.5279
7.2600
7.2247
4.9102
4.9057
4.9011
3.2088
3.1516
3.1470
3.1424
1.9684
1.9561
1.7487
1.7413
1.6191
1.2977
1.2693
1.2015
0.9163

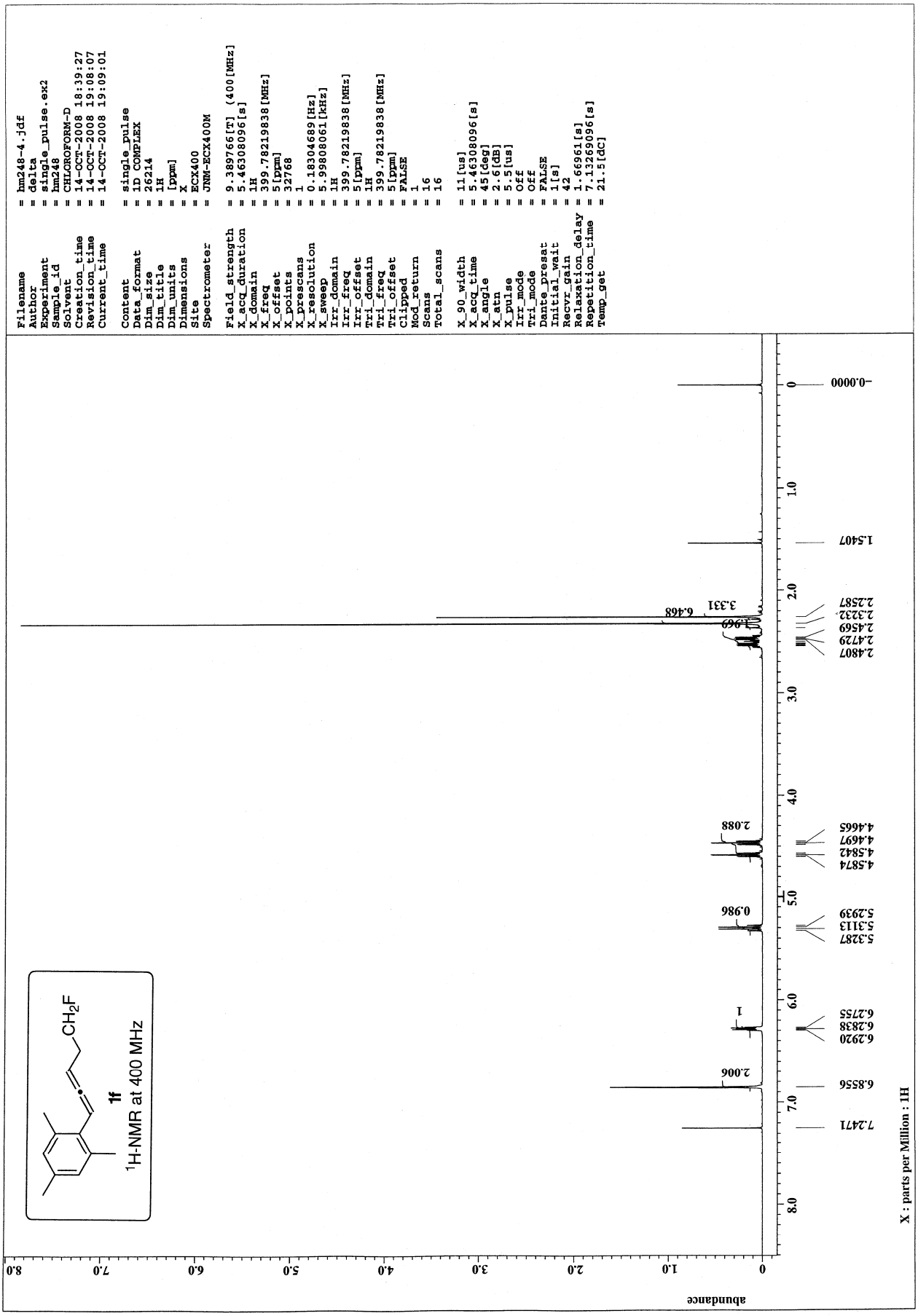

Filename = hm137-5.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm137
Solvent = CHLOROFORM-D
Creation_time = 2-SEP-2008 20:15:49
Revision_time = 18-NOV-2008 17:05:55
Current_time = 18-NOV-2008 17:05:59
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.525303333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 50
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 23.3[dC]
(CH2)12
SO2Ph
F
SO2Ph
3m
13C-NMR at 101 MHz
204.9373
130.9442
130.9299
130.9204
128.8752
128.8275
117.3765
114.6782
95.0942
95.0751
92.6486
72.4591
28.3712
27.9851
27.6895
27.2986
26.4738
X : parts per Million : 13C
abundance

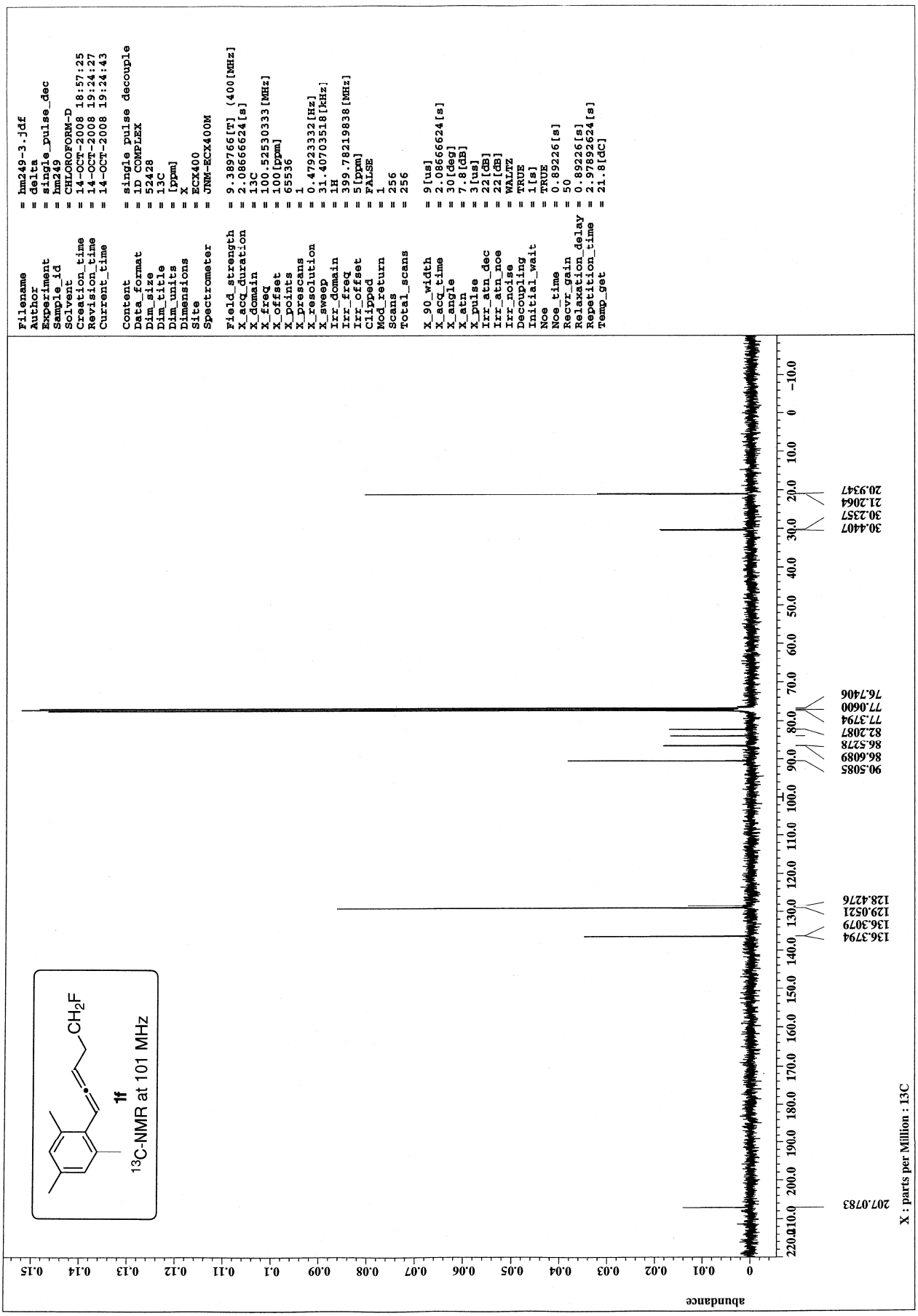

Filename = hm139-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm139
Solvent = CHLOROFORM-D
Creation_time = 3-SEP-2008 13:18:15
Revision_time = 3-SEP-2008 13:22:55
Current_time = 3-SEP-2008 13:23:38
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.35127296[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -150[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 2.846789[Hz]
X_sweep = 46.64179104[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.35127296[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 8[s]
Repetition_time = 8.35127296[s]
Temp_get = 23.9[dC]
(CH2)12
SO2Ph
F
SO2Ph
3m
19F-NMR at 373 MHz
abundance
X : parts per Million : 19F
-143.6874
-143.7409
-143.8021

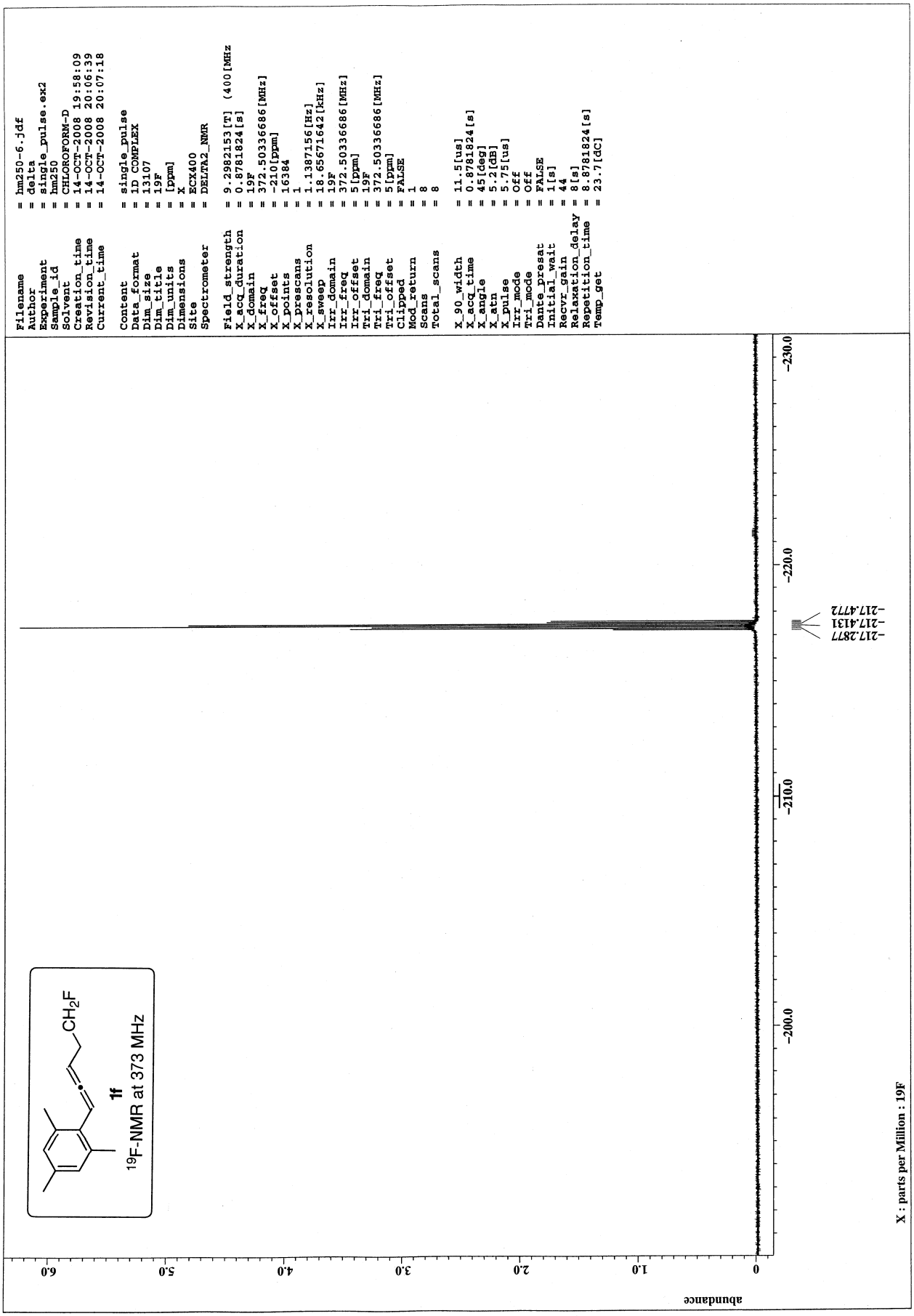

Filename = hm254-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm254
Solvent = CHLOROFORM-D
Creation_time = 16-OCT-2008 18:16:52
Revision_time = 16-OCT-2008 18:29:05
Current_time = 16-OCT-2008 18:29:29
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 5.51550976[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.1813069[Hz]
X_sweep = 5.94106464[kHz]
Irr_domain = 1H
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.51550976[s]
X_angle = 45[deg]
X_atn = 9[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 1.60236[s]
Repetition_time = 7.11786976[s]
Temp_get = 23.6[dC]
CH2F
Ph
1b
1H-NMR at 400 MHz
6.396
4.46
2.17
2
4.082
0.967
0.0000
1.3355
1.4312
1.5324
2.3091
2.3151
2.3288
2.3348
4.2748
4.3934
4.4099
4.2908
4.8711
4.9498
4.9668
7.3002
7.3185
7.3290
7.3323
abundance
X : parts per Million : 1H

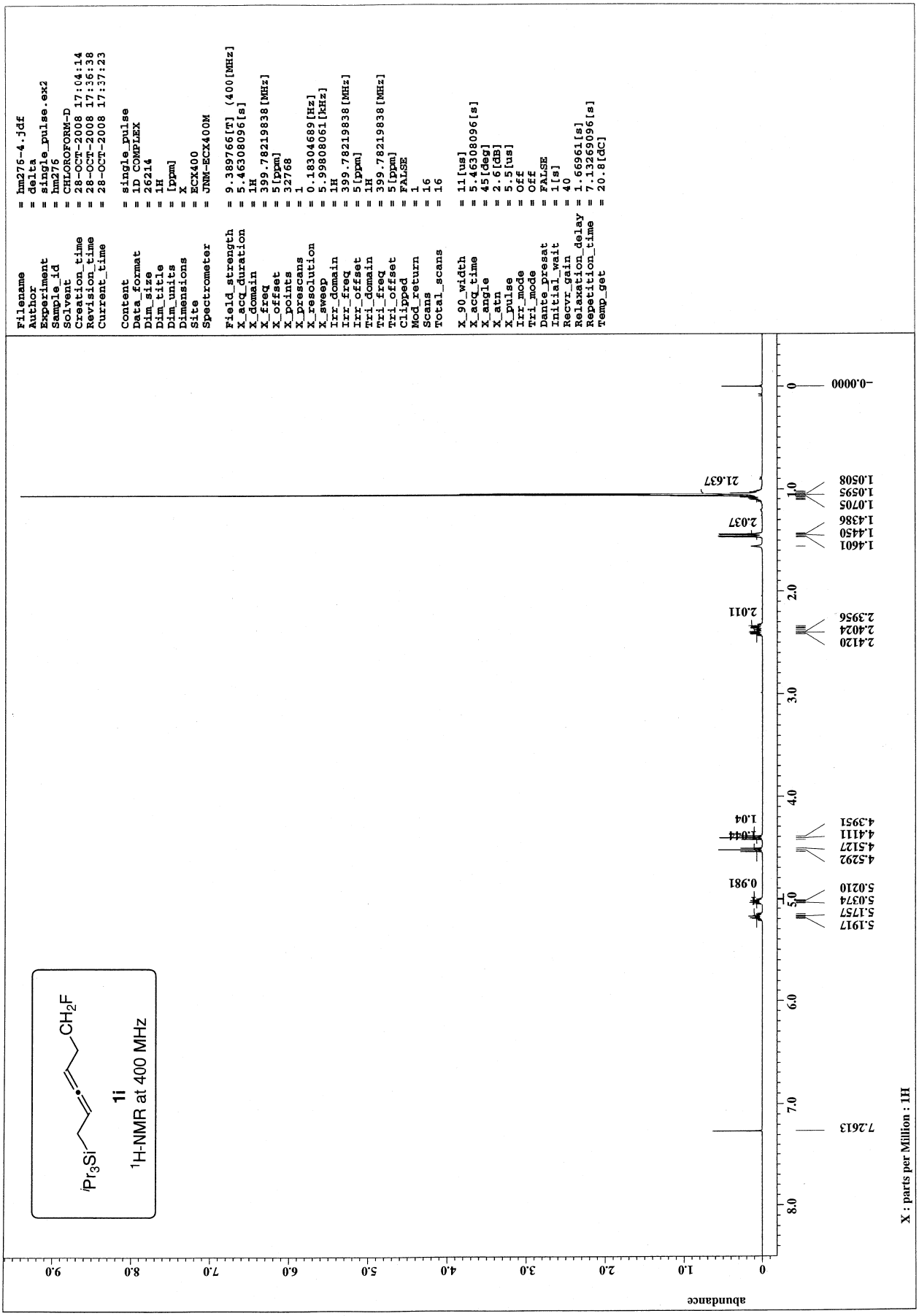

Filename = hm255-3.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm255
Solvent = CHLOROFORM-D
Creation_time = 16-OCT-2008 18:48:19
Revision_time = 16-OCT-2008 19:15:32
Current_time = 16-OCT-2008 19:15:55
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.525303333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 50
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 21.5[dC]
Ph
CH2F
1b
13C-NMR at 101 MHz
206.1153
148.6838
128.0843
125.9533
125.6435
88.1487
84.6543
84.5685
77.3794
77.0600
76.7406
44.1943
38.2018
30.0879
29.8829
28.7531
28.2477
X : parts per Million : 13C
abundance

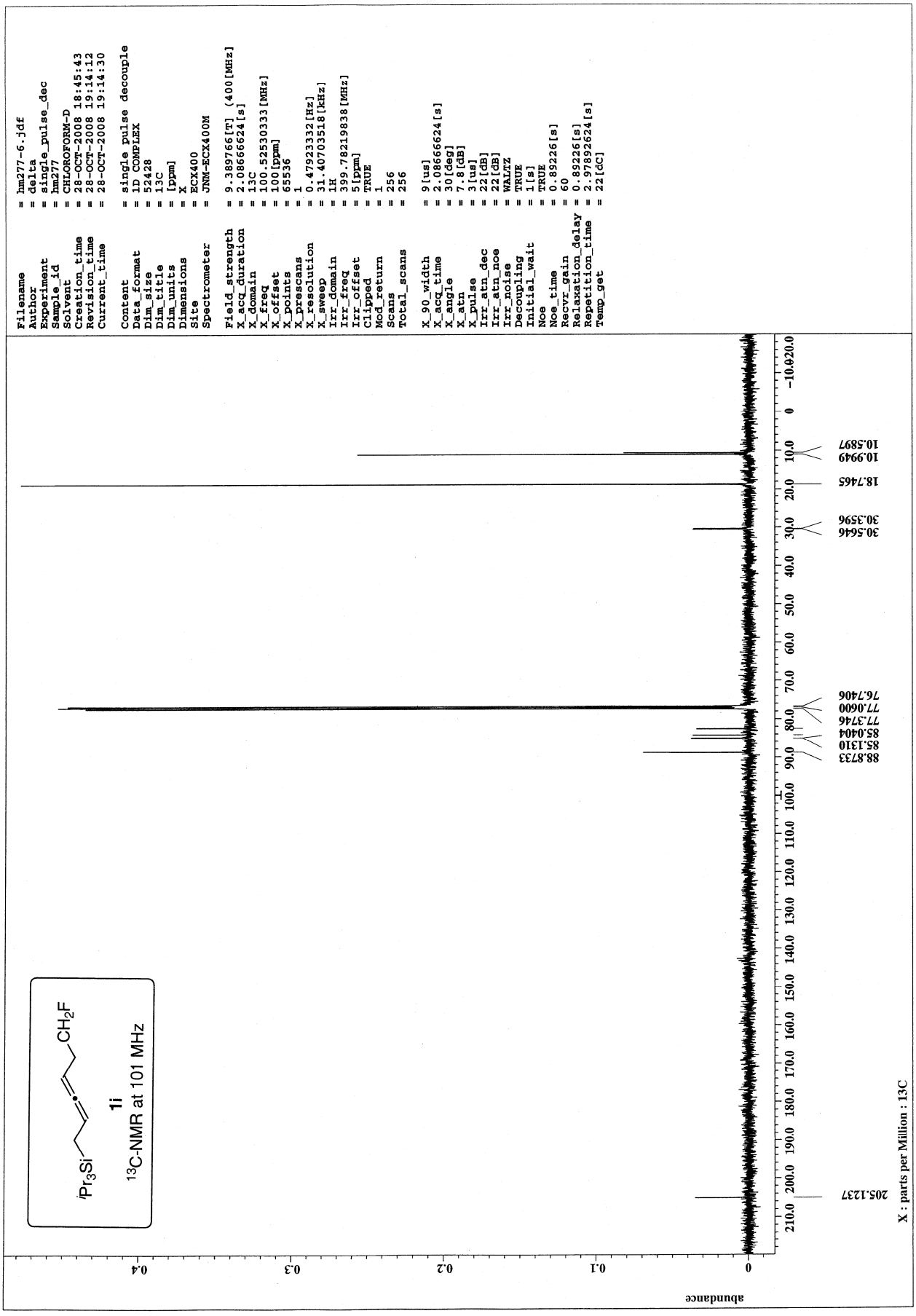

Filename = hm255-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm255
Solvent = CHLOROFORM-D
Creation_time = 16-OCT-2008 18:21:07
Revision_time = 16-OCT-2008 18:32:07
Current_time = 16-OCT-2008 18:32:08
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.702554592[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -210[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 1.4233945[Hz]
X_sweep = 23.32089552[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.702554592[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 8[s]
Repetition_time = 8.702554592[s]
Temp_get = 23.5[dC]
Ph
CH2F
1b
19F-NMR at 373 MHz
abundance
X : parts per Million : 19F
-190.0
-200.0
-210.0
-220.0
-230.0
-217.3481
-217.4742
-217.5353

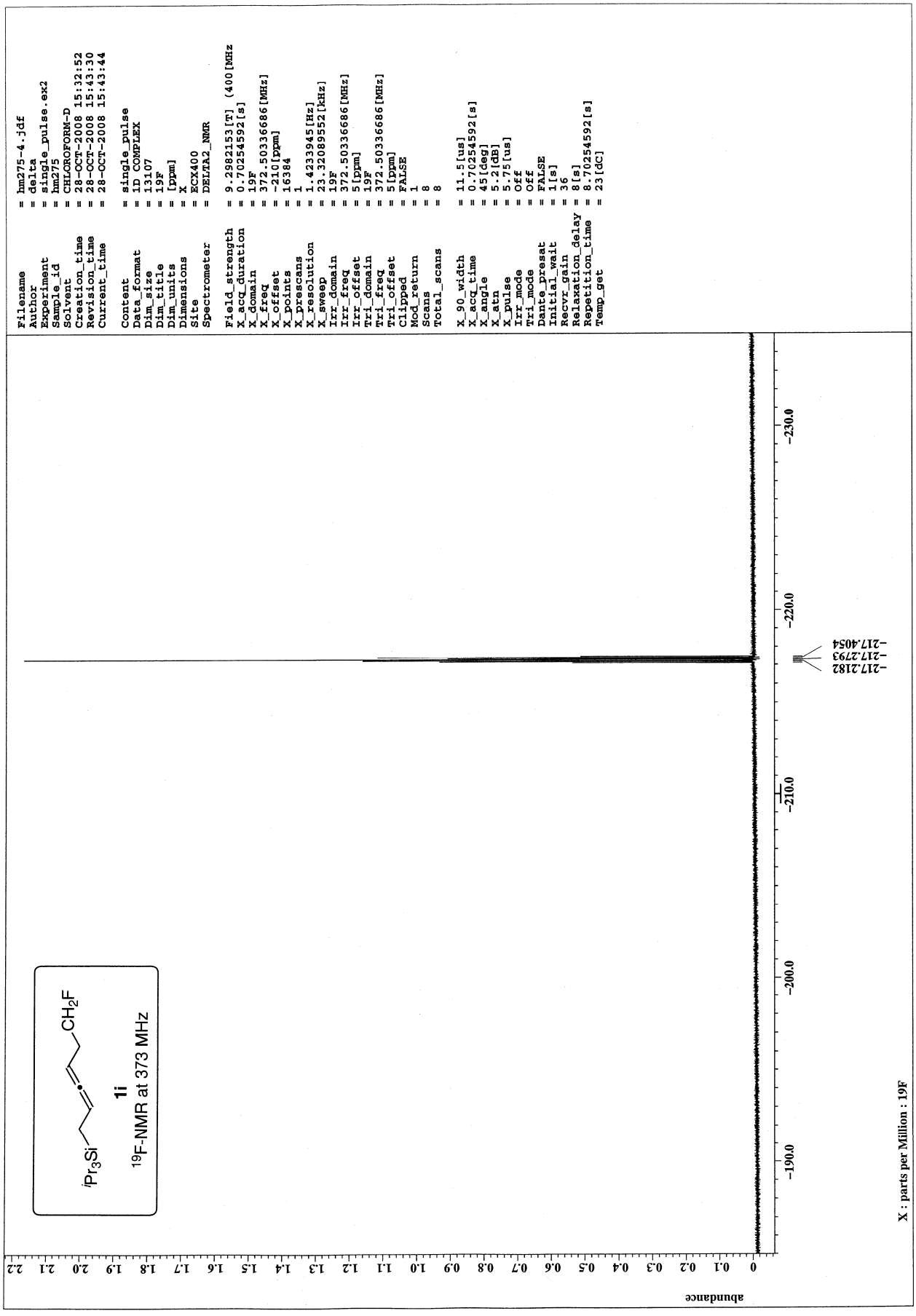

Filename = hm248-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm248
Solvent = CHLOROFORM-D
Creation_time = 14-OCT-2008 18:39:27
Revision_time = 14-OCT-2008 19:08:07
Current_time = 14-OCT-2008 19:09:01
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 21.5[dC]
1f
1H-NMR at 400 MHz
CH2F
abundance
X : parts per Million : 1H
7.2471
6.8556
6.2920
6.2838
6.2755
5.3287
5.3113
5.2939
4.5874
4.5842
4.4697
4.4665
2.4807
2.4729
2.4569
2.3232
2.2587
1.5407
-0.0000
2.006
1
0.986
2.088
3.331
6.468
2.969

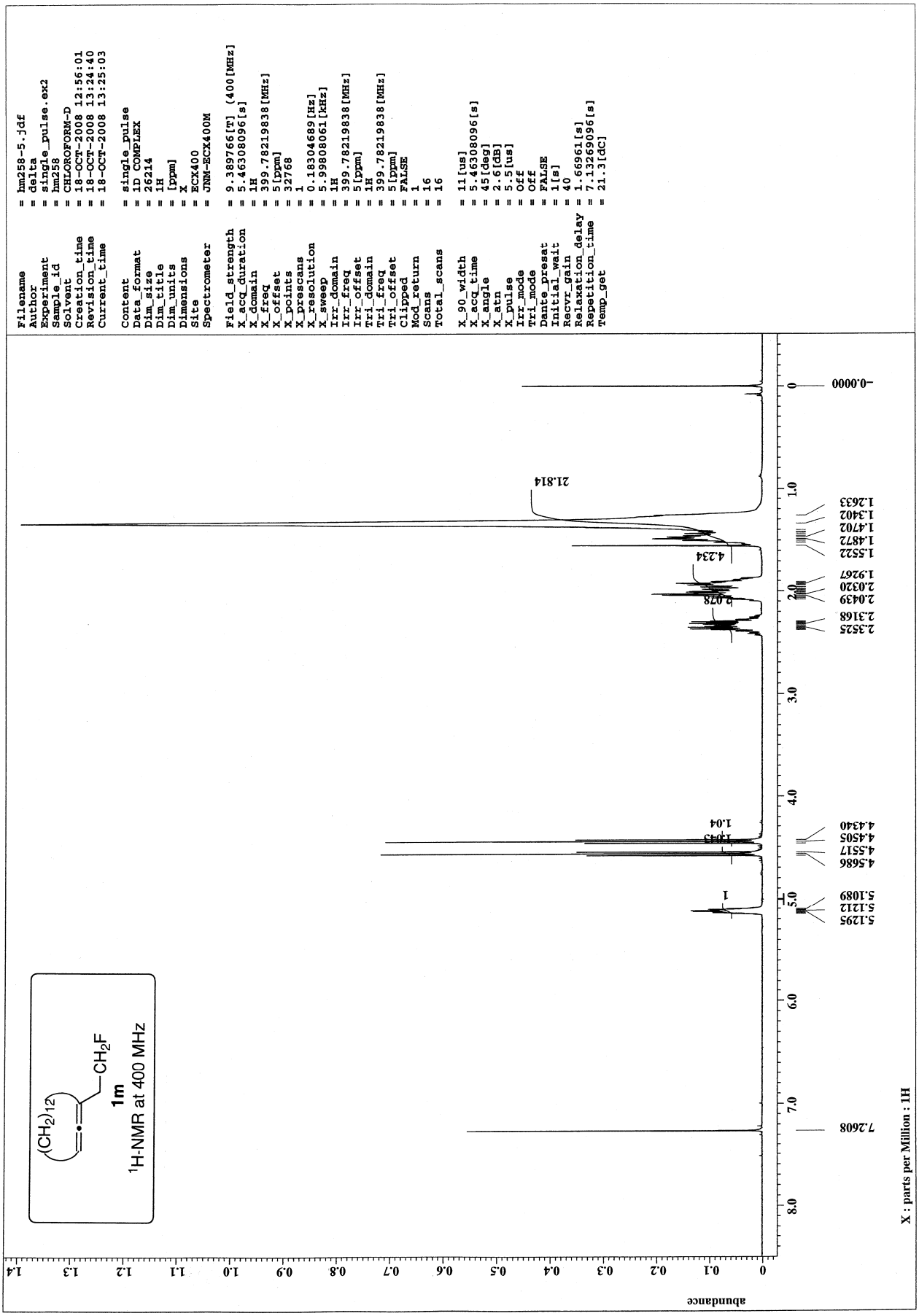

Filename = hm249-3.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm249
Solvent = CHLOROFORM-D
Creation_time = 14-OCT-2008 18:57:25
Revision_time = 14-OCT-2008 19:24:27
Current_time = 14-OCT-2008 19:24:43
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 50
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 21.8[dC]
CH2F
1f
13C-NMR at 101 MHz
abundance
X : parts per Million : 13C
207.0783
136.3794
136.3079
129.0521
128.4276
90.5085
86.6089
86.5278
82.2087
77.3794
77.0600
76.7406
30.4407
30.2357
21.2064
20.9347

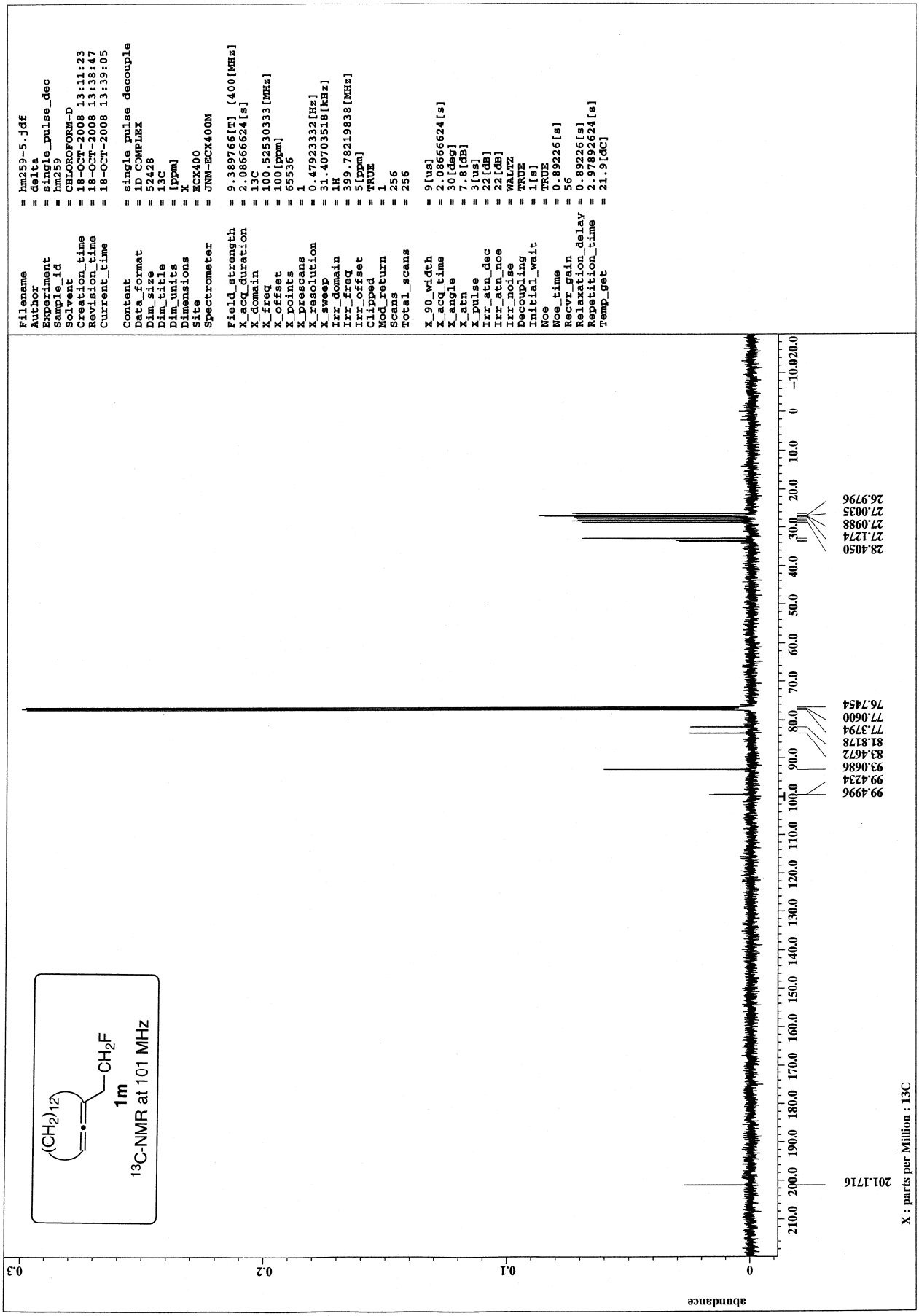

Filename = hm250-6.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm250
Solvent = CHLOROFORM-D
Creation_time = 14-OCT-2008 19:58:09
Revision_time = 14-OCT-2008 20:06:39
Current_time = 14-OCT-2008 20:07:18
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.8781824[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -210[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 1.1387156[Hz]
X_sweep = 18.65671642[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.8781824[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 8[s]
Repetition_time = 8.8781824[s]
Temp_get = 23.7[dC]
CH2F
1f
19F-NMR at 373 MHz
abundance
6.0
5.0
4.0
3.0
2.0
1.0
0
-200.0
-210.0
-220.0
-230.0
-217.2877
-217.4131
-217.4772
X : parts per Million : 19F

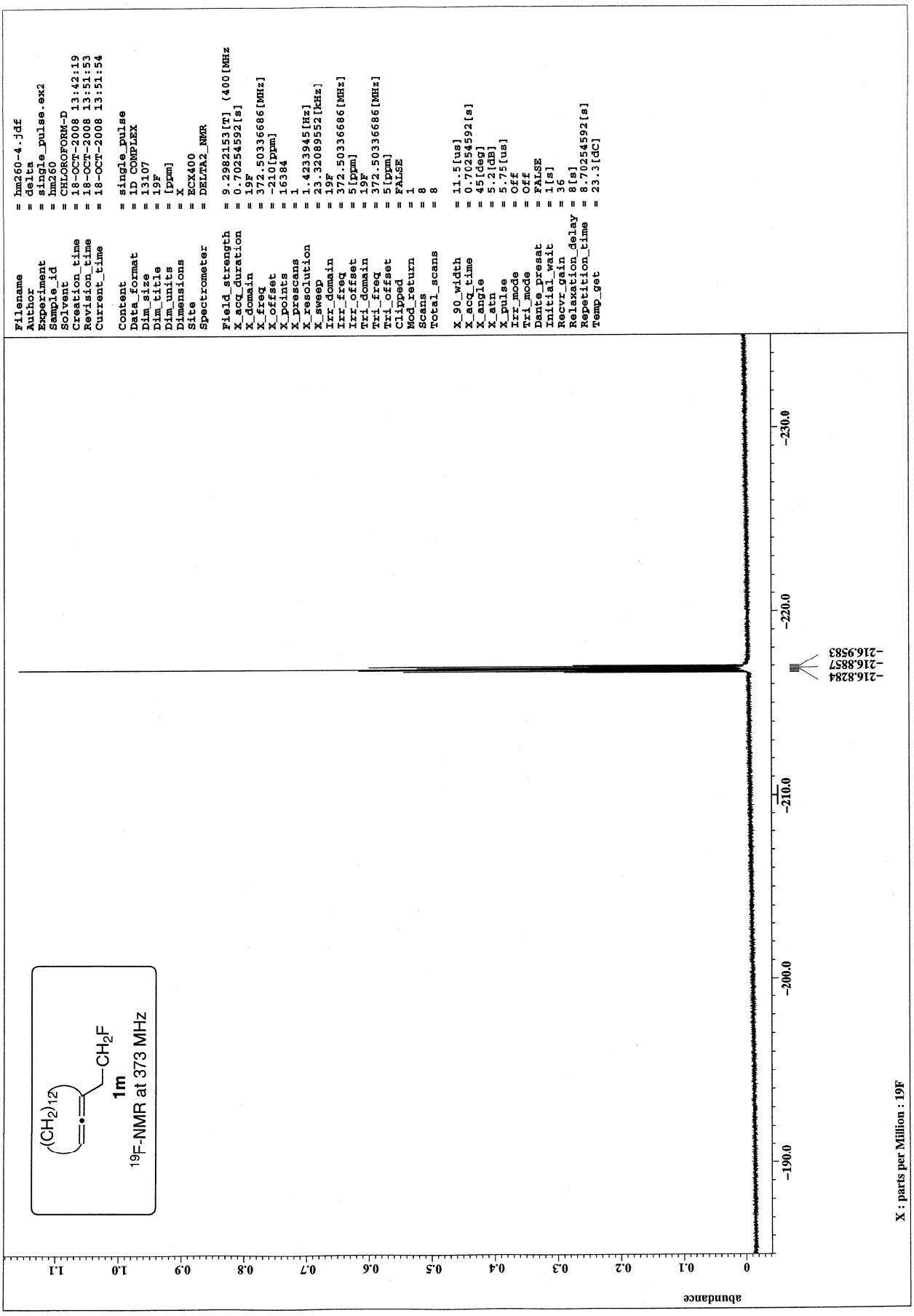

Filename = hm276-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm276
Solvent = CHLOROFORM-D
Creation_time = 28-OCT-2008 17:04:14
Revision_time = 28-OCT-2008 17:36:38
Current_time = 28-OCT-2008 17:37:23
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 20.8[dC]
iPr3Si
CH2F
1i
1H-NMR at 400 MHz
abundance
X : parts per Million : 1H
21.637
2.037
2.011
1.04
0.981
7.2613
5.1917
5.1757
5.0374
5.0210
4.5292
4.5127
4.4111
4.3951
2.4120
2.4024
2.3956
1.4601
1.4450
1.4386
1.0705
1.0595
1.0508
0.0000


Filename = hm277-6.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm277
Solvent = CHLOROFORM-D
Creation_time = 28-OCT-2008 18:45:43
Revision_time = 28-OCT-2008 19:14:12
Current_time = 28-OCT-2008 19:14:30
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recvr_gain = 60
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 22[dC]
$^{i}Pr_3Si$
CH_2F
1i
^{13}C-NMR at 101 MHz
205.1237
88.8733
85.1310
85.0404
77.3746
77.0600
76.7406
30.5646
30.3596
18.7465
10.9949
10.5897
abundance
X : parts per Million : 13C


Filename = hm275-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm275
Solvent = CHLOROFORM-D
Creation_time = 28-OCT-2008 15:32:52
Revision_time = 28-OCT-2008 15:43:30
Current_time = 28-OCT-2008 15:43:44
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DEFTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.70254592[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -210[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 1.4233945[Hz]
X_sweep = 23.32089552[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.70254592[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 8[s]
Repetition_time = 8.70254592[s]
Temp_get = 23[dC]
iPr3Si
CH2F
1i
19F-NMR at 373 MHz
abundance
X : parts per Million : 19F
-190.0
-200.0
-210.0
-220.0
-230.0
-217.2182
-217.2793
-217.4054


Filename = hm258-5.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm258
Solvent = CHLOROFORM-D
Creation_time = 18-OCT-2008 12:56:01
Revision_time = 18-OCT-2008 13:24:40
Current_time = 18-OCT-2008 13:25:03
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 5.46308096[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 32768
X_prescans = 1
X_resolution = 0.18304689[Hz]
X_sweep = 5.99808061[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 = 16
Total_scans = 16
X_90_width = 11[us]
X_acq_time = 5.46308096[s]
X_angle = 45[deg]
X_atn = 2.6[dB]
X_pulse = 5.5[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 1.66961[s]
Repetition_time = 7.13269096[s]
Temp_get = 21.3[dC]
(CH2)12
CH2F
1m
1H-NMR at 400 MHz
abundance
X : parts per Million : 1H
21.814
4.234
2.078
1.045
1.04
1
7.2608
5.1295
5.1212
5.1089
4.5686
4.5517
4.4505
4.4340
2.3525
2.3168
2.0439
2.0320
1.9267
1.5522
1.4872
1.4702
1.3402
1.2633
-0.0000


Filename = hm259-5.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = hm259
Solvent = CHLOROFORM-D
Creation_time = 18-OCT-2008 13:11:23
Revision_time = 18-OCT-2008 13:38:47
Current_time = 18-OCT-2008 13:39:05
Content = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 52428
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = JNM-ECX400M
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.08666624[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 65536
X_prescans = 1
X_resolution = 0.47923332[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 256
Total_scans = 256
X_90_width = 9[us]
X_acq_time = 2.08666624[s]
X_angle = 30[deg]
X_atn = 7.8[dB]
X_pulse = 3[us]
Irr_atn_dec = 22[dB]
Irr_atn_noe = 22[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 0.89226[s]
Recyr_gain = 56
Relaxation_delay = 0.89226[s]
Repetition_time = 2.97892624[s]
Temp_get = 21.9[dC]
(CH2)12
CH2F
1m
13C-NMR at 101 MHz
abundance
X : parts per Million : 13C
201.1716
99.4996
99.4234
93.0686
83.4672
81.8178
77.3794
77.0600
76.7454
28.4050
27.1274
27.0988
27.0035
26.9796


Filename = hm260-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = hm260
Solvent = CHLOROFORM-D
Creation_time = 18-OCT-2008 13:42:19
Revision_time = 18-OCT-2008 13:51:53
Current_time = 18-OCT-2008 13:51:54
Content = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 19F
Dim_units = [ppm]
Dimensions = X
Site = ECX400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 0.70254592[s]
X_domain = 19F
X_freq = 372.50336686[MHz]
X_offset = -210[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 1.42339945[Hz]
X_sweep = 23.32089552[kHz]
Irr_domain = 19F
Irr_freq = 372.50336686[MHz]
Irr_offset = 5[ppm]
Tri_domain = 19F
Tri_freq = 372.50336686[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.5[us]
X_acq_time = 0.70254592[s]
X_angle = 45[deg]
X_atn = 5.2[dB]
X_pulse = 5.75[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 8[s]
Repetition_time = 8.70254592[s]
Temp_get = 23.3[dC]
(CH2)12
CH2F
1m
19F-NMR at 373 MHz
abundance
X : parts per Million : 19F
-216.8284
-216.8857
-216.9583