

Supplementary Information for Synthesis of 2-Imidazolones and 2-Iminoimidazoles

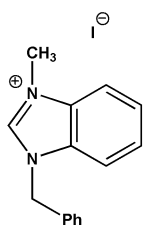
Heather M. Lima and Carl J. Lovely*

Department of Chemistry and Biochemistry, The University of Texas at Arlington,

Arlington, TX 76019

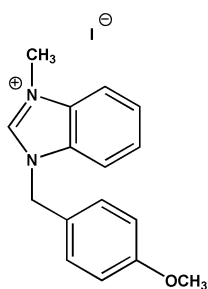
1. Experimental procedures and characterization data for **15a-j**, **16a-j**, **18** and **21-25** (S1-S12)
2. Copies of ^1H and ^{13}C NMR spectra for **15a-j**, **16a-j**, **18** and **21-25** (S13-S64)

1-Benzyl-3-methyl-1*H*-benzimidazol-3-ium iodide (**15a**):



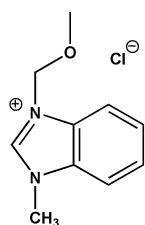
1-Benzyl-1*H*-benzimidazole (1.00 g, 4.80 mmol) in toluene (30 mL) was added MeI (1.50 mL, 24.0 mmol) and heated to 110 °C for 18 h at which time aliquots of MeI were added until starting material was no longer detected by TLC. The resulting solids were filtered and washed with EtOAc to give **15a** as a pale, yellow solid (1.55 g, 92%). mp: 157-159 °C (lit. 138 °C)¹; ¹H NMR (500 MHz, CDCl₃): δ = 11.01 (s, 1H), 7.72 (d, *J* = 8.6 Hz, 1H), 7.62-7.58 (m, 2H), 7.54-7.51 (m, 3H), 7.35-7.30 (m, 3H), 5.81 (s, 2H), 4.24 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ = 142.3, 132.5, 132.2, 131.1, 129.5, 129.4, 128.6, 127.5, 113.9, 113.2, 51.6, 34.4; IR (cm⁻¹): 3005, 1561, 1462, 1432, 1344, 1191, 749, 702; HR-ESIMS (*m/z*): Calcd. for [M]⁺ C₁₅H₁₅N₂ is 223.1230 found 223.1236.

1-(4-methoxybenzyl)-3-methyl-1*H*-benzimidazol-3-ium iodide (**15b**):



1-(4-Methoxybenzyl)-1*H*-benzimidazole (1.00 g, 4.20 mmol) in toluene (60 mL) was added MeI (0.50 mL, 8.4 mmol) and heated to 110 °C for 18 h at which time aliquots of MeI were added until starting material was no longer detected by TLC. The precipitated solids were filtered and washed with EtOAc and then Et₂O to give **15b** as a beige solid (1.30 g, 82%). mp: 197-200 °C; ¹H NMR (300 MHz, CD₃OD): δ = 9.45 (s, 1H), 7.95-7.87 (m, 2H), 7.73-7.62 (m, 2H), 7.44 (d, *J* = 8.9 Hz, 2H), 6.97 (d, *J* = 8.6 Hz, 2H), 5.64 (s, 2H), 4.13 (s, 3H), 3.78 (s, 3H); ¹³C NMR (125 MHz, CD₃OD): δ = 160.6, 142.0, 132.6, 131.3, 130.0, 126.9, 126.8, 124.9, 114.4, 113.5, 113.1, 54.5, 50.1, 32.7; IR (cm⁻¹): 2974, 1610, 1567, 1516, 1451, 1248, 1185, 1020, 783, 761; HR-ESIMS (*m/z*): Calcd. for [M]⁺ C₁₆H₁₇N₂O is 253.1335 found 253.1329.

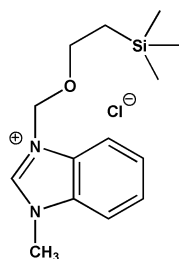
3-Methoxymethyl-1-methyl-1*H*-benzimidazol-3-ium chloride (**15c**):



1-Methyl-1*H*-benzimidazole (0.50 g, 3.8 mmol) in THF was added MOMCl (0.34 mL, 4.5 mmol) and stirred at rt for 18 h. The solvent was removed by rotary evaporation and the resulting solids were suspended in Et₂O, filtered and washed with Et₂O to give **15c** as a white, hygroscopic solid (0.73 g, 91%) that was stored at rt under N₂. mp: 115-118 °C (lit.

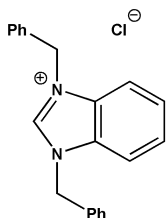
88-90 °C)²; ¹H NMR (500 MHz, CD₃OD): δ = 9.67 (s, 1H), 8.01-7.97 (m, 2H), 7.76-7.71 (m, 2H), 5.87 (s, 2H), 4.18 (s, 3H), 3.44 (s, 3H); ¹³C NMR (125 MHz, CD₃OD): δ = 142.7, 132.7, 131.0, 127.3, 127.2, 113.6, 113.2, 78.5, 56.4, 32.7; IR (cm⁻¹): 3351, 3048, 1563, 1467, 1099, 1060, 1005, 765.

1-Methyl-3-trimethylethoxymethyl-1*H*-benzimidazol-3-ium chloride (15d):



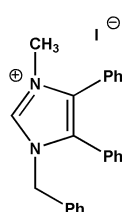
1-Methyl-1*H*-benzimidazole (0.50 g, 3.8 mmol) in THF (15 mL) was added SEM-Cl (0.80 mL, 4.5 mmol) and stirred at rt for 18h. The solvent was removed by rotary evaporation and the resulting white solid was suspended in Et₂O, filtered and washed with Et₂O to give **15d** as a white solid (1.09 g, 96%). mp: 114-115 °C; ¹H NMR (300 MHz, CDCl₃): δ = 11.47 (s, 1H), 7.87-7.84 (m, 1H), 7.74-7.71 (m, 1H), 7.67-7.62 (m, 2H), 6.04 (s, 2H), 4.29 (s, 3H), 3.69 (t, *J* = 7.9 Hz, 2H), 0.90 (t, *J* = 8.2 Hz, 2H), -0.08 (s, 9H); ¹³C NMR (75 MHz, CDCl₃): δ = 143.8, 132.4, 130.8, 127.5, 114.3, 112.9, 68.3, 34.0, 17.9, -1.3; IR (cm⁻¹): 3442, 3367, 3027, 2954, 1569, 1420, 1250, 1113, 834, 763; HR-ESIMS (*m/z*): Calcd. for [M]⁺ C₁₄H₂₃N₂OSi is 263.1574 found 263.1573.

1,3-Dibenzyl-1*H*-benzimidazol-3-ium chloride (15e):



1-Benzyl-1*H*-benzimidazole (0.75 g, 3.6 mmol) was suspended in toluene (30 mL) and benzyl chloride (0.50 mL, 4.3 mmol) was added and heated to reflux for 18 h. The solids were filtered and washed with Et₂O to give **15e** as an off-white solid (0.65 g, 54%). mp: 211-212 °C (lit. 210-211 °C)³; ¹H NMR (300 MHz, CD₃OD): δ = 9.73 (s, 1H), 7.87-7.84 (m, 2H), 7.64-7.61 (m, 2H), 7.48-7.38 (m, 10H), 4.87 (s, 4H); ¹³C NMR (125 MHz, CD₃OD): δ = 142.0, 133.3, 131.7, 129.1, 129.0, 128.1, 127.1, 113.7, 50.7; IR (cm⁻¹): 3419, 3355, 3036, 2954, 1557, 1460, 1426, 1374, 1189, 1016, 756, 740, 701.

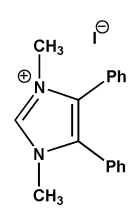
1-Benzyl-3-methyl-4,5-diphenyl-1*H*-imidazol-3-ium iodide (15f):



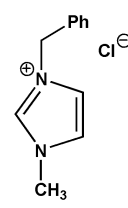
1-Benzyl-4,5-diphenyl-1*H*-imidazole (0.15 g, 0.48 mmol) in THF (10 mL) was added Mel (0.10 mL, 1.4 mmol) and stirred at 70 °C for 18h. An additional aliquot of Mel (3 eq) was added and heating resumed for 3h. The solids were filtered and washed with EtOAc to give

15f as a white solid (0.18 g, 81%). mp: 223-225 °C; ¹H NMR (300 MHz, CDCl₃): δ = 10.36 (s, 1H), 7.45-7.34 (m, 6H), 7.31-7.25 (m, 5H), 7.22-7.19 (m, 4H), 5.40 (s, 2H), 3.91 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ = 136.7, 133.0, 132.8, 132.0, 131.1, 130.6, 130.5, 129.3, 128.9, 124.9, 124.5, 51.5, 35.5; IR (cm⁻¹): 3033, 1561, 1497, 1438, 1076, 766, 728, 702; HR-ESIMS (*m/z*): Calcd. for [M]⁺ C₂₃H₂₁N₂ is 325.1749 found 325.1695.

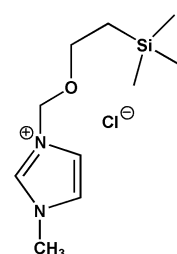
1,3-Dimethyl-4,5-diphenyl-1*H*-imidazol-3-ium iodide (**15g**):

 1-Methyl-4,5-diphenyl-1*H*-imidazole (0.15 g, 0.64 mmol) in toluene (5 mL) was added MeI (0.20 mL, 3.2 mmol) and stirred at 125 °C for 3h. The solution was cooled to rt and the solids were filtered and washed with EtOAc to give **15g** as a pale yellow solid (0.22 g, 92%). mp: 214-216 °C; ¹H NMR (500 MHz, CDCl₃): δ = 10.37 (s, 1H), 7.44-7.37 (m, 6H), 7.30-7.27 (m, 4H), 3.91 (s, 6H); ¹³C NMR (125 MHz, CDCl₃): δ = 137.3, 132.4, 130.7, 130.5, 129.3, 124.7, 35.3; IR (cm⁻¹): 3067, 1577, 1468, 1218, 849, 766, 706; HR-ESIMS (*m/z*): Calcd. for [M]⁺ C₁₇H₁₇N₂ is 249.1386 found 249.1392.

3-Benzyl-1-methyl-1*H*-imidazol-3-ium chloride (**15h**):

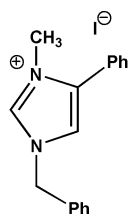
 1-Methylimidazole (1.00 mL, 12.5 mmol) in THF (50 mL) was added BnCl (7.20 mL, 62.7 mmol) and heated to reflux overnight. The solvent was decanted and the resulting oil was triturated with Et₂O and dried under vacuum to give **15h** as an off-white semi-solid (2.20 g, 84%). ¹H NMR (500 MHz, CDCl₃): δ = 10.65 (s, 1H), 7.45-7.42 (m, 3H), 7.34-7.31 (m, 4H), 5.54 (s, 2H), 4.02 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ = 138.0, 133.3, 129.5, 129.5, 129.0, 123.6, 121.8, 53.4, 36.7.

1-Methyl-3-trimethylsilyloxyethyl-1*H*-imidazol-3-ium chloride (**15i**):

 1-Methylimidazole (0.25 mL, 3.1 mmol) in THF (5 mL) was added SEM-Cl (0.66 mL, 3.7 mmol) and stirred at rt. Within minutes, a second layer was observed, and after 30 minutes the layers were allowed to separate. The top layer was drawn off with a pipet, and the resulting oil was dried under vacuum to give **15i** as a clear, colorless oil (0.71 g,

91%). ^1H NMR (500 MHz, CDCl_3): δ = 10.81 (s, 1H), 7.46 (s, 1H), 7.42 (s, 1H), 5.73 (s, 2H), 4.12 (s, 3H), 3.65 (t, J = 8.0 Hz, 2H), 0.93 (t, J = 8.0 Hz), -0.02 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3): δ = 138.5, 123.7, 120.7, 78.9, 68.6, 36.9, 18.0, -1.3; IR (cm^{-1}): 2953, 1575, 1557, 1248, 1157, 1096, 857, 833, 739; HR-ESIMS (m/z): Calcd. for $[\text{M}]^+$ $\text{C}_{10}\text{H}_{21}\text{N}_2\text{OSi}$ is 231.1418 found 213.1424.

1-Benzyl-3-methyl-4-phenyl-1*H*-imidazol-3-ium iodide (15j):



1-Benzyl-4-phenyl-imidazole (0.20 g, 0.85 mmol) in THF (10 mL) was added Mel (0.16 mL, 2.6 mmol) and heated at reflux overnight. The solvent was removed and the resulting residue triturated with EtOAc, then Et_2O to give **15j** as a yellow semi-solid (0.30 g, 94%). ^1H NMR (300 MHz, CDCl_3): δ = 10.31 (s, 1H), 7.59-7.56 (m, 2H), 7.50-7.45 (m, 3H), 7.47-7.43 (m, 4H), 7.39-7.36 (m, 4H), 7.30 (d, J = 1.7 Hz, 1H), 5.62 (s, 2H), 3.90 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3): δ = 137.3, 136.0, 132.8, 130.8, 129.7, 129.6, 129.5, 129.5, 124.6, 119.1, 53.6, 35.4; IR (cm^{-1}): 3027, 1556, 1495, 1443, 1146, 762, 741, 697; HR-ESIMS (m/z): Calcd. for $[\text{M}]^+$ $\text{C}_{17}\text{H}_{17}\text{N}_2$ is 249.1386 found 249.1395.

General procedure for oxidation of 1-Benzyl-3-methyl-1*H*-benzimidazol-3-ium iodide (15a):

Method A: Benzimidazolium salt (0.29 mmol) in THF (10 mL) was cooled to 0 °C and NaH (60% dispersion in mineral oil, 0.017 g, 0.43 mmol) was added and stirred under N_2 at 0 °C for 10 min. NCS (0.050 g, 0.37 mmol) was added and stirred for 20 min. 2M NaOH (5 mL) was added and the reaction mixture was allowed to come to room temp. and stir for 10 min. The reaction was diluted with water (10 mL) and the aqueous layer extracted with EtOAc (2x15 mL). The combined organics were washed with water (10 mL), followed by brine (10 mL), dried (anhyd. Na_2SO_4), and concentrated.

Method B: Benzimidazolium salt (0.29 mmol) in THF (10 mL) was added 1M $\text{K}_2\text{CO}_3/\text{Na}_2\text{CO}_3$ or 2M NaOH (1.1 mmol) followed by NCS (0.050 g, 0.37 mmol) and stirred at room temp for 1 h (except in the case of Na_2CO_3 which required stirring for 18 h). The reaction was diluted

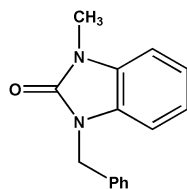
with water (10 mL) and the aqueous layer extracted with EtOAc (2x15 mL). The combined organics were washed with water (10 mL), followed by brine (10 mL), dried (anhyd. Na₂SO₄), and concentrated.

Method C: Benzimidazolium salt (0.34 mmol) in THF (10 mL) was cooled to 0 °C and 5% NaOCl (5 mL) was added. The reaction was allowed to come to room temp and stir for 10 min. The reaction was diluted with water (10 mL) and the aqueous layer extracted with EtOAc (2 x 15 mL). The combined organics were washed with water (10 mL), followed by brine (10 mL), dried (anhyd. Na₂SO₄), and concentrated.

General procedure for the oxidation of 1-Benzyl-3-methyl-4,5-diphenyl-1*H*-imidazol-3-ium iodide (15f):

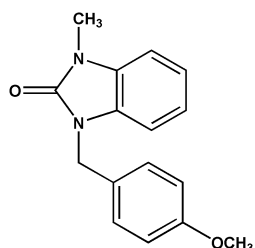
Method D: Imidazolium salt (0.10 g, 0.22 mmol) in THF (5 mL) was added 1M NaOH (1.0 mL, 0.88 mmol) followed by slow, dropwise addition of 5% NaOCl (0.40 mL) over about 10 minutes at room temp. The reaction was diluted with water and extracted with EtOAc (2 x 10 mL). The combined organics were washed with water (10 mL), followed by brine (10 mL), dried (anhyd. Na₂SO₄), and concentrated.

1-Benzyl-3-methyl-1,3-dihydro-2*H*-benzimidazol-2-one (16a):



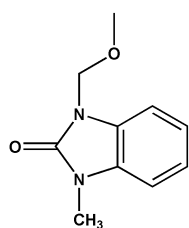
From **15a** (0.12 g, 0.34 mmol) following Method C and purified by column chromatography (4:6 EtOAc/Hexane), **16a** was obtained as a white solid (0.070 g, 85%). mp: 87-89 °C (lit. 87-88 °C)⁴; ¹H NMR (500 MHz, CDCl₃): δ = 7.34-7.29 (m, 4H), 7.27-7.25 (m, 1H), 7.09-7.06 (m, 1H), 7.02-6.97 (m, 2H), 6.87 (d, *J* = 7.5 Hz, 1H), 5.08 (s, 2H), 3.46 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ = 154.7, 136.5, 130.2, 129.3, 128.8, 127.8, 127.6, 121.4, 121.3, 108.3, 107.5, 45.0, 27.3; IR (cm⁻¹): 3043, 2946, 1705, 1494, 1435, 1398, 1246, 1121, 1003, 731.

1-(4-methoxybenzyl)-3-methyl-1,3-dihydro-2H-benzimidazol-2-one (**16b**):



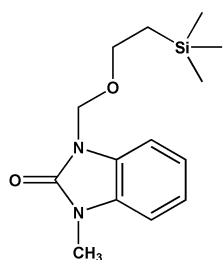
From **15b** (0.12 g, 0.31 mmol) following Method C and purified by column chromatography (6:4 EtOAc/Hexane), **16b** was obtained as a white solid (0.069 g, 81%). mp: 102-104 °C; ¹H NMR (500 MHz, CDCl₃): δ = 7.27 (d, *J* = 8.6 Hz, 2H), 7.08-7.05 (m, 1H), 7.02-6.95 (m, 2H), 6.89 (d, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 8.6 Hz, 2H), 5.01 (s, 2H), 3.76 (s, 3H), 3.45 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ = 159.2, 154.6, 130.2, 129.2, 129.0, 128.6, 121.3, 114.2, 108.3, 107.5, 55.3, 44.5, 27.3; IR (cm⁻¹): 2972, 1699, 1609, 1513, 1499, 1245, 1170, 1023, 740, 724; HR-ESIMS (*m/z*): Calcd. for [M+Na]⁺ C₁₆H₁₆N₂O₂Na is 291.1104 found 291.1115, Calcd. for [2M+Na]⁺ is 559.2316 found 559.2346.

3-Methoxymethyl-1-methyl-1,3-dihydro-2H-benzimidazol-2-one (**16c**):



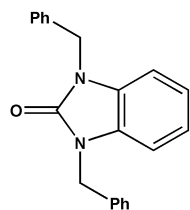
From **15c** (0.10 g, 0.47 mmol) following Method C and purified by column chromatography (1:1 EtOAc/Hexane), **16c** was obtained as a white solid (0.073 g, 81%). mp: 68-70 °C; ¹H NMR (300 MHz, CDCl₃): δ = 7.18-7.10 (m, 3H), 7.01-6.98 (m, 1H), 5.30 (s, 2H), 3.43 (s, 3H), 3.36 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ = 154.6, 130.2, 128.7, 122.1, 121.7, 108.7, 107.7, 72.6, 56.4, 27.2; IR (cm⁻¹): 2937, 1689, 1622, 1501, 1380, 1031, 907, 750, 721, 636; HR-ESIMS (*m/z*): Calcd. for [M+Na]⁺ C₁₀H₁₂N₂O₂Na is 215.0791 found 215.0782; Calcd. for [2M+Na]⁺ C₂₀H₂₄N₄O₄Na is 407.1690 found 407.1708.

1-Methyl-3-trimethylsilyloxyethyl-1,3-dihydro-2H-benzimidazol-2-one (**16d**):



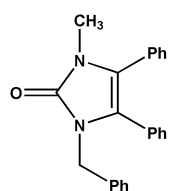
From **15d** (0.036 g, 0.12 mmol) following Method C and purified by column chromatography (2:8 EtOAc/Hexane), **16d** was obtained as a colorless oil⁴ (0.026 g, 79%): ¹H NMR (300 MHz, CDCl₃): δ = 7.18-7.09 (m, 3H), 6.99-6.96 (m, 1H), 5.31 (s, 2H), 3.60 (t, *J* = 8.3 Hz, 2H), 3.41 (s, 3H), 0.91 (t, *J* = 8.3 Hz, 2H), -0.04 (s, 9H); ¹³C NMR (75 MHz, CDCl₃): δ = 154.5, 130.2, 128.8, 122.0, 121.6, 108.8, 107.5, 70.8, 66.2, 27.2, 17.9, -1.3; IR (cm⁻¹): 2951, 1694, 1449, 1374, 1247, 1072, 832, 695.

1,3-Dibenzyl-1,3-dihydro-2H-benzimidazol-2-one (16e):



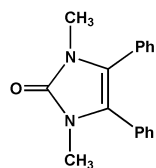
From **15e** (0.15 g, 0.45 mmol) following Method C and purified by column chromatography (3:7 EtOAc/Hexane), **16e** was obtained as an off-white solid (0.12 g, 88%). mp: 110-112 °C (lit. 110 °C)⁵; ¹H NMR (500 MHz, CDCl₃): δ = 7.35-7.30 (m, 8H), 7.28-7.26 (m, 2H), 6.99-6.96 (m, 2H), 6.89-6.86 (m, 2H), 5.12 (s, 4H); ¹³C NMR (125 MHz, CDCl₃): δ = 154.7, 136.4, 129.4, 128.9, 127.8, 127.6, 121.5, 108.4, 45.1; IR (cm⁻¹): 3025, 2926, 1691, 1489, 1436, 1407, 1356, 1164, 750, 696, 659.

1-Benzyl-3-methyl-4,5-diphenyl-1,3-dihydro-2H-imidazol-2-one (16f):



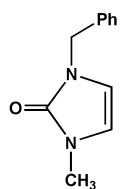
From **15f** (0.10 g, 0.22 mmol) following Method D and purified by column chromatography (4:6 EtOAc/Hexane), **16f** was obtained as a white solid (0.059 g, 79%). mp: 122-124 °C; ¹H NMR (500 MHz, CDCl₃): δ = 7.25-7.19 (m, 9H), 7.16-7.14 (m, 2H), 7.07-7.06 (m, 2H), 7.03-7.01 (m, 2H), 4.85 (s, 2H), 3.29 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ = 154.0, 138.0, 130.7, 130.1, 129.1, 129.1, 128.5, 128.2, 128.0, 127.6, 127.3, 121.6, 121.1, 45.4, 29.3; IR (cm⁻¹): 3060, 2948, 1674, 1600, 1498, 1450, 1387, 748, 703; HR-ESIMS (*m/z*): Calcd. for [M+H]⁺ C₂₃H₂₁N₂O is 341.1648 found 341.1633; Calcd. for [M+Na]⁺ C₂₃H₂₀N₂O₂Na is 363.1468 found 363.1472; Calcd. for [2M+Na]⁺ C₄₆H₄₀N₄O₂Na is 703.3043 found 703.3056.

1,3-Dimethyl-4,5-diphenyl-1,3-dihydro-2H-imidazol-2-one (16g):



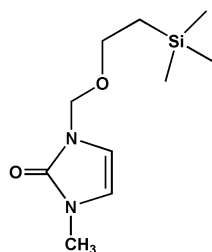
From **15g** (0.060 g, 0.16 mmol) following Method D and purified by column chromatography (silica gel was neutralized with Et₃N) (8:2 EtOAc/Hexane to 100% EtOAc), **16g** was obtained as a white, crystalline solid (0.030 g, 71%). mp: 186-189 °C (lit. 203 °C⁶, 183-184 °C⁷); ¹H NMR (500 MHz, CDCl₃): δ = 7.29-7.26 (m, 6H), 7.16-7.14 (m, 4H), 3.24 (2, 6H); ¹³C NMR (125 MHz, CDCl₃): δ = 154.0, 130.2, 129.2, 128.6, 128.0, 121.3, 29.1; IR (cm⁻¹): 2873, 1680, 1458, 1418, 1379, 1021, 778, 767, 746, 709; HR-ESIMS (*m/z*): Calcd. for [M+H]⁺ C₁₇H₁₆N₂O is 265.1335 found 265.1331.

3-Benzyl-1-methyl-1,3-dihydro-2H-imidazol-2-one (16h):



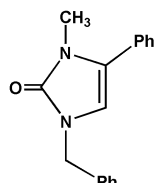
From **15h** (0.20 g, 0.96 mmol) following Method D and purified by column chromatography (100% EtOAc), **16h** was obtained as a white solid (0.070 g, 39%). mp: 60-61 °C (lit. 63-64 °C)⁴; ¹H NMR (500 MHz, CDCl₃): δ = 7.34-7.31 (m, 2H), 7.29-7.27 (m, 2H), 7.25-7.23 (m, 1H), 6.15 (d, *J* = 2.9 Hz, 1H), 6.10 (d, *J* = 2.9 Hz, 1H), 4.77 (s, 2H), 3.27 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ = 153.3, 137.0, 128.8, 127.9, 127.8, 111.8, 110.0, 47.3, 30.6; IR (cm⁻¹): 3118, 2944, 1659, 1643, 1477, 1450, 1408, 1373, 1241, 810, 739.

1-Methyl-3-trimethylsilyloxyethyl-1,3-dihydro-2H-imidazol-2-one (16i):



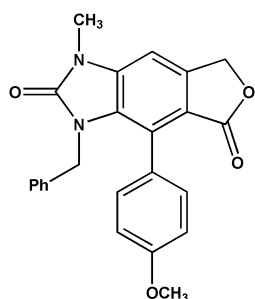
From **15i** (0.15 g, 0.60 mmol) following Method D and purified by column chromatography (1:1 EtOAc/Hexane), **16i** was obtained as a colorless oil⁴ (0.050 g, 36%). ¹H NMR (500 MHz, CDCl₃): δ = 6.31 (d, *J* = 2.9 Hz, 1H), 6.17 (d, *J* = 2.9 Hz, 1H), 4.98 (s, 2H), 3.56 (t, *J* = 8.0 Hz, 2H), 3.24 (s, 3H), 0.90 (t, *J* = 8.0 Hz, 2H), -0.03 (s, 9H); ¹³C NMR (125 MHz, CDCl₃): δ = 153.6, 112.4, 109.8, 72.7, 66.1, 30.4, 17.9, -1.3; IR (cm⁻¹): 2951, 1675, 1467, 1412, 1246, 1080, 917, 857, 833, 761.

1-Benzyl-3-methyl-4-phenyl-1,3-dihydro-2H-imidazol-2-one (16j):



From **15j** (0.30 g, 0.80 mmol) following Method D and purified by column chromatography (6:4 EtOAc/Hexane), **16j** was obtained as a yellow oil (0.14 g, 67%). ¹H NMR (300 MHz, CDCl₃): δ = 7.40-7.30 (m, 10 H), 6.16 (s, 1H), 4.85 (s, 2H), 3.33 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ = 154.0, 137.0, 128.9, 128.1, 128.0, 127.9, 127.7, 125.2, 107.7, 107.5, 47.3, 29.4; IR (cm⁻¹): 3031, 2929, 1668, 1453, 1403, 1174, 724, 695; HR-ESIMS (*m/z*): Calcd for [M+Na]⁺ is C₁₇H₁₆N₂O₂ is 287.1155 found 287.1168.

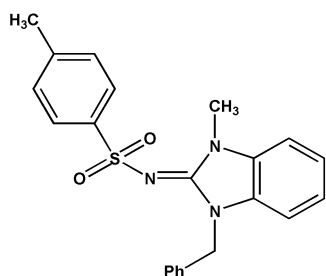
3-Benzyl-4-(4-methoxyphenyl)-1-methyl-3,7-dihydro-1H-furo[3,4-*f*]benzimidazole-2,5-dione (18):



From **17** (1.0 g, 1.9 mmol) following Method C and purified by column chromatography (7:3 EtOAc/Hexane), **18** was obtained as an off-white solid (0.58 g, 75%). mp: 185-187 °C; ¹H NMR (500 MHz, CDCl₃): δ = 7.12-7.09 (m, 3H), 7.03

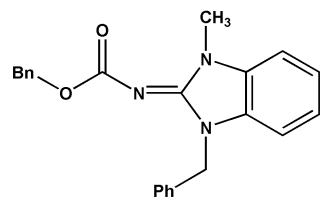
(s, 1H), 6.94 (d, $J = 8.6$ Hz, 2H), 6.77 (d, $J = 8.9$, 2H), 6.58-6.56 (m, 2H), 5.23 (s, 2H), 4.79 (s, 2H), 3.83 (s, 3H), 3.57 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): $\delta = 169.8, 159.7, 155.6, 141.8, 136.4, 136.2, 131.3, 128.2, 127.8, 127.2, 126.0, 124.0, 123.6, 117.1, 113.1, 99.5, 67.7, 55.3, 45.8, 27.8$; IR (cm^{-1}): 1748, 1705, 1609, 1517, 1496, 1352, 1244, 1028; HR-ESIMS (m/z): Calcd. for $[\text{M}+\text{Na}]^+$ $\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_4\text{Na}$ is 423.1315, found 423.1316.

1-Benzyl-2-*tert*-butoxycarbonylimino-3-methyl-1,3-dihydro-2*H*-benzimidazole (21):



15a (0.075 g, 0.21 mmol) in DMF (3 mL) was added chloramine-T trihydrate (0.13 g, 0.47 mmol) and stirred at rt for 1 h. The reaction was diluted with water (5 mL) and extracted with EtOAc (2 x 5 mL). The combined organics were washed with 2M NaOH (5 mL), water (5 mL), and then brine (5 mL). The organics were dried (anhyd. Na_2SO_4) and concentrated. The resulting solids were recrystallized from CH_2Cl_2 /hexane to provide **21** as pale yellow crystals (0.080 g, 95%). mp: 165-167 °C; ^1H NMR (500 MHz, CDCl_3): $\delta = 7.82$ (s, 1H), 7.81 (s, 1H), 7.26-7.24 (m, 5H), 7.20-7.16 (m, 5H), 7.06 (d, $J = 8.0$ Hz, 1H), 5.18 (s, 2H), 3.94 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): $\delta = 148.6, 142.7, 141.5, 135.1, 131.3, 129.7, 129.2, 128.9, 128.0, 127.5, 125.9, 123.7, 123.4, 110.3, 109.9, 47.0, 32.4, 21.5$; IR (cm^{-1}): 1579, 1567, 1445, 1245, 1132, 1088; HR-ESIMS (m/z): Calcd. for $[\text{M}+\text{H}]^+$ $\text{C}_{22}\text{H}_{22}\text{N}_3\text{O}_2\text{S}$ is 392.1427 found 392.1420.

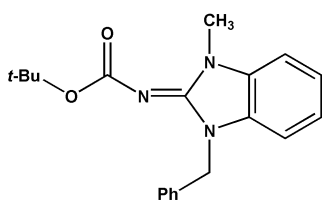
1-Benzyl-2-benzyloxycarbonylimino-3-methyl-1,3-dihydro-2*H*-benzimidazole (22):



Benzyl carbamate (0.095 g, 0.63 mmol) in CH_2Cl_2 (10 mL) was added *t*-BuOCl (0.080 mL, 0.71 mmol) and stirred at rt for 30 min. The reaction was cooled to 0 °C and DBU (0.13 mL, 0.86 mmol) was added followed by **15a** (0.10 g, 0.29 mmol) and stirred at rt for 30 min. The reaction was quenched with water (10 mL), the layers were separated and the aqueous layer extracted with CH_2Cl_2 (5 mL). The combined organics were washed with 2M NaOH (5 mL), water (5 mL) and brine (5 mL). The organic layer was dried (anhyd. Na_2SO_4), concentrated, and purified by column chromatography (7:3 EtOAc/Hexane) to give **22** as a white solid (0.090 g, 85%). mp: 76-77 °C; ^1H NMR (500 MHz, CDCl_3): $\delta =$

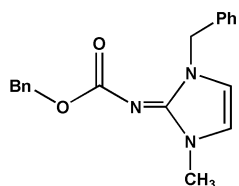
7.44 (d, $J = 7.5$ Hz, 2H), 7.32 (t, $J = 6.9$ Hz, 2H), 7.29-7.26 (m, 3H), 7.25-7.18 (m, 5H), 7.14 (dd, $J = 2.3$ Hz, $J = 7.5$ Hz, 1H), 5.29 (s, 2H), 5.20 (s, 2H), 3.57 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): $\delta = 159.0, 153.4, 137.9, 135.3, 131.5, 130.2, 128.9, 128.4, 128.1, 128.0, 127.6, 127.5, 123.1, 123.0, 110.1, 109.3, 67.2, 47.0, 31.0$; IR (cm^{-1}): 3031, 2947, 1651, 1575, 1493, 1427, 1376, 1308, 1261, 1222, 1174; HR-ESIMS (m/z): Calcd. for $[\text{M}+\text{H}]^+ \text{C}_{23}\text{H}_{22}\text{N}_3\text{O}_2$ is 372.1707 found 372.1709.

1-Benzyl-2-*tert*-butylcarbonylimino-3-methyl-1,3-dihydro-2*H*-benzimidazole (23):



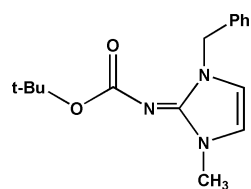
Prepared following the same procedure as **22** from **15a** (0.074 g, 0.63 mmol) and purified by column chromatography (1:1 EtOAc/Hexane) to give **23** as a white solid (0.069 g, 72%). mp: 141-142 °C; ^1H NMR (500 MHz, CDCl_3): $\delta = 7.29-7.26$ (m, 3H), 7.25-7.23 (m, 2H), 7.18-7.16 (m, 2H), 7.11-7.07 (m, 1H), 6.97 (d, $J = 8.6$ Hz, 1H), 5.30 (s, 2H), 3.58 (s, 3H), 1.53 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3): $\delta = 159.0, 153.2, 135.5, 131.6, 130.3, 128.8, 127.8, 127.5, 122.8, 122.7, 110.0, 109.0, 78.2, 46.9, 31.1, 28.5$; IR (cm^{-1}): 3061, 2972, 1647, 1581, 1495, 1457, 1361, 1320, 1151, 1056; HR-ESIMS (m/z): Calcd. for $[\text{M}+\text{H}]^+ \text{C}_{20}\text{H}_{24}\text{N}_3\text{O}_2$ is 338.1863 found 338.1858; Calcd. for $[\text{M}+\text{Na}]^+ \text{C}_{20}\text{H}_{23}\text{N}_3\text{O}_2\text{Na}$ is 360.1682 found 360.1684.

1-Benzyl-2-benzyloxycarbonylimino-3-methyl-2,3-dihydro-1*H*-imidazole (24):



Prepared following the same procedure as **22** from **15h** (0.15 g 0.72 mmol) and purified by column chromatography (8% MeOH in EtOAc) to give **24** as a white solid (0.082g, 36%). mp: 93-95 °C (lit. 93-95 °C)⁸; ^1H NMR (500 MHz, CDCl_3): $\delta = 7.43$ (d, $J = 7.5$ Hz, 2H), 7.33-7.29 (m, 5H), 7.24-7.21 (m, 3H), 6.49 (d, $J = 2.9$ Hz, 1H), 6.37 (d, $J = 2.9$ Hz, 1H), 5.16 (s, 2H), 4.98 (s, 2H), 3.46 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): $\delta = 159.4, 150.9, 138.5, 135.2, 129.0, 128.5, 128.4, 128.3, 127.9, 127.4, 116.4, 114.3, 66.8, 50.0, 34.2$; IR (cm^{-1}): 3031, 2944, 1631, 1549, 1486, 1454, 1381, 1313, 1233, 1165, 1066.

1-Benzyl-2-tert-butylcarbonylimino-3-methyl-2,3-dihydro-1H-imidazole (25):



Prepared following the same procedure as **22** from **15h** (0.15 g, 0.72 mmol) and purified by column chromatography (8% MeOH in EtOAc) to give **25** as a clear, colorless oil (0.15 g, 71%). (lit. mp: 88-91 °C)⁸; ¹H NMR (500 MHz, CDCl₃): δ = 7.32-7.29 (m, 3H), 7.24-7.22 (m, 2H); 6.46 (d, *J* = 2.3 Hz, 1H), 6.31 (d, *J* = 2.3 Hz,

1H), 4.98 (s, 2H), 3.46 (s, 3H), 1.50 (s, 9H); ¹³C NMR (125 MHz, CDCl₃): δ = 159.5, 150.9, 135.5, 129.0, 128.5, 128.3, 116.2, 114.0, 77.0, 49.9, 34.2, 28.7; IR (cm⁻¹): 2973, 1626, 1548, 1483, 1453, 1361, 1318, 1240, 1153, 1066.

¹ Reddy, S. P.;Veeranagaiah, V.; Ratnam, C. V. *Proc. Indian Acad. Sci., Sec. A* **1975**, *81*, 124-131.

² Medvedeva, M. M., Pozharskii, A.F. *Khim. Geterotsikl. Soedin.* **1982**, *8*, 1086-1088.

³ Bostai, B.; Novak, Z.; Benyei, A.C.; Kotschy, A. *Org. Lett.* **2007**, *17*, 3437-3439.

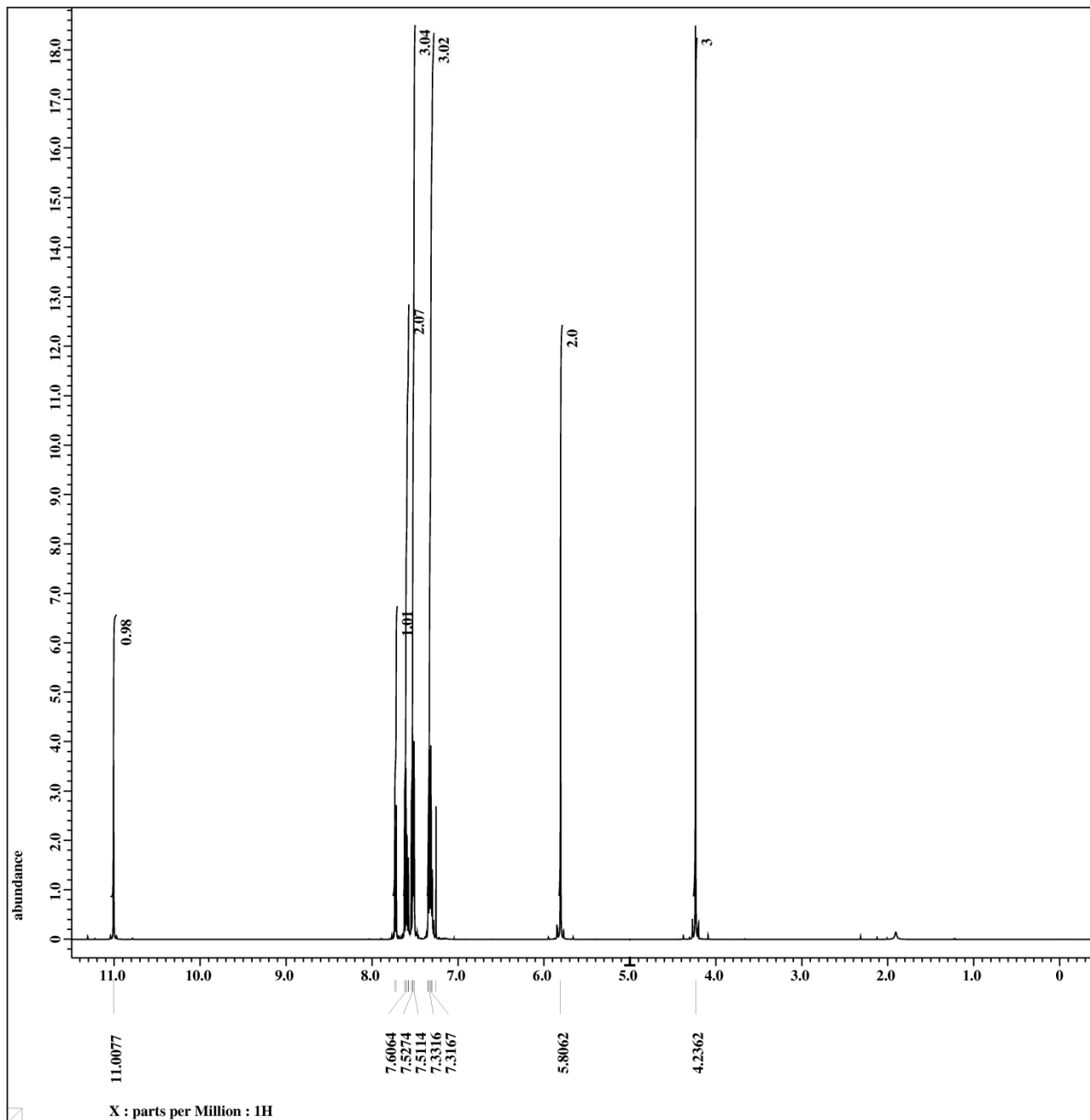
⁴ Nakamura, S.; Tsuno, N.; Yamashita, M.; Kawasaki, I.; Ohta, S.; Ohishi, Y. *J. Chem. Soc., Perkin Trans.* **2001**, *1*, 429-436.

⁵ Vernin, G.; Domlog, H.; Siv, C.; Metzger, J.; El-Shafei, A. K. *J. Heterocycl. Chem.* **1981**, *18*, 85-89.

⁶ Chawla, H. M.; Pathak, M. *Tetrahedron* **1990**, *4*, 1331-1342.

⁷ Pozharskii, A. F.; Kuz'menko, V. V.; Kashparov, I. S.; Sokolov, V. I.; Medvedeva, M. M. *Khim. Geterotsikl. Soedin.* **1976**, *3*, 356-364.

⁸ Kawasaki, I.; Nakamura, S.; Yanagitani, S.; Kakuno, A.; Yamahita, M.; Ohta, S. *J. Chem. Soc., Perkins Trans.* **2001**, *1*, 3095-3099.

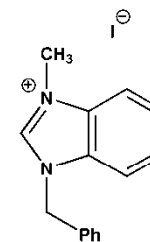


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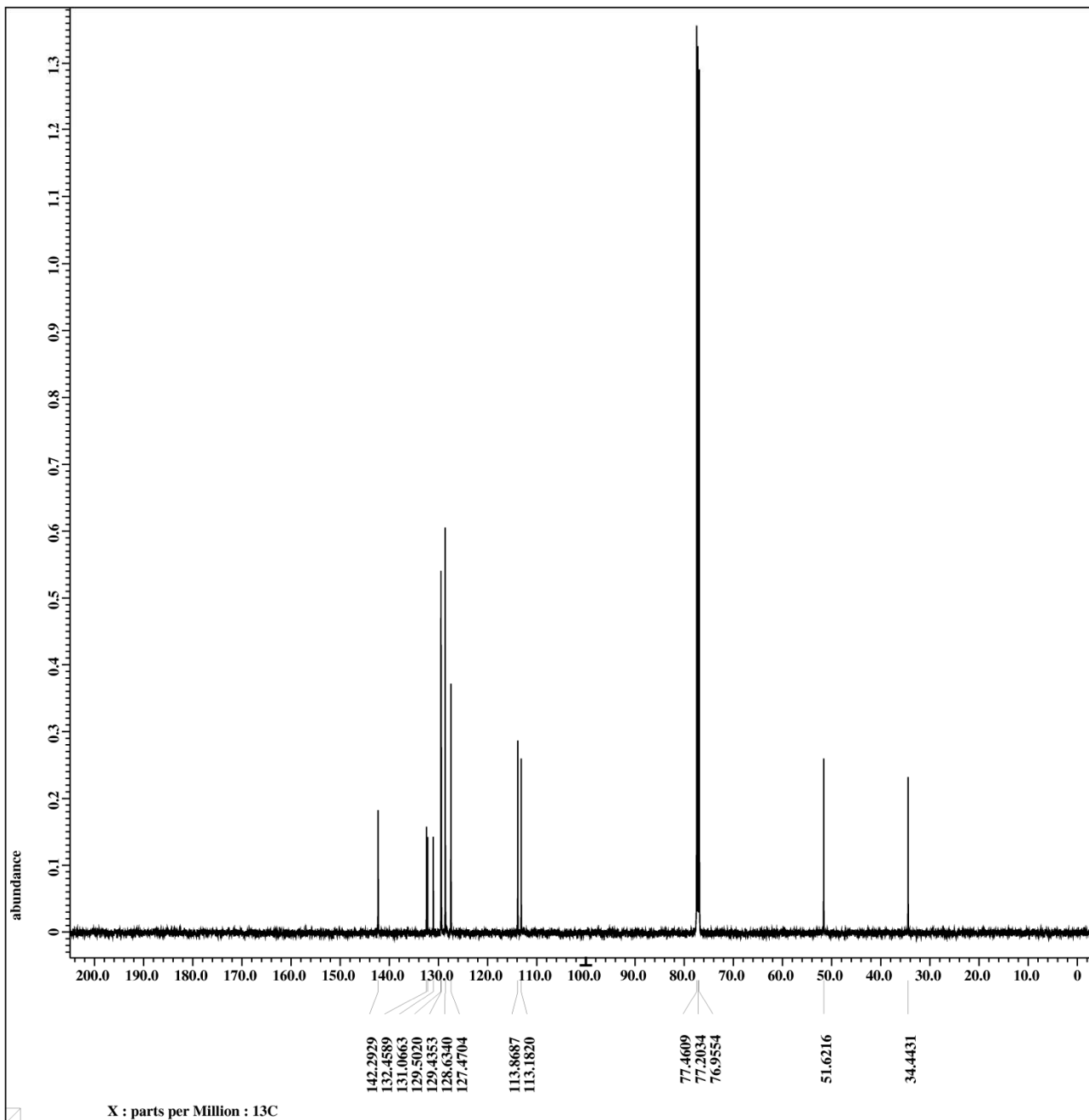
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15a



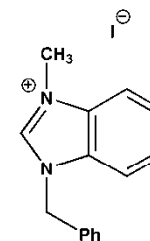
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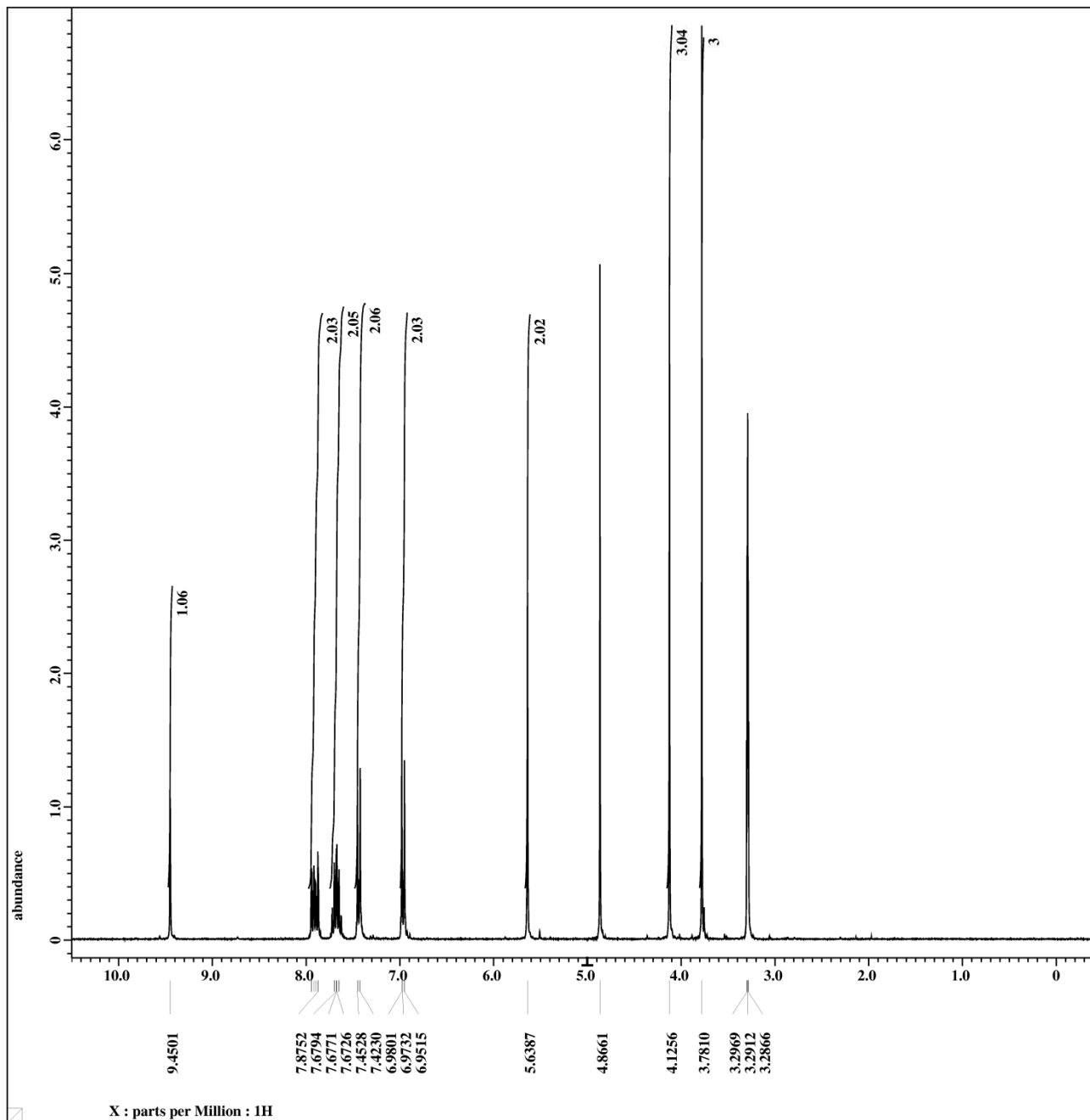
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15a



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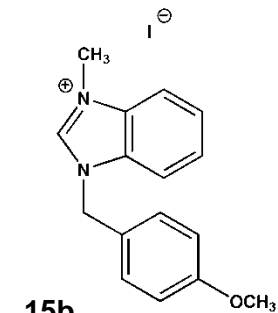
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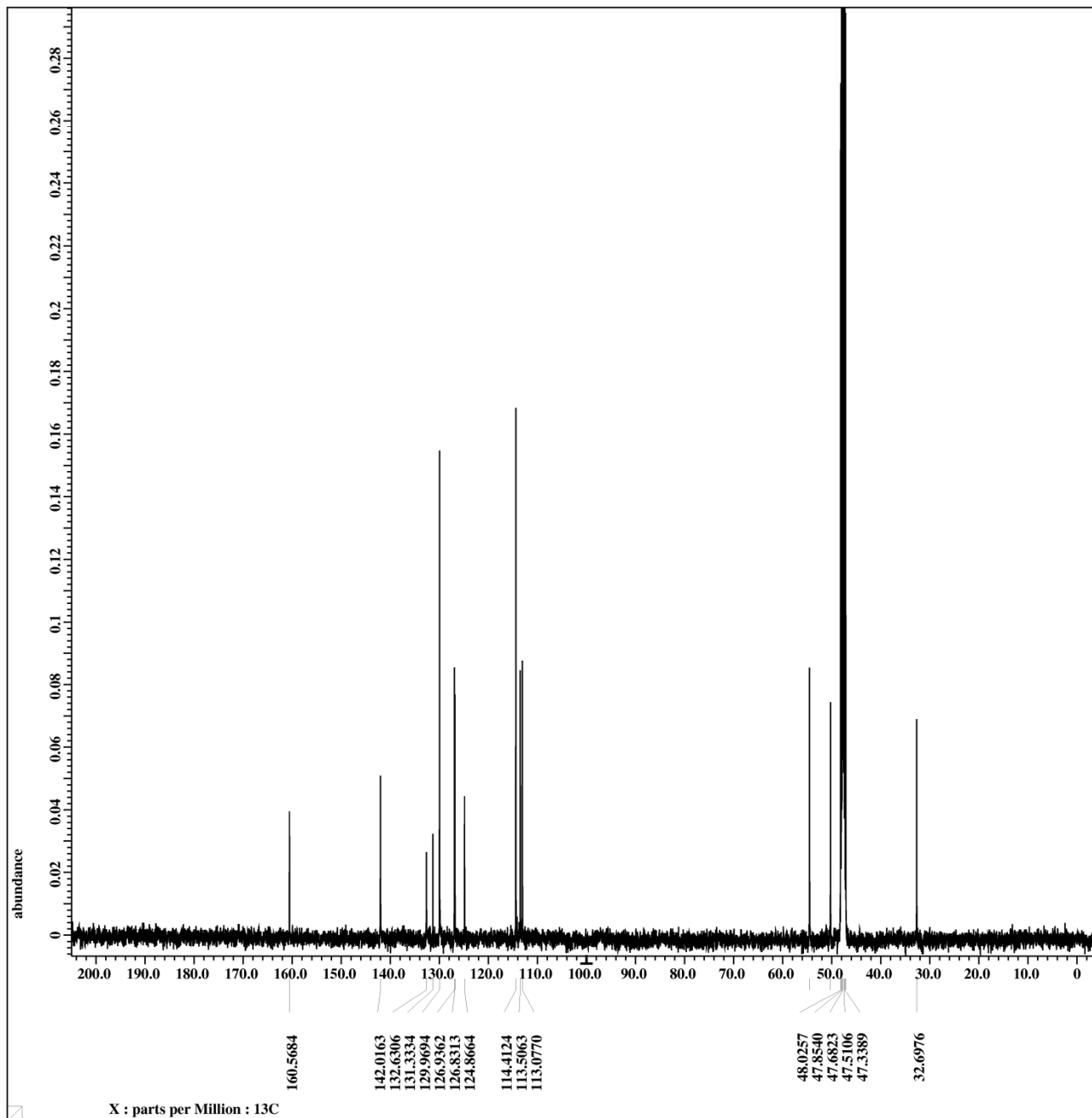
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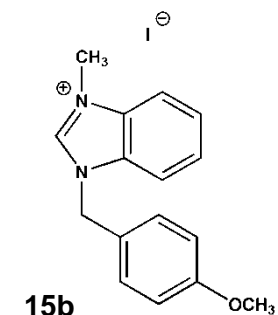
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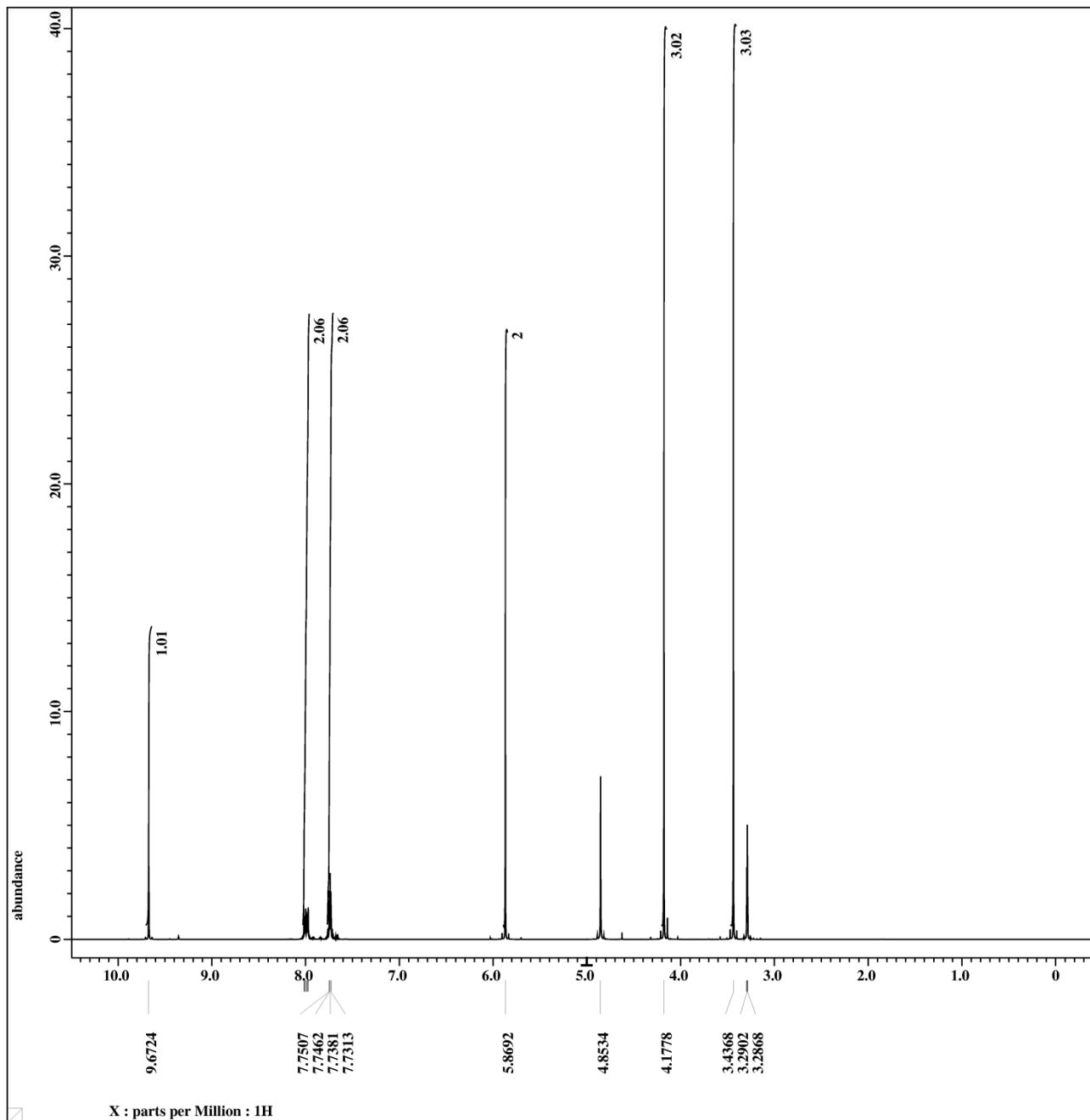
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X_freq         = 125.76529768[MHz]
X_offset       = 100[ppm]
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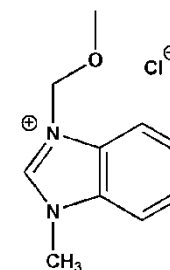
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Sample_id    = S#604804
Solvent      = METHANOL-D3
Creation_time = 17-FEB-2011 07:50:38
Revision_time = 20-FEB-2011 17:46:55
Current_time  = 20-FEB-2011 17:47:51

Comment      = single_pulse
Data_format  = 1D_COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

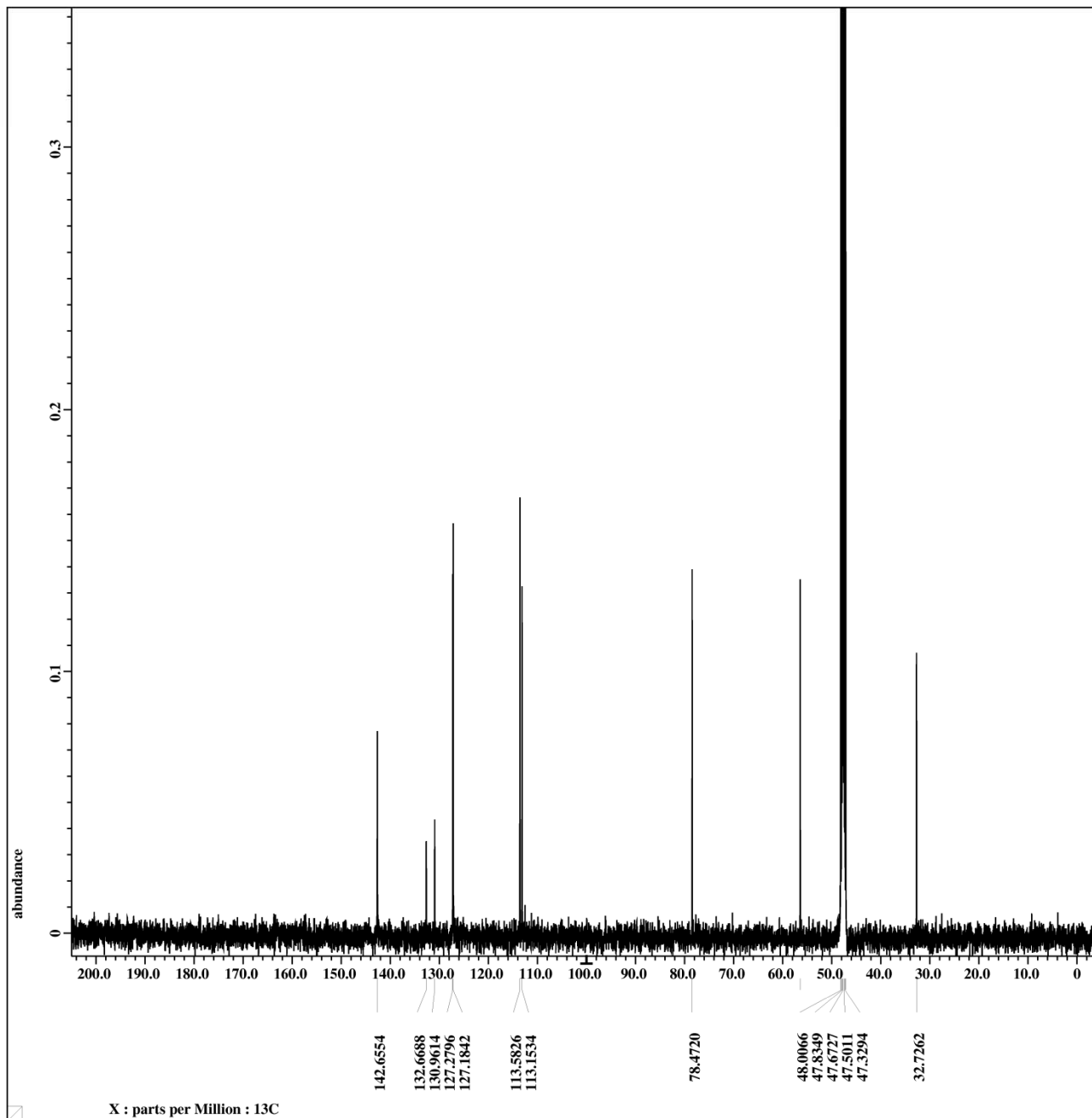
Field_strength = 11.7473579[T] (500[MH]
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans     = 0
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width    = 12.54[us]
X_acq_time    = 1.74587904[s]
X_angle       = 45[deg]
X_atn         = 4[dB]
X_pulse       = 6.27[us]
Irr_mode      = Off
Tri_mode      = Off
Dante_presat  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 46
Relaxation_delay = 5[s]
Repetition_time = 6.74587904[s]
Temp_get      = 21[dC]

```



15c



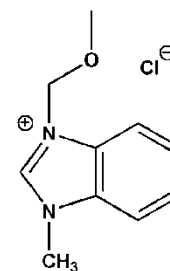
```

Filename      = HMF_III_108-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#607271
Solvent      = METHANOL-D3
Creation_time = 17-FEB-2011 08:16:00
Revision_time = 20-FEB-2011 17:49:29
Current_time  = 20-FEB-2011 17:50:27

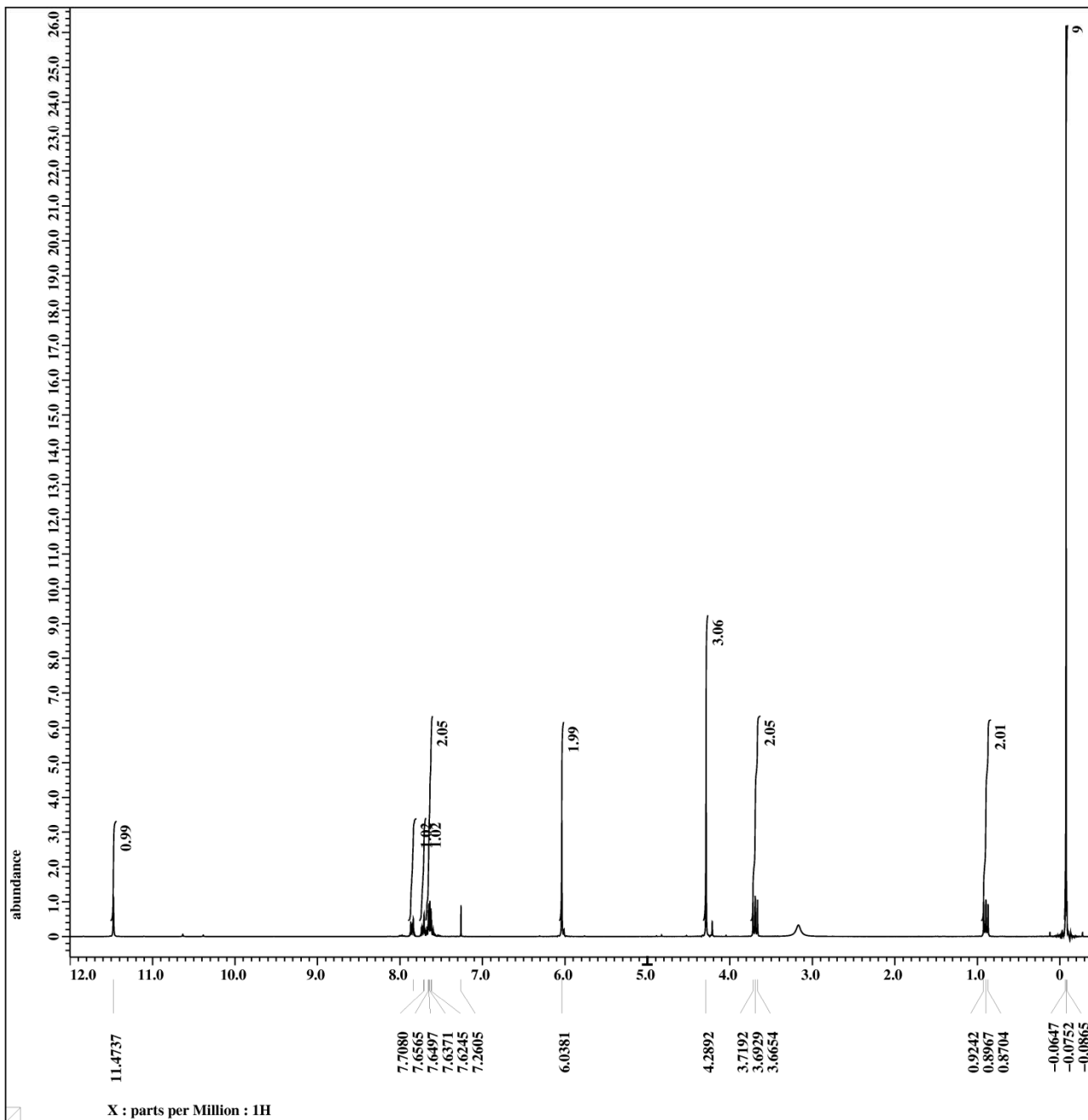
Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034[Hz]
X_sweep        = 39.3081761[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 350
Total_scans    = 350

X_90_width    = 10.73[us]
X_acq_time    = 0.83361792[s]
X_angle       = 30[deg]
X_atn         = 9[dB]
X_pulse       = 3.57666667[us]
Irr_atn_dec   = 20[dB]
Irr_atn_noe   = 20[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 3[s]
Recvr_gain    = 50
Relaxation_delay = 3[s]
Repetition_time = 3.83361792[s]
Temp_get      = 21.8[dC]
  
```



15c

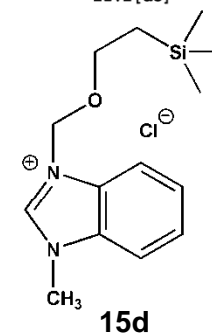


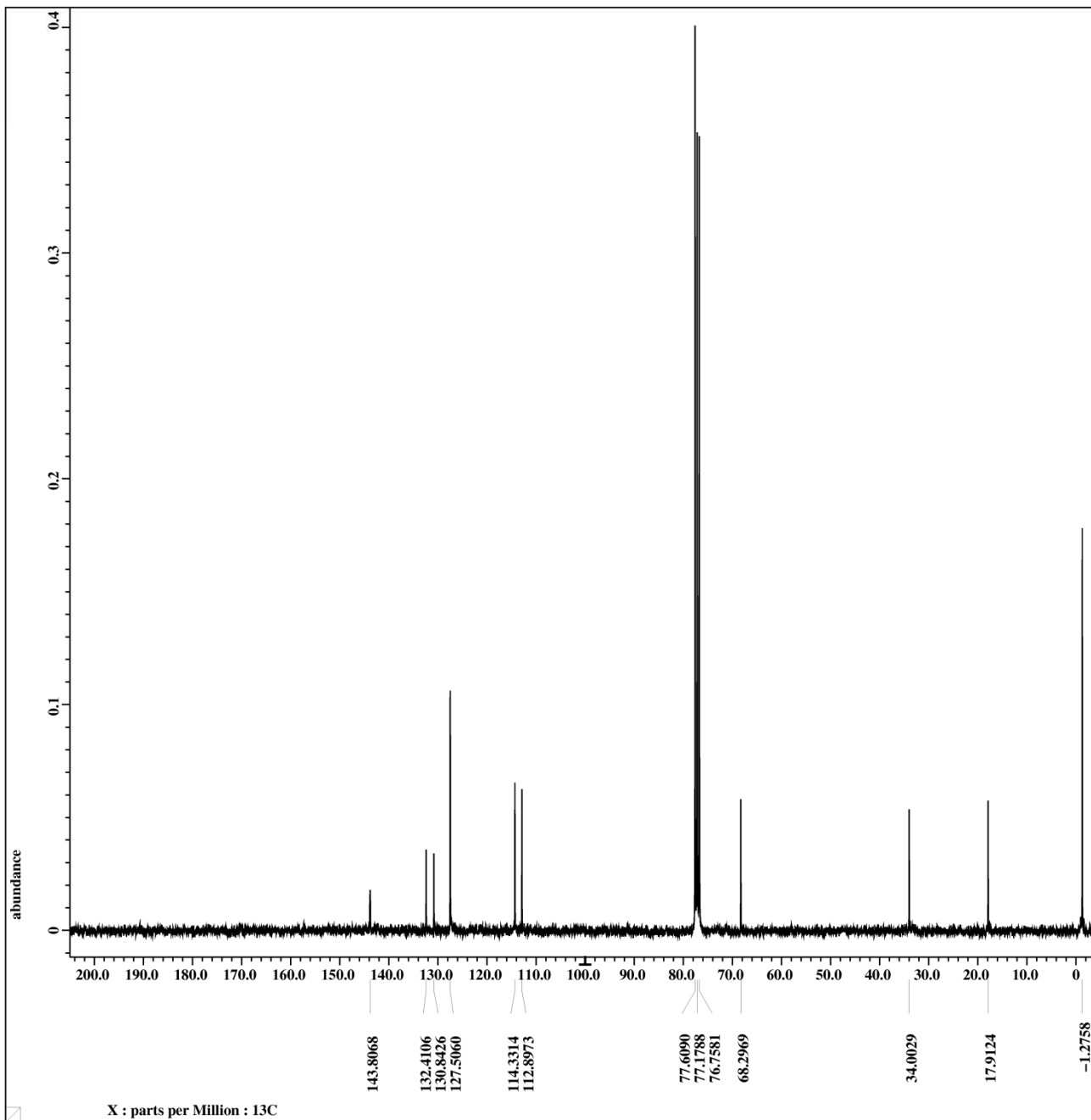
Filename = HMF_II_289-7.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#481543
 Solvent = CHLOROFORM-D
 Creation_time = 9-SEP-2010 13:02:58
 Revision_time = 7-OCT-2010 15:33:59
 Current_time = 7-OCT-2010 15:34:20

Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 300
 Spectrometer = DELTA2_NMR

Field_strength = 7.0586013[T] (300[MHz])
 X_acq_duration = 2.90717696[s]
 X_domain = 1H
 X_freq = 300.52965592[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.34397631[Hz]
 X_sweep = 5.63570784[kHz]
 Irr_domain = 1H
 Irr_freq = 300.52965592[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 300.52965592[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 24
 Total_scans = 24

X_90_width = 13.01[us]
 X_acq_time = 2.90717696[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.505[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 38
 Relaxation_delay = 5[s]
 Repetition_time = 7.90717696[s]
 Temp_get = 21.2[dc]





```

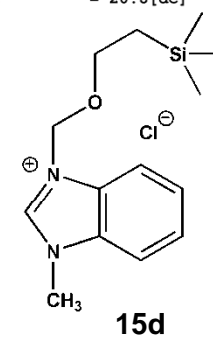
Filename      = HMF_II_289-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#499773
Solvent      = CHLOROFORM-D
Creation_time = 9-SEP-2010 14:41:39
Revision_time = 7-OCT-2010 15:41:36
Current_time  = 7-OCT-2010 15:44:45

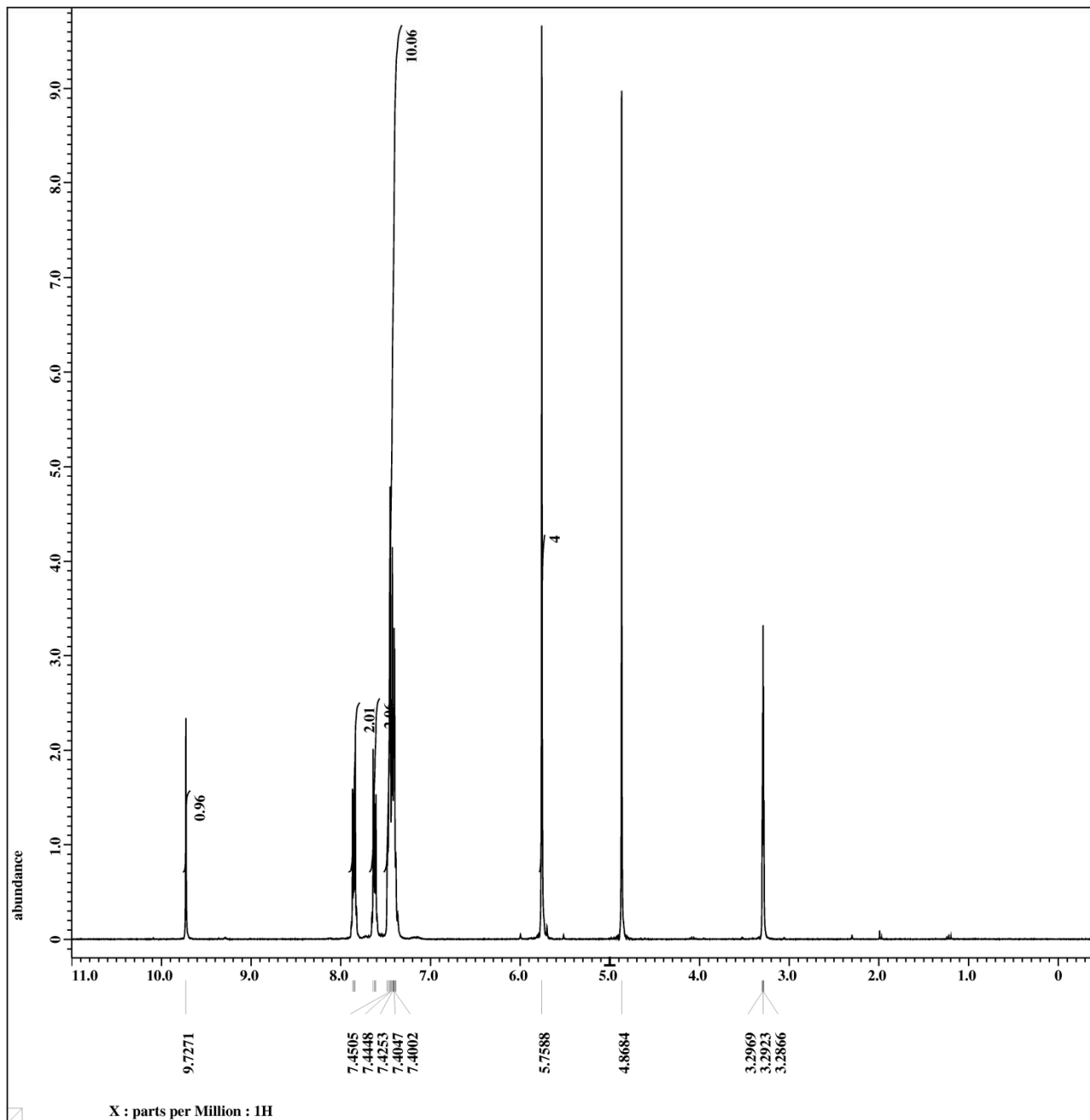
Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECX 300
Spectrometer = DELTA2_NMR

Field_strength = 7.0586013[T] (300[MHz]
X_acq_duration = 1.38412032[s]
X_domain       = 13C
X_freq         = 75.56823426[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans    = 4
X_resolution   = 0.72248054[Hz]
X_sweep        = 23.67424242[kHz]
Irr_domain    = 1H
Irr_freq      = 300.52965592[MHz]
Irr_offset    = 5[ppm]
Clipped       = FALSE
Mod_return    = 10
Scans         = 800
Total_scans   = 800

X_90_width    = 9.75[us]
X_acq_time    = 1.38412032[s]
X_angle       = 30[deg]
X_atn         = 8[dB]
X_pulse       = 3.25[us]
Irr_atn_dec   = 25[dB]
Irr_atn_noe   = 25[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 4[s]
Recvr_gain    = 50
Relaxation_delay = 4[s]
Repetition_time = 5.38412032[s]
Temp_get      = 20.8[dC]

```





```

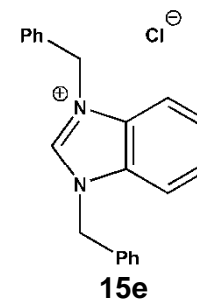
Filename      = HMF_II_295-4.jdf
Author        = delta
Experiment    = single_pulse.ex2
Sample_id     = S#495759
Solvent       = METHANOL-D3
Creation_time = 16-SEP-2010 13:26:01
Revision_time = 7-OCT-2010 15:11:28
Current_time  = 7-OCT-2010 15:12:19

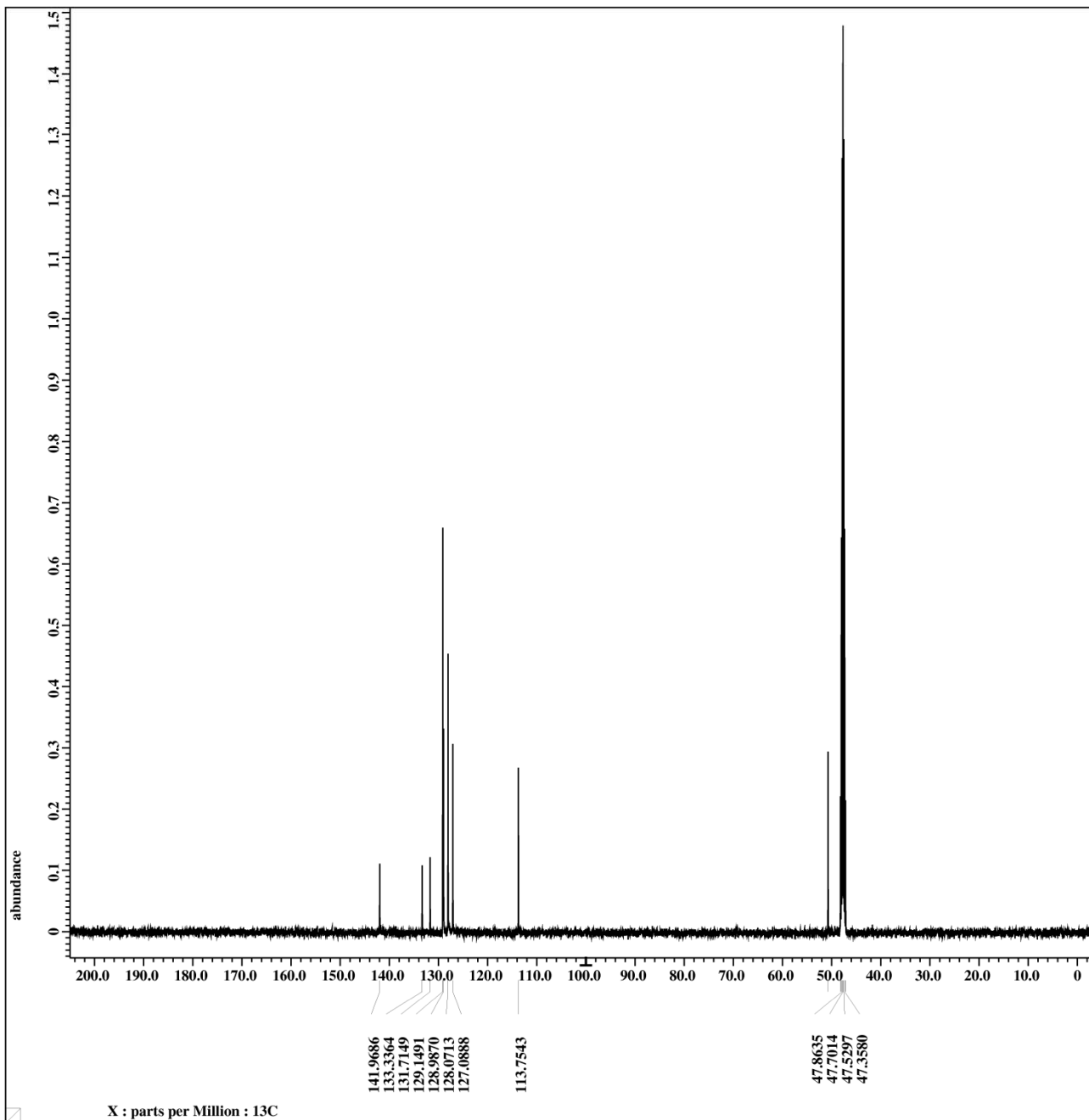
Comment       = single_pulse
Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECX 300
Spectrometer  = DELTA2_NMR

Field_strength = 7.0586013[T] (300[MHz]
X_acq_duration = 2.90717696[s]
X_domain       = 1H
X_freq         = 300.52965592[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 0
X_resolution   = 0.34397631[Hz]
X_sweep        = 5.63570784[kHz]
Irr_domain    = 1H
Irr_freq       = 300.52965592[MHz]
Irr_offset     = 5[ppm]
Tri_domain    = 1H
Tri_freq       = 300.52965592[MHz]
Tri_offset     = 5[ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 24
Total_scans   = 24

X_90_width    = 13.01[us]
X_acq_time    = 2.90717696[s]
X_angle       = 45[deg]
X_atn         = 4[dB]
X_pulse       = 6.505[us]
Irr_mode      = Off
Tri_mode      = Off
Dante_presat  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 50
Relaxation_delay = 5[s]
Repetition_time = 7.90717696[s]
Temp_get      = 21.1[dc]

```





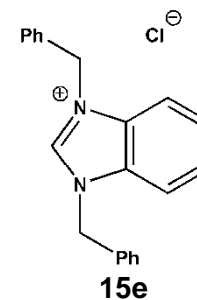
```

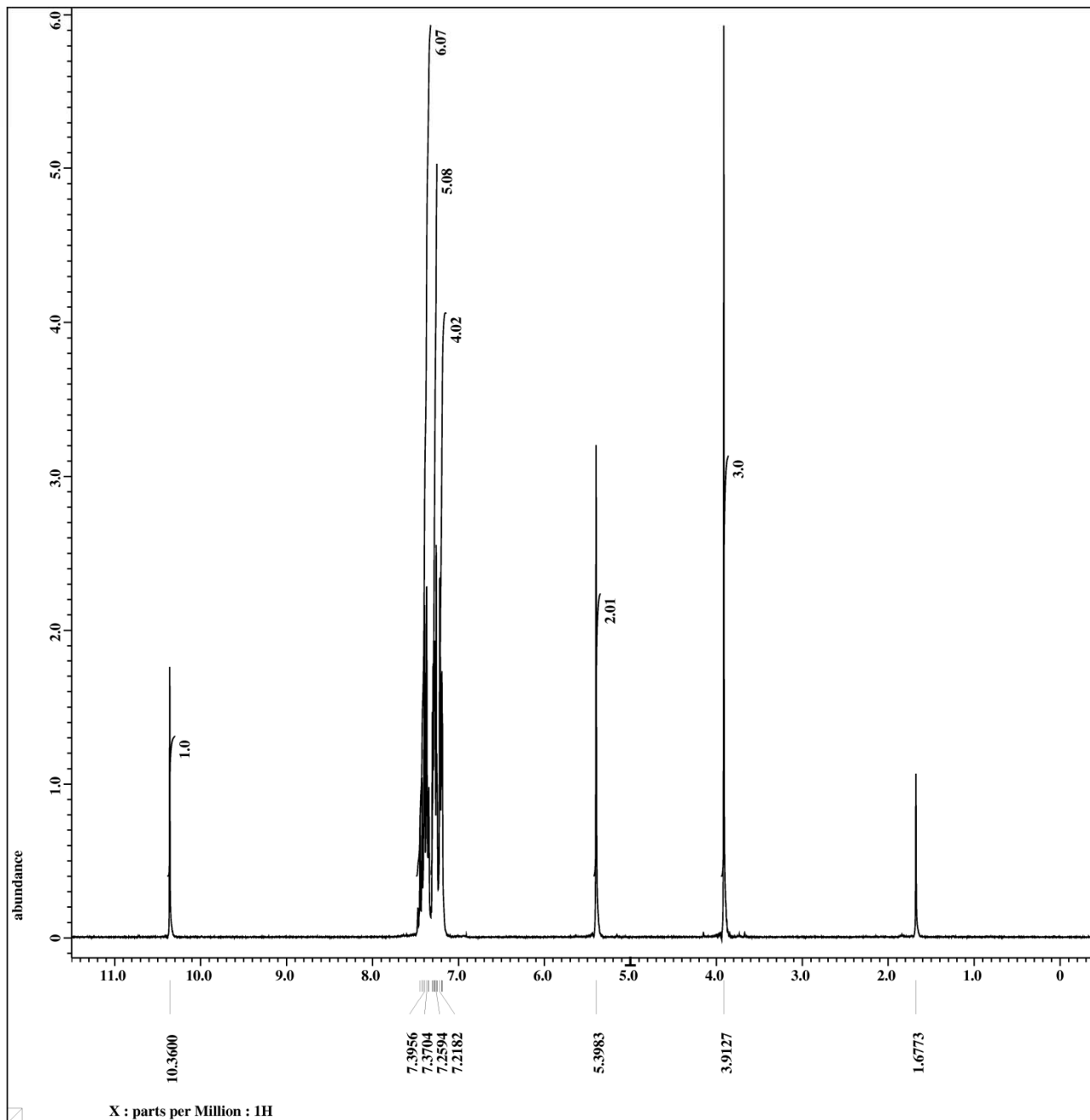
Filename      = HMF_II_295-2.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#609546
Solvent      = METHANOL-D3
Creation_time = 12-JAN-2011 08:09:03
Revision_time = 12-JAN-2011 10:18:48
Current_time  = 12-JAN-2011 10:19:30

Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 170
Total_scans    = 170

X_90_width    = 10.73 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 9 [dB]
X_pulse        = 3.57666667 [us]
Irr_atn_dec    = 20 [dB]
Irr_atn_noe    = 20 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 4 [s]
Recvr_gain     = 50
Relaxation_delay = 4 [s]
Repetition_time = 4.83361792 [s]
Temp_get       = 21.7 [dC]
  
```



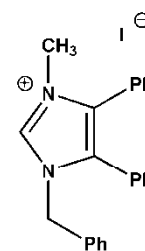


Filename = HMF_II_309-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#607383
 Solvent = CHLOROFORM-D
 Creation_time = 24-SEP-2010 16:36:18
 Revision_time = 8-OCT-2010 10:51:37
 Current_time = 8-OCT-2010 10:52:33

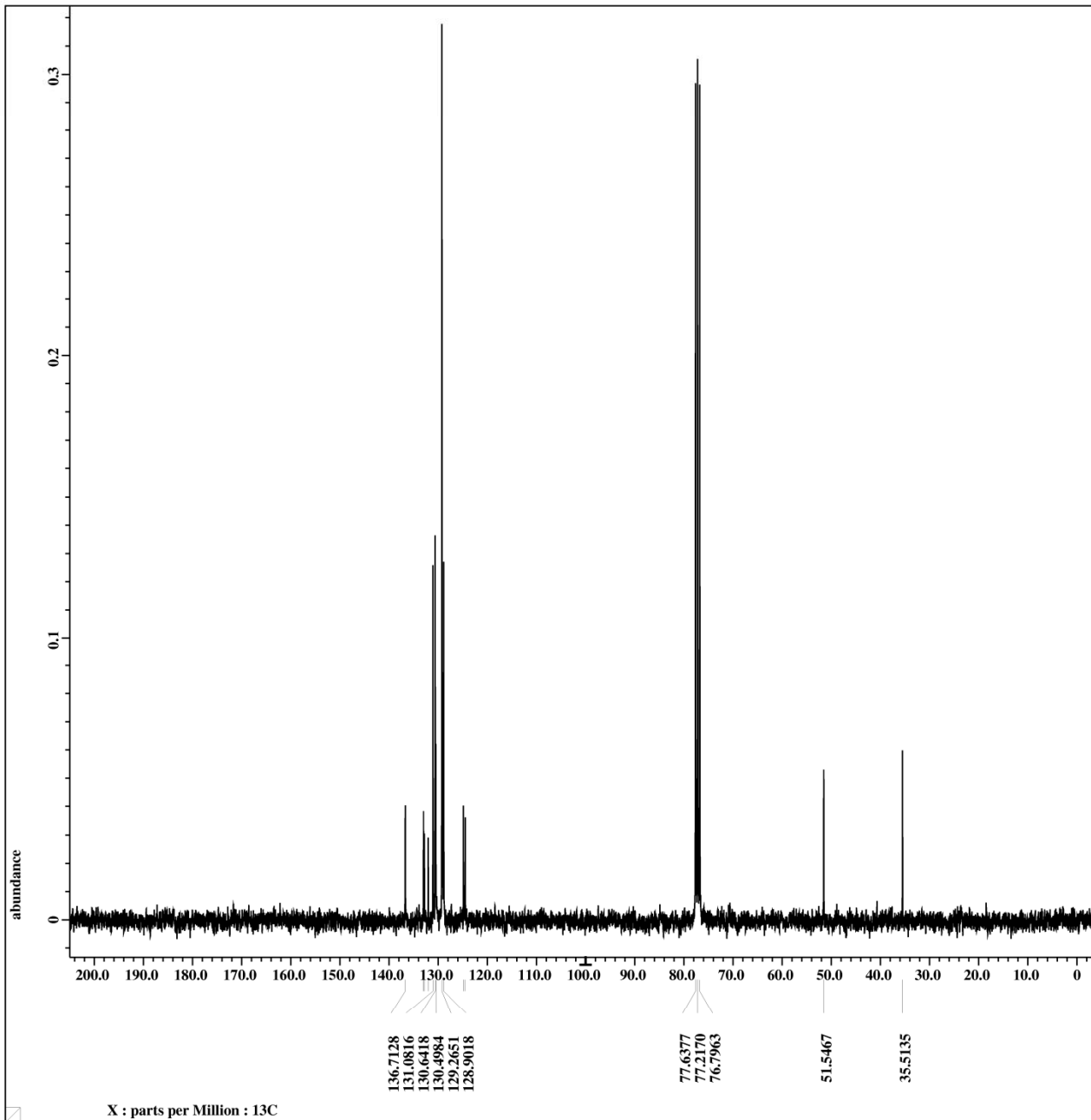
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 300
 Spectrometer = DELTA2_NMR

Field_strength = 7.0586013[T] (300[MHz])
 X_acq_duration = 2.90717696[s]
 X_domain = 1H
 X_freq = 300.52965592[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.34397631[Hz]
 X_sweep = 5.63570784[kHz]
 Irr_domain = 1H
 Irr_freq = 300.52965592[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 300.52965592[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 24
 Total_scans = 24

X_90_width = 13.01[us]
 X_acq_time = 2.90717696[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.505[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 7.90717696[s]
 Temp_get = 20.7[dc]



15f

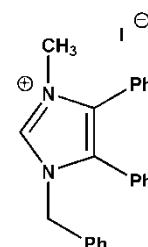


Filename = HMF_II_309-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#495800
 Solvent = CHLOROFORM-D
 Creation_time = 8-OCT-2010 13:44:16
 Revision_time = 19-NOV-2010 23:45:05
 Current_time = 19-NOV-2010 23:46:58

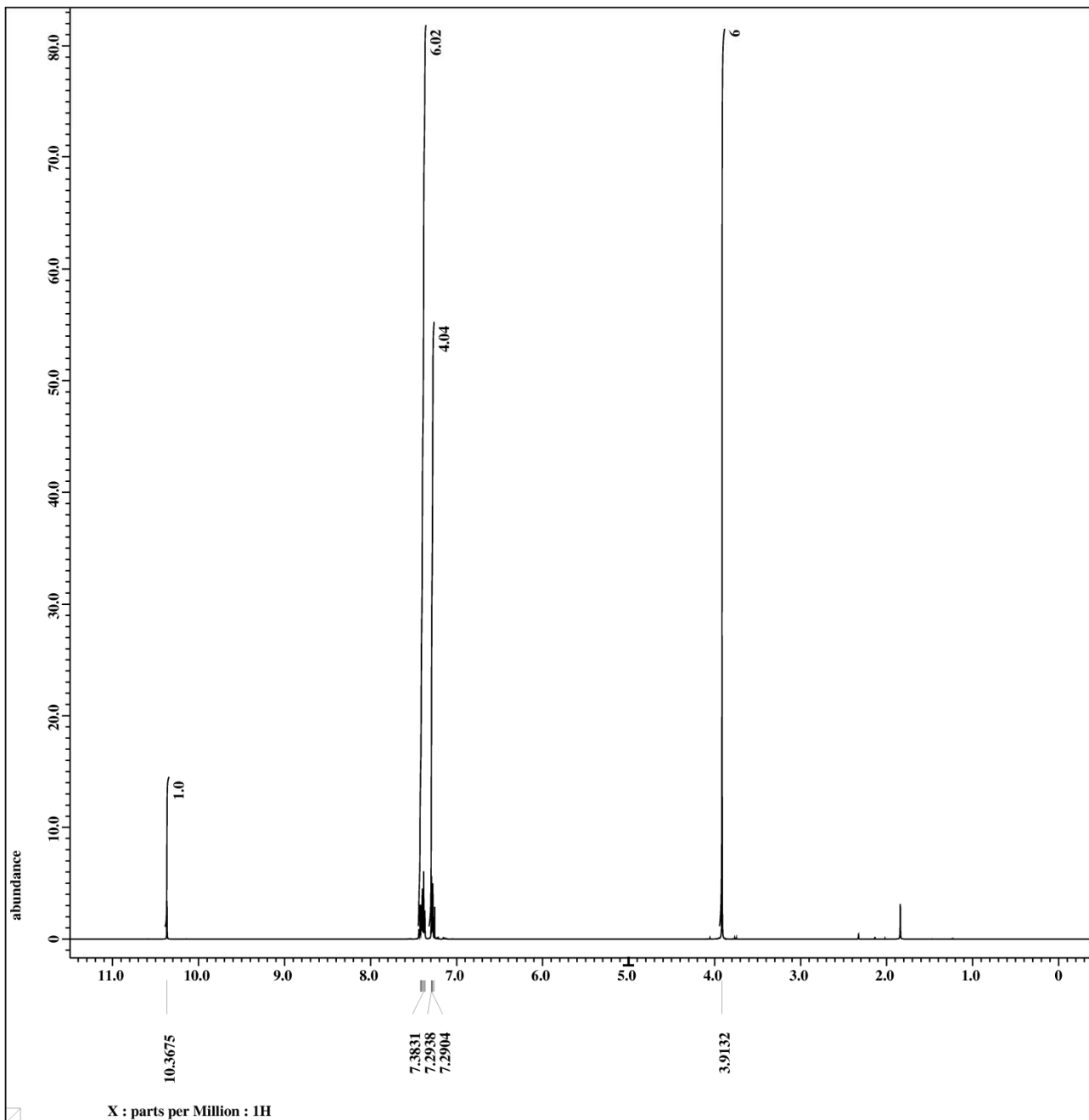
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 300
 Spectrometer = DELTA2_NMR

Field_strength = 7.0586013[T] (300[MHz]
 X_acq_duration = 1.38412032[s]
 X_domain = 13C
 X_freq = 75.56823426[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.72248054[Hz]
 X_sweep = 23.67424242[kHz]
 Irr_domain = 1H
 Irr_freq = 300.52965592[MHz]
 Irr_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 10
 Scans = 220
 Total_scans = 220

X_90_width = 9.75[us]
 X_acq_time = 1.38412032[s]
 X_angle = 30[deg]
 X_atn = 8[dB]
 X_atn = 3.25[us]
 Irr_pulse_dec = 25[dB]
 Irr_atn_noe = 25[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 3[s]
 Recvr_gain = 50
 Relaxation_delay = 3[s]
 Repetition_time = 4.38412032[s]
 Temp_get = 21.3[dC]



15f



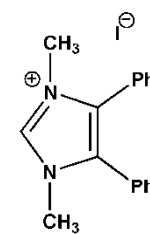
```

Filename      = HMF_III_190-4.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = S#399345
Solvent      = CHLOROFORM-D
Creation_time = 25-MAY-2011 01:12:10
Revision_time = 24-MAY-2011 11:50:59
Current_time  = 24-MAY-2011 11:52:39

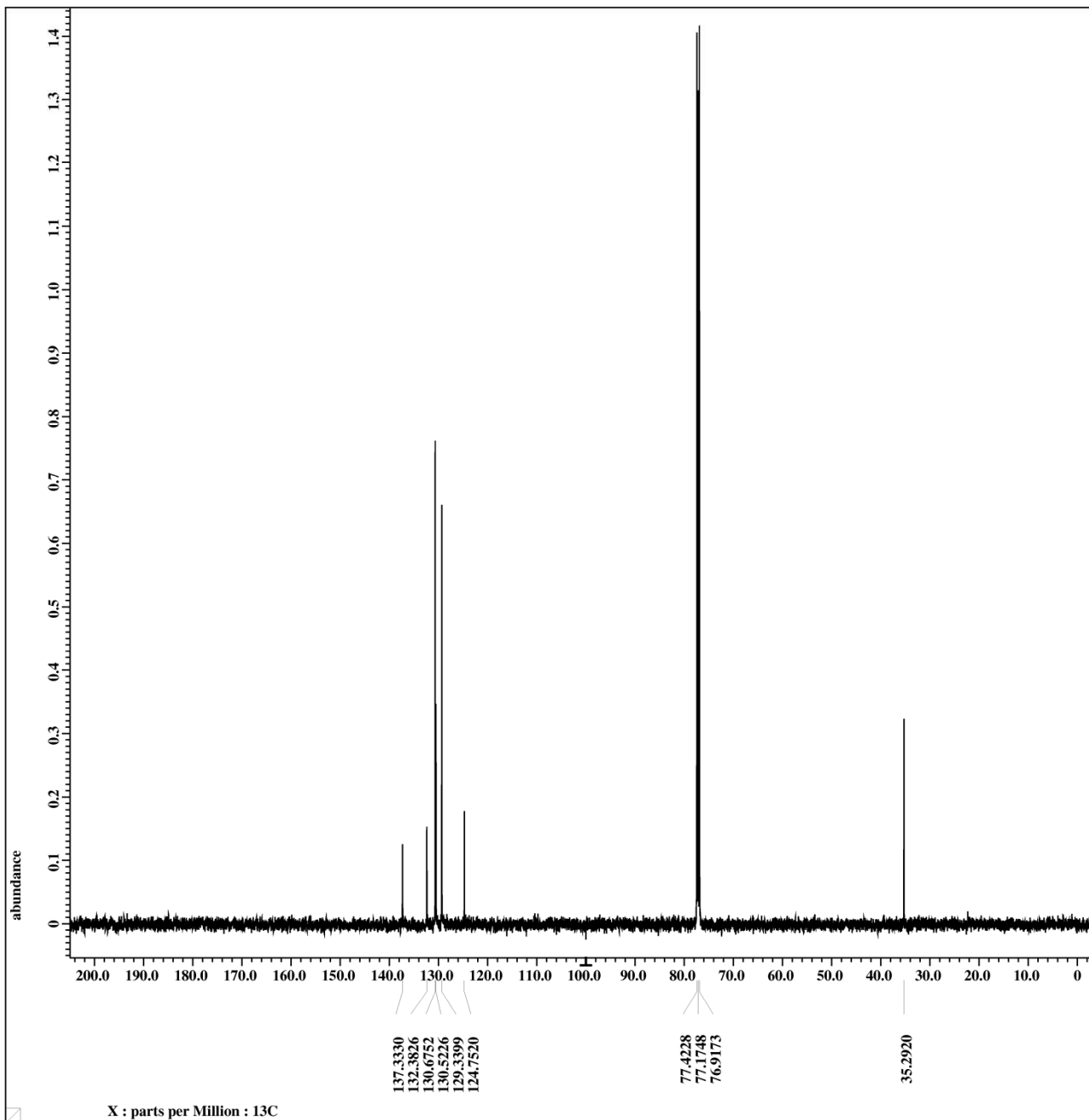
Comment      = single_pulse
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH]
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans     = 0
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width    = 12.54[us]
X_acq_time     = 1.74587904[s]
X_angle       = 45[deg]
X_atn         = 4[dB]
X_pulse       = 6.27[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 42
Relaxation_delay = 5[s]
Repetition_time = 6.74587904[s]
Temp_get       = 21.1[dC]
  
```



15g



```

Filename      = HMF_III_190-2.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#402135
Solvent      = CHLOROFORM-D
Creation_time = 25-MAY-2011 01:22:00
Revision_time = 24-MAY-2011 11:58:44
Current_time  = 24-MAY-2011 11:59:25

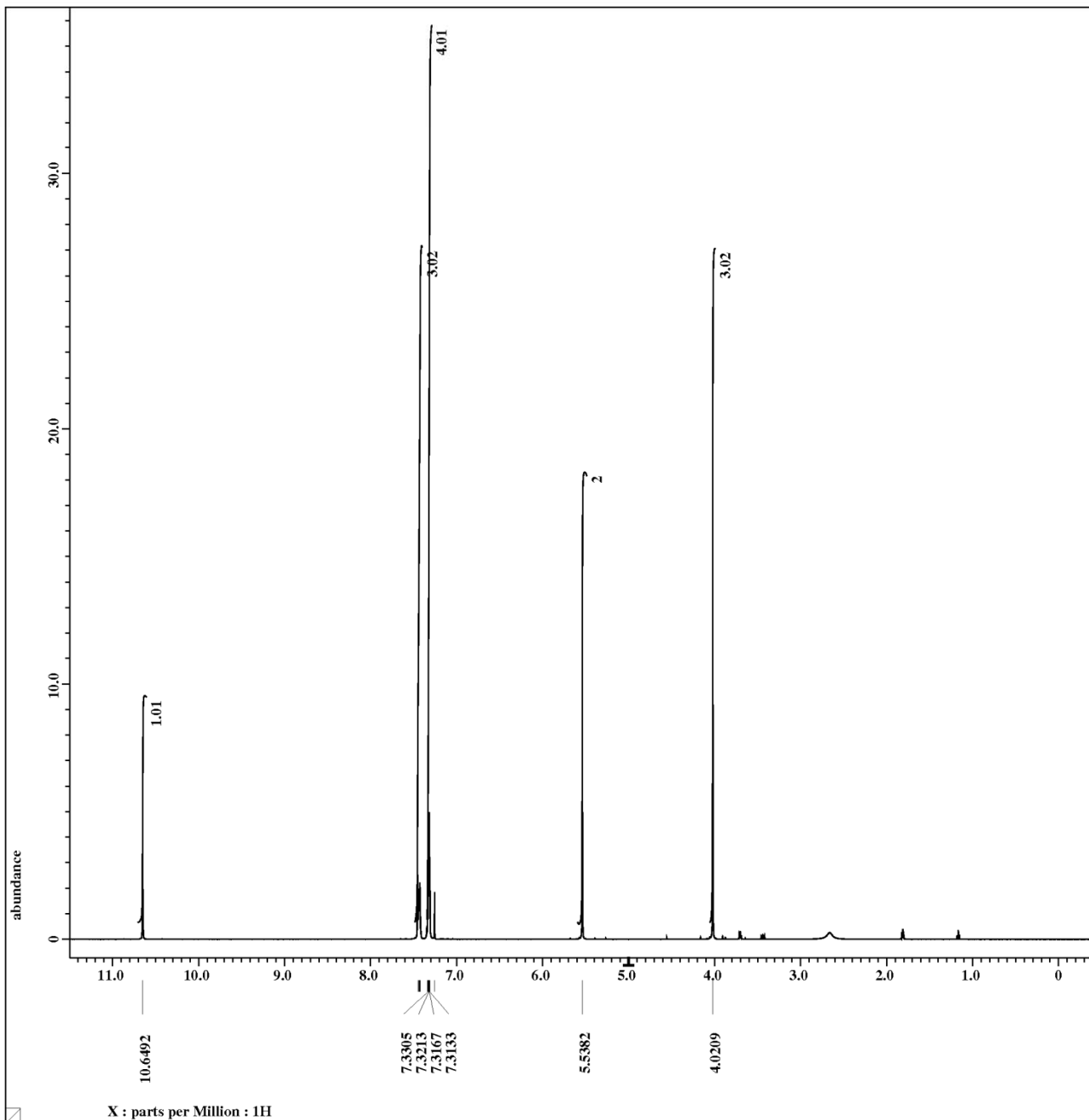
Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 90
Total_scans    = 90

X_90_width    = 10.73[us]
X_acq_time    = 0.83361792[s]
X_angle       = 30[deg]
X_atn         = 9[dB]
X_pulse       = 3.57666667[us]
Irr_atn_dec   = 20[dB]
Irr_atn_noe   = 20[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 4[s]
Recvr_gain    = 50
Relaxation_delay = 4[s]
Repetition_time = 4.83361792[s]
Temp_get      = 21.6[dC]
  
```



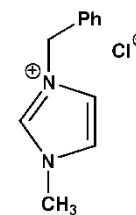
15g



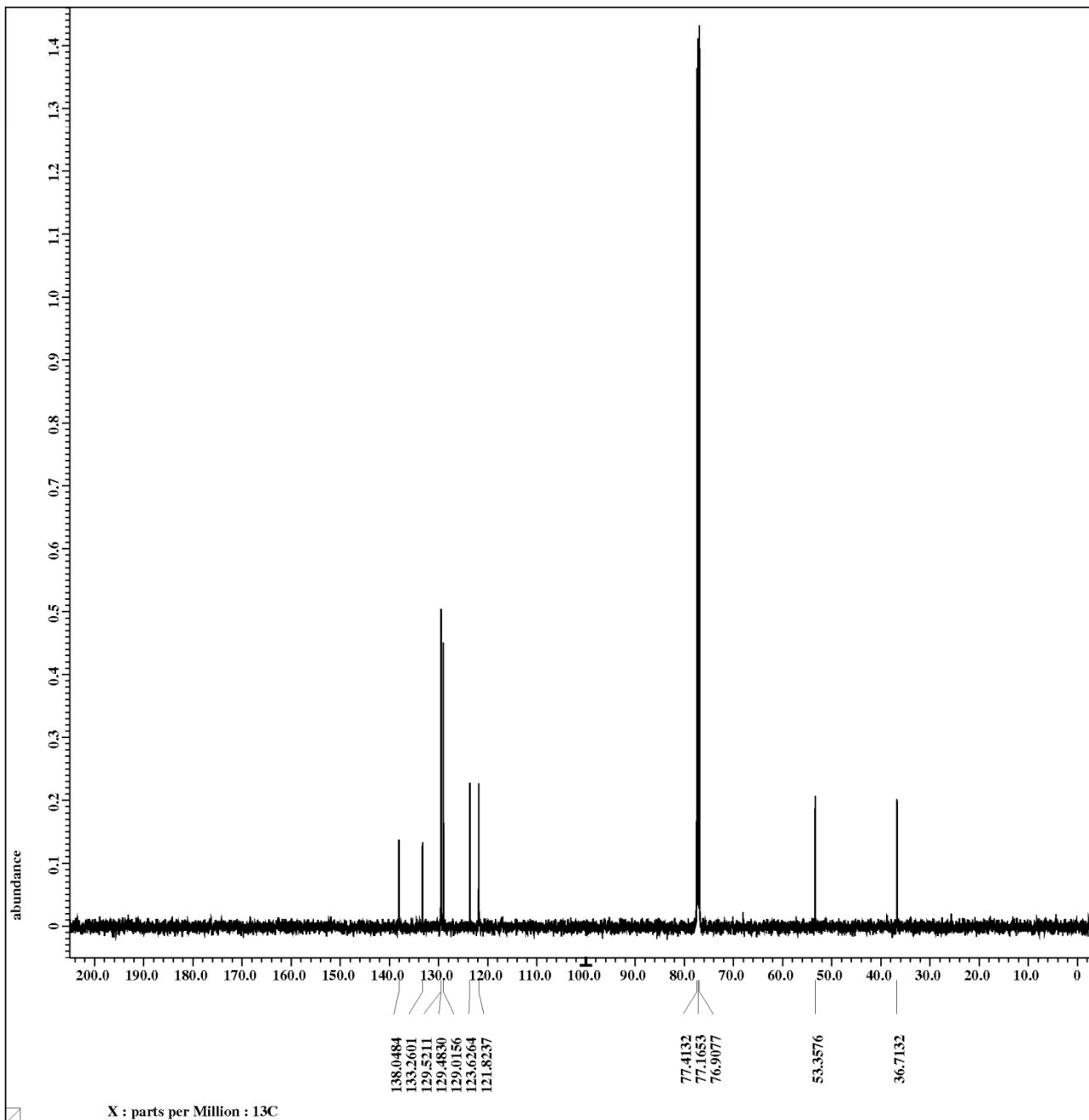
Filename = HMF_III_208-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#505468
 Solvent = CHLOROFORM-D
 Creation_time = 4-JUL-2011 04:11:20
 Revision_time = 12-JUL-2011 11:04:15
 Current_time = 12-JUL-2011 11:05:02

Comment = single pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 40
 Relaxation_delay = 5[s]
 Repetition_time = 6.74587904[s]
 Temp_get = 21[dc]



15h



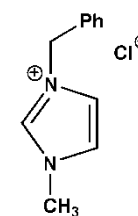
```

Filename      = HMF_III_208-2.jdf
Author        = delta
Experiment    = single_pulse_dec
Sample_id     = S#507375
Solvent       = CHLOROFORM-D
Creation time  = 4-JUL-2011 04:19:42
Revision time  = 12-JUL-2011 11:05:24
Current_time  = 12-JUL-2011 11:05:57

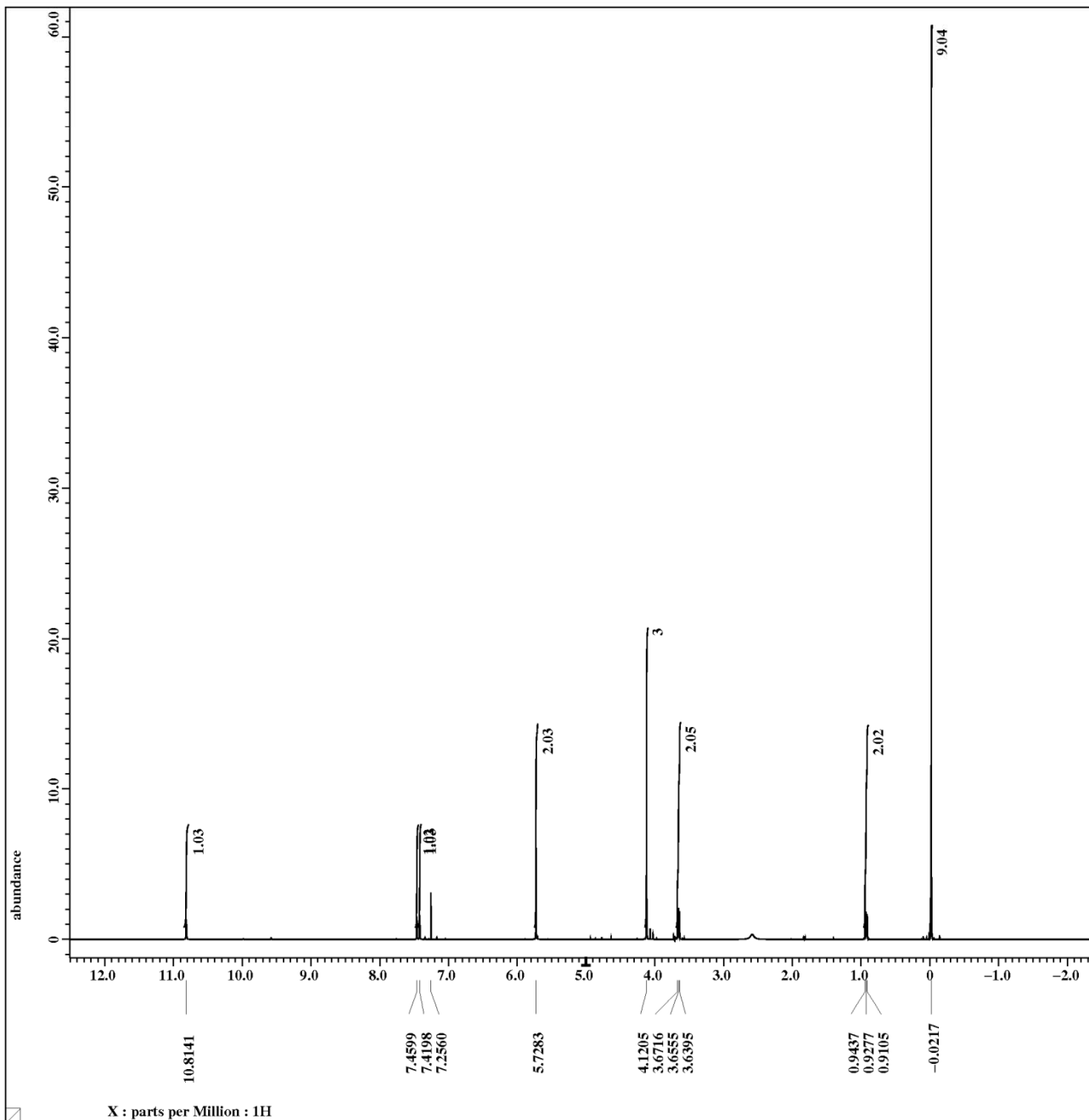
Comment       = single pulse decouple
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034[Hz]
X_sweep        = 39.3081761[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 90
Total_scans    = 90

X_90_width    = 10.73[us]
X_acq_time    = 0.83361792[s]
X_angle       = 30[deg]
X_atn         = 9[dB]
X_pulse       = 3.57666667[us]
Irr_atn_dec   = 20[dB]
Irr_atn_noe   = 20[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 4[s]
Recvr_gain    = 50
Relaxation_delay = 4[s]
Repetition_time = 4.83361792[s]
Temp_get      = 21.4[dC]
  
```



15h

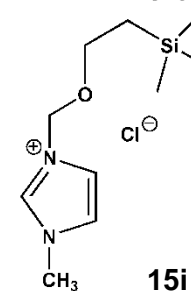


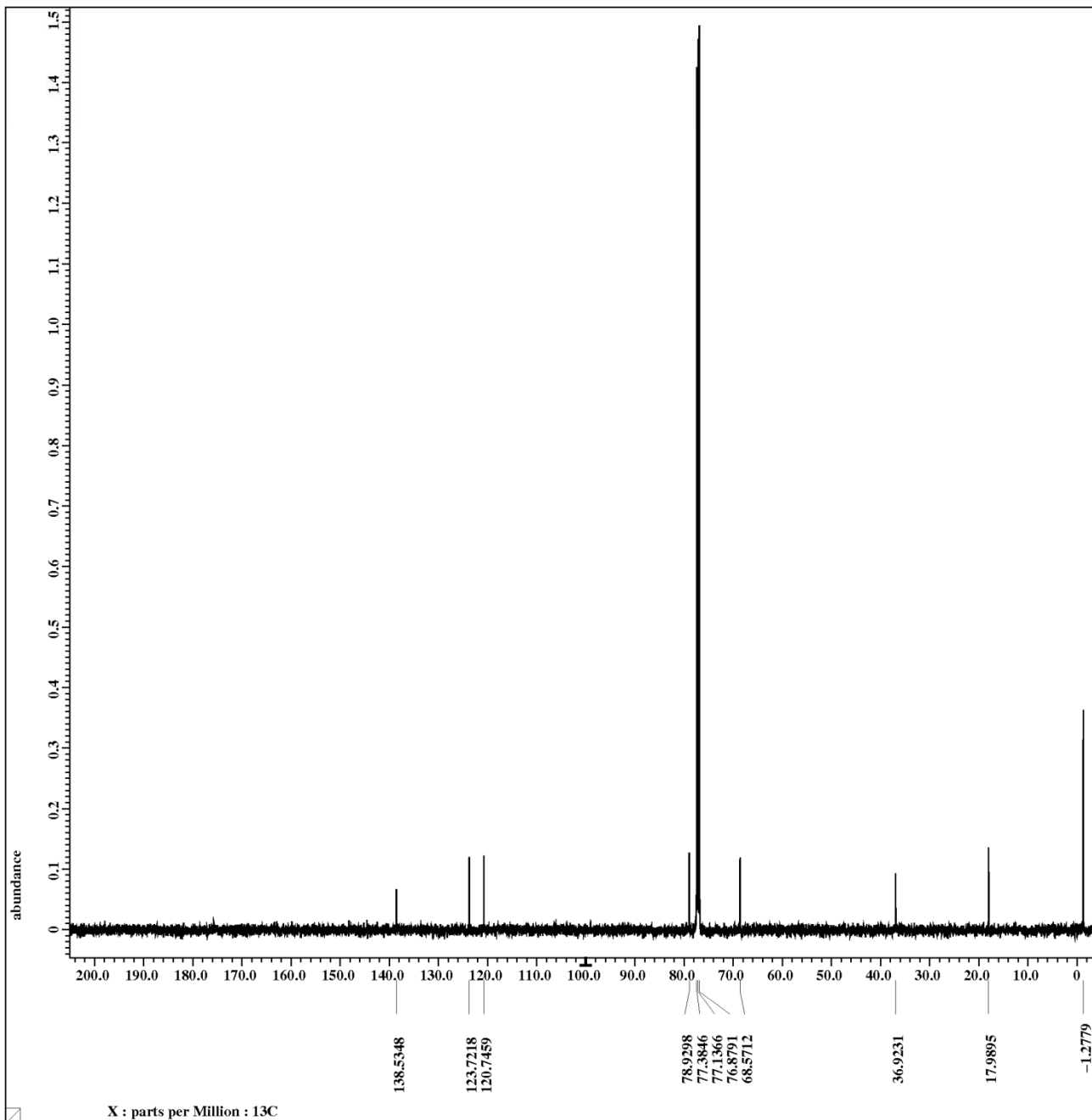
Filename = HMF_IV_15-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#611017
 Solvent = CHLOROFORM-D
 Creation_time = 14-JUL-2011 07:07:20
 Revision_time = 14-JUL-2011 14:03:39
 Current_time = 14-JUL-2011 14:04:07

Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 42
 Relaxation_delay = 5[s]
 Repetition_time = 6.74587904[s]
 Temp_get = 21.3[dC]



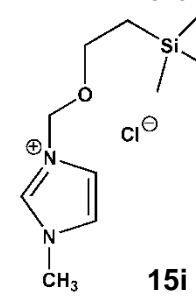


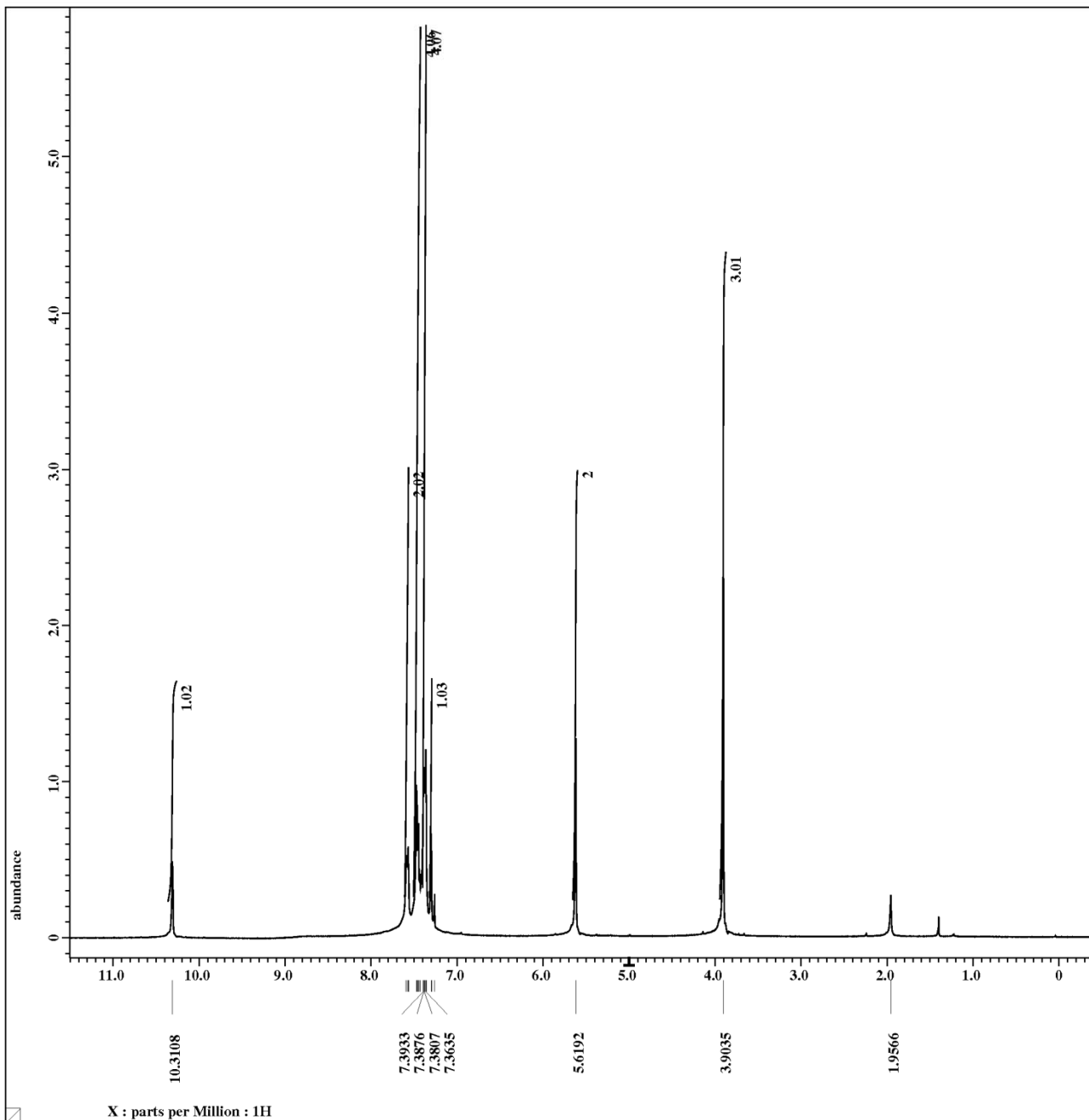
Filename = HMF_IV_15-2.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#612821
 Solvent = CHLOROFORM-D
 Creation_time = 14-JUL-2011 07:18:45
 Revision_time = 14-JUL-2011 14:04:24
 Current_time = 14-JUL-2011 14:04:54

Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 0.83361792[s]
 X_domain = 13C
 X_freq = 125.76529768 [MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.19959034 [Hz]
 X_sweep = 39.3081761 [kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 10
 Scans = 130
 Total_scans = 130

X_90_width = 10.73 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 9 [dB]
 X_pulse = 3.57666667 [us]
 Irr_atn_dec = 20 [dB]
 Irr_atn_noe = 20 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 4 [s]
 Recvr_gain = 50
 Relaxation_delay = 4 [s]
 Repetition_time = 4.83361792 [s]
 Temp_get = 21.7 [dC]



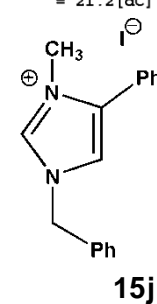


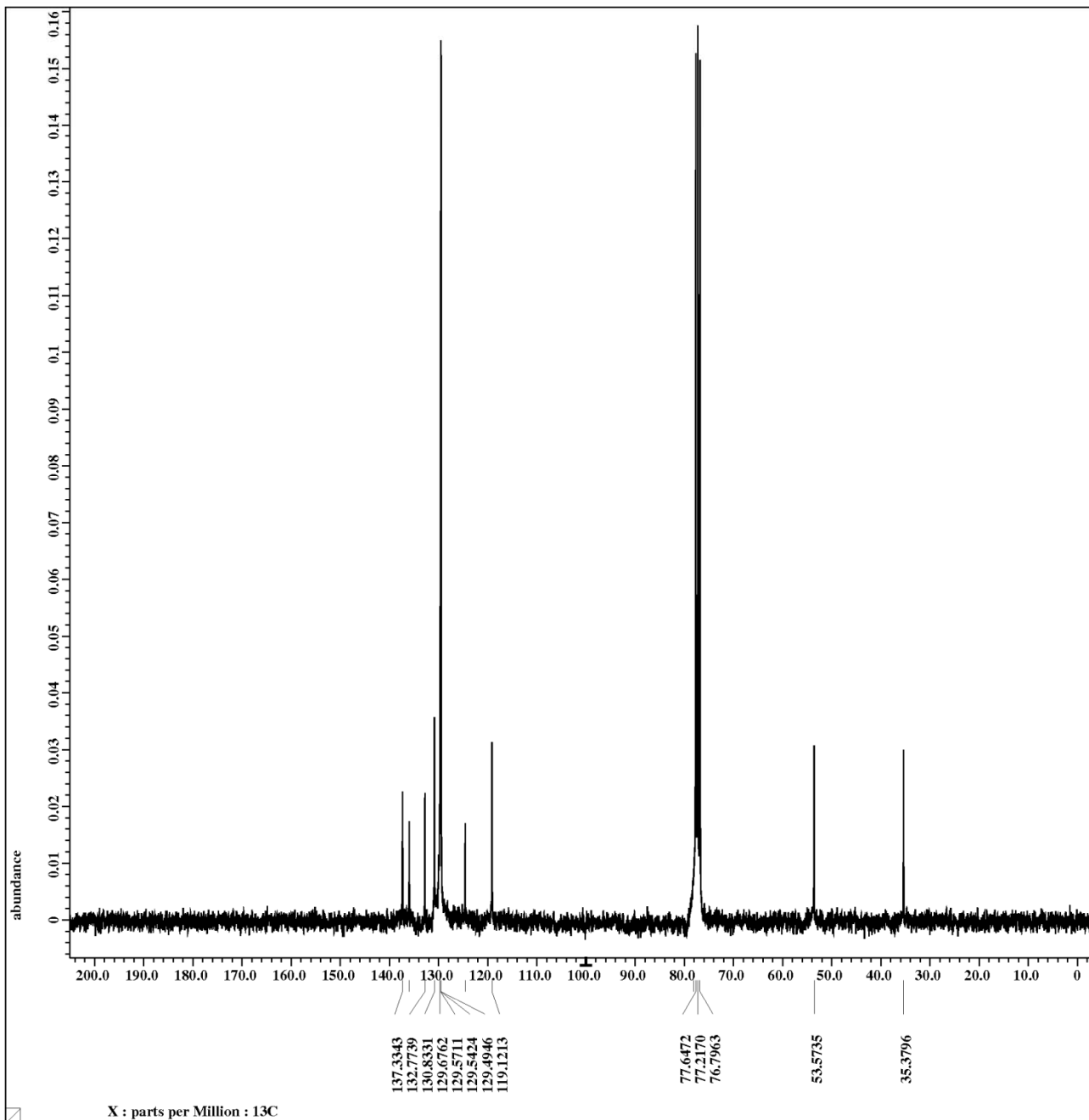
Filename = HMF_IV_27-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#657294
 Solvent = CHLOROFORM-D
 Creation_time = 15-AUG-2011 17:57:06
 Revision_time = 15-AUG-2011 20:07:45
 Current_time = 15-AUG-2011 20:08:15

Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 300
 Spectrometer = DELTA2_NMR

Field_strength = 7.0586013[T] (300[MHz])
 X_acq_duration = 2.90717696[s]
 X_domain = 1H
 X_freq = 300.52965592[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.34397631[Hz]
 X_sweep = 5.63570784[kHz]
 Irr_domain = 1H
 Irr_freq = 300.52965592[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 300.52965592[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 24
 Total_scans = 24

X_90_width = 13.01[us]
 X_acq_time = 2.90717696[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.505[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 40
 Relaxation_delay = 5[s]
 Repetition_time = 7.90717696[s]
 Temp_get = 21.2[dc]





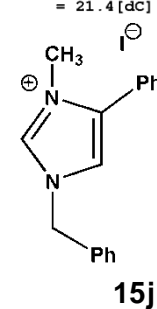
```

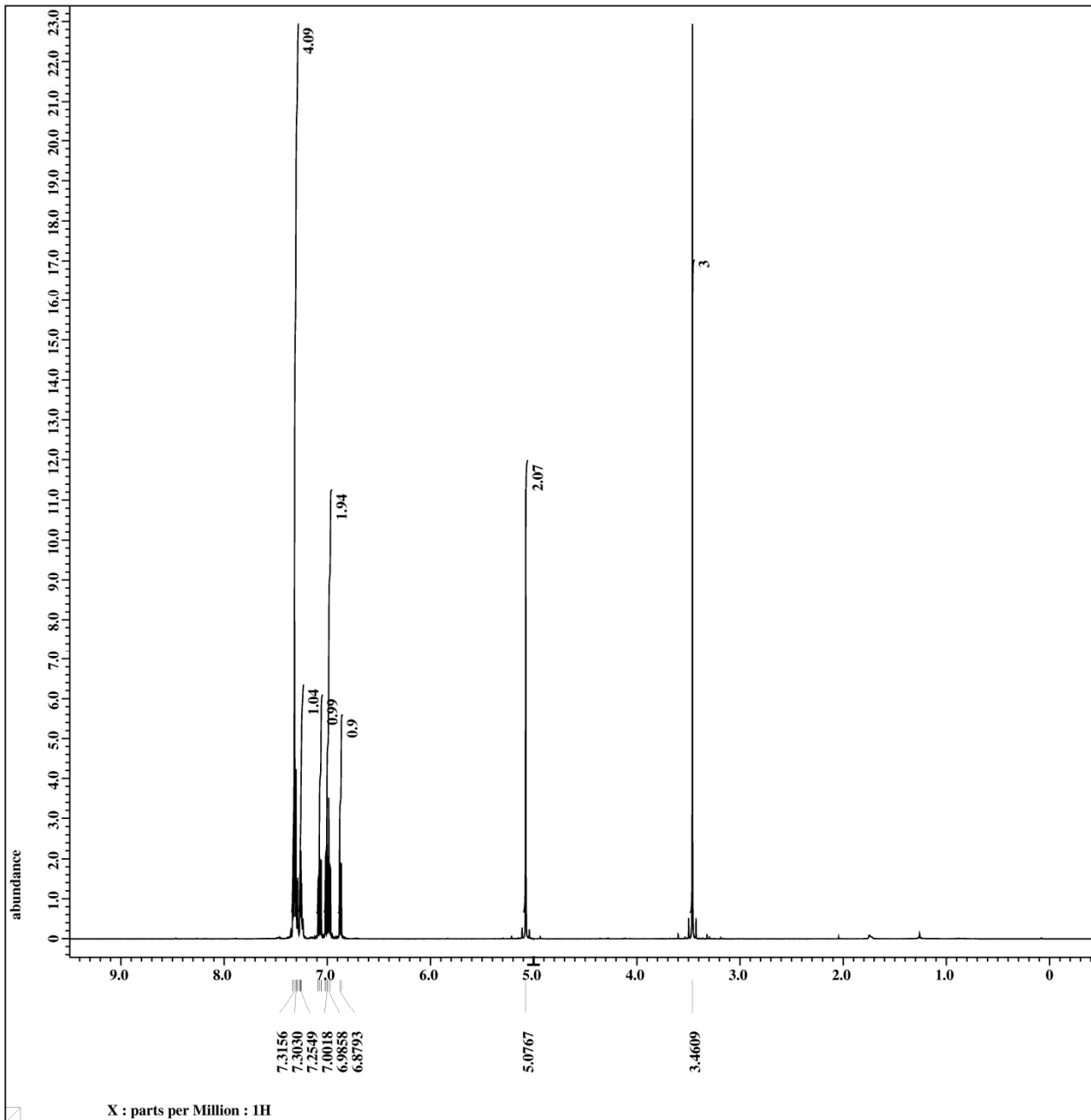
Filename      = HMF_IV_27-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#660147
Solvent      = CHLOROFORM-D
Creation_time = 15-AUG-2011 19:17:57
Revision_time = 15-AUG-2011 20:09:01
Current_time  = 15-AUG-2011 20:10:06

Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECX 300
Spectrometer = DELTA2_NMR

Field_strength = 7.0586013[T] (300[MHz])
X_acq_duration = 1.38412032[s]
X_domain       = 13C
X_freq         = 75.56823426[MHz]
X_offset      = 100[ppm]
X_points       = 32768
X_prescans    = 4
X_resolution   = 0.72248054[Hz]
X_sweep       = 23.67424242[kHz]
Irr_domain    = 1H
Irr_freq      = 300.52965592[MHz]
Irr_offset    = 5[ppm]
Clipped       = FALSE
Mod_return    = 10
Scans         = 1090
Total_scans   = 1090

X_90_width    = 9.75[us]
X_acq_time    = 1.38412032[s]
X_angle       = 30[deg]
X_atn         = 8[dB]
X_pulse       = 3.25[us]
Irr_atn_dec   = 25[dB]
Irr_atn_noe   = 25[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 3[s]
Recvr_gain    = 50
Relaxation_delay = 3[s]
Repetition_time = 4.38412032[s]
Temp_get      = 21.4[dc]
  
```



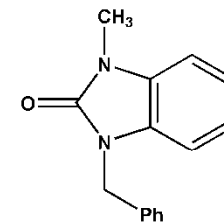


Filename = HMF_III_26-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#587187
 Solvent = CHLOROFORM-D
 Creation_time = 6-JAN-2011 07:20:07
 Revision_time = 5-JAN-2011 16:56:03
 Current_time = 5-JAN-2011 16:56:57

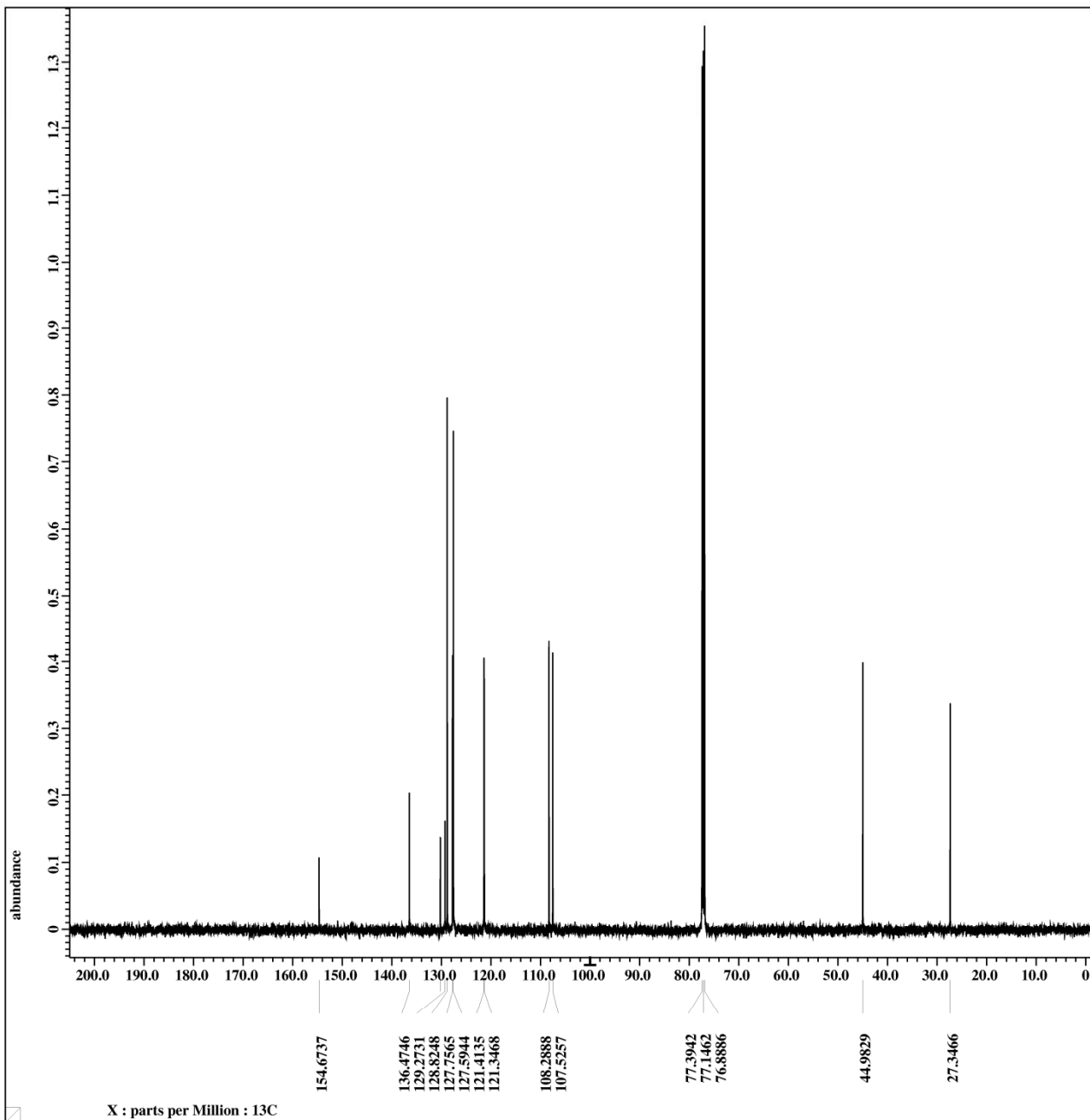
Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 38
 Relaxation_delay = 5[s]
 Repetition_time = 6.74587904[s]
 Temp_get = 21.3[dc]



16a

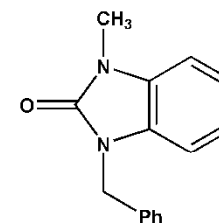


Filename = HMF_III_26-4.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#589288
 Solvent = CHLOROFORM-D
 Creation_time = 6-JAN-2011 07:34:25
 Revision_time = 5-JAN-2011 17:03:18
 Current_time = 5-JAN-2011 17:04:43

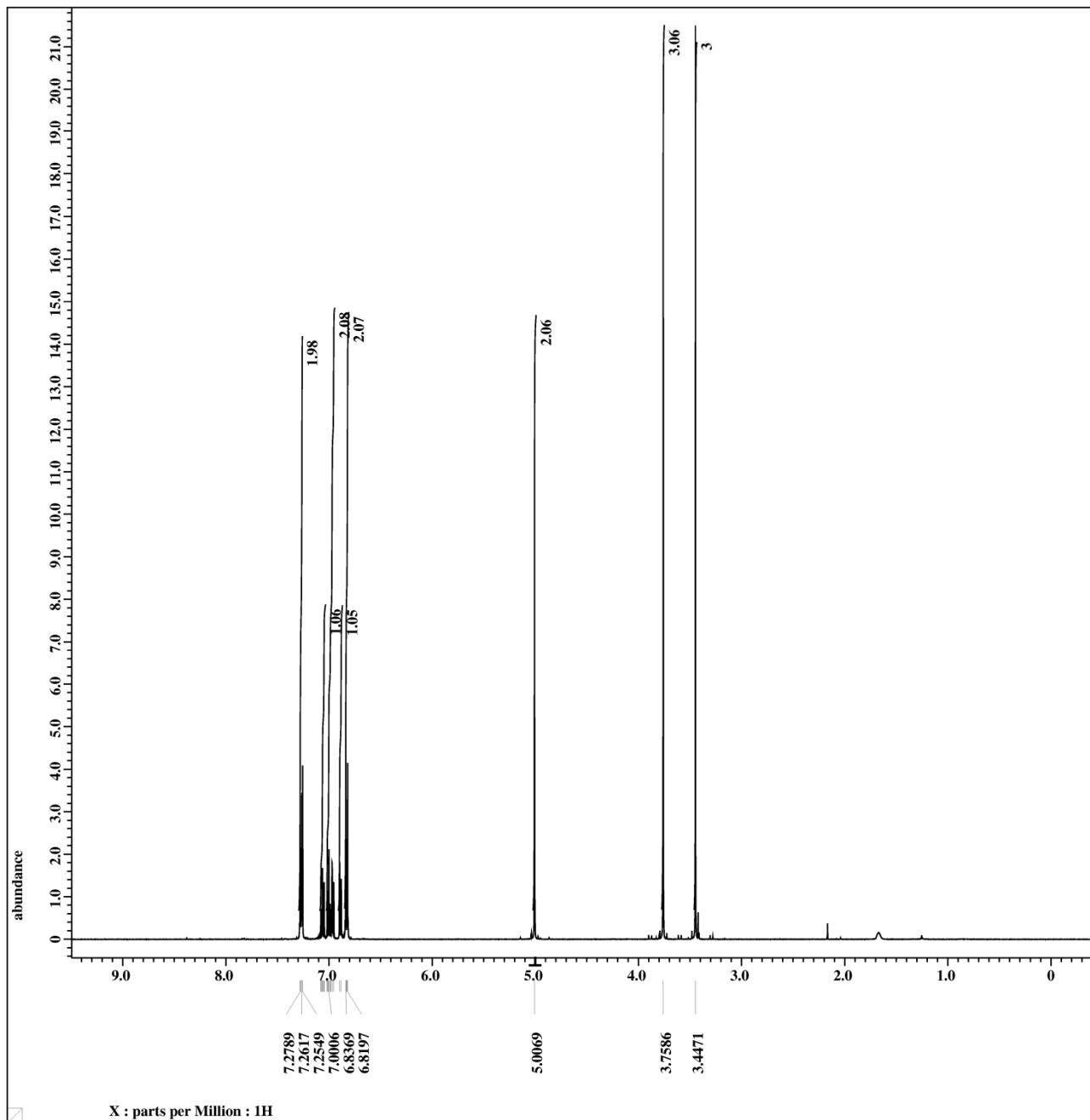
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 0.83361792[s]
 X_domain = 13C
 X_freq = 125.76529768[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.19959034[Hz]
 X_sweep = 39.3081761[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 10
 Scans = 160
 Total_scans = 160

X_90_width = 10.73[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 9[dB]
 X_pulse = 3.57666667[us]
 Irr_atn_dec = 20[dB]
 Irr_atn_noe = 20[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 4[s]
 Recvr_gain = 50
 Relaxation_delay = 4[s]
 Repetition_time = 4.83361792[s]
 Temp_get = 21.8[dC]



16a



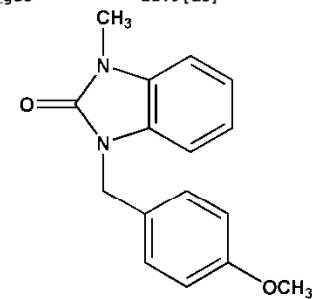
```

Filename      = HMF_III_8-4.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = S#581766
Solvent      = CHLOROFORM-D
Creation_time = 2-OCT-2010 06:06:25
Revision_time = 7-OCT-2010 17:12:06
Current_time  = 7-OCT-2010 17:12:42

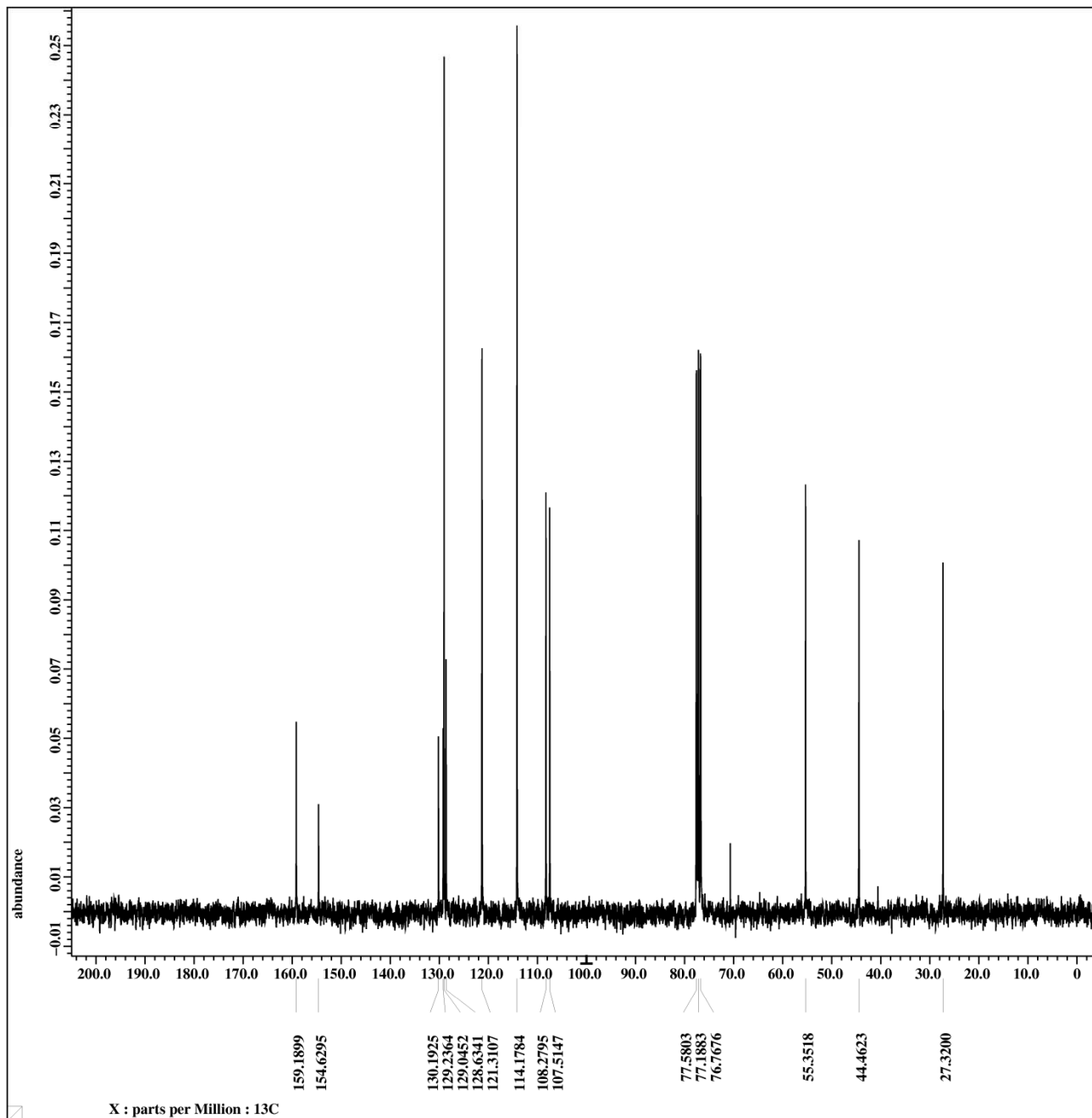
Comment      = single_pulse
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans     = 0
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width    = 12.54[us]
X_acq_time    = 1.74587904[s]
X_angle       = 45[deg]
X_atn         = 4[dB]
X_pulse       = 6.27[us]
Irr_mode      = Off
Tri_mode      = Off
Dante_presat  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 56
Relaxation_delay = 5[s]
Repetition_time = 6.74587904[s]
Temp_get      = 21.9[degC]
  
```



16b



```

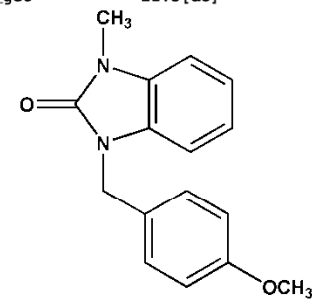
Filename      = HMF_III_8-4.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#522800
Solvent      = CHLOROFORM-D
Creation_time = 7-OCT-2010 14:30:20
Revision_time = 7-OCT-2010 16:47:40
Current_time  = 7-OCT-2010 16:54:02

Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECX 300
Spectrometer = DELTA2_NMR

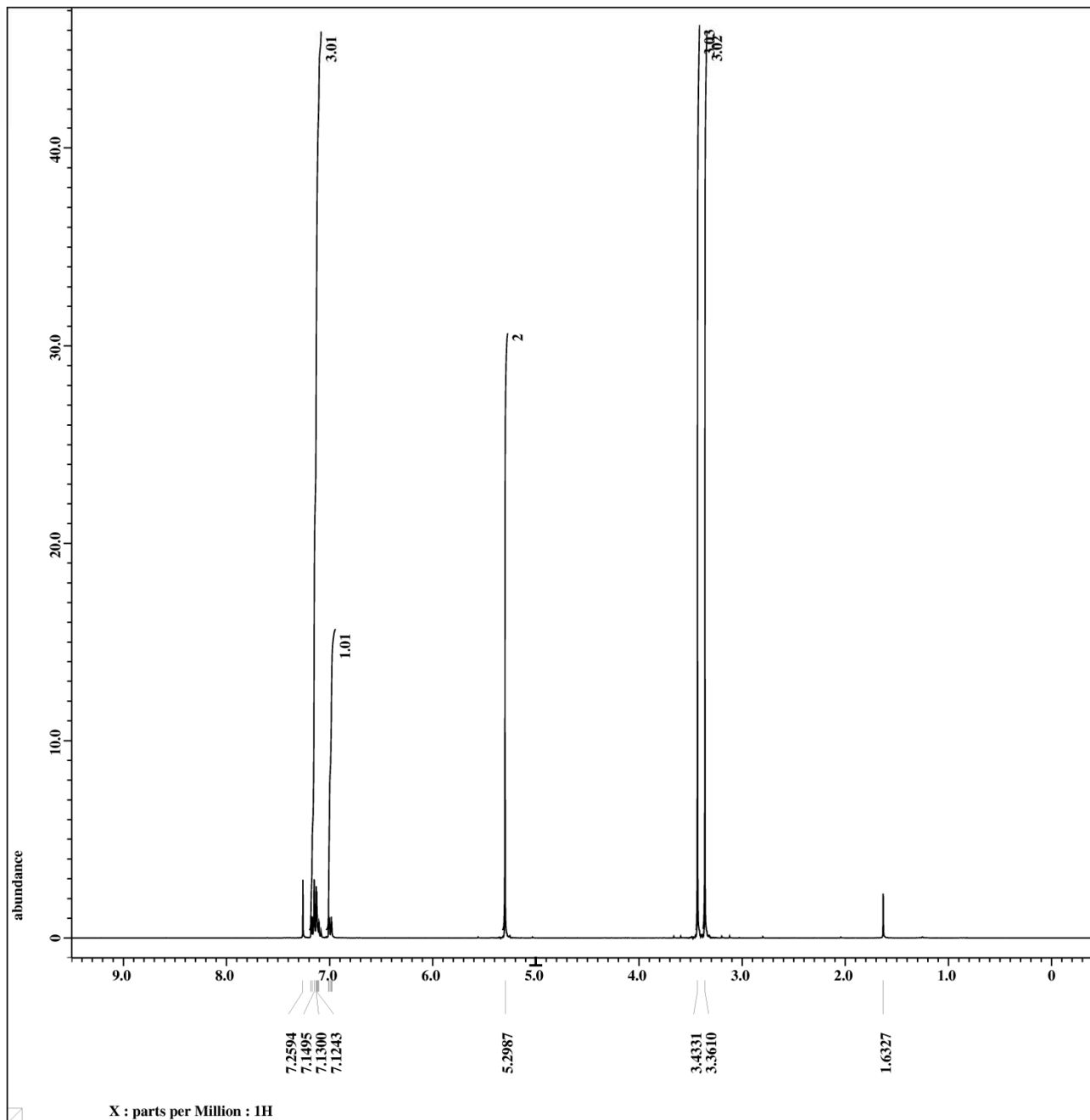
Field_strength = 7.0586013[T] (300[MHz]
X_acq_duration = 1.38412032[s]
X_domain       = 13C
X_freq         = 75.56823426[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans    = 4
X_resolution   = 0.72248054[Hz]
X_sweep        = 23.67424242[kHz]
Irr_domain     = 1H
Irr_freq       = 300.52965592[MHz]
Irr_offset     = 5[ppm]
Clipped       = FALSE
Mod_return    = 10
Scans         = 250
Total_scans   = 250

X_90_width    = 9.75[us]
X_acq_time    = 1.38412032[s]
X_angle       = 30[deg]
X_atn         = 8[dB]
X_pulse       = 3.25[us]
Irr_atn_dec   = 25[dB]
Irr_atn_noe   = 25[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 3[s]
Recvr_gain    = 50
Relaxation_delay = 3[s]
Repetition_time = 4.38412032[s]
Temp_get      = 21.3[dC]

```



16b

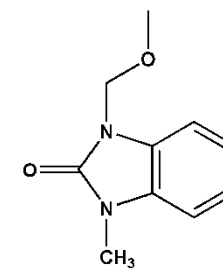


Filename = HMF_III_13_1-11.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#590482
 Solvent = CHLOROFORM-D
 Creation_time = 5-OCT-2010 16:07:57
 Revision_time = 25-MAY-2011 15:54:32
 Current_time = 25-MAY-2011 15:55:14

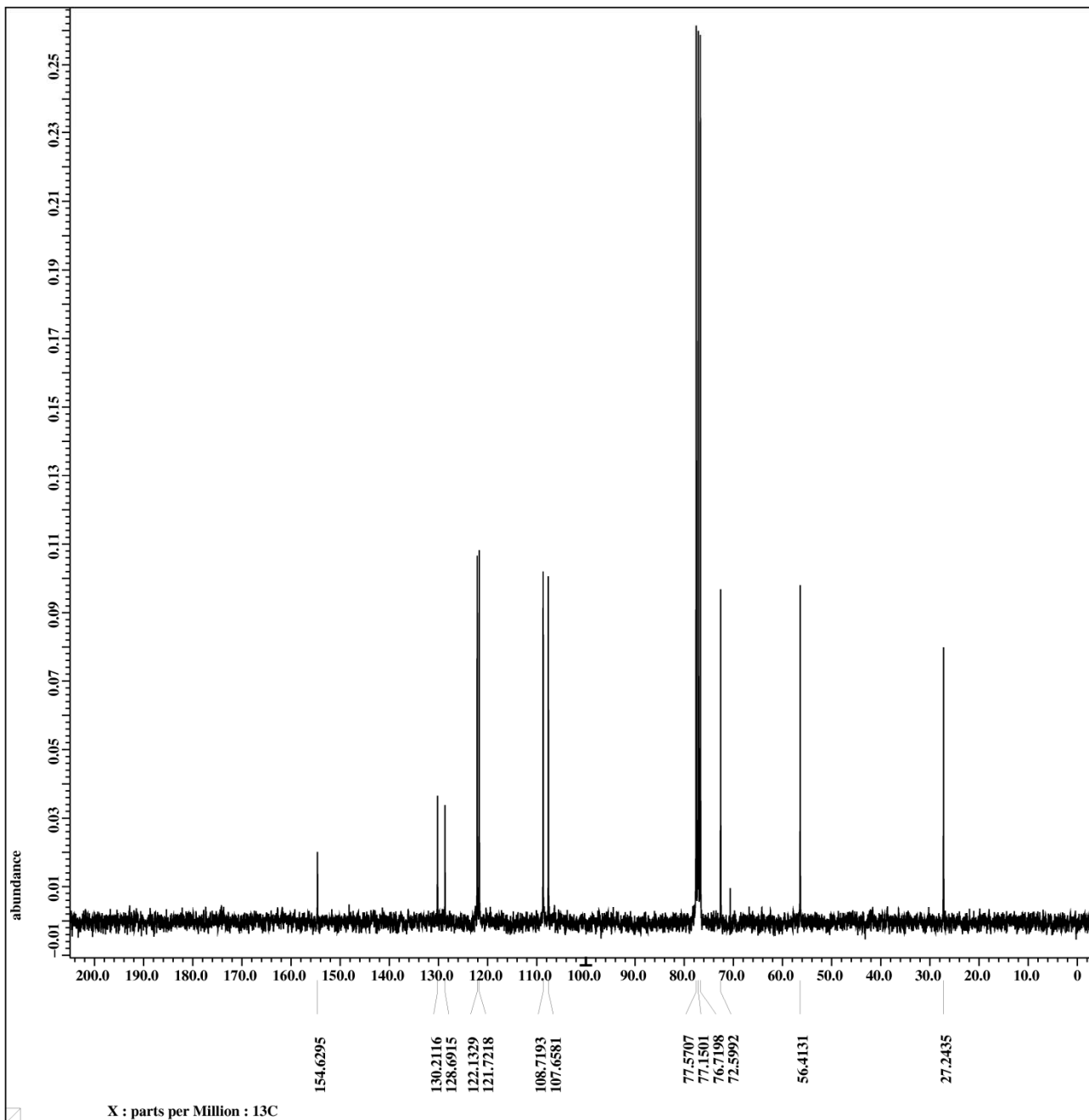
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 300
 Spectrometer = DELTA2_NMR

Field_strength = 7.0586013[T] (300[MHz])
 X_acq_duration = 2.90717696[s]
 X_domain = 1H
 X_freq = 300.52965592[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.34397631[Hz]
 X_sweep = 5.63570784[kHz]
 Irr_domain = 1H
 Irr_freq = 300.52965592[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 300.52965592[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 24
 Total_scans = 24

X_90_width = 13.01[us]
 X_acq_time = 2.90717696[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.505[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 50
 Relaxation_delay = 5[s]
 Repetition_time = 7.90717696[s]
 Temp_get = 20.3[dc]



16c



```

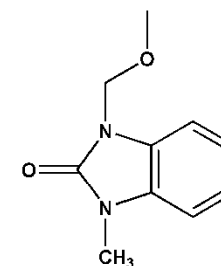
Filename      = HMF_III_13-2.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#644569
Solvent      = CHLOROFORM-D
Creation_time = 7-OCT-2010 18:03:31
Revision_time = 7-OCT-2010 21:11:21
Current_time = 7-OCT-2010 21:12:10

Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECX 300
Spectrometer = DELTA2_NMR

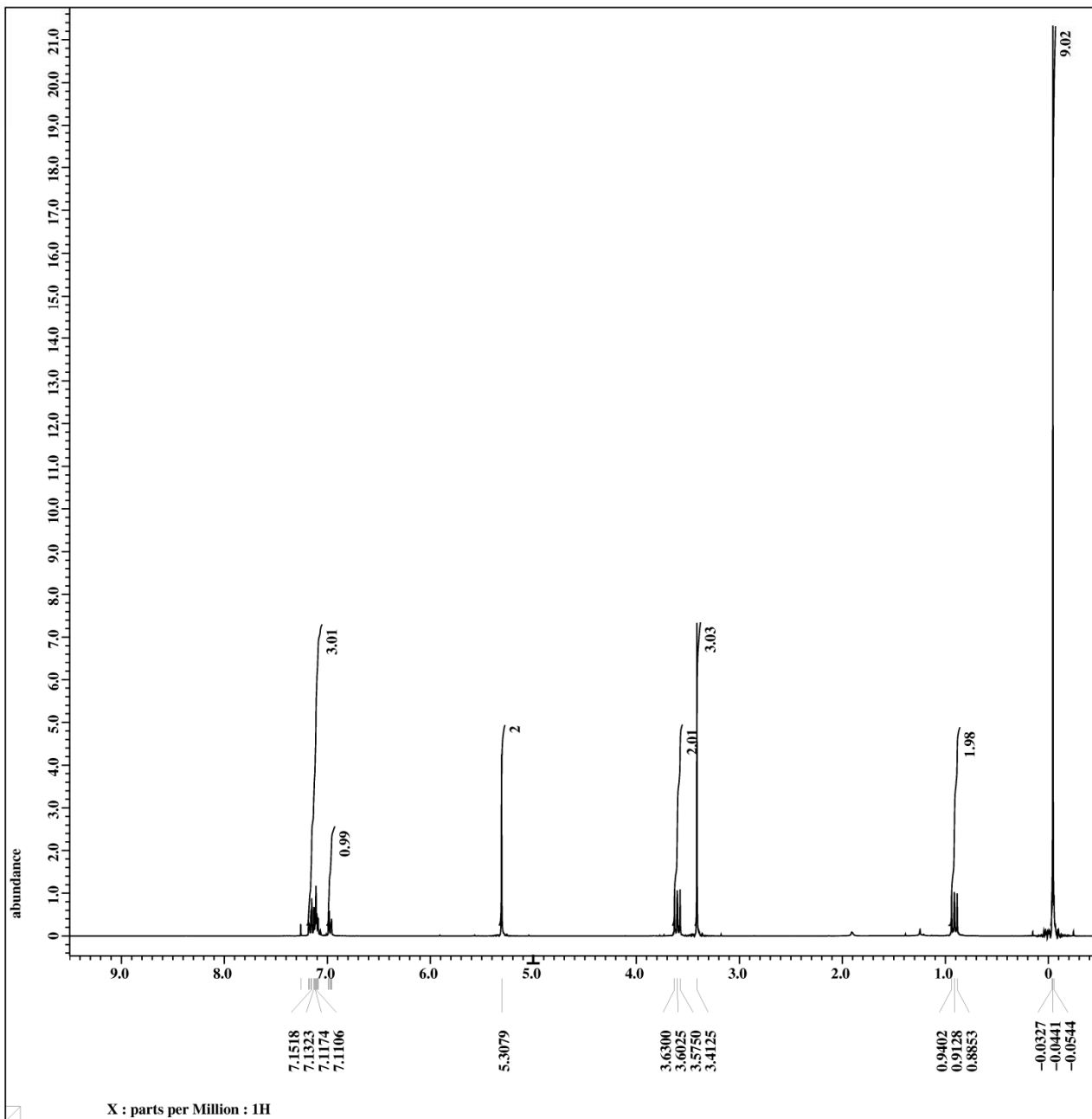
Field_strength = 7.0586013[T] (300[MHz]
X_acq_duration = 1.38412032[s]
X_domain       = 13C
X_freq        = 75.56823426[MHz]
X_offset      = 100[ppm]
X_points      = 32768
X_prescans    = 4
X_resolution  = 0.72248054[Hz]
X_sweep       = 23.67424242[kHz]
Irr_domain    = 1H
Irr_freq      = 300.52965592[MHz]
Irr_offset    = 5[ppm]
Clipped       = FALSE
Mod_return    = 10
Scans         = 390
Total_scans   = 390

X_90_width   = 9.75[us]
X_acq_time   = 1.38412032[s]
X_angle      = 30[deg]
X_atn        = 8[dB]
X_pulse      = 3.25[us]
Irr_atn_dec  = 25[dB]
Irr_atn_noe  = 25[dB]
Irr_noise    = WALTZ
Decoupling   = TRUE
Initial_wait = 1[s]
Noe          = TRUE
Noe_time     = 3[s]
Recvr_gain   = 50
Relaxation_delay = 3[s]
Repetition_time = 4.38412032[s]
Temp_get     = 21.1[dC]

```



16c

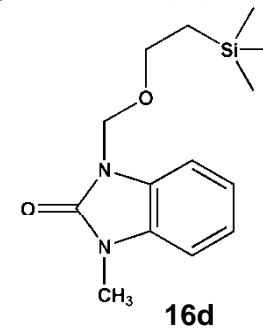


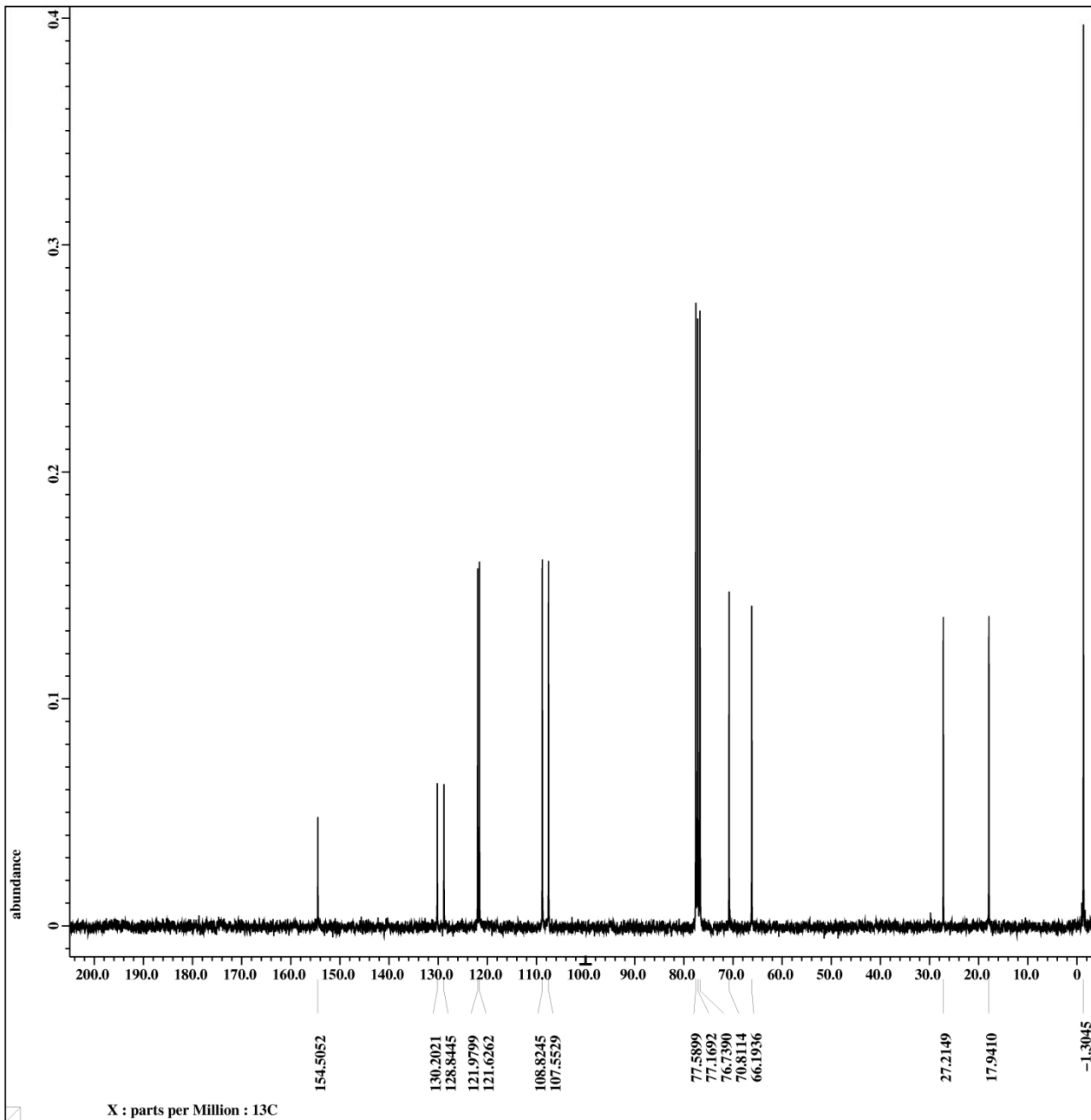
Filename = HMF_III_27-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#618345
 Solvent = CHLOROFORM-D
 Creation_time = 19-NOV-2010 16:55:12
 Revision_time = 19-NOV-2010 21:31:45
 Current_time = 19-NOV-2010 21:33:05

Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECX 300
 Spectrometer = DELTA2_NMR

Field_strength = 7.0586013[T] (300[MHz]
 X_acq_duration = 2.90717696[s]
 X_domain = 1H
 X_freq = 300.52965592[MHz]
 X_offset = 5[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.34397631[Hz]
 X_sweep = 5.63570784[kHz]
 Irr_domain = 1H
 Irr_freq = 300.52965592[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 300.52965592[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 24
 Total_scans = 24

X_90_width = 13.01[us]
 X_acq_time = 2.90717696[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.505[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 30
 Relaxation_delay = 5[s]
 Repetition_time = 7.90717696[s]
 Temp_get = 20.3[dC]





```

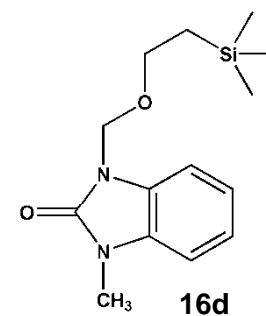
Filename      = HMF_III_27-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#620897
Solvent      = CHLOROFORM-D
Creation_time = 19-NOV-2010 17:30:11
Revision_time = 19-NOV-2010 21:37:24
Current_time  = 19-NOV-2010 21:37:41

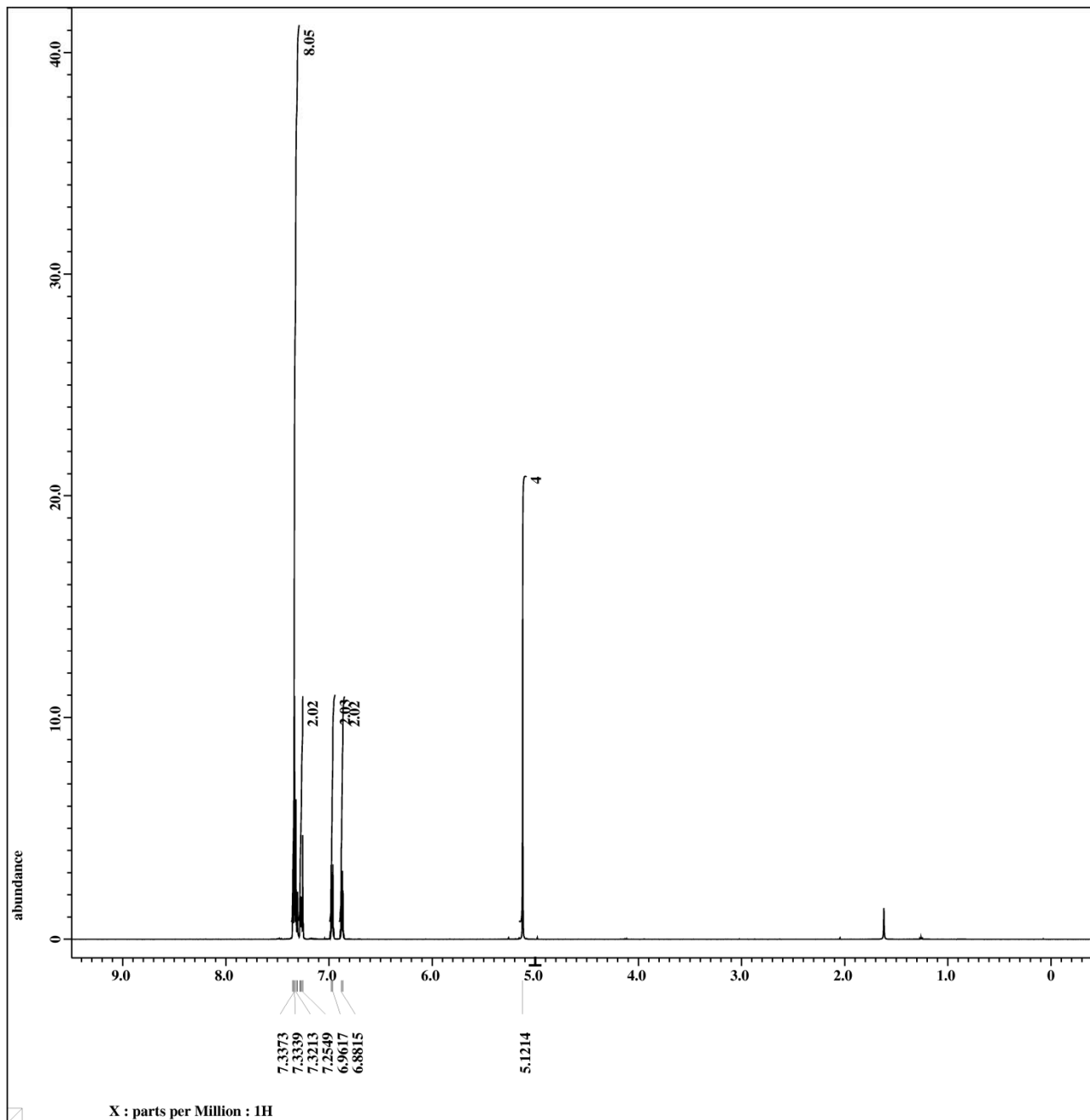
Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECX 300
Spectrometer = DELTA2_NMR

Field_strength = 7.0586013[T] (300[MHz]
X_acq_duration = 1.38412032[s]
X_domain       = 13C
X_freq         = 75.56823426[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 0.72248054[Hz]
X_sweep        = 23.67424242[kHz]
Irr_domain     = 1H
Irr_freq       = 300.52965592[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 450
Total_scans    = 450

X_90_width    = 9.75[us]
X_acq_time    = 1.38412032[s]
X_angle       = 30[deg]
X_atn         = 8[dB]
X_pulse       = 3.25[us]
Irr_atn_dec   = 25[dB]
Irr_atn_noe   = 25[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 3[s]
Recvr_gain    = 50
Relaxation_delay = 3[s]
Repetition_time = 4.38412032[s]
Temp_get      = 21.2[dC]

```





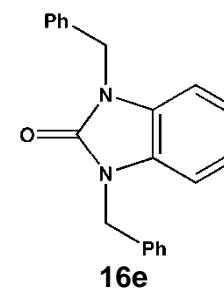
```

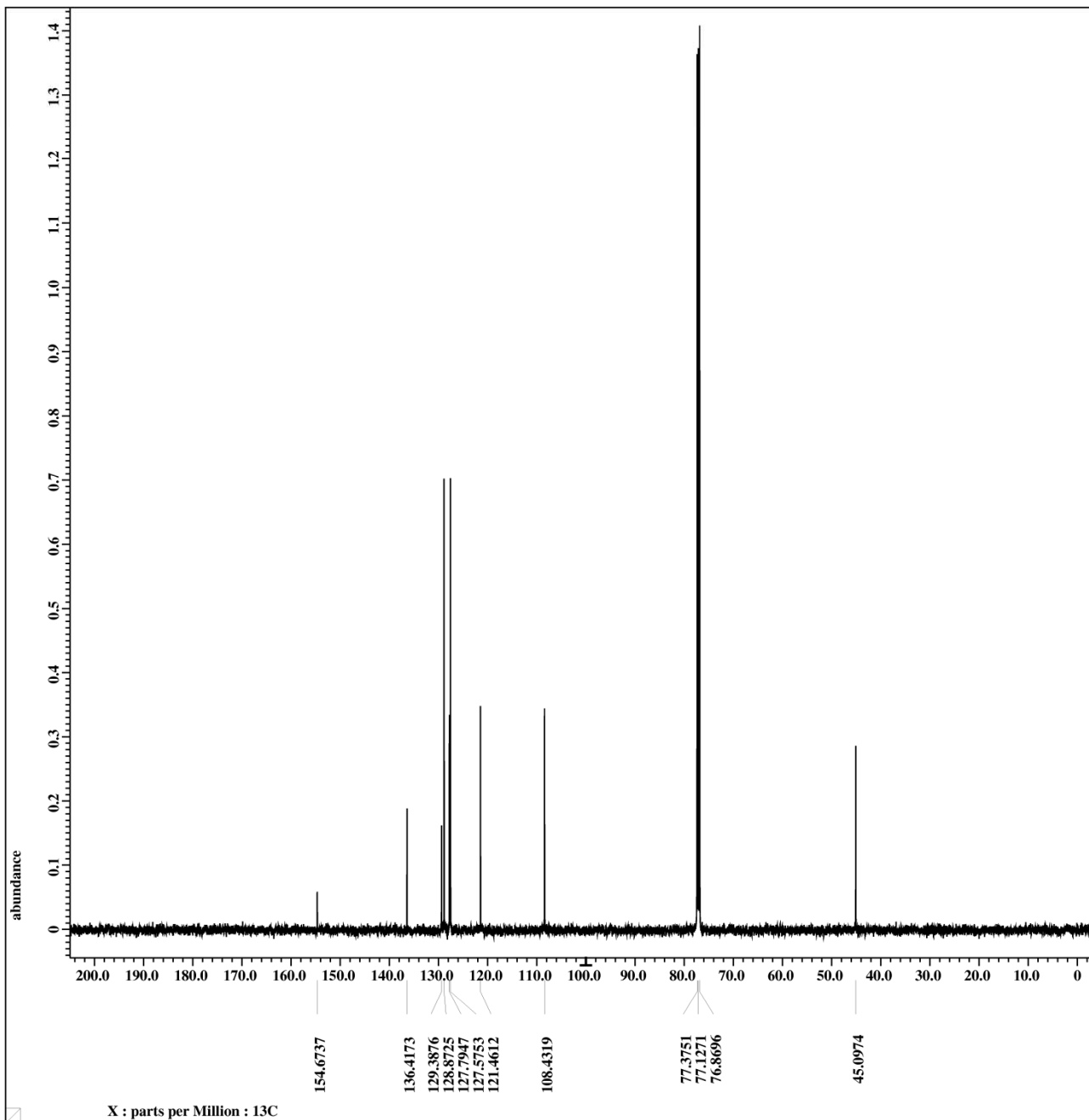
Filename      = HMF_III_14-4.jdf
Author        = delta
Experiment    = single_pulse.ex2
Sample_id     = S#416202
Solvent       = CHLOROFORM-D
Creation_time = 26-MAY-2011 01:40:17
Revision_time = 25-MAY-2011 15:45:30
Current_time  = 25-MAY-2011 15:45:51

Comment       = single_pulse
Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans     = 0
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width    = 12.54[us]
X_acq_time     = 1.74587904[s]
X_angle        = 45[deg]
X_atn          = 4[dB]
X_pulse        = 6.27[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 42
Relaxation_delay = 5[s]
Repetition_time = 6.74587904[s]
Temp_get       = 21.1[dC]
  
```





```

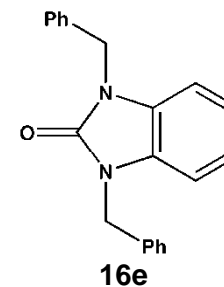
Filename      = HMF_III_14-2.jdf
Author        = delta
Experiment    = single_pulse_dec
Sample_id     = S#417885
Solvent       = CHLOROFORM-D
Creation_time = 26-MAY-2011 01:53:54
Revision_time = 25-MAY-2011 15:46:05
Current_time  = 25-MAY-2011 15:46:40

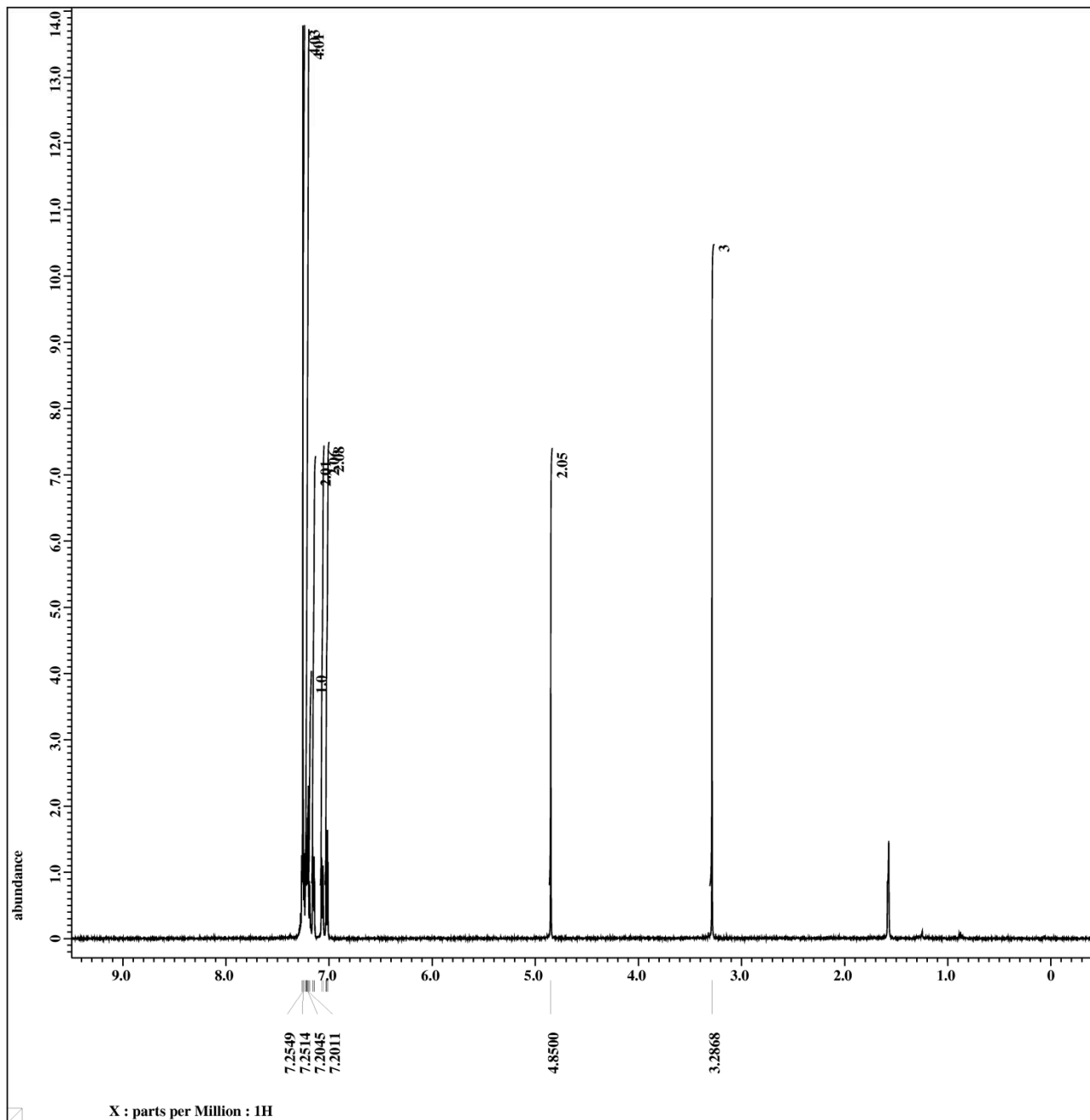
Comment       = single pulse decouple
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 160
Total_scans    = 160

X_90_width    = 10.73 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 9 [dB]
X_pulse        = 3.57666667 [us]
Irr_atn_dec    = 20 [dB]
Irr_atn_noe    = 20 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 4 [s]
Recvr_gain     = 50
Relaxation_delay = 4 [s]
Repetition_time = 4.83361792 [s]
Temp_get       = 21.6 [dC]

```

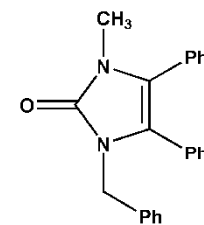




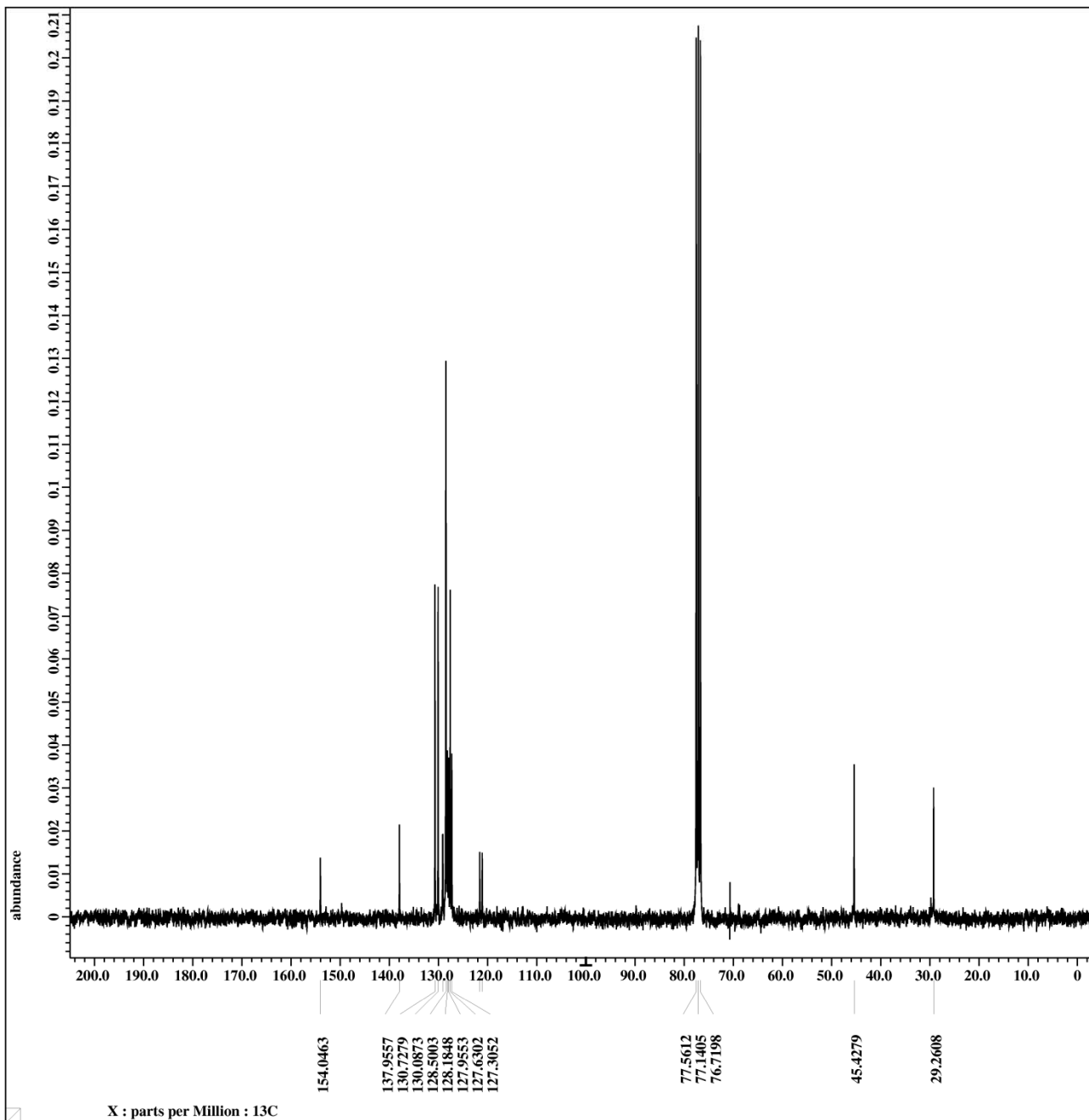
Filename = HMF_III_3-9.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#571504
 Solvent = CHLOROFORM-D
 Creation_time = 2-OCT-2010 05:49:20
 Revision_time = 24-MAY-2011 13:14:09
 Current_time = 24-MAY-2011 14:45:33

Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 66
 Relaxation_delay = 5[s]
 Repetition_time = 6.74587904[s]
 Temp_get = 21.6[dC]



16f



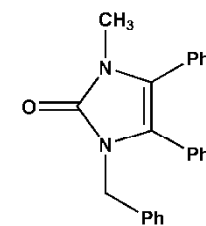
```

Filename      = HMF_III_3-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#403574
Solvent      = CHLOROFORM-D
Creation_time = 7-OCT-2010 11:56:56
Revision_time = 7-OCT-2010 17:37:48
Current_time  = 7-OCT-2010 17:38:18

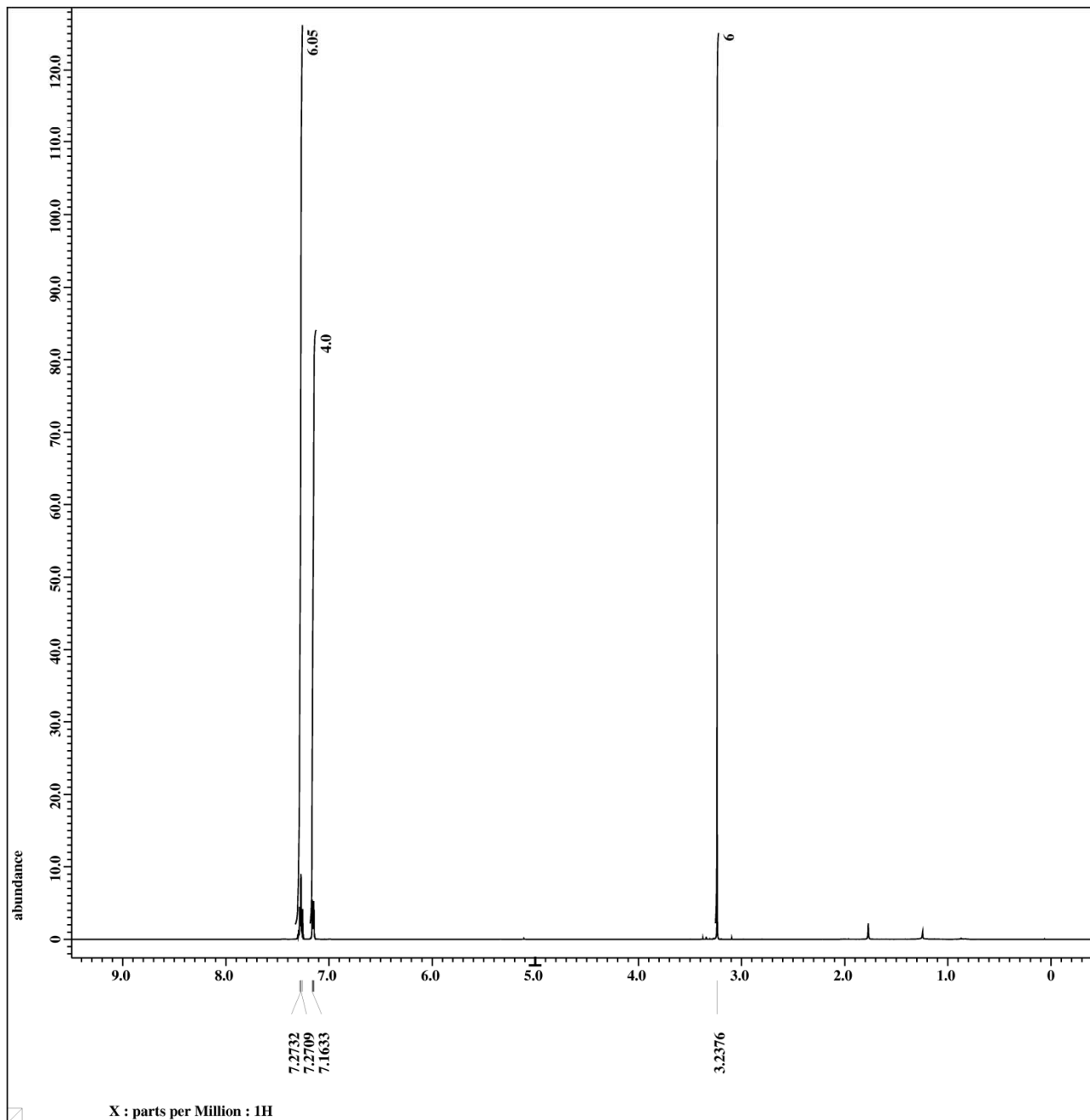
Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECX 300
Spectrometer = DELTA2_NMR

Field_strength = 7.0586013[T] (300[MHz])
X_acq_duration = 1.38412032[s]
X_domain      = 13C
X_freq       = 75.56823426[MHz]
X_offset     = 100[ppm]
X_points     = 32768
X_prescans   = 4
X_resolution = 0.72248054[Hz]
X_sweep      = 23.67424242[kHz]
Irr_domain   = 1H
Irr_freq     = 300.52965592[MHz]
Irr_offset   = 5[ppm]
Clipped      = FALSE
Mod_return   = 10
Scans        = 870.0
Total_scans  = 870.0

X_90_width   = 9.75[us]
X_acq_time   = 1.38412032[s]
X_angle      = 30[deg]
X_atn        = 8[dB]
X_pulse      = 3.25[us]
Irr_atn_dec  = 25[dB]
Irr_atn_noe  = 25[dB]
Irr_noise    = WALTZ
Decoupling   = TRUE
Initial_wait = 1[s]
Noe          = TRUE
Noe_time     = 3[s]
Recvr_gain   = 50
Relaxation_delay = 3[s]
Repetition_time = 4.38412032[s]
Temp_get     = 21.4[dC]
  
```



16f



```

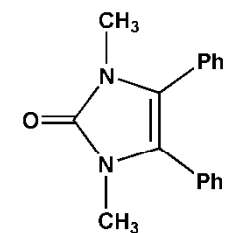
Filename      = HMF_III_191-4.jdf
Author        = delta
Experiment    = single_pulse.ex2
Sample_id     = S#388288
Solvent       = CHLOROFORM-D
Creation_time = 25-MAY-2011 00:54:28
Revision_time = 24-MAY-2011 12:10:48
Current_time  = 24-MAY-2011 12:12:56

Comment       = single_pulse
Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

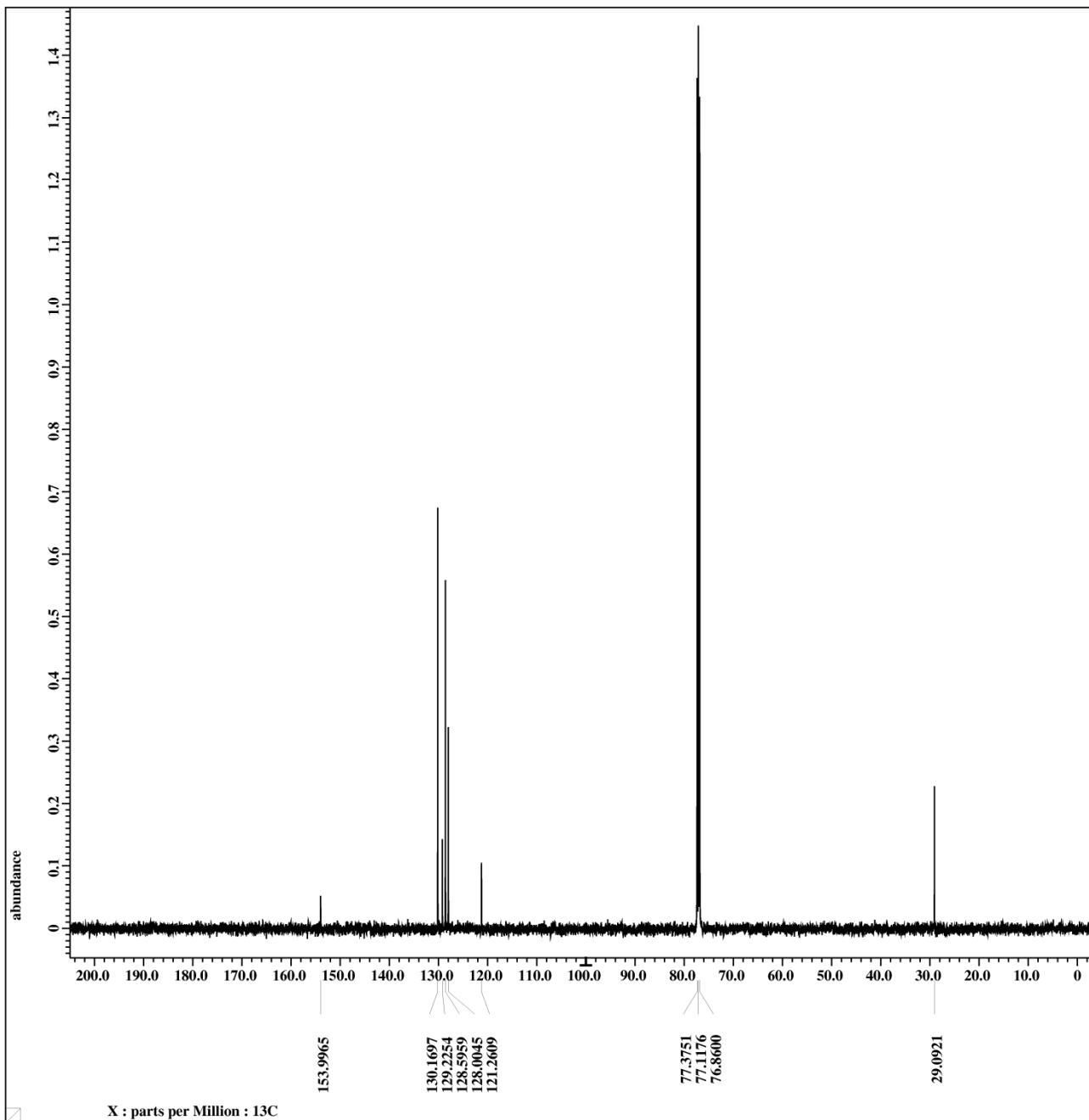
Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans     = 0
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 12.54[us]
X_acq_time     = 1.74587904[s]
X_angle        = 45[deg]
X_atn          = 4[dB]
X_pulse        = 6.27[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 44
Relaxation_delay = 5[s]
Repetition_time = 6.74587904[s]
Temp_get       = 21.1[dC]

```



16g



```

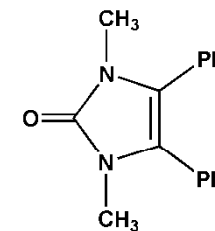
Filename      = HMF_III_191-2.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#390503
Solvent      = CHLOROFORM-D
Creation_time = 25-MAY-2011 01:04:14
Revision_time = 24-MAY-2011 12:14:07
Current_time  = 24-MAY-2011 12:14:40

Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site        = ECA 500
Spectrometer = JNM-ECA500

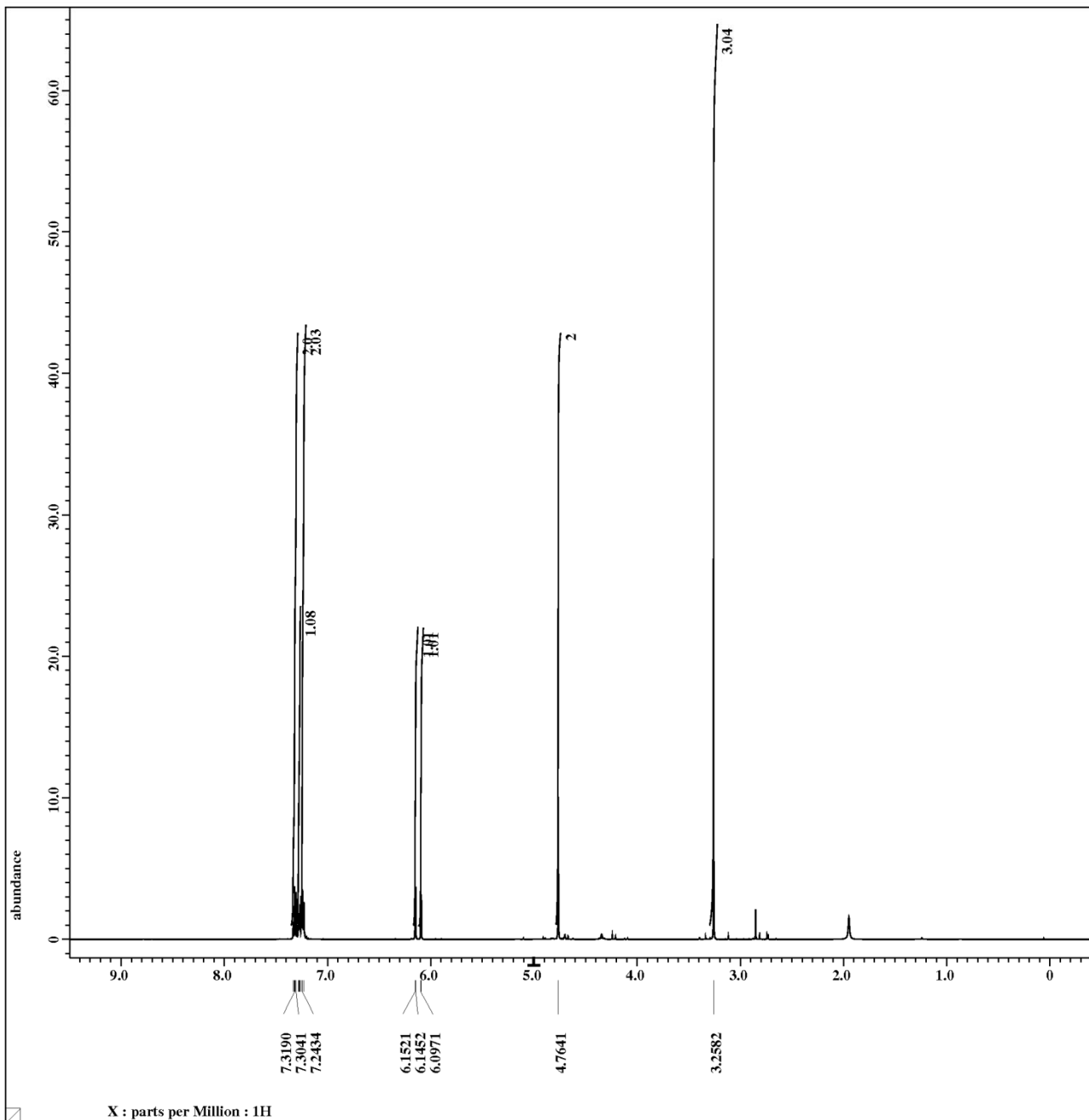
Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 110
Total_scans    = 110

X_90_width    = 10.73 [us]
X_acq_time    = 0.83361792 [s]
X_angle       = 30 [deg]
X_atn         = 9 [dB]
X_pulse       = 3.57666667 [us]
Irr_atn_dec   = 20 [dB]
Irr_atn_noe   = 20 [dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1 [s]
Noe           = TRUE
Noe_time      = 4 [s]
Recvr_gain    = 50
Relaxation_delay = 4 [s]
Repetition_time = 4.83361792 [s]
Temp_get      = 21.5 [dC]

```



16g

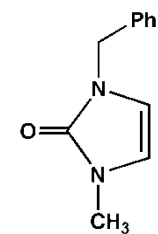


Filename = HMF_IV_12-8.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#634558
 Solvent = CHLOROFORM-D
 Creation_time = 20-JUL-2011 07:46:37
 Revision_time = 8-AUG-2011 22:38:56
 Current_time = 8-AUG-2011 22:39:47

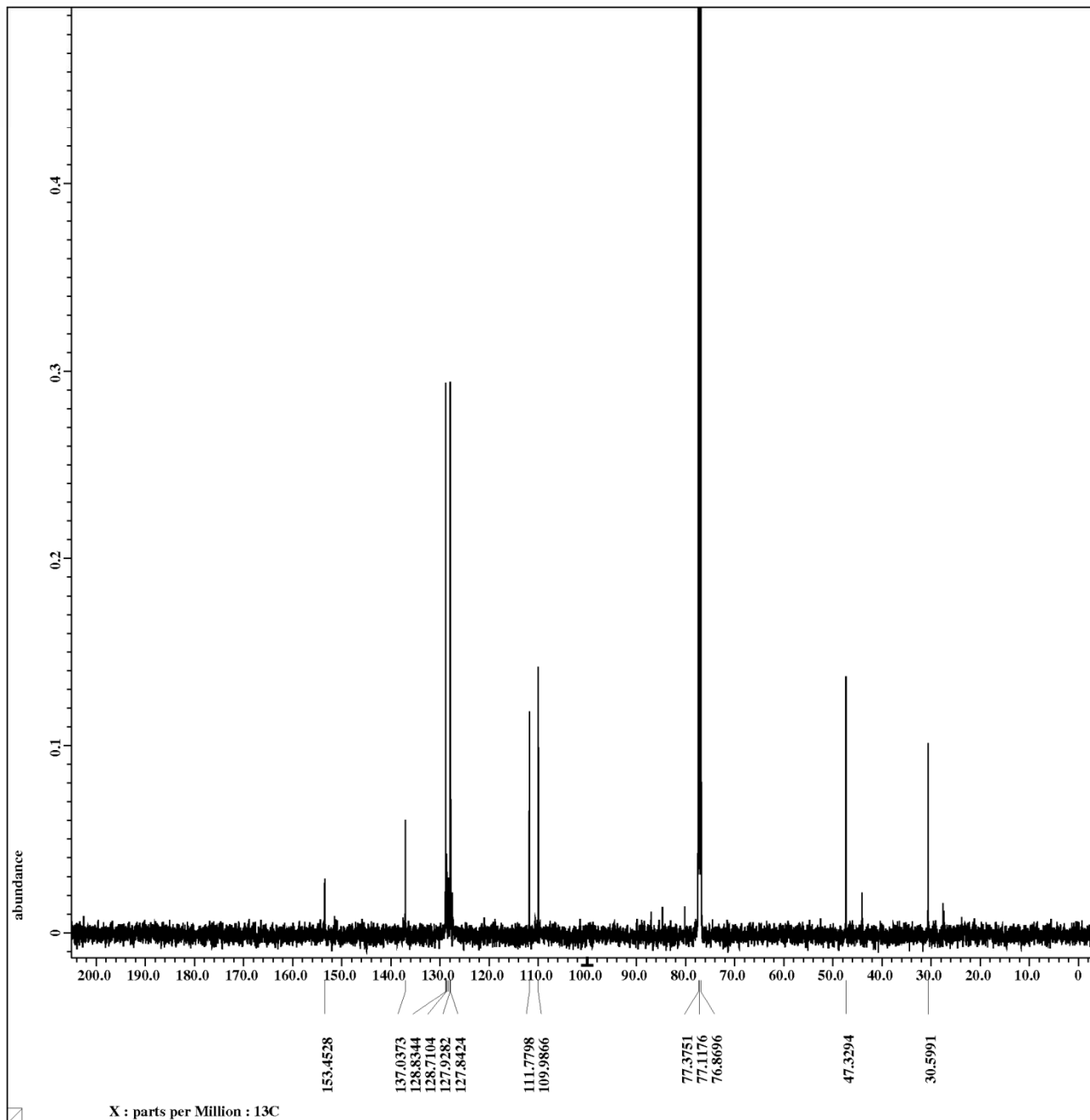
Comment = single pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 40
 Relaxation_delay = 5[s]
 Repetition_time = 6.74587904[s]
 Temp_get = 21.2[dC]



16h

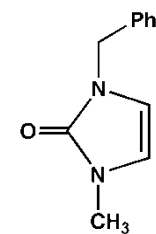


Filename = HMF_IV_12_crude-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#588738
 Solvent = CHLOROFORM-D
 Creation_time = 4-JUL-2011 06:52:13
 Revision_time = 8-AUG-2011 22:42:46
 Current_time = 8-AUG-2011 22:43:39

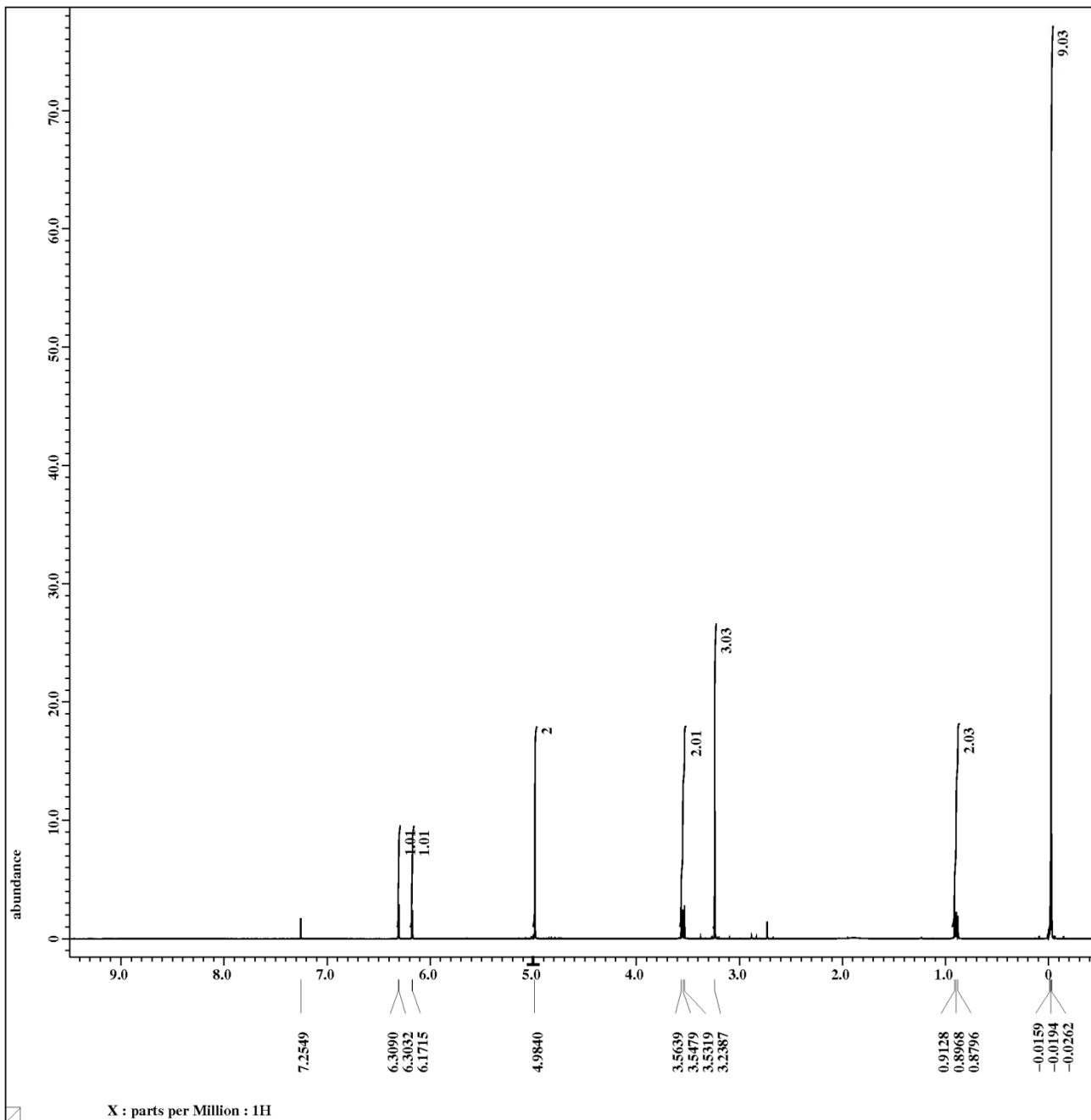
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 0.83361792[s]
 X_domain = 13C
 X_freq = 125.76529768[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.19959034[Hz]
 X_sweep = 39.3081761[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 10
 Scans = 300
 Total_scans = 300

X_90_width = 10.73[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 9[dB]
 X_pulse = 3.57666667[us]
 Irr_atn_dec = 20[dB]
 Irr_atn_noe = 20[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 4[s]
 Recvr_gain = 50
 Relaxation_delay = 4[s]
 Repetition_time = 4.83361792[s]
 Temp_get = 21.8[dC]



16h

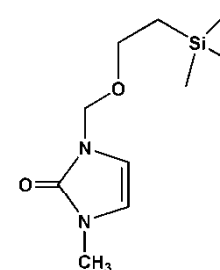


Filename = HMF_IV_20-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#443938
 Solvent = CHLOROFORM-D
 Creation_time = 21-SEP-2011 02:06:06
 Revision_time = 20-SEP-2011 15:28:00
 Current_time = 20-SEP-2011 15:29:06

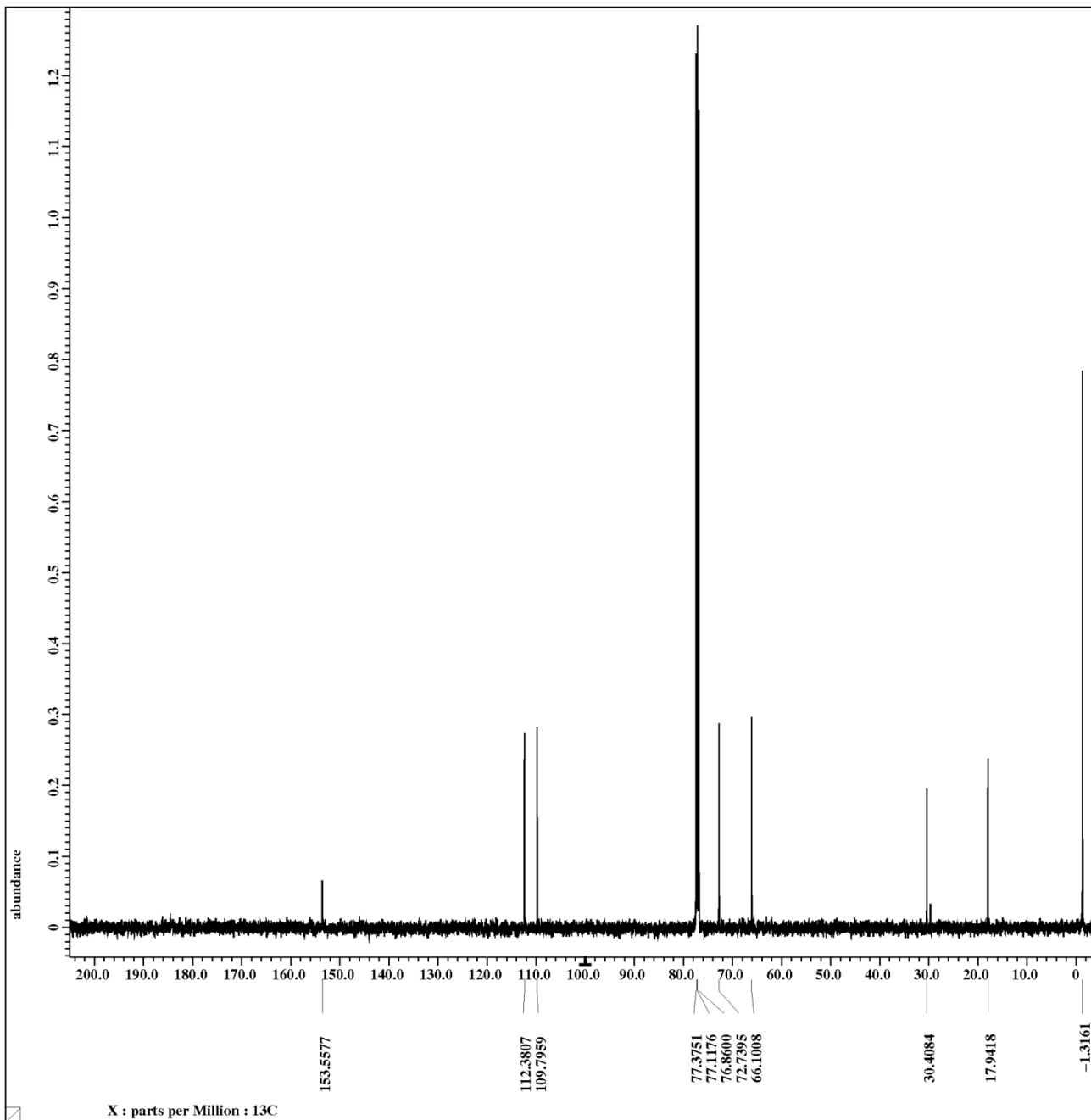
Comment = single pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 36
 Relaxation_delay = 5[s]
 Repetition_time = 6.74587904[s]
 Temp_get = 22.1[dc]



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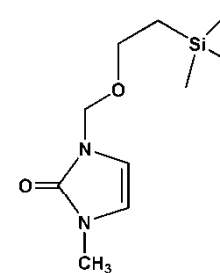
```

Filename      = HMF_IV_20-2.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#445637
Solvent      = CHLOROFORM-D
Creation time = 21-SEP-2011 02:13:11
Revision time = 20-SEP-2011 15:31:04
Current_time = 20-SEP-2011 15:31:34

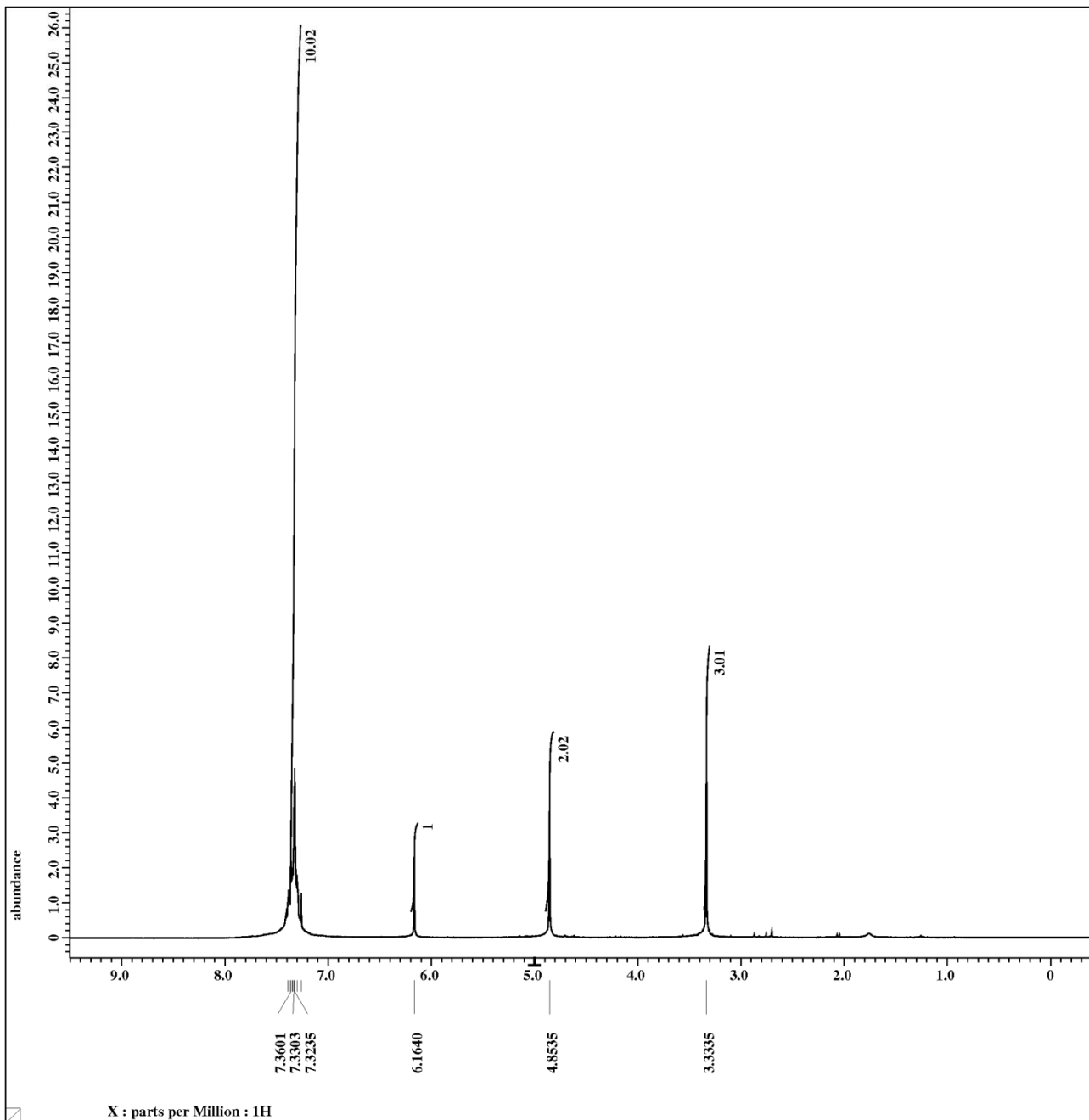
Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 100
Total_scans    = 100

X_90_width    = 10.73 [us]
X_acq_time    = 0.83361792 [s]
X_angle       = 30 [deg]
X_atn         = 9 [dB]
X_pulse       = 3.57666667 [us]
Irr_atn_dec   = 20 [dB]
Irr_atn_noe   = 20 [dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1 [s]
Noe           = TRUE
Noe_time      = 3 [s]
Recvr_gain    = 50
Relaxation_delay = 3 [s]
Repetition_time = 3.83361792 [s]
Temp_get      = 22.6 [dC]
  
```



16i



```

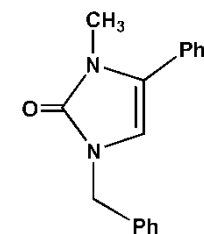
Filename      = HMF_IV_33-4.jdf
Author        = delta
Experiment    = single_pulse.ex2
Sample_id     = S#583292
Solvent       = CHLOROFORM-D
Creation_time = 4-AUG-2011 15:52:38
Revision_time = 8-AUG-2011 19:21:55
Current_time  = 8-AUG-2011 19:23:41

Comment       = single_pulse
Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECX 300
Spectrometer  = DELTA2_NMR

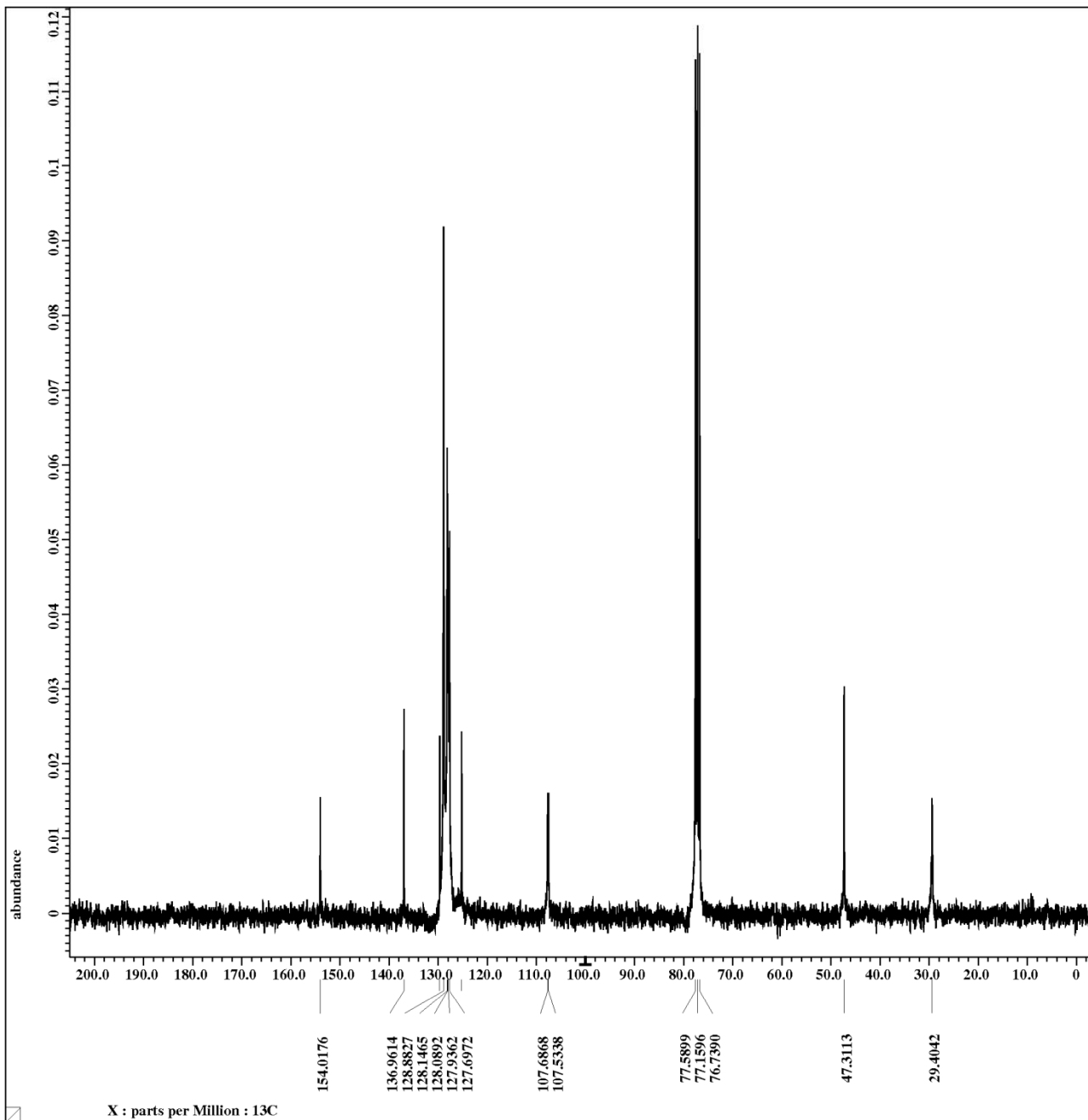
Field_strength = 7.0586013[T] (300[MHz]
X_acq_duration = 2.90717696[s]
X_domain       = 1H
X_freq         = 300.52965592[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 0
X_resolution   = 0.34397631[Hz]
X_sweep        = 5.63570784[kHz]
Irr_domain     = 1H
Irr_freq       = 300.52965592[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 300.52965592[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 18
Total_scans    = 18

X_90_width     = 13.01[us]
X_acq_time     = 2.90717696[s]
X_angle        = 45[deg]
X_atn          = 4[dB]
X_pulse        = 6.505[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 50
Relaxation_delay = 5[s]
Repetition_time = 7.90717696[s]
Temp_get       = 21.1[dc]

```



16j



```

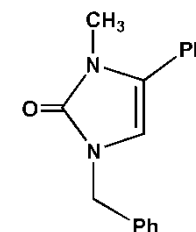
Filename      = HMF_IV_33-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#674535
Solvent      = CHLOROFORM-D
Creation time = 8-AUG-2011 20:37:05
Revision time = 9-AUG-2011 14:14:03
Current_time = 9-AUG-2011 14:14:38

Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECX 300
Spectrometer = DELTA2_NMR

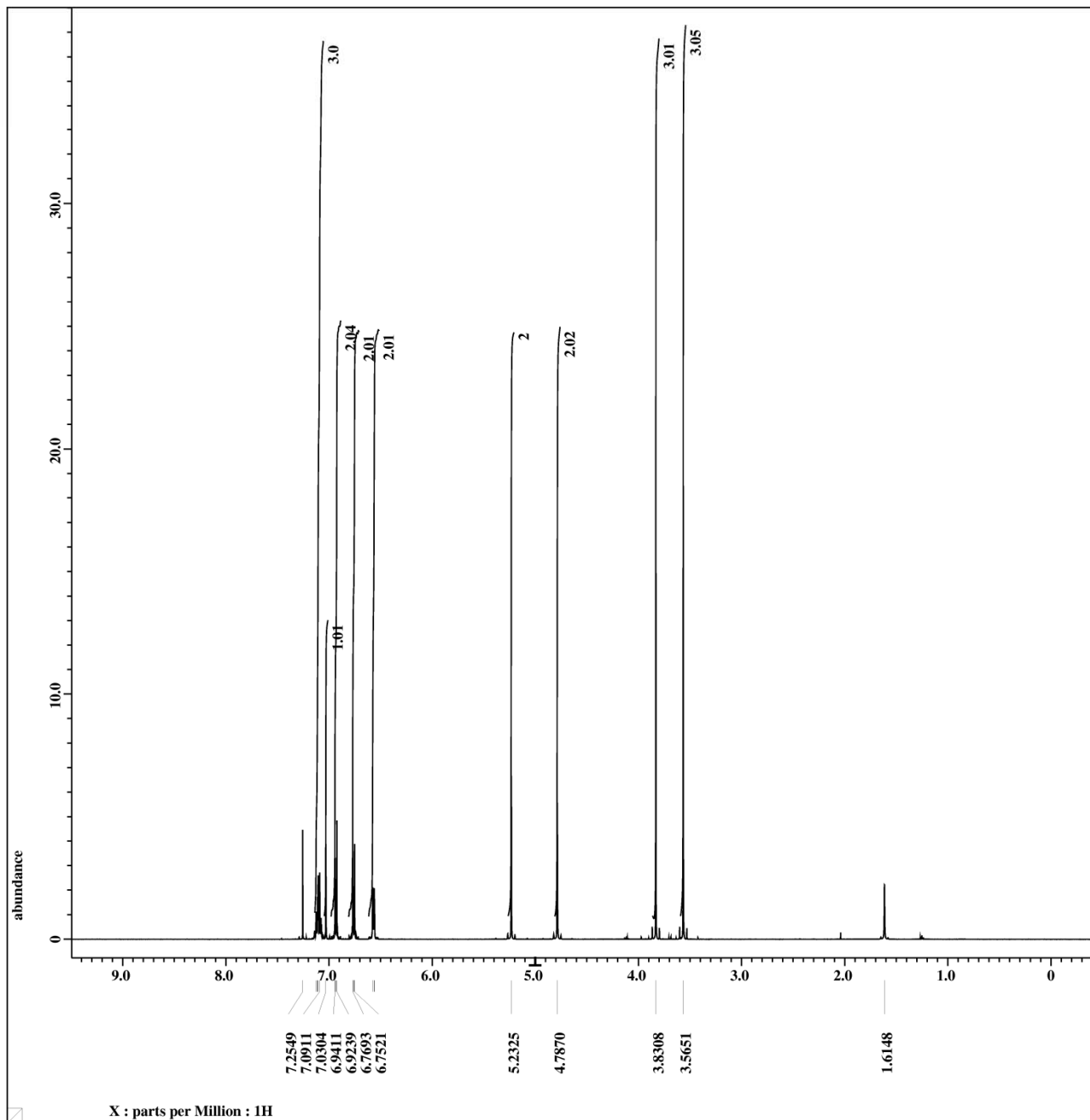
Field_strength = 7.0586013[T] (300[MHz]
X_acq_duration = 1.38412032[s]
X_domain       = 13C
X_freq         = 75.56823426[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 0.72248054[Hz]
X_sweep        = 23.67424242[kHz]
Irr_domain     = 1H
Irr_freq       = 300.52965592[MHz]
Irr_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 1500
Total_scans    = 1500

X_90_width    = 9.75[us]
X_acq_time    = 1.38412032[s]
X_angle       = 30[deg]
X_atn         = 8[dB]
X_pulse       = 3.25[us]
Irr_atn_dec   = 25[dB]
Irr_atn_noe   = 25[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 4[s]
Recvr_gain    = 50
Relaxation_delay = 4[s]
Repetition_time = 5.38412032[s]
Temp_get      = 21.2[dc]

```



16j

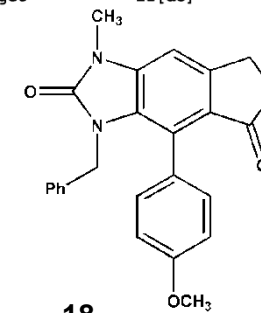


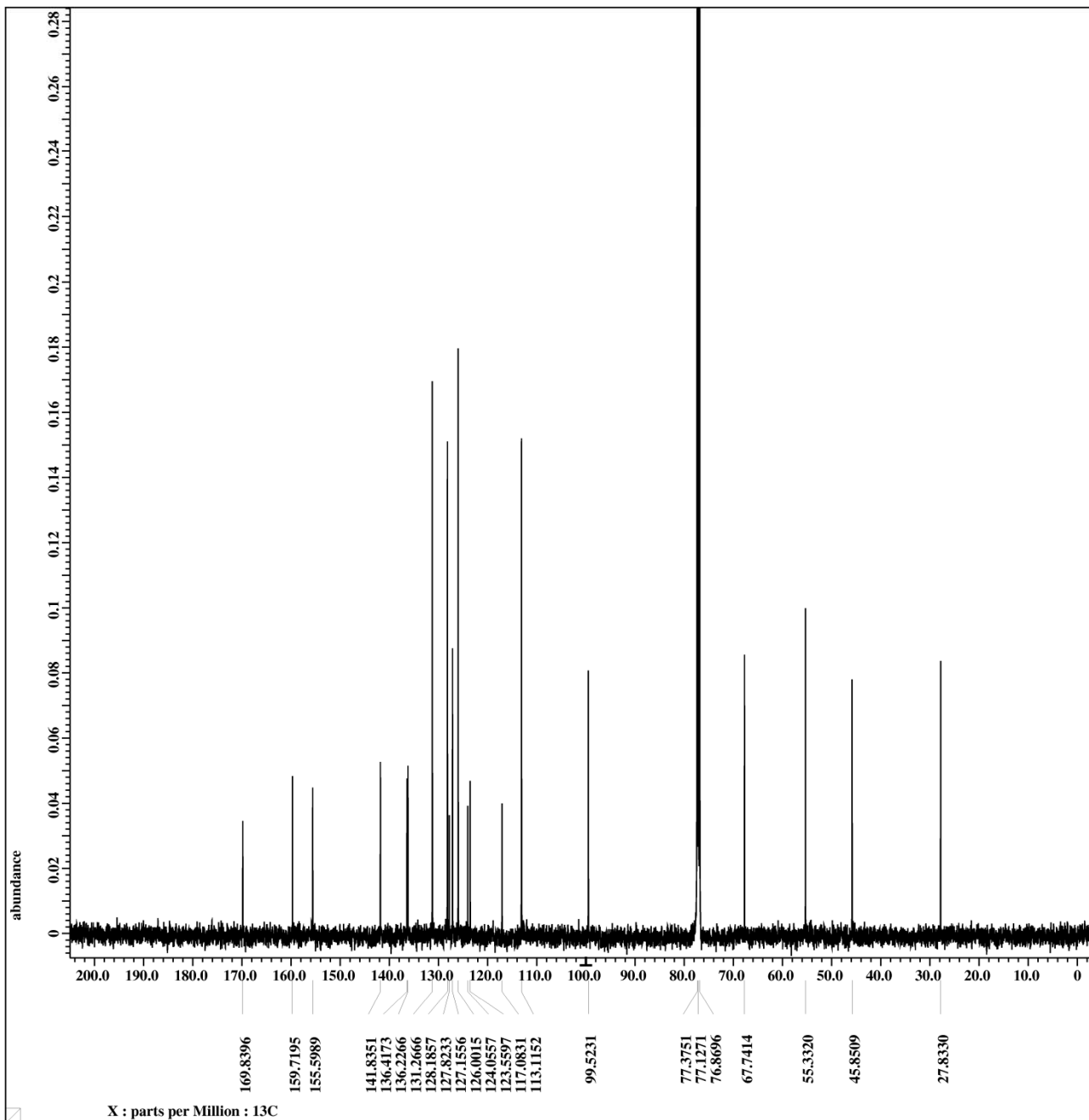
Filename = HMF_III_118-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#533042
 Solvent = CHLOROFORM-D
 Creation_time = 21-FEB-2011 05:51:17
 Revision_time = 20-FEB-2011 17:58:26
 Current_time = 20-FEB-2011 17:59:23

Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 44
 Relaxation_delay = 5[s]
 Repetition_time = 6.74587904[s]
 Temp_get = 21[dC]





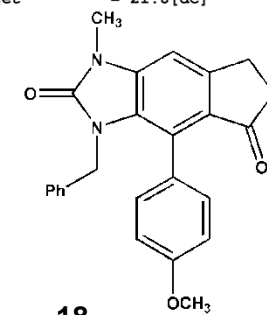
```

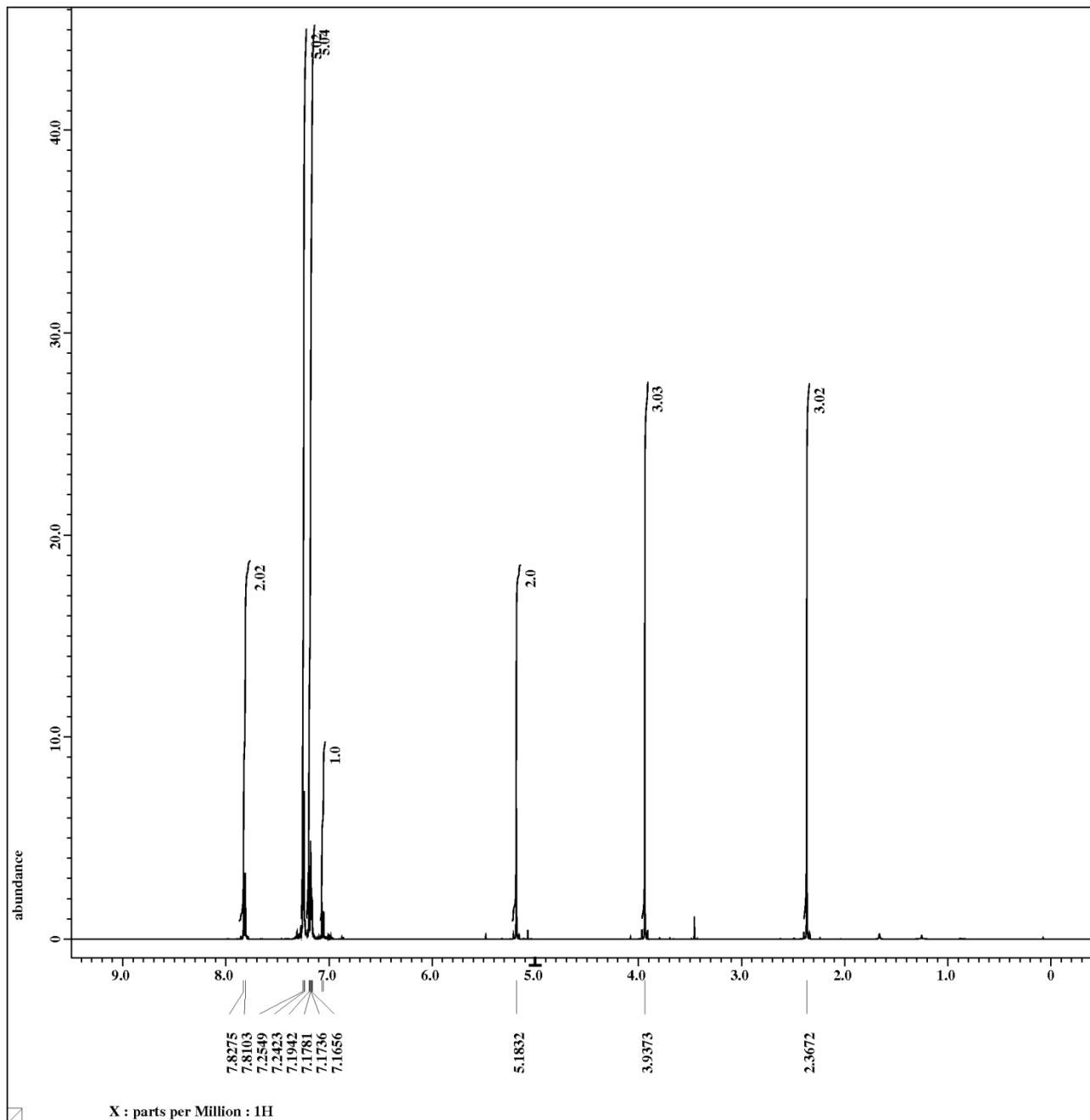
Filename      = HMF_III_118-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#534813
Solvent      = CHLOROFORM-D
Creation_time = 21-FEB-2011 06:31:39
Revision_time = 20-FEB-2011 17:59:50
Current_time  = 20-FEB-2011 18:00:26

Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset      = 100 [ppm]
X_points      = 32768
X_prescans    = 4
X_resolution   = 1.19959034 [Hz]
X_sweep       = 39.3081761 [kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521 [MHz]
Irr_offset    = 5.0 [ppm]
Clipped       = FALSE
Mod_return    = 10
Scans         = 490
Total_scans   = 490

X_90_width   = 10.73 [us]
X_acq_time    = 0.83361792 [s]
X_angle       = 30 [deg]
X_atn         = 9 [dB]
X_pulse      = 3.57666667 [us]
Irr_atn_dec  = 20 [dB]
Irr_atn_noe  = 20 [dB]
Irr_noise    = WALTZ
Decoupling   = TRUE
Initial_wait = 1 [s]
Noe          = TRUE
Noe_time     = 4 [s]
Recvr_gain   = 50
Relaxation_delay = 4 [s]
Repetition_time = 4.83361792 [s]
Temp_get     = 21.8 [dC]
  
```





```

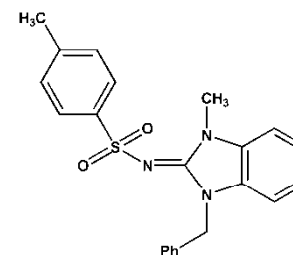
Filename      = HMF_III_98-6.jdf
Author       = delta
Experiment   = single_pulse.ex2
Sample_id    = S#382466
Solvent      = CHLOROFORM-D
Creation_time = 22-JAN-2011 01:38:28
Revision_time = 8-AUG-2011 23:00:47
Current_time  = 8-AUG-2011 23:01:04

Comment      = single_pulse
Data_format  = 1D_COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

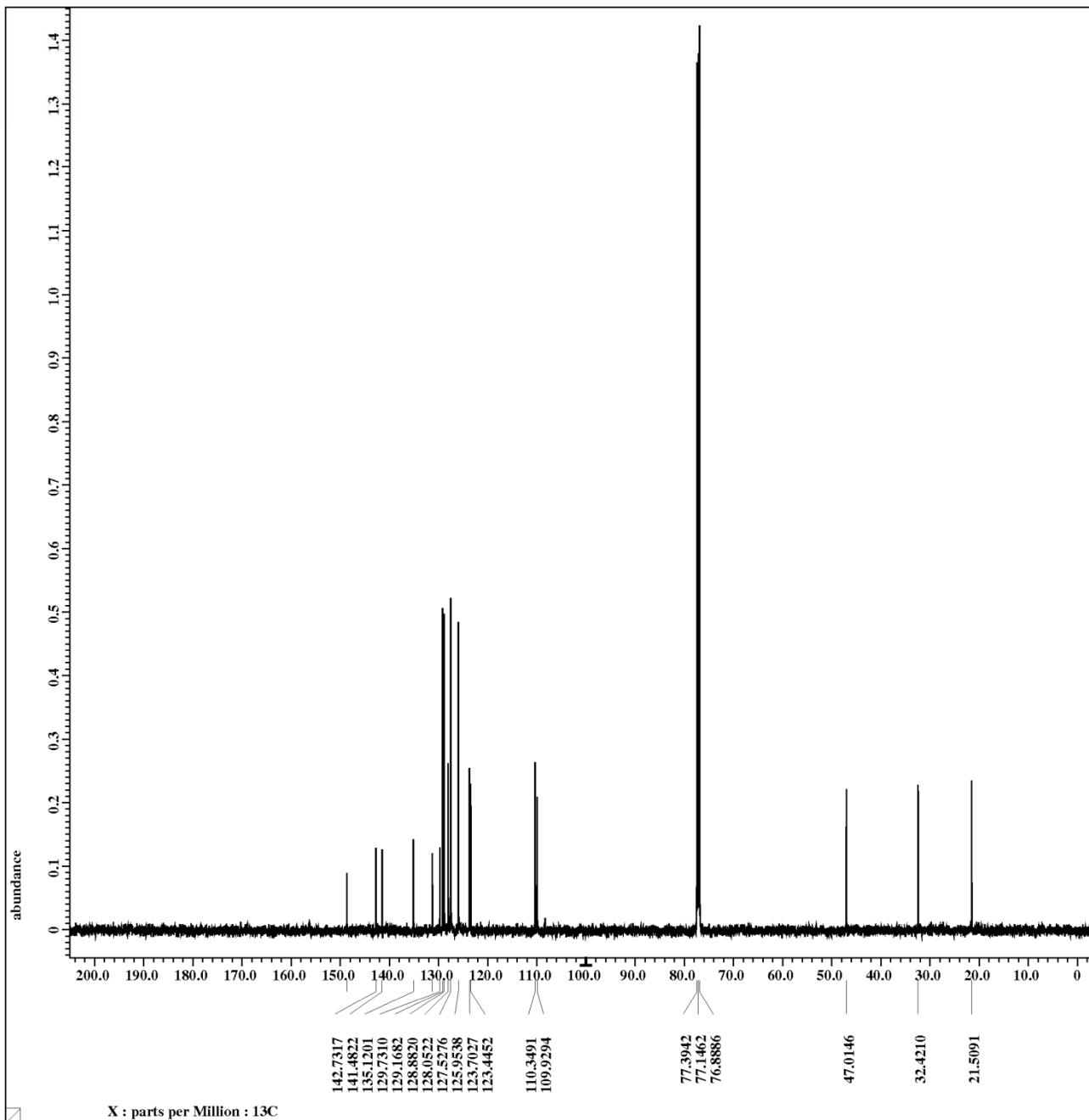
Field_strength = 11.7473579[T] (500[MH]
X_acq_duration = 1.74587904[s]
X_domain       = 1H
X_freq         = 500.15991521[MHz]
X_offset       = 5.0[ppm]
X_points       = 16384
X_prescans     = 0
X_resolution   = 0.57277737[Hz]
X_sweep        = 9.38438438[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521[MHz]
Tri_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 11
Total_scans    = 11

X_90_width    = 12.54[us]
X_acq_time     = 1.74587904[s]
X_angle        = 45[deg]
X_atn          = 4[dB]
X_pulse        = 6.27[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 38
Relaxation_delay = 5[s]
Repetition_time = 6.74587904[s]
Temp_get       = 21.2[dC]

```



21

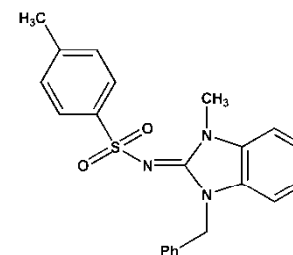


Filename = HMF_III_98-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#383851
 Solvent = CHLOROFORM-D
 Creation_time = 22-JAN-2011 01:52:09
 Revision_time = 8-AUG-2011 23:01:32
 Current_time = 8-AUG-2011 23:02:15

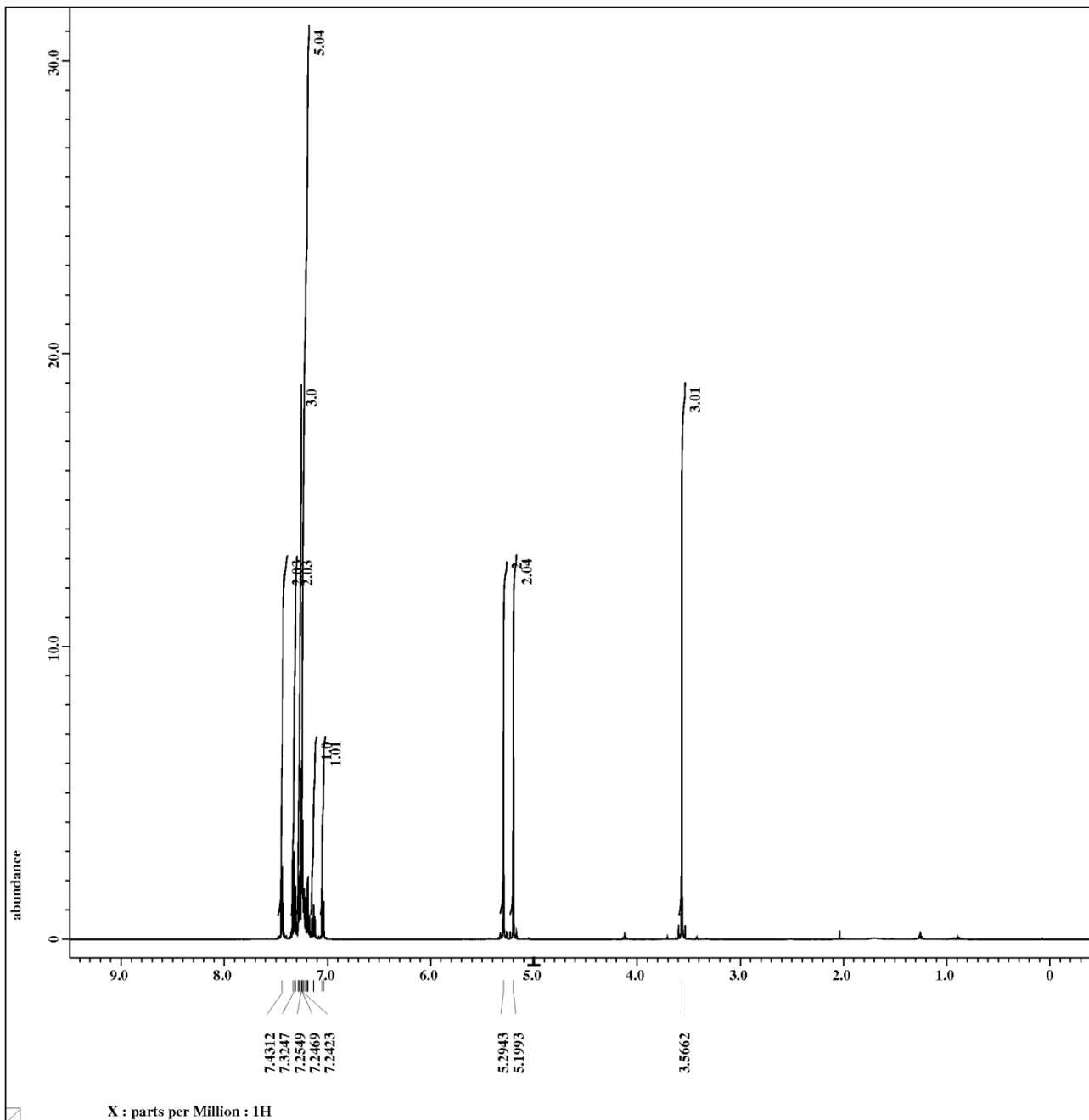
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 0.83361792[s]
 X_domain = 13C
 X_freq = 125.76529768 [MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.19959034 [Hz]
 X_sweep = 39.3081761 [kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521 [MHz]
 Irr_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 10
 Scans = 160
 Total_scans = 160

X_90_width = 10.73 [us]
 X_acq_time = 0.83361792 [s]
 X_angle = 30 [deg]
 X_atn = 9 [dB]
 X_pulse = 3.57666667 [us]
 Irr_atn_dec = 20 [dB]
 Irr_atn_noe = 20 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Noe = TRUE
 Noe_time = 4 [s]
 Recvr_gain = 50
 Relaxation_delay = 4 [s]
 Repetition_time = 4.83361792 [s]
 Temp_get = 21.7 [dC]



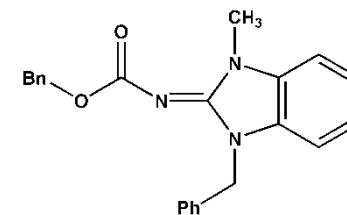
21



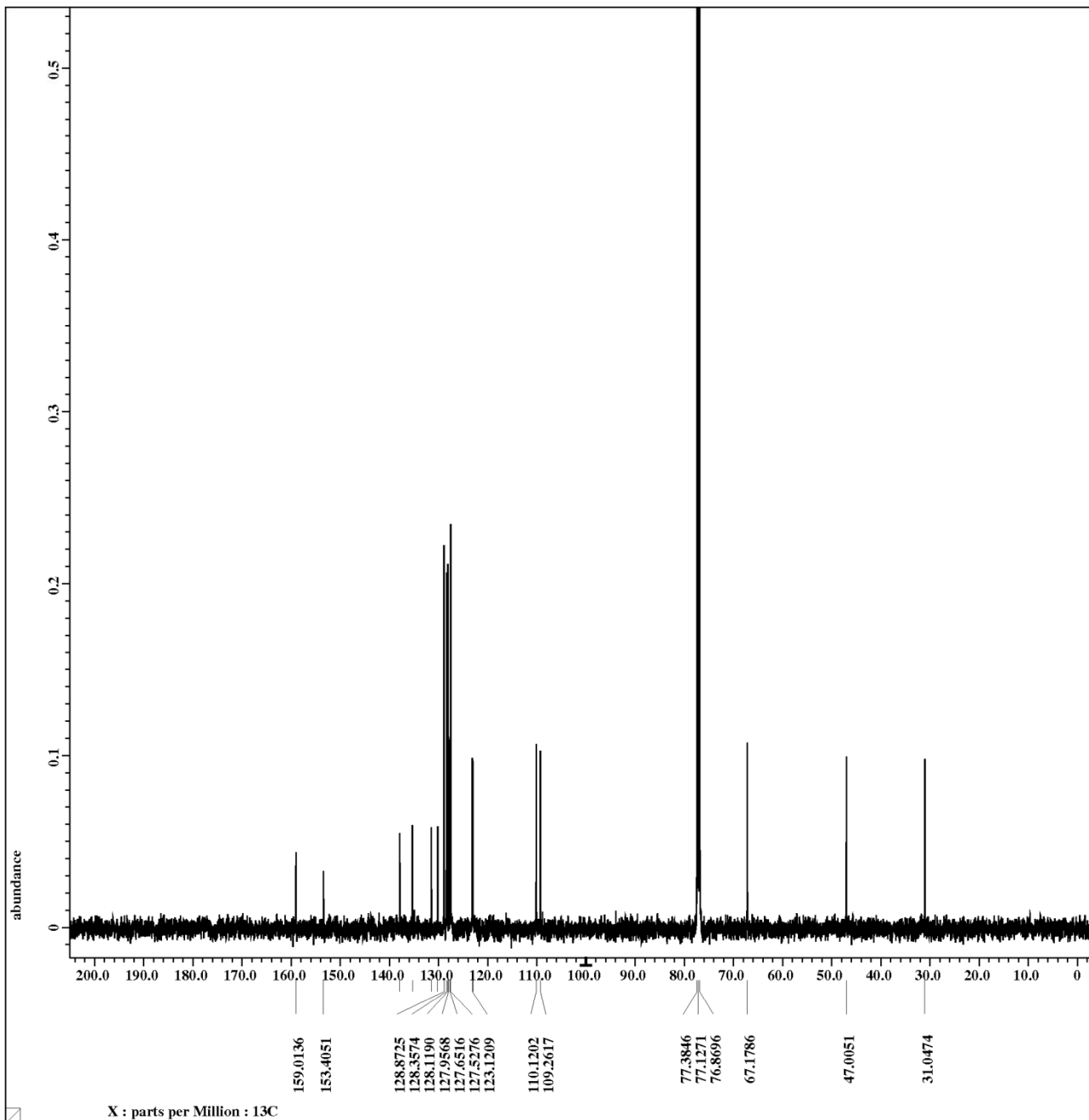
Filename = HMF_III_120-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#500510
 Solvent = CHLOROFORM-D
 Creation_time = 12-FEB-2011 04:56:59
 Revision_time = 27-JUL-2011 21:56:20
 Current_time = 27-JUL-2011 21:57:10

Comment = single pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16
 X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 40
 Relaxation_delay = 5[s]
 Repetition_time = 6.74587904[s]
 Temp_get = 25.5[dc]



22



```

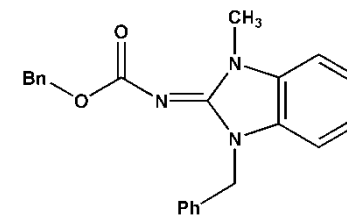
Filename      = HMF_III_120-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#502240
Solvent      = CHLOROFORM-D
Creation time = 12-FEB-2011 05:06:42
Revision time = 27-JUL-2011 22:05:18
Current_time = 27-JUL-2011 22:05:59

Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

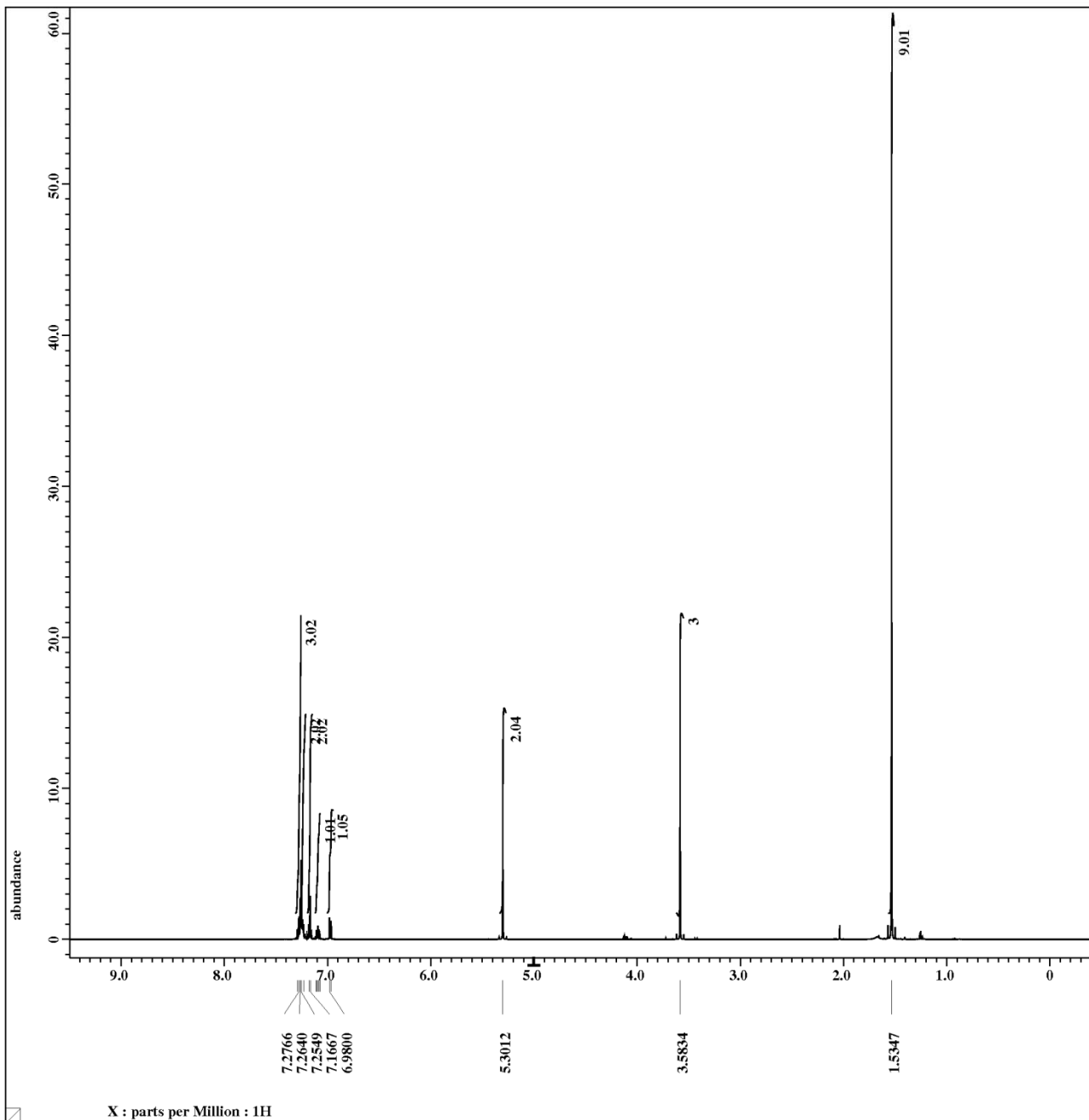
Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768[MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034[Hz]
X_sweep        = 39.3081761[kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521[MHz]
Irr_offset     = 5.0[ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 110
Total_scans    = 110

X_90_width    = 10.73[us]
X_acq_time    = 0.83361792[s]
X_angle       = 30[deg]
X_atn         = 9[dB]
X_pulse       = 3.57666667[us]
Irr_atn_dec   = 20[dB]
Irr_atn_noe   = 20[dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1[s]
Noe           = TRUE
Noe_time      = 4[s]
Recvr_gain    = 50
Relaxation_delay = 4[s]
Repetition_time = 4.83361792[s]
Temp_get      = 25.9[dC]

```



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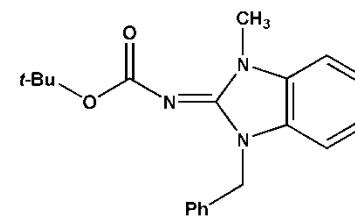


Filename = HMF_III_123-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#575446
 Solvent = CHLOROFORM-D
 Creation_time = 18-FEB-2011 07:02:09
 Revision_time = 27-JUL-2011 22:52:33
 Current_time = 27-JUL-2011 22:53:27

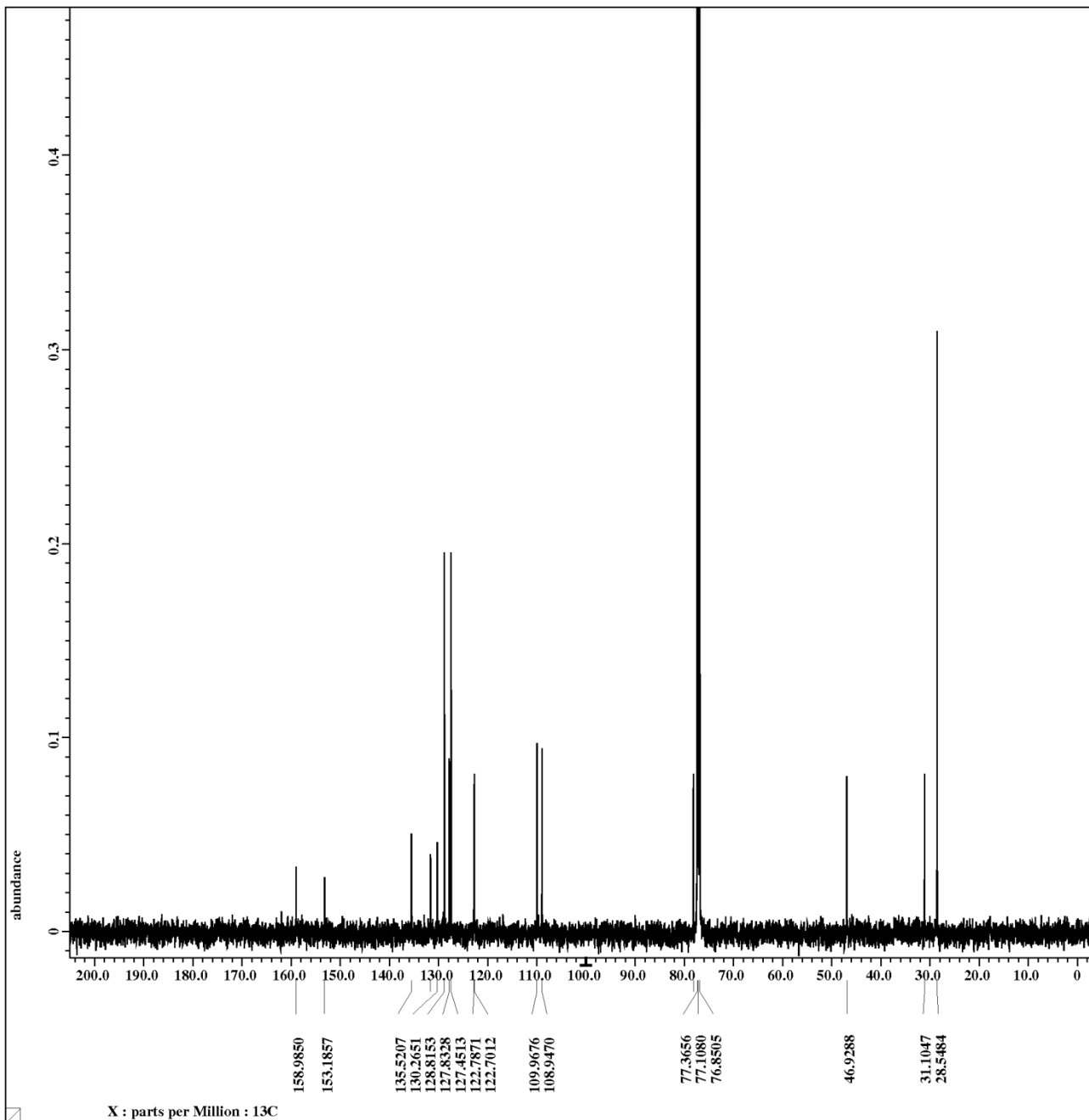
Comment = single pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 42
 Relaxation_delay = 5[s]
 Repetition_time = 6.74587904[s]
 Temp_get = 21.2[dc]



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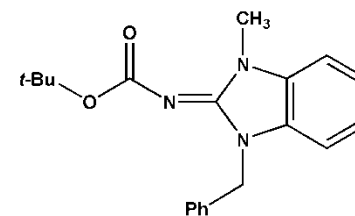


Filename = HMF_IV_30-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#615413
 Solvent = CHLOROFORM-D
 Creation_time = 27-SEP-2011 07:09:13
 Revision_time = 27-SEP-2011 14:50:17
 Current_time = 27-SEP-2011 14:51:17

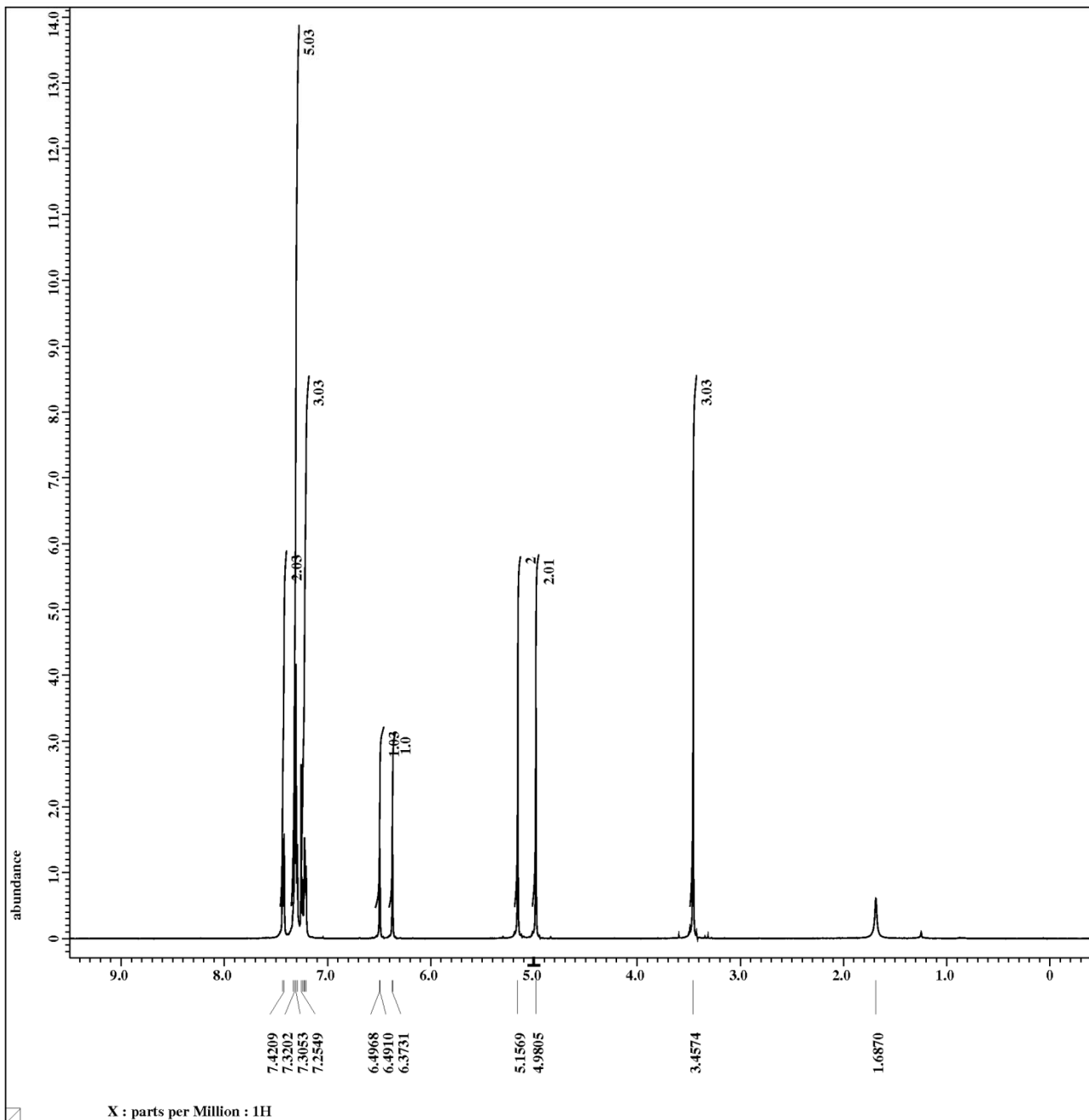
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 0.83361792[s]
 X_domain = 13C
 X_freq = 125.76529768[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.19959034[Hz]
 X_sweep = 39.3081761[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 10
 Scans = 240
 Total_scans = 240

X_90_width = 10.73[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 9[dB]
 X_pulse = 3.57666667[us]
 Irr_atn_dec = 20[dB]
 Irr_atn_noe = 20[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 4[s]
 Recvr_gain = 50
 Relaxation_delay = 4[s]
 Repetition_time = 4.83361792[s]
 Temp_get = 22.6[dC]



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```

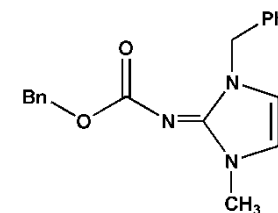
Filename      = HMF_IV_34-4.jdf
Author        = delta
Experiment    = single_pulse.ex2
Sample_id     = S#484608
Solvent       = CHLOROFORM-D
Creation_time = 29-SEP-2011 03:14:36
Revision_time = 28-SEP-2011 14:09:11
Current_time  = 28-SEP-2011 14:09:50

Comment      = single_pulse
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

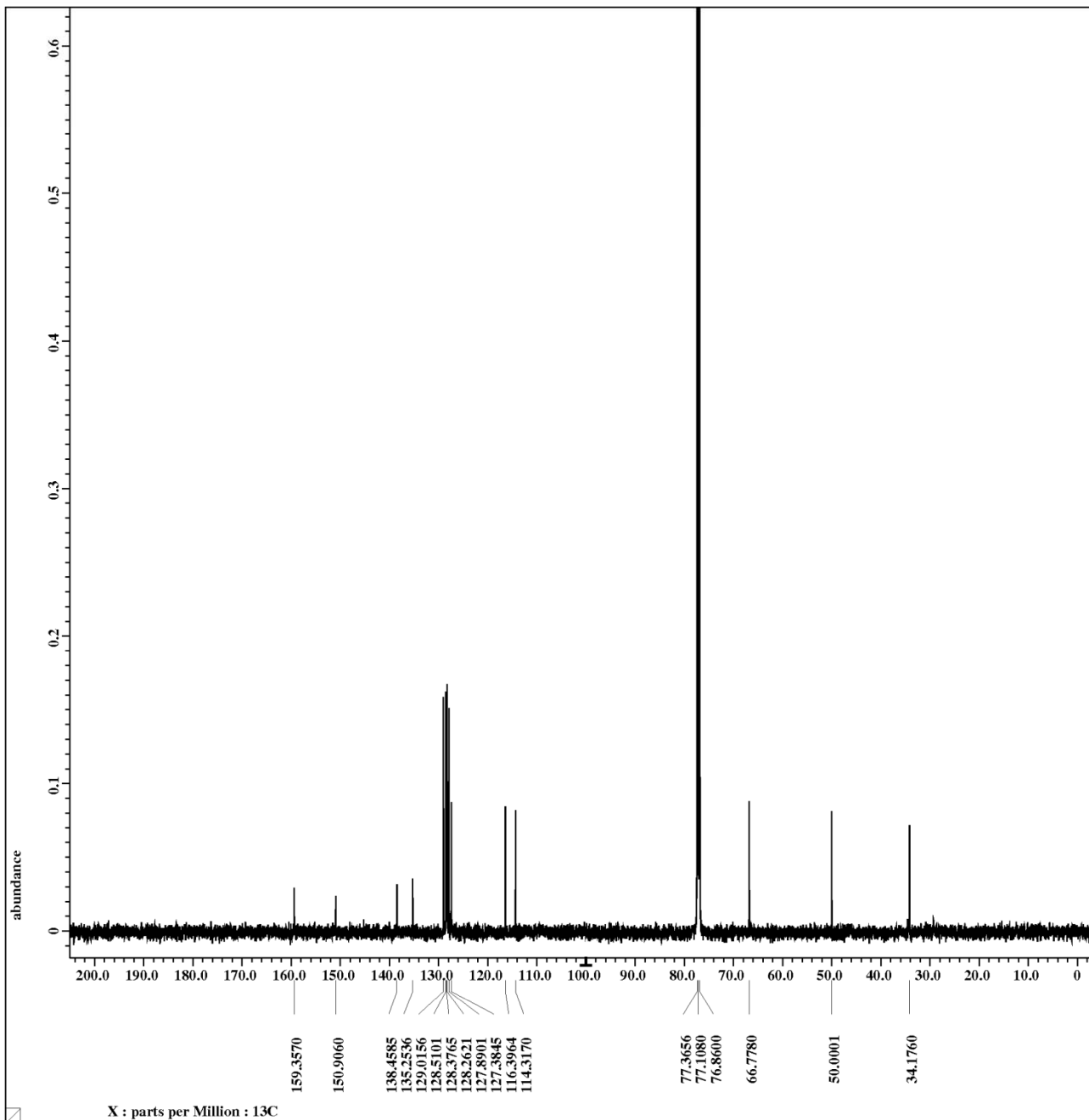
Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 1.74587904[s]
X_domain      = 1H
X_freq        = 500.15991521[MHz]
X_offset      = 5.0[ppm]
X_points      = 16384
X_prescans    = 0
X_resolution  = 0.57277737[Hz]
X_sweep       = 9.38438438[kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521[MHz]
Irr_offset    = 5.0[ppm]
Tri_domain    = 1H
Tri_freq      = 500.15991521[MHz]
Tri_offset    = 5.0[ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 16
Total_scans   = 16

X_90_width   = 12.54[us]
X_acq_time    = 1.74587904[s]
X_angle       = 45[deg]
X_atn         = 4[dB]
X_pulse       = 6.27[us]
Irr_mode      = Off
Tri_mode      = Off
Dante_presat  = FALSE
Initial_wait  = 1[s]
Recvr_gain    = 46
Relaxation_delay = 5[s]
Repetition_time = 6.74587904[s]
Temp_get      = 23.2[dC]

```



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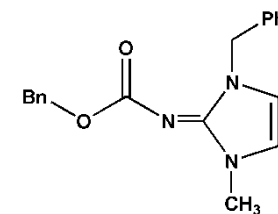


Filename = HMF_IV_34-3.jdf
 Author = delta
 Experiment = single_pulse_dec
 Sample_id = S#486376
 Solvent = CHLOROFORM-D
 Creation_time = 29-SEP-2011 03:40:59
 Revision_time = 28-SEP-2011 14:10:12
 Current_time = 28-SEP-2011 14:10:46

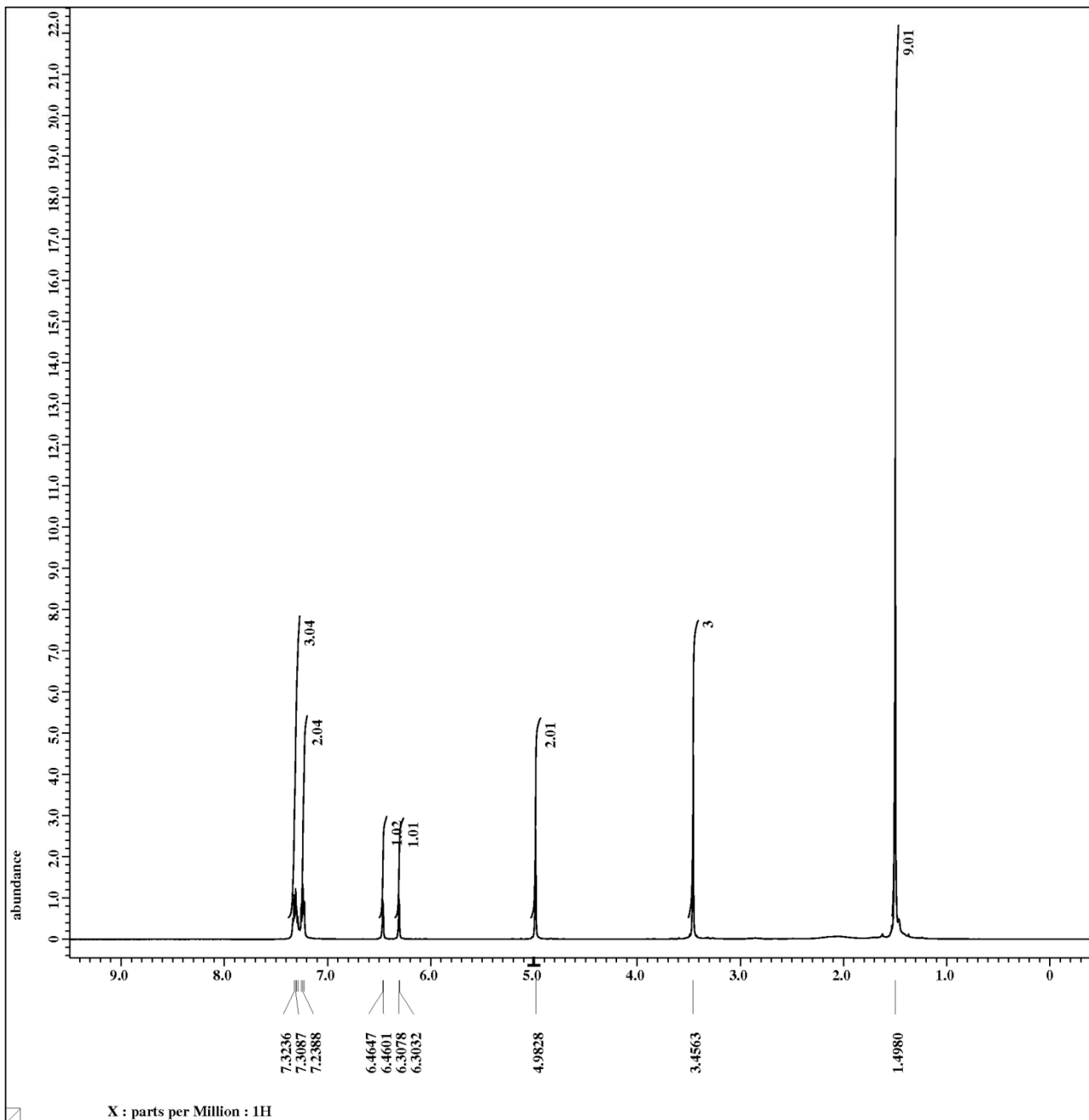
Comment = single pulse decouple
 Data_format = 1D COMPLEX
 Dim_size = 26214
 Dim_title = 13C
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 0.83361792[s]
 X_domain = 13C
 X_freq = 125.76529768[MHz]
 X_offset = 100[ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 1.19959034[Hz]
 X_sweep = 39.3081761[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 10
 Scans = 400
 Total_scans = 400

X_90_width = 10.73[us]
 X_acq_time = 0.83361792[s]
 X_angle = 30[deg]
 X_atn = 9[dB]
 X_pulse = 3.57666667[us]
 Irr_atn_dec = 20[dB]
 Irr_atn_noe = 20[dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1[s]
 Noe = TRUE
 Noe_time = 3[s]
 Recvr_gain = 50
 Relaxation_delay = 3[s]
 Repetition_time = 3.83361792[s]
 Temp_get = 23.8[dC]



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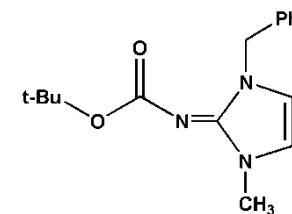


Filename = HMF_IV_35-4.jdf
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#638136
 Solvent = CHLOROFORM-D
 Creation_time = 20-SEP-2011 07:29:46
 Revision_time = 20-SEP-2011 16:27:41
 Current_time = 20-SEP-2011 16:28:21

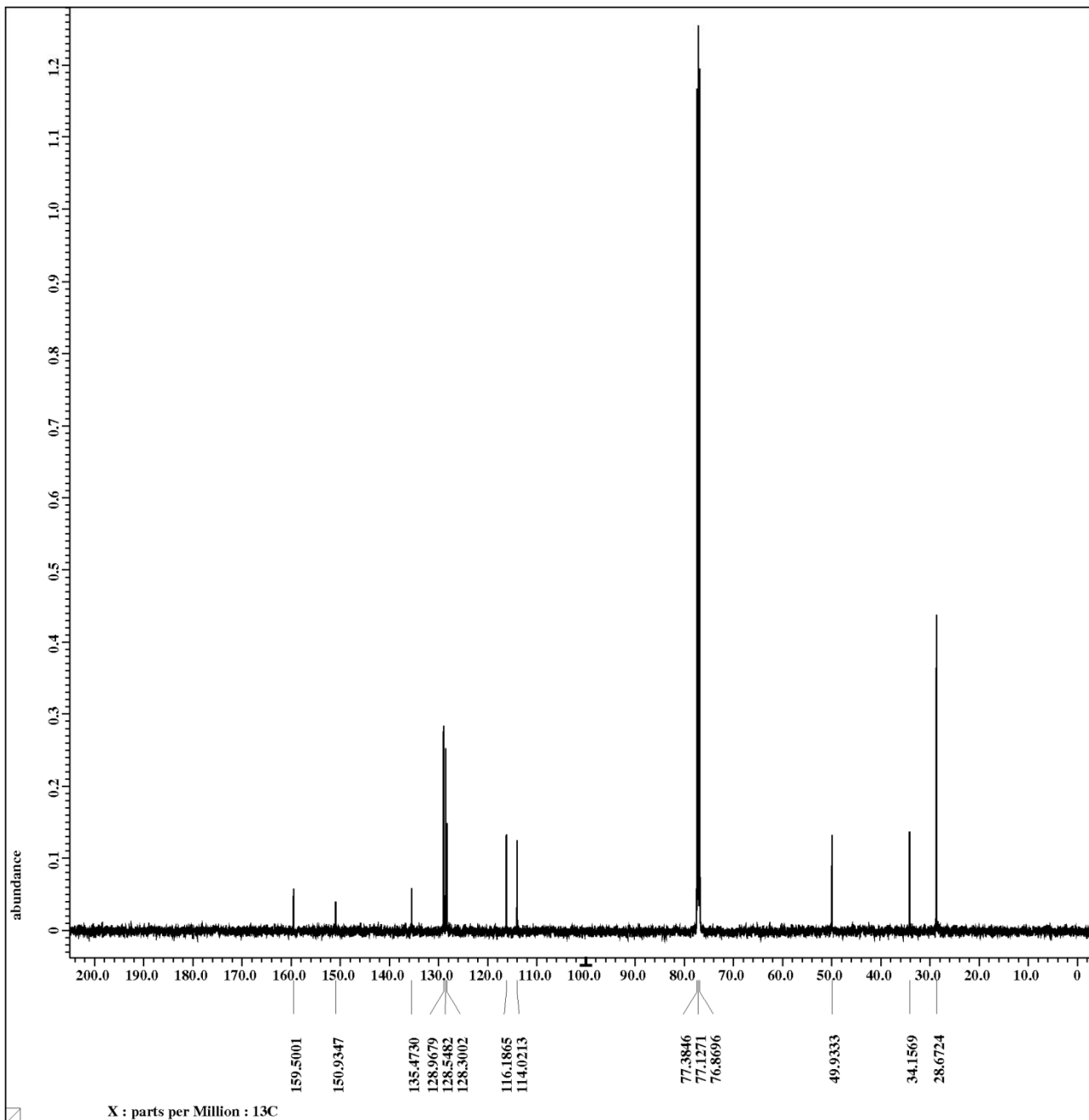
Comment = single_pulse
 Data_format = 1D_COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 500
 Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
 X_acq_duration = 1.74587904[s]
 X_domain = 1H
 X_freq = 500.15991521[MHz]
 X_offset = 5.0[ppm]
 X_points = 16384
 X_prescans = 0
 X_resolution = 0.57277737[Hz]
 X_sweep = 9.38438438[kHz]
 Irr_domain = 1H
 Irr_freq = 500.15991521[MHz]
 Irr_offset = 5.0[ppm]
 Tri_domain = 1H
 Tri_freq = 500.15991521[MHz]
 Tri_offset = 5.0[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 16
 Total_scans = 16

X_90_width = 12.54[us]
 X_acq_time = 1.74587904[s]
 X_angle = 45[deg]
 X_atn = 4[dB]
 X_pulse = 6.27[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 40
 Relaxation_delay = 5[s]
 Repetition_time = 6.74587904[s]
 Temp_get = 22.1[dc]



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```

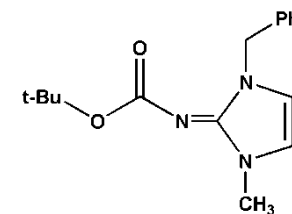
Filename      = HMF_IV_35-3.jdf
Author       = delta
Experiment   = single_pulse_dec
Sample_id    = S#639878
Solvent      = CHLOROFORM-D
Creation_time = 20-SEP-2011 07:49:07
Revision_time = 20-SEP-2011 16:28:44
Current_time  = 20-SEP-2011 16:29:11

Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECA 500
Spectrometer = JNM-ECA500

Field_strength = 11.7473579[T] (500[MH
X_acq_duration = 0.83361792[s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100[ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 10
Scans          = 230.0
Total_scans    = 230.0

X_90_width    = 10.73 [us]
X_acq_time    = 0.83361792 [s]
X_angle       = 30 [deg]
X_atn         = 9 [dB]
X_pulse       = 3.57666667 [us]
Irr_atn_dec   = 20 [dB]
Irr_atn_noe   = 20 [dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1 [s]
Noe           = TRUE
Noe_time      = 4 [s]
Recvr_gain    = 50
Relaxation_delay = 4 [s]
Repetition_time = 4.83361792 [s]
Temp_get      = 22.7 [dC]

```



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