Supporting Information

First synthesis and reactivity of 1,3-dialkyl-5-(polyfluoroalkyl)pyrimido[4,5-b]quinoline-2,4(1H,3H)-diones (5-RF-5-deazaalloxazines)

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Table of Contents

1 General: analytical equipment, chemicals and work technique

NMR Spectroscopy: ^{1}H NMR spectra (250.13, 300.13 and 500.13 MHz) and ^{13}C NMR spectra (62.90, 75.47 and 125.77 MHz) were recorded on Bruker instruments AVANCE 250, ARX 300, and AVANCE 500 respectively using CDCl3, DMSO-d_6 and CF_3COOD as solvents. The spectra were calibrated according to the solvent signals ($CDCl_3$: ^{1}H = 7.26, ^{13}C = 77.36; DMSO-d_6: ^{1}H = 2.54, ^{13}C = 40.45; CF_3COOD: ^{1}H = 11.50, ^{13}C = 116.60 (q, $^{1}J_{(C-F)}$ = 283.19 Hz) and 164.20 (q, $^{2}J_{(C-F)}$ = 43.99 Hz)). ^{19}F-NMR spectra were recorded at 235.33 or 282.38 MHz on AVANCE 250 and ARX 300 respectively considering $CFCl_3$-signal as a zero point of the scale. All chemical shifts are given in ppm. All coupling constants *J* are indicated in Hz. Multiplicities are given as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad signal. More complex coupling patterns are represented by combinations of the respective symbols. For example, td indicates a triplet of doublets with the larger coupling constant associated with the first symbol (here: triplet). The ^{1}H and ^{13}C NMR signals were assigned by DEPT and two-dimensional ^{1}H-^{1}H COSY, ^{1}H-^{1}H NOESY and ^{1}H-^{13}C correlation spectra (HMBC and HSQC).

Mass spectrometry (MS):

a) Finnigan MAT 95 XP (Thermo Electron Corporation), EI, 70 eV;

b) GC 6890/ MS D 5973 (Agilent Technologies), MS(GC), 70 eV.

High resolution MS (HRMS):

a) Finnigan MAT 95 XP (Thermo Electron Corporation), EI, 70 eV;

b) 6210 Time-of-Flight LC/MS (Agilent Technologies), ESI.

Only the measurements with an average deviation from the theoretical mass of ± 2 µDa were accounted as correct.

Infrared spectroscopy (IR): Nicolet 380 FT-IR spectrometer with ATR sampling technique for solids as well as liquids. Signal characterization: (w) = weak, (m) = medium, (s) = strong.

Elemental analysis (EA): Flash EA 1112 (Thermoquest).

X-ray crystallography: Bruker Apex Kappa-II diffraktometer with CCD camera (Mo-K_α radiation and graphite monochromator, λ = 0.71073 Å). The space group is determined by the XPREP program and the structures were solved via the SHELX-97 program package. Refinements were carried out according to the minimum square error method.

UV/Vis spectroscopy: Lambda 2 (Perkin Elmer). Cuvette length *l* = 1 cm.

Fluorescence spectroscopy: HITACHI F-4010. Cuvette length l = 1 cm, cuvette width w = = 1 cm.

Thin layer chromatography (TLC): Merck HPTLC silica gel 60 F_{254} (aluminium sheets 20x20 cm). Detection with UV light at 254 and 366 nm; afterwards development with vanillin-sulfuric acid solution (1 g of vanillin, 14 mL of acetic acid and 1 mL of conc. sulfuric acid in 85 mL of methanol).

Melting Points: All the measurements were carried out on the FP900 Thermosystem (Mettler) using a polarized light microscope Laborlux 12 POL S (Leitz). The melting points are uncorrected.

Column chromatography: Separation on Acros or Merck silica gel 60 Å (0.060-0.200 mm, 70-230 mesh). Eluents were distilled before use.

All chemicals were purchased from the standard chemical suppliers, such as Sigma-Aldrich®, Arcos®, Merck® and others.

2 Experimental procedures and description of products

2.1 Synthesis of 6-amino-1,3-dialkylpyrimidine-2,4(1*H*,3*H*)-diones

General procedure for the synthesis of 6-amino-1,3-dialkylpyrimidine-2,4(1*H*,3*H*)-diones 2.

Method A (for simple anilines): In a Schlenk tube were placed 1 eq of 6-chloro-1,3-dialkyluracil and 2,2 eq of amine. Then the reaction mass was heated under argon at 180 °C for 3 hours. After cooling to 100 °C the mixture was treated by hot water, cooled to r.t. and triturated with diethyl ether. The formed solid was filtered off by suction, washed twice with water and diethyl ether and dried in a high vacuum.

Method B (for anilines with two amino groups): In a Schlenk tube were placed 1 eq of amine and 1.2 eq of 6-chloro-1,3-dimethyluracil (molar ratio = 1 : 2.4). Then 1 eq of quinoline was added and the reaction mass was heated under argon at 180 °C for 3 hours. After cooling to 70 °C the mixture was treated by hot ethanol and boiled few minutes under reflux. The precipitate was filtered off by suction, washed twice with ethanol and dried in a high vacuum.

Method C (for inactive amines): In a Schlenk flask was prepared solution of amine (2.2 eq) in dry THF. Then 2.2 eq of *n*-butyl lithium (2.5 M solution in hexane) was added at –78 °C under argon. To obtained lithium salt previously prepared solution of 6-chloro-1,3-dialkyluracil (1 eq) in THF was added dropwise and afterwards the reaction mixture was allowed to warm to r.t.. The next day the solution was acidified with acetic acid and the solvent was evaporated. The solid rest was triturated with water and diethyl ether, filtered off by suction, washed twice and dried in a high vacuum.

1,3-Dimethyl-6-{[3-(trifluoromethyl)phenyl]amino}pyrimidine-2,4(1*H*,3*H*)-dione (2f). The product was prepared according to **Method A**, starting from 1.1 g of 6-chloro-1,3-dimethyluracil and 2.233 g of 3-(trifluoromethyl)aniline. Yield 1.587 g (84%), white solid, mp 198-200 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.25 (s, 3H, CH_3), 3.53 (s, 3H, CH_3), 4.91 (s, 1H, H-5), 7.25 (br s, 1H, NH), 7.28-7.35 (m, 1H, CH_{Ar}), 7.36 (s, 1H, CH_{Ar}), 7.39-7.47 (m, 2H, CH_{Ar}). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 28.3 (CH_3), 30.1 (CH_3), 79.7 (CH-5), 121.6 (q, $^{3}J_{(C-F)}$ = 3.8 Hz, CH), 123.1 (q, $^{3}J_{(C-F)}$ = 3.8 Hz, CH), 123.8 (q, $^{1}J_{(C-F)}$ = 272.7 Hz, CF_3), 128.0 (CH), 130.5 (CH), 132.5 (q, $^{2}J_{(C-F)}$ = 32.9 Hz), 138.5, 152.2, 153.1, 163.6. ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –62.9 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 300 ($[M+H]^+$, 15), 299 ($[M]^+$, 100), 280 (16), 241 (15), 214 (18), 213 (67), 212 (11), 200 (33), 199 (33), 186 (20), 185 (35), 172 (20), 145 (69), 127 (46), 126 (12), 95 (10), 82 (35), 55 (21), 54 (10), 42 (13). HRMS (ESI): Calcd. for $C_{13}H_{13}F_3N_3O_2$ $[M+H]^+$: 300.09544, found: 300.09553. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3307 (w), 3066 (w), 1699 (m), 1633 (s), 1605 (s), 1591 (m), 1537 (s), 1493 (s), 1471 (m), 1443 (m), 1421 (m), 1383 (m), 1362 (m), 1331 (s), 1315 (s), 1281 (m), 1265 (m), 1213 (w), 1171 (s), 1124 (s), 1093 (s), 1066 (s), 1003 (m), 933 (m), 920 (m), 891 (m), 816 (m), 777 (s), 750 (s), 743 (s), 702 (s), 673 (w), 662 (s), 648 (m), 638 (m), 582

(m).

6-[(4-Methoxyphenyl)amino]-1,3-dipropylpyrimidine-2,4(1*H*,3*H*)-dione (2j). The product was prepared according to the **Method A**, starting from 1.2 g of 6-chloro-1,3-dipropyluracil and 1.409 g of *p*-anisidine. Yield 1.133 g (69%), pinkish solid, mp 109-111 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 0.86 (t, 3H, ^{3}J = 6.99 Hz), 0.95 (t, 3H, ^{3}J = 7.09 Hz), 1.46-1.82 (m, 4H, CH_2), 3.68-3.88 (m, 5H, CH_2, MeO), 3.96 (t, 1H, ^{3}J = 6.99 Hz), 4.66 (s, 1H, H-5), 6.78 (br s, 1H, NH), 6.84 (d, 2H, ^{3}J = 6.84 Hz, CH_{Ph}), 7.01 (d, 2H, ^{3}J = 6.84 Hz, CH_{Ph}). ^{13}C NMR (75.48 MHz, $CDCl_3$): δ = 11.4 (CH_3), 11.6 (CH_3), 21.4 (CH_2), 21.9 (CH_2), 42.9 (CH_2), 44.2 (CH_2), 55.8 (MeO), 78.1 (CH-5), 115.1 (CH_{Ar}), 128.0 (CH_{Ar}), 129.8, 151.9, 153.8, 158.7, 163.3. MS (GC, 70 eV): *m/z* (%) = 318 ([M+H]$^{+}$, 19), 317 ([M]$^{+}$, 99), 275 (46), 274 (49), 260 (12), 233 (20), 190 (31), 189 (20), 175 (17), 174 (20), 162 (22), 153 (10), 149 (18), 148 (25), 147 (27), 146 (15), 134 (13), 133 (18), 132 (18), 123 (100), 121 (13), 108 (16), 77 (11), 68 (15), 43 (15), 41 (19). HRMS (ESI): Calcd. for $C_{17}H_{24}N_3O_3$ [M+H]$^{+}$: 318.18122, found: 318.18072. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3273 (w), 2958 (m), 2875 (w), 2837 (w), 1687 (s), 1606 (s), 1587 (s), 1531 (s), 1506 (s), 1479 (s), 1456 (s), 1437 (s), 1412 (s), 1392 (s), 1379 (s), 1360 (s), 1335 (m), 1319 (m), 1286 (s), 1267 (m), 1242 (s), 1205 (m), 1178 (s), 1165 (s), 1105 (m), 1049 (m), 1032 (s), 1011 (m), 937 (m), 895 (m), 878 (m), 831 (m), 777 (s), 764 (s), 750 (s), 737 (s), 712 (m), 673 (m), 644 (m), 629 (s), 552 (s).

6,6'-[Biphenyl-4,4'-diyldi(imino)]bis(1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione) (2k). The product was prepared according to the **Method B**, starting from 0.455 g of 6-chloro-1,3-dimethyluracil, 0.2 g of benzidine and 0.404 g of quinoline. Yield 0.452 g (91%), grey solid, mp >375 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.17 (s, 6H, CH_3), 3.50 (s, 6H, CH_3), 4.82 (s, 2H, H5, H5'), 7.38 (d, 4H, ^{3}J = 8.59 Hz, CH_{Ar}), 7.80 (d, 4H, ^{3}J = 8.59 Hz, CH_{Ar}), 8.63 (s, 2H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.2 (CH_3), 31.1 (CH_3), 78.6 (CH-5, CH-5'), 125.8 (CH), 128.3 (CH), 137.2, 138.8, 152.5, 154.0, 162.5. MS (EI, 70 eV): *m/z* (%) = 461 ([M+H]$^{+}$, 23), 460 ([M]$^{+}$, 100), 374 (11). HRMS (EI): Calcd. for $C_{24}H_{24}O_4N_6$ [M]$^{+}$: 460.18535, found: 460.185839. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3219 (m), 3109 (w), 3043 (w), 2958 (w), 2895 (w), 1701 (s), 1624 (s), 1597 (s), 1581 (s), 1525 (s), 1497 (s), 1466 (s), 1429 (s), 1383 (s), 1363 (s), 1321 (m), 1288 (s), 1275 (s), 1254 (s), 1192 (m), 1051 (m), 1009 (m), 997 (m), 912 (m), 818 (s), 775 (s), 754 (s), 729 (m), 698 (m), 669 (m), 654 (m), 642 (m), 602 (s), 538 (m).

6,6'-[Methylenebis(4,1-phenyleneimino)]bis(1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione) (2l). The product was prepared according to the **Method B**, starting from 0.442 g of 6-chloro-1,3-dimethyluracil, 0.209 g of 4,4'-diaminodiphenylmethane and 0.392 g of quinoline. Yield 0.387 g (77%), brownish solid, mp 308-310 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.14 (s, 6H, CH_3), 3.46 (s, 6H, CH_3), 4.02 (s, 2H, CH_2), 4.63 (s, 2H, H5, H5'), 7.22 (d, 4H, ^{3}J = 8.50 Hz, CH_{Ar}), 7.33 (d, 4H, ^{3}J = 8.50 Hz, CH_{Ar}), 8.50 (s, 2H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.1 (CH_3), 30.9 (CH_3), 40.8 (CH_2), 77.8 (CH-5, CH-5'), 126.2 (CH), 130.6 (CH), 137.2, 139.7, 152.5, 154.3, 162.5. MS (GC, 70 eV): *m/z* (%) = 475

([M+H]$^+$, 20), 474 ([M]$^+$, 72), 473 (100), 334 (13), 229 (10), 145 (12), 104 (16), 82 (12), 40 (11). HRMS (ESI): Calcd. for $C_{25}H_{27}N_6O_4$ [M+H]$^+$: 475.20883, found: 475.20938. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3209 (w), 2953 (w), 1695 (s), 1622 (s), 1589 (s), 1525 (s), 1510 (s), 1462 (s), 1441 (s), 1431 (s), 1414 (s), 1381 (s), 1360 (s), 1282 (s), 1257 (s), 1192 (m), 1178 (m), 1107 (m), 1020 (m), 999 (m), 912 (m), 860 (m), 812 (m), 777 (s), 752 (s), 723 (m), 667 (m), 648 (s), 635 (s), 577 (m), 542 (s).

1,3-Dimethyl-6-[(3-methyl-1-phenyl-1*H*-pyrazol-5-yl)amino]pyrimidine-2,4(1*H*,3*H*)-dione (2n). The product was prepared according to the **Method C**, using a solution of 5-amino-3-methyl-1-phenylpyrazole (0.764 g) in dry THF (7 mL), 1.76 mL of *n*-butyl lithium (2.5 M solution in hexane) and a solution of 6-chloro-1,3-dimethyluracil (0.35 g) in dry THF (7 mL). Yield 0.51 g (82%), white solid, mp 125-126 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 2.32 (s, 3H, CH_3-3'), 3.10 (s, 3H, CH_3), 3.39 (s, 3H, CH_3), 4.38 (s, 1H, H-5), 6.36 (s, 1H, H-4'), 7.34-7.42 (m, 1H, $CH_{p\text{-}Ph}$), 7.46-7.60 (m, 4H, CH_{Ph}), 8.83 (br s, 1H, NH). ^{13}C NMR (75.48 MHz, DMSO-d_6): δ = 14.8 (CH_3-3'), 28.2 (CH_3), 30.9 (CH_3), 78.0 (CH-5), 105.9, 123.6 (CH_{Ph}), 128.1 (CH_{Ph}), 130.1 (CH_{Ph}), 136.5, 139.2, 149.4, 152.1, 153.8, 162.3. MS (GC, 70 eV): *m/z* (%) = 312 ([M+H]$^+$, 19), 311 ([M]$^+$, 100), 184 (18), 82 (13), 77 (23), 55 (19). HRMS (ESI): Calcd. for $C_{16}H_{18}N_5O_2$ [M+H]$^+$: 312.14550, found: 312.14612. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3452 (w), 3331 (w), 3138 (w), 3030 (w), 2902 (w), 1701 (s), 1651 (s), 1633 (s), 1605 (s), 1593 (s), 1549 (s), 1497 (s), 1471 (s), 1435 (s), 1417 (s), 1381 (s), 1362 (m), 1313 (m), 1286 (m), 1230 (m), 1198 (m), 1173 (m), 1144 (m), 1076 (m), 1049 (w), 1022 (m), 1014 (m), 995 (m), 908 (w), 854 (w), 837 (w), 798 (w), 783 (s), 752 (s), 743 (s), 712 (m), 692 (s), 667 (m), 650 (m), 619 (s), 602 (s), 575 (s).

6-(2,3-Dihydro-1*H*-indol-1-yl)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (2p). The product was prepared according to the **Method A**, starting from 0.7 g of 6-chloro-1,3-dimethyluracil and 1.051 g of indoline. Yield 0.714 g (69%), white solid, mp 148-149 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.15 (t, 2H, ^3J = 7.93 Hz, CH_2-3'), 3.36 (s, 3H, CH_3), 3.40 (s, 3H, CH_3), 3.77 (t, 2H, ^3J = 7.93 Hz, CH_2-2'), 5.56 (s, 1H, H-5), 6.67 (d, 1H, ^3J = 7.93 Hz, H-7'), 6.89-6.98 (m, 1H, H-5'), 7.09-7.18 (m, 1H, H-6'), 7.23 (d, 1H, ^3J = 7.37 Hz, H-4'). ^{13}C NMR (75.48 MHz, $CDCl_3$): δ = 28.2 (CH_3), 29.1 (CH_2-3'), 33.6 (CH_3), 54.3 (CH_2-2'), 89.7 (CH-5), 112.8 (CH_{Ar}), 122.6 (CH_{Ar}), 125.7 (CH_{Ar}), 127.8 (CH_{Ar}), 131.9, 145.6, 153.2, 154.5, 163.6. MS (GC, 70 eV): *m/z* (%) = 258 ([M+H]$^+$, 15), 257 ([M]$^+$, 100), 256 (19), 119 (50), 118 (31), 117 (10), 82 (47). HRMS (EI): Calcd. for $C_{14}H_{15}N_3O_2$ [M]$^+$: 257.11588, found: 257.11583. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3049 (w), 2949 (w), 2860 (w), 1695 (s), 1651 (s), 1635 (s), 1614 (s), 1605 (s), 1591 (s), 1504 (w), 1485 (s), 1435 (s), 1381 (m), 1362 (m), 1354 (m), 1336 (m), 1302 (m), 1292 (m), 1265 (s), 1230 (m), 1217 (m), 1169 (m), 1159 (w), 1149 (w), 1093 (w), 1065 (w), 1047 (w), 1024 (w), 989 (m), 937 (w), 924 (w), 879 (w), 868 (w), 827 (w), 806 (w), 797 (s), 756 (s), 748 (s), 725 (m), 716 (m), 694 (m), 683 (m), 671 (m), 604 (w), 554 (m), 538 (m).

6-(3,4-Dihydroquinolin-1(2*H*)-yl)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (2q). The product was

prepared according to the **Method C**, using a solution of 1,2,3,4-tetrahydroquinoline (1.846 g) in dry THF (22 mL), 5.5 mL of *n*-butyl lithium (2.5 M solution in hexane) and a solution of 6-chloro-1,3-dimethyluracil (1.1 g) in dry THF (22 mL). Yield 1.494 g (87%), brownish oil. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 2.00-2.13 (m, 2H, CH_2-3'), 2.86 (t, 2H, ^{3}J = 6.71 Hz, CH_2-4'), 3.25 (s, 3H, CH_3), 3.37 (s, 3H, CH_3), 3.46 (t, 2H, ^{3}J = 5.86 Hz, CH_2-2'), 5.51 (s, 1H, H-5), 6.55 (d, 1H, ^{3}J = 8.12 Hz, H-8'), 6.86-6.96 (m, 1H, H-6'), 7.01-7.09 (m, 1H, H-7'), 7.11 (d, 1H, ^{3}J = 7.74 Hz, H-5'). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 22.5 (CH_2), 26.8 (CH_2), 28.3 (CH_3), 32.5 (CH_3), 49.8 (CH_2-2'), 95.3 (CH-5), 117.7 (CH_{Ar}), 122.3 (CH_{Ar}), 126.5, 127.3 (CH_{Ar}), 130.0 (CH_{Ar}), 141.3, 153.1, 156.3, 163.6. MS (GC, 70 eV): *m/z* (%) = 272 ($[M+H]^+$, 16), 271 ($[M]^+$, 100), 270 (69), 254 (34), 186 (12), 185 (55), 133 (19), 132 (35), 130 (21), 117 (27), 82 (58), 77 (11). HRMS (ESI): Calcd. for $C_{15}H_{18}N_3O_2$ $[M+H]^+$: 272.13935, found: 272.13934. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2932 (m), 2859 (w), 1697 (m), 1644 (s), 1615 (s), 1598 (s), 1587 (s), 1491 (s), 1425 (s), 1389 (m), 1368 (m), 1296 (m), 1253 (m), 1229 (m), 1192 (m), 1171 (m), 1114 (w), 1072 (w), 1020 (w), 996 (m), 941 (w), 910 (w), 888 (w), 875 (w), 850 (w), 806 (m), 749 (s), 716 (m), 700 (m), 690 (m), 654 (w), 645 (w), 596 (w), 547 (m).

2.2 Synthesis of 5-(polyfluoroacyl)-6-amino-1,3-dialkyl-pyrimidine-2,4(1*H*,3*H*)-diones

General procedure for the synthesis of 5-(polyfluoroacyl)-6-amino-1,3-dialkyl-pyrimidine-2,4(1*H*,3*H*)-diones 3a-w and 5a-e. To a solution of 6-amino-1,3-dialkyl-pyrimidine-2,4(1*H*,3*H*)-dione **2** (0.4 g) in 4 mL of dry dioxane was added dry pyridine (1.2 eq) and corresponding anhydride (or chloroanhydride, if R_F = *n*-C_3F_7) of polyfluorocarboxylic acid (2 eq). Then the solution was allowed to stand at r.t. overnight. The next day the solvent was evaporated and the residue was dried in high vacuum at 100 °C. Then the crude product was triturated with water, filtered off by suction and dried in a high vacuum.

6-Anilino-1,3-dimethyl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione (3a). The product was prepared according to the general procedure from 0.4 g of 6-anilino-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.164 g of pyridine and 0.727 g of trifluoroacetic anhydride in 4 mL of dry dioxane. Yield 0.524 g (93%), white solid, mp 143-145 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.09 (s, 3H, CH_3), 3.23 (s, 3H, CH_3), 7.22-7.40 (m, 3H, CH_{Ph}), 7.40-7.51 (m, 2H, ^{3}J = 7.27 Hz, $CH_{m\text{-}Ph}$), 11.10 (br s, 1H, NH). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –71.4 (s, CF_3). ^{13}C NMR (75.47 MHz, DMSO-d_6): δ = 28.6 (CH_3), 36.1 (CH_3), 93.3, 117.7 (q, $^{1}J_{(C\text{-}F)}$ = 288.6 Hz, CF_3), 124.2 (CH), 127.1 (CH), 130.5 (CH), 139.4, 151.6, 159.0, 160.7, 179.0 (q, $^{2}J_{(C\text{-}F)}$ = 35.8 Hz, CO). MS (EI, 70 eV): *m/z* (%) = 328 ($[M+H]^+$, 10), 327 ($[M]^+$, 69), 309 (40), 259 (27), 258 (100), 230 (11), 201 (64), 197 (53), 133 (11), 92 (12), 77 (20), 69 (11). HRMS (ESI): Calcd. for $C_{14}H_{13}F_3N_3O_3$ $[M+H]^+$: 328.09035, found: 328.09031. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3057 (w), 2955 (w), 1726 (m), 1668 (s), 1651 (s), 1614 (s), 1585 (s), 1514 (s), 1495 (s), 1446 (s), 1416 (m), 1387 (m), 1325 (m), 1308 (s), 1284 (m), 1240 (m), 1203 (s), 1173 (s), 1155 (s), 1084 (s), 1053 (m), 1028

(m), 1014 (m), 995 (s), 926 (m), 872 (w), 860 (w), 845 (w), 824 (m), 795 (s), 760 (s), 748 (s), 719 (m), 696 (s), 687 (s), 662 (s), 615 (m), 594 (m), 567 (m), 530 (s).

6-Anilino-5-(2,2,3,3,4,4,4-heptafluorobutanoyl)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3b). The product was prepared according to the general procedure from 0.4 g of 6-anilino-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.164 g of pyridine and 0.804 g of heptafluorobutyryl chloride in 4 mL of dry dioxane. Yield 0.712 g (96%), white solid, mp 127-128 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.08 (s, 3H, CH_3), 3.23 (s, 3H, CH_3), 7.27 (t, 1H, ^{3}J = 7.27 Hz, $CH_{p\text{-Ph}}$), 7.19 (d, 2H, ^{3}J = 7.55 Hz, $CH_{o\text{-Ph}}$), 7.40-7.49 (m, 2H, $CH_{m\text{-Ph}}$), 10.84 (br s, 1H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.7 (CH_3), 36.2 (CH_3), 94.7 (C-5), 124.1 (CH), 127.0 (CH), 130.5 (CH), 139.3, 151.7, 158.5, 160.7, 181.9 (t, $^{2}J_{(C\text{-}F)}$ = 26.6 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –121.2 (s, CF_2), –111.0 (q, J = 10.22 Hz, CF_2), –79.9 (t, J = 9.70 Hz, CF_3). MS (GC, 70 eV): *m/z* (%) = 427 ([M]$^{+}$, 7.8), 259 (16), 258 (100), 201 (30), 92 (11), 77 (12). HRMS (EI): Calcd. for $C_{16}H_{12}O_3N_3F_7$ [M]$^{+}$: 427.07614, found: 427.076505. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3014 (w), 2956 (w), 1720 (m), 1666 (s), 1624 (s), 1576 (s), 1495 (s), 1444 (s), 1408 (m), 1379 (m), 1336 (s), 1311 (m), 1282 (s), 1213 (s), 1176 (s), 1147 (s), 1122 (s), 1088 (m), 1078 (m), 1065 (m), 1028 (m), 1005 (m), 951 (m), 932 (m), 914 (m), 893 (s), 860 (m), 808 (m), 789 (s), 777 (s), 754 (s), 721 (s), 694 (s), 685 (s), 654 (s), 615 (m), 594 (s), 567 (m), 528 (s).

6-[(2,4-Dimethylphenyl)amino]-1,3-dimethyl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione (3c). The product was prepared according to the general procedure from 0.39 g of 6-[(2,4-dimethylphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.143 g of pyridine and 0.632 g of trifluoroacetic anhydride in 3.9 mL of dry dioxane. Yield 0.481 g (90%), white solid, mp 136-138 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 2.31 (s, 3H, Ar-CH_3), 2.32 (s, 3H, Ar-CH_3), 2.96 (s, 3H, N-CH_3), 3.22 (s, 3H, N-CH_3), 7.10 (d, 1H, ^{3}J = 8.12 Hz, CH_{Ar}), 7.17-7.23 (m, 2H, CH_{Ar}), 11.43 (br s, 1H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 17.5 (Ar-CH_3), 20.4 (Ar-CH_3), 27.7 (N-CH_3), 35.2 (N-CH_3), 91.7 (C-5), 117.0 (q, $^{1}J_{(C\text{-}F)}$ = 287.8 Hz, CF_3), 124.9 (CH), 127.4 (CH), 131.7 (CH), 132.0, 134.0, 136.8, 150.5, 159.1, 159.4, 177.6 (q, $^{2}J_{(C\text{-}F)}$ = 35.8 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –71.1 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 355 ([M]$^{+}$, 31), 287 (13), 286 (100), 229 (12), 128 (14), 120 (11), 69 (13). HRMS (EI): Calcd. for C16H16O3N3F3 [M]$^{+}$: 355.11383, found: 355.11345. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2962 (w), 2359 (w), 1726 (m), 1668 (s), 1645 (m), 1614 (s), 1583 (s), 1514 (s), 1504 (s), 1454 (s), 1441 (s), 1387 (m), 1379 (m), 1317 (s), 1281 (m), 1246 (m), 1228 (m), 1213 (s), 1196 (s), 1173 (s), 1155 (s), 1080 (s), 1057 (m), 1036 (m), 995 (s), 947 (m), 893 (m), 883 (w), 852 (m), 824 (m), 795 (s), 773 (m), 758 (s), 733 (s), 706 (m), 685 (m), 650 (m), 581 (m), 569 (m), 557 (m), 532 (m).

6-[(2,4-Dimethylphenyl)amino]-1,3-dimethyl-5-(2,2,3,3,3-pentafluoropropanoyl)pyrimidine-2,4(1*H*,3*H*)-dione (3d). The product was prepared according to the general procedure from 0.35 g of 6-[(2,4-dimethylphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.128 g of pyridine and 0.837 g

of pentafluoropropionic anhydride in 3.5 mL of dry dioxane. Yield 0.481 g (88%), yellowish solid, mp 193-195 °C. ^{1}H NMR (250.13 MHz, DMSO-d_6): δ = 2.30 (s, 3H, Ar-CH_3), 2.32 (s, 3H, Ar-CH_3), 2.91 (s, 3H, N-CH_3), 3.23 (s, 3H, N-CH_3), 7.10 (d, 1H, ^{3}J = 8.04 Hz, CH_{Ar}), 7.18-7.25 (m, 2H, CH_{Ar}), 11.42 (br s, 1H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 18.5 (CH_3), 21.4 (CH_3), 28.8 (CH_3), 36.4 (CH_3), 94.1 (C-5), 126.0 (CH), 128.4 (CH), 132.6 (CH), 133.0, 134.8, 137.8, 151.5, 160.2, 160.3, 181.0 (t, $^{2}J_{(C\text{-}F)}$ = 27.1 Hz, CO). ^{19}F NMR (235.33 MHz, DMSO-d_6): δ = –115.2 (s, CF_2), –78.5 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 405 ([M]$^{+}$, 65), 387 (18), 287 (27), 286 (100), 275 (14), 258 (17), 229 (24), 120 (11). HRMS (ESI): Calcd. for $C_{17}H_{17}F_5N_3O_3$ [M+H]$^{+}$: 406.11846, found: 406.11903. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2962 (w), 2929 (w), 2351 (w), 1724 (s), 1668 (s), 1614 (s), 1583 (s), 1516 (s), 1504 (s), 1454 (s), 1444 (s), 1385 (m), 1363 (s), 1315 (s), 1279 (m), 1225 (s), 1173 (s), 1140 (s), 1111 (s), 1061 (m), 1030 (m), 960 (s), 939 (s), 889 (m), 852 (m), 816 (s), 804 (m), 787 (s), 760 (s), 739 (s), 729 (s), 704 (m), 687 (s), 656 (m), 642 (s), 586 (m), 569 (m), 561 (m), 536 (m).

6-[(2,4-Dimethylphenyl)amino]-5-(2,2,3,3,4,4,4-heptafluorobutanoyl)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3e). The product was prepared according to the general procedure from 0.35 g of 6-[(2,4-dimethylphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.128 g of pyridine and 0.627 g of heptafluorobutyryl chloride in 3.5 mL of dry dioxane. Yield 0.535 g (87%), white solid, mp 130 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 2.31 (s, 3H, Ar-CH_3), 2.32 (s, 3H, Ar-CH_3), 2.95 (s, 3H, N-CH_3), 3.22 (s, 3H, N-CH_3), 7.10 (d, 1H, ^{3}J = 8.12 Hz, CH_{Ar}), 7.18-7.23 (m, 2H, CH_{Ar}), 11.14 (br s, 1H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 18.5 (CH_3), 21.4 (CH_3), 28.7 (CH_3), 36.2 (CH_3), 94.0 (C-5), 125.9 (CH), 128.4 (CH), 132.6 (CH), 133.0, 134.9, 137.7, 151.6, 159.7, 160.5, 181.6 (t, $^{2}J_{(C\text{-}F)}$ = 26.3 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –120.8 (s, CF_2), –110.3 (q, *J* = 169.62 Hz, CF_2), –79.8 (t, *J* = 9.70 Hz, CF_3). MS (GC, 70 eV): *m/z* (%) = 455 ([M]$^{+}$, 22), 287 (18), 286 (100), 258 (11), 229 (13). HRMS (EI): Calcd. for $C_{18}H_{16}O_3N_3F_7$ [M]$^{+}$: 455.10744, found: 455.107556. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2956 (w), 2928 (w), 2145 (w), 1724 (m), 1672 (s), 1606 (s), 1574 (s), 1502 (s), 1443 (s), 1406 (m), 1387 (m), 1333 (m), 1315 (s), 1282 (m), 1267 (m), 1254 (m), 1221 (s), 1207 (s), 1198 (s), 1165 (s), 1140 (s), 1120 (s), 1086 (m), 1066 (s), 1055 (s), 1039 (m), 1007 (m), 959 (m), 951 (m), 933 (s), 924 (s), 893 (m), 856 (m), 816 (s), 802 (m), 787 (s), 758 (s), 743 (s), 725 (s), 706 (m), 685 (s), 675 (s), 640 (s), 596 (m), 561 (m), 546 (m).

6-[(4-Ethylphenyl)amino]-1,3-dimethyl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione (3f). The product was prepared according to the general procedure from 0.3 g of 6-[(4-ethylphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.11 g of pyridine and 0.486 g of trifluoroacetic anhydride in 3 mL of dry dioxane. Yield 0.362 g (88%), grey solid, mp 141-143 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 1.21 (t, 3H, ^{3}J = 7.55 Hz, Et), 2.64 (q, 2H, ^{3}J = 7.55 Hz, Et), 3.06 (s, 3H, CH_3), 3.23 (s, 3H, CH_3), 7.26 (d, 2H, ^{3}J = 8.78 Hz, CH_{Ar}), 7.29 (d, 2H, ^{3}J = 8.78 Hz, CH_{Ar}), 11.22 (br s, 1H, NH). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –71.3 (s, CF_3). ^{13}C NMR (75.47 MHz, DMSO-d_6): δ = 16.4 ($CH_{3(Et)}$), 28.5

(CH_2), 28.6 (CH_3), 36.3 (CH_3), 93.1, 117.8 (q, $^1J_{(C-F)}$ = 288.5 Hz, CF_3), 124.4 (CH), 129.8 (CH), 136.8, 143.0, 151.6, 159.2, 160.6, 178.7 (q, $^2J_{(C-F)}$ = 35.8 Hz, CO). MS (EI, 70 eV): *m/z* (%) = 355 ($[M]^+$, 41), 337 (52), 327 (22), 322 (12), 309 (16), 287 (13), 286 (100), 272 (13), 259 (15), 258 (90), 229 (13), 225 (36), 201 (23), 197 (17), 128 (15), 91 (11), 82 (19), 77 (12), 66 (27), 65 (15), 39 (15). HRMS (ESI): Calcd. for $C_{16}H_{17}F_3N_3O_3$ $[M+H]^+$: 356.12165, found: 356.12154. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3045 (w), 2972 (w), 2879 (w), 1722 (s), 1666 (s), 1622 (s), 1589 (s), 1558 (m), 1539 (m), 1514 (s), 1506 (s), 1456 (s), 1446 (s), 1435 (s), 1414 (m), 1389 (m), 1373 (m), 1311 (s), 1282 (m), 1244 (m), 1236 (m), 1211 (s), 1182 (s), 1174 (s), 1155 (s), 1119 (m), 1086 (s), 1061 (m), 1020 (m), 995 (s), 957 (m), 874 (m), 837 (m), 791 (s), 760 (s), 733 (s), 721 (m), 687 (s), 654 (m), 633 (m), 584 (m), 554 (m), 542 (m), 532 (m).

5-[Chloro(difluoro)acetyl]-6-[(4-ethylphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3g). The product was prepared according to the general procedure from 0.3 g of 6-[(4-ethylphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.11 g of pyridine and 0.562 g of chlorodifluoroacetic anhydride in 3 mL of dry dioxane. Yield 0.417 g (97%), grey solid, mp 133-135 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 1.20 (t, 3H, ^3J = 7.55 Hz, Et), 2.63 (q, 2H, ^3J = 7.55 Hz, Et), 3.10 (s, 3H, CH_3), 3.22 (s, 3H, CH_3), 7.22 (d, 2H, ^3J = 8.50 Hz, CH_{Ar}), 7.28 (d, 2H, ^3J = 8.50 Hz, CH_{Ar}), 10.90 (br s, 1H, NH). ^{13}C NMR (125.77 MHz, DMSO-d_6): δ = 16.4 (CH_3), 28.5 (CH_2), 28.7 (CH_3), 35.9 (CH_3), 92.3 (C-5), 121.3 (t, $^1J_{(C-F)}$ = 302.0 Hz, $CClF_2$), 124.2 (CH), 129.8 (CH), 137.0, 142.8, 151.6, 158.9, 160.3, 180.8 (t, $^2J_{(C-F)}$ = 29.9 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –59.9 (s, $CClF_2$). MS (GC, 70 eV): *m/z* (%) = 371 ($[M]^+$, ^{35}Cl, 5.2), 320 (19), 319 (100), 305 (16), 304 (77), 247 (10), 207 (38), 192 (10), 82 (13). HRMS (ESI): Calcd. for $C_{16}H_{17}ClF_2N_3O_3$ $[M+H, {}^{35}Cl]^+$: 372.09210, found: 372.09257. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2962 (w), 2931 (w), 2874 (w), 1720 (m), 1660 (s), 1622 (s), 1574 (s), 1504 (s), 1452 (s), 1441 (s), 1404 (s), 1367 (s), 1311 (m), 1279 (s), 1254 (m), 1174 (s), 1134 (s), 1095 (m), 1070 (s), 1059 (m), 1005 (s), 953 (m), 930 (s), 914 (s), 870 (s), 841 (m), 825 (s), 804 (s), 793 (s), 773 (s), 756 (s), 743 (s), 716 (m), 669 (s), 646 (s), 625 (s), 567 (m), 534 (s).

6-[(4-Ethylphenyl)amino]-1,3-dimethyl-5-(2,2,3,3,3-pentafluoropropanoyl)pyrimidine-2,4(1*H*,3*H*)-dione (3h). The product was prepared according to the general procedure from 0.35 g of 6-[(4-ethylphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.128 g of pyridine and 0.837 g of pentafluoropropionic anhydride in 3.5 mL of dry dioxane. Yield 0.516 g (94%), greyish solid, mp 161-163 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 1.21 (t, 3H, ^3J = 7.59 Hz, Et), 2.64 (q, 2H, ^3J = 7.59 Hz, Et), 3.02 (s, 3H, CH_3), 3.23 (s, 3H, CH_3), 7.29 (s, 4H, CH_{Ar}), 11.23 (br s, 1H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 16.4 (CH_3), 28.5 (CH_2), 28.7 (CH_3), 36.7 (CH_3), 94.6 (C-5), 124.5 (CH), 129.7 (CH), 136.6, 143.1, 151.7, 159.2, 160.4, 181.1 (t, $^2J_{(C-F)}$ = 27.0 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –115.6 (s, CF_2), –78.7 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 405 ($[M]^+$, 41), 387 (16), 287 (30), 286 (100), 275 (13), 229 (25). HRMS (EI): Calcd. for $C_{17}H_{16}O_3N_3F_5$ $[M]^+$: 405.11063, found: 405.11084. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2966 (w), 2935 (w), 2874 (w), 1728 (m), 1670 (s), 1591 (s), 1576 (s), 1504 (s), 1454

(s), 1441 (s), 1408 (m), 1375 (s), 1315 (s), 1281 (s), 1254 (m), 1215 (s), 1176 (s), 1147 (s), 1117 (s), 1065 (m), 1030 (m), 1020 (m), 959 (s), 933 (s), 874 (m), 839 (m), 820 (m), 810 (s), 795 (s), 760 (s), 735 (s), 714 (m), 685 (s), 656 (m), 646 (s), 629 (s), 567 (m), 538 (m).

6-[(2-Methoxyphenyl)amino]-1,3-dimethyl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione (3i). The product was prepared according to the general procedure from 0.3 g of 6-[(2-methoxyphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.109 g of pyridine and 0.482 g of trifluoroacetic anhydride in 3 mL of dry dioxane. Yield 0.369 g (90%), greyish solid, mp 174-176 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.97 (s, 3H, CH_3), 3.23 (s, 3H, CH_3), 3.90 (s, 3H, OMe), 7.00-7.10 (m, 1H, CH_{Ar}), 7.21 (d, 1H, ^{3}J = 8.69 Hz, CH_{Ar}), 7.29-7.38 (m, 2H, CH_{Ar}), 11.51 (br s, 1H, NH). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –71.0 (s, CF_3). ^{13}C NMR (75.47 MHz, DMSO-d_6): δ = 28.7 (CH_3), 36.5 (CH_3), 56.9 (OMe), 93.2, 113.2 (CH), 118.0 (q, $^{1}J_{(C-F)}$ = 287.6 Hz, CF_3), 121.7 (CH), 126.0 (CH), 126.8, 129.2 (CH), 151.5, 152.8, 159.8, 160.3, 178.3 (q, $^{2}J_{(C-F)}$ = 35.9 Hz, CO). MS (EI, 70 eV): *m/z* (%) = 358 ($[M+H]^+$, 13), 357 ($[M]^+$, 100), 339 (21), 338 (11), 326 (15), 289 (13), 288 (96), 274 (11), 273 (86), 128 (12). HRMS (ESI): Calcd. for $C_{15}H_{15}F_3N_3O_4$ $[M+H]^+$: 358.10092, found: 358.10099. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2976 (w), 2841 (w), 1734 (m), 1714 (m), 1660 (s), 1622 (s), 1585 (s), 1520 (s), 1498 (s), 1464 (s), 1441 (s), 1417 (m), 1385 (m), 1327 (m), 1296 (s), 1269 (m), 1242 (m), 1232 (m), 1217 (s), 1207 (s), 1188 (s), 1174 (s), 1144 (s), 1115 (s), 1082 (s), 1049 (m), 1020 (s), 995 (s), 949 (m), 872 (w), 858 (w), 824 (m), 793 (s), 756 (s), 733 (s), 712 (m), 692 (m), 675 (m), 660 (s), 598 (m), 577 (m), 550 (m), 527 (s).

5-[Chloro(difluoro)acetyl]-6-[(2-methoxyphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3j). The product was prepared according to the general procedure from 0.3 g of 6-[(2-methoxyphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.109 g of pyridine and 0.558 g of chlorodifluoroacetic anhydride in 3 mL of dry dioxane. Yield 0.395 g (92%), greyish solid, mp 163-165 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.00 (s, 3H, CH_3), 3.23 (s, 3H, CH_3), 3.89 (s, 3H, OMe), 7.04 (dd, 1H, $^{3}J_1$ = 7.57 Hz, $^{3}J_2$ = 7.55 Hz, CH_{Ar}), 7.19 (d, 1H, ^{3}J = 8.67 Hz, CH_{Ar}), 7.29-7.38 (m, 2H, CH_{Ar}), 11.26 (br s, 1H, NH). ^{13}C NMR (125.77 MHz, DMSO-d_6): δ = 28.7 (CH_3), 36.4 (CH_3), 56.9 (CH_3), 92.4 (C-5), 113.2 (CH), 121.4 (t, $^{1}J_{(C-F)}$ = 301.3 Hz, $CClF_2$), 121.7 (CH), 125.9 (CH), 126.9, 129.0 (CH), 151.5, 152.8, 159.6, 160.1, 180.5 (t, $^{2}J_{(C-F)}$ = 29.8 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –59.7 (s, $CClF_2$). MS (GC, 70 eV): *m/z* (%) = 375 ($[M]^+$, ^{37}Cl, 5.5), 373 ($[M]^+$, ^{35}Cl, 18), 338 (10), 289 (16), 288 (100), 274 (11), 273 (79), 244 (10), 81 (17). HRMS (EI): Calcd. for $C_{15}H_{14}O_4N_3ClF_2$ [M, ^{37}Cl]$^+$: 373.06354, found: 373.063406. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3005 (w), 2953 (w), 2845 (w), 1724 (s), 1660 (s), 1628 (s), 1599 (s), 1576 (s), 1520 (s), 1497 (s), 1454 (s), 1443 (s), 1392 (s), 1362 (s), 1325 (m), 1290 (s), 1267 (s), 1232 (s), 1194 (m), 1171 (s), 1136 (s), 1115 (s), 1072 (s), 1045 (s), 1030 (s), 1005 (s), 978 (m), 935 (m), 920 (s), 866 (m), 851 (m), 800 (s), 775 (s), 748 (s), 717 (s), 685 (m), 665 (s), 656 (s), 619 (s), 590 (m), 571 (m), 552 (m).

5-(2,2,3,3,4,4,4-Heptafluorobutanoyl)-6-[(3-methoxyphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3m). The product was prepared according to the general procedure from 0.4 g of 6-[(3-methoxyphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.145 g of pyridine and 0.712 g of heptafluorobutyryl chloride in 4 mL of dry dioxane. Yield 0.658 g (94%), grey solid, mp 136-138 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.11 (s, 3H, CH_3), 3.23 (s, 3H, CH_3), 3.78 (s, 3H, OMe), 6.84 (d, 1H, ^{3}J = 8.31 Hz, CH_{Ar}), 6.89 (d, 1H, ^{3}J = 7.93 Hz, CH_{Ar}), 6.98 (s, 1H, H-2'), 7.33 (dd, 1H, $^{3}J_1$ = 8.31 Hz, $^{3}J_2$ = 7.93 Hz, H-5'), 10.78 (br s, 1H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.7 (CH_3), 36.0 (CH_3), 56.2 (CH_3), 94.8 (C-5), 109.5 (CH), 112.9 (CH), 116.1 (CH), 131.2 (CH), 140.5, 151.7, 158.3, 160.7, 161.1, 182.0 (t, $^{2}J_{(C-F)}$ = 26.4 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –121.1 (s, CF_2), –110.8 (q, J = 10.22 Hz, CF_2), –80.0 (t, J = 9.70 Hz, CF_3). MS (GC, 70 eV): *m/z* (%) = 440 (11), 439 (55), 411 (11), 328 (15), 327 (100), 270 (14). HRMS (ESI): Calcd. for C17H15F7N3O4 $[M+H]^+$: 458.0945, found: 458.0943. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2949 (w), 2847 (w), 2046 (w), 1795 (w), 1716 (m), 1662 (s), 1628 (s), 1605 (m), 1587 (s), 1564 (s), 1495 (s), 1441 (s), 1408 (m), 1377 (m), 1335 (s), 1317 (m), 1294 (s), 1259 (m), 1211 (s), 1182 (s), 1144 (s), 1122 (s), 1088 (s), 1051 (s), 1012 (m), 960 (m), 920 (w), 897 (m), 876 (s), 820 (m), 797 (m), 781 (s), 756 (s), 729 (s), 689 (s), 671 (s), 650 (s), 594 (s), 575 (m), 548 (m).

1,3-Dimethyl-5-(trifluoroacetyl)-6-{[3-(trifluoromethyl)phenyl]amino}pyrimidine-2,4(1*H*,3*H*)-dione (3n). The product was prepared according to the general procedure from 0.4 g of **2f**, 0.127 g of pyridine and 0.561 g of trifluoroacetic anhydride in 4 mL of dry dioxane. Yield 0.523 g (99%), pinkish amorphous solid. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.24 (s, 3H, CH_3), 3.27 (s, 3H, CH_3), 7.50-7.58 (m, 2H, CH_{Ar}), 7.61-7.71 (m, 2H, CH_{Ar}), 10.40 (br s, 1H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.6 (CH_3), 34.7 (CH_3), 93.3 (C-5), 117.0 (q, $^{1}J_{(C-F)}$ = 289.4 Hz, CF_3), 119.7 (CH), 122.7 (CH), 124.7 (q, $^{1}J_{(C-F)}$ = 272.5 Hz, CF_3), 127.5 (CH), 131.2 (q, $^{2}J_{(C-F)}$ = 32.1 Hz), 131.7 (CH), 141.2, 151.6, 158.3, 161.0, 179.9 (q, $^{2}J_{(C-F)}$ = 36.1 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –72.4 (s, CF_3), –61.4 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 395 ($[M]^+$, 27), 377 (26), 327 (27), 326 (100), 269 (39), 265 (57), 201 (32), 145 (15), 128 (12), 82 (12), 69 (11). HRMS (EI): Calcd. for $C_{15}H_{11}O_3N_3F_6$ $[M]^+$: 395.06991, found: 395.07016. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3078 (w), 2964 (w), 1790 (w), 1722 (m), 1668 (s), 1585 (s), 1514 (m), 1504 (s), 1495 (s), 1441 (s), 1402 (m), 1371 (m), 1327 (s), 1240 (m), 1159 (s), 1124 (s), 1068 (s), 995 (s), 976 (s), 924 (m), 906 (m), 887 (m), 858 (w), 822 (m), 795 (s), 756 (s), 733 (m), 725 (s), 698 (s), 658 (s), 635 (m), 594 (m), 565 (m), 532 (m).

1,3-Dimethyl-6-[(4-nitrophenyl)amino]-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione (3o). The product was prepared according to the general procedure from 0.336 g of 1,3-dimethyl-6-[(4-nitrophenyl)amino]pyrimidine-2,4(1*H*,3*H*)-dione, 0.115 g of pyridine and 0.511 g of trifluoroacetic anhydride in 3.4 mL of dry dioxane. Yield 0.359 g (79%), brownish solid, mp 256-258 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.25 (s, 3H, CH_3), 3.27 (s, 3H, CH_3), 7.39 (d, 2H, ^{3}J = 9.26 Hz, CH-2', CH-6'), 8.25 (d, 2H, ^{3}J = 9.26 Hz, CH-3', CH-5'), 10.40 (br s, 1H, NH). ^{13}C NMR (75.48 MHz, DMSO-

d$_6$): δ = 28.7 (CH_3), 34.6 (CH_3), 96.5 (C-5), 116.9 (q, $^1J_{(C-F)}$ = 290.1 Hz, CF_3), 121.4 (CH_{Ar}), 126.3 (CH_{Ar}), 143.8, 147.4, 151.6, 157.1, 160.9, 180.3 (q, $^2J_{(C-F)}$ = 36.3 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-*d*$_6$): δ = –72.3 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 277 (14), 276 (100), 275 (45), 218 (17), 191 (10), 190 (42), 174 (30), 163 (16), 162 (23), 149 (12), 147 (26), 145 (11), 144 (18), 131 (12), 127 (62), 116 (10), 90 (41), 89 (16), 82 (49), 76 (20), 75 (12), 63 (21), 55 (38), 56 (16), 50 (14), 42 (15). HRMS (ESI): Calcd. for $C_{14}H_{10}F_3N_4O_5$ $[M+H]^+$: 371.06123, found: 371.06123. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3247 (m), 3078 (w), 2913 (w), 1711 (w), 1691 (w), 1660 (w), 1640 (w), 1633 (m), 1616 (m), 1602 (m), 1578 (m), 1539 (s), 1528 (s), 1520 (s), 1479 (m), 1471 (s), 1434 (m), 1383 (w), 1371 (w), 1341 (s), 1292 (s), 1265 (m), 1194 (s), 1176 (m), 1143 (m), 1107 (m), 1183 (w), 1064 (w), 1008 (w), 992 (w), 916 (w), 883 (w), 859 (m), 838 (m), 821 (m), 791 (s), 759 (s), 736 (s), 716 (s), 645 (s), 667 (m), 632 (s), 578 (m), 537 (s).

6-[(4-Bromophenyl)amino]-1,3-dimethyl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione (3p). The product was prepared according to the general procedure from 1.2 g of 6-[(4-bromophenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.367 g of pyridine and 1.625 g of trifluoroacetic anhydride in 12 mL of dry dioxane. Yield 94%, violet solid, mp 186 °C. ^{1}H NMR (300.13 MHz, DMSO-*d*$_6$): δ = 3.15 (s, 3H, CH_3), 3.23 (s, 3H, CH_3), 7.27 (d, 2H, ^3J = 8.88 Hz, CH-2', CH-6'), 7.62 (d, 2H, ^3J = 8.88 Hz, CH-3', CH-5'), 10.75 (br s, 1H, NH). ^{13}C NMR (62.90 MHz, DMSO-*d*$_6$): δ = 28.6 (CH_3), 35.7 (CH_3), 93.5 (C-5), 117.4 (q, $^1J_{(C-F)}$ = 289.0 Hz, CF_3), 119.1, 125.9 (CH_{Ar}), 133.3 (CH_{Ar}), 139.1, 151.6, 158.6, 160.7, 179.2 (q, $^2J_{(C-F)}$ = 35.9 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-*d*$_6$): δ = –71.7 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 407 ($[M]^+$, ^{81}Br, 40), 405 ($[M]^+$, ^{79}Br, 40), 389 (33), 387 (40), 339 (15), 338 (97), 337 (16), 336 (100), 321 (18), 319 (20), 291 (12), 281 (34), 279 (27), 277 (43), 275 (42), 257 (19), 229 (16), 224 (11), 223 (10), 211 (10), 209 (21), 208 (15), 207 (43), 178 (15), 172 (23), 171 (13), 170 (16), 157 (12), 155 (13), 145 (15), 128 (32), 127 (13), 91 (12), 82 (25), 81 (15), 80 (11), 76 (14), 75 (15), 69 (23), 63 (13), 60 (12), 44 (13), 32 (35). HRMS (ESI): Calcd. for $C_{14}H_{12}BrF_3N_3O_3$ $[M+H, ^{79}Br]^+$: 406.00087, found: 406.00136. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3293 (w), 3191 (w), 3099 (w), 2962 (w), 1766 (w), 1722 (m), 1672 (s), 1639 (s), 1568 (s), 1503 (s), 1490 (s), 1454 (s), 1443 (s), 1384 (m), 1319 (m), 1301 (m), 1278 (m), 1244 (m), 1217 (s), 1193 (s), 1176 (s), 1151 (s), 1088 (m), 1071 (s), 1054 (m), 1015 (m), 998 (s), 960 (m), 941 (m), 871 (m), 825 (s), 814 (s), 796 (s), 783 (s), 755 (s), 733 (s), 718 (s), 681 (s), 671 (s), 628 (m), 608 (m), 575 (s), 529 (m).

6-[(4-Ethoxyphenyl)amino]-1,3-dimethyl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione (3q). The product was prepared according to the general procedure from 0.37 g of 6-[(4-ethoxyphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.127 g of pyridine and 0.565 g of trifluoroacetic anhydride in 3.7 mL of dry dioxane. Yield 0.416 g (82%), brownish solid, mp 119-121 °C. ^{1}H NMR (300.13 MHz, DMSO-*d*$_6$): δ = 1.36 (t, 3H, ^3J = 6.99 Hz, EtO), 3.03 (s, 3H, CH_3), 3.22 (s, 3H, CH_3), 4.07 (q, 2H, ^3J = 6.99 Hz, EtO), 7.00 (d, 2H, ^3J = 8.88 Hz, CH_{Ar}), 7.29 (d, 2H, ^3J = 8.88 Hz, CH_{Ar}), 11.34 (br s, 1H, NH). ^{13}C NMR (125.77 MHz, DMSO-*d*$_6$): δ = 15.4 ($CH_{3(EtO)}$), 28.6 (CH_3), 36.3 (CH_3), 64.3 ($CH_{2(EtO)}$), 92.7 (C-

5), 116.1 (CH), 117.9 (q, $^{1}J_{(C\text{-}F)}$ = 287.9 Hz, CF_3), 126.3 (CH), 131.5, 151.7, 157.9, 159.4, 160.6, 178.4 (q, $^{2}J_{(C\text{-}F)}$ = 35.7 Hz, CO). MS (GC, 70 eV): *m/z* (%) = 371 ($[M]^+$, 11), 353 (10), 276 (21), 275 (100), 274 (19), 247 (10), 246 (73), 189 (16), 162 (10), 161 (14), 148 (20), 147 (22), 134 (15), 133 (15), 132 (17), 82 (24). HRMS (EI): Calcd. for C16H16O4N3F3 $[M]^+$: 371.10874, found: 371.10840. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2982 (w), 1722 (m), 1668 (s), 1614 (s), 1576 (s), 1504 (s), 1485 (s), 1454 (s), 1441 (s), 1408 (m), 1389 (m), 1315 (s), 1304 (m), 1281 (m), 1257 (s), 1242 (s), 1211 (s), 1188 (s), 1169 (s), 1151 (s), 1113 (s), 1080 (s), 1045 (s), 995 (s), 957 (m), 932 (m), 922 (m), 874 (m), 833 (s), 824 (m), 795 (s), 758 (s), 737 (s), 721 (m), 689 (s), 656 (s), 633 (m), 586 (m), 567 (s), 534 (m).

5-(Difluoroacetyl)-6-[(4-ethoxyphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (3r). The product was prepared according to the general procedure from 0.04 g of 6-[(4-ethoxyphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione, 0.14 g of pyridine and 0.506 g of difluoroacetic anhydride in 4 mL of dry dioxane. Yield 0.508 g (99%), brownish solid, mp 144-146 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 1.37 (t, 3H, ^{3}J = 6.90 Hz, EtO), 2.91 (s, 3H, CH_3), 3.24 (s, 3H, CH_3), 4.08 (q, 2H, ^{3}J = 6.90 Hz, EtO), 7.03 (d, 2H, ^{3}J = 8.88 Hz, CH_{Ar}), 7.17 (t, 1H, $^{2}J_{(H\text{-}F)}$ = 54.01 Hz, CHF_2), 7.35 (d, 2H, ^{3}J = 8.88 Hz, CH_{Ar}), 12.54 (br s, 1H, NH). ^{13}C NMR (75.48 MHz, DMSO-d_6): δ = 15.5 ($CH_{3(EtO)}$), 28.7 (CH_3), 37.1 (CH_3), 64.3 ($CH_{2(EtO)}$), 94.0 (C-5), 109.2 (t, $^{1}J_{(C\text{-}F)}$ = 242.3 Hz, CHF_2), 116.1 (CH_{Ar}), 126.6 (CH_{Ar}), 131.0, 151.6, 158.1, 159.8, 162.0, 185.5 (t, $^{2}J_{(C\text{-}F)}$ = 23.8 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –125.7 (s, CHF_2). MS (EI, 70 eV): *m/z* (%) = 354 ($[M+H]^+$, 21), 353 ($[M]^+$, 92), 333 (21), 304 (56), 303 (23), 302 (100), 275 (21), 274 (86), 245 (20), 217 (19), 182 (29), 160 (15), 108 (12), 82 (19), 81 (10). HRMS (EI): Calcd. for $C_{16}H_{17}F_2N_3O_4$ $[M]^+$: 353.11816, found: 353.11822. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3334 (w), 3080 (w), 2977 (w), 1724 (w), 1651 (m), 1592 (s), 1582 (s), 1549 (w), 1510 (s), 1445 (s), 1396 (w), 1319 (w), 1319 (w), 1305 (m), 1291 (w), 1240 (s), 1189 (w), 1176 (w), 1142 (m), 1116 (m), 1080 (m), 1043 (s), 1004 (s), 943 (w), 918 (w), 899 (m), 867 (m), 844 (m), 818 (m), 807 (s), 777 (s), 769 (s), 760 (s), 751 (s), 712 (w), 694 (m), 666 (m), 628 (w), 579 (m), 556 (m), 534 (m).

6-[(4-Methoxyphenyl)amino]-5-(2,2,3,3,3-pentafluoropropanoyl)-1,3-dipropylpyrimidine-2,4(1*H*,3*H*)-dione (3t). The product was prepared according to the general procedure from 0.35 g of **2j**, 0.105 g of pyridine and 0.684 g of pentafluoropropionic anhydride in 3.5 mL of dry dioxane. Yield 0.439 g (86%), pinkish solid, mp 85-87 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 0.72 (t, 3H, ^{3}J = 7.37 Hz, CH_3), 0.91 (t, 3H, ^{3}J = 7.46 Hz, CH_3), 1.42-1.72 (m, 4H, CH_2), 3.70-3.89 (m, 7H, CH_2, MeO), 7.00 (d, 2H, ^{3}J = 8.87 Hz, CH_{Ar}), 7.29 (d, 2H, ^{3}J = 8.87 Hz, CH_{Ar}), 10.61 (br s, 1H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 11.5 (CH_3), 12.0 (CH_3), 21.3 (CH_2), 21.4 (CH_2), 43.3 (CH_2), 47.2 (CH_2), 56.3 (MeO), 93.3 (C-5), 115.7 (CH_{Ar}), 126.4 (CH_{Ar}), 131.8, 151.2, 158.0, 158.8, 160.2, 181.6 (t, $^{2}J_{(C\text{-}F)}$ = 26.8 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –116.0 (s, CF_2), –78.7 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 464 ($[M+H]^+$, 15), 463 ($[M]^+$, 85), 445 (15), 403 (18), 345 (20), 344 (100), 302 (24), 260 (56), 243 (14), 214 (12), 123 (18), 43 (16), 41 (11). HRMS (ESI): Calcd. for $C_{20}H_{23}F_5N_3O_4$ $[M+H]^+$: 464.16032, found:

464.16109. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2964 (w), 2877 (w), 1716 (m), 1670 (s), 1593 (s), 1504 (s), 1443 (s), 1416 (s), 1385 (s), 1360 (m), 1329 (m), 1300 (s), 1279 (s), 1246 (s), 1213 (s), 1184 (s), 1171 (s), 1144 (s), 1109 (s), 1086 (m), 1061 (m), 1032 (s), 962 (s), 953 (s), 932 (s), 910 (m), 870 (m), 845 (m), 831 (s), 808 (m), 797 (s), 775 (s), 750 (s), 729 (s), 687 (s), 654 (m), 638 (s), 629 (s), 548 (m).

6,6'-[Biphenyl-4,4'-diyldi(imino)]bis[1,3-dimethyl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione] (3u). The product was prepared from 0.25 g of **72k**, 0.103 g of pyridine and 0.456 g of trifluoroacetic anhydride in 5 mL of dry dioxane according to the general procedure, except that the synthesis was carried out in a pressure tube at 80 °C for 3 h. Yield 0.329 g (93%), beige solid, mp 246 °C (dec.). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.15 (s, 6H, CH_3), 3.24 (s, 6H, CH_3), 7.42 (d, 4H, ^{3}J = 8.60 Hz, CH_{Ar}), 7.79 (d, 4H, ^{3}J = 8.60 Hz, CH_{Ar}), 11.07 (br s, 2H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.7 (CH_3), 36.2 (CH_3), 93.6 (C-5, C-5'), 117.6 (q, $^{1}J_{(C-F)}$ = 286.2 Hz, CF_3), 124.4 (CH), 128.5 (CH), 137.4, 138.9, 151.7, 158.8, 160.7, 179.0 (q, $^{2}J_{(C-F)}$ = 35.8 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –71.4 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 652 ($[M]^+$, 3.6), 634 (15), 617 (31), 616 (100), 565 (15), 504 (26), 496 (12). HRMS (EI): Calcd. for $C_{28}H_{22}O_6N_6F_6$ $[M]^+$: 652.14995, found: 652.14898. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2958 (w), 2359 (w), 1730 (m), 1674 (s), 1605 (s), 1587 (s), 1514 (s), 1498 (s), 1441 (s), 1404 (m), 1387 (m), 1335 (m), 1298 (m), 1286 (m), 1267 (m), 1238 (m), 1209 (s), 1194 (s), 1163 (s), 1082 (s), 995 (s), 872 (m), 825 (s), 797 (s), 756 (s), 727 (m), 708 (m), 694 (m), 667 (m), 640 (m), 594 (m), 571 (m), 534 (m).

6,6'-[Methylenebis(4,1-phenyleneimino)]bis[1,3-dimethyl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione] (3v). The product was prepared according to the general procedure from 0.333 g of **2l**, 0.133 g of pyridine and 0.59 g of trifluoroacetic anhydride in 6.6 mL of dry dioxane. Yield 0.458 g (98%), beige solid, mp 129-131 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.07 (s, 6H, CH_3), 3.22 (s, 6H, CH_3), 3.98 (s, 2H, CH_2), 7.26 (d, 4H, ^{3}J = 8.69 Hz, CH_{Ar}), 7.29 (d, 4H, ^{3}J = 8.69 Hz, CH_{Ar}), 11.05 (br s, 2H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.6 (CH_3), 36.0 (CH_3), 40.7 (CH_2), 93.0 (C-5, C-5'), 120.3 (q, $^{1}J_{(C-F)}$ = 288.5 Hz, CF_3), 124.4 (CH), 130.8 (CH), 137.4, 140.1, 151.6, 159.0, 160.7, 178.9 (q, $^{2}J_{(C-F)}$ = 35.5 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –71.4 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 631 (38), 630 (100), 553 (11), 552 (35), 518 (13), 498 (18), 203 (12). HRMS (ESI): Calcd. for $C_{29}H_{25}F_6N_6O_6$ $[M+H]^+$: 667.17343, found: 667.17425. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2962 (w), 1724 (m), 1668 (s), 1593 (s), 1512 (s), 1506 (s), 1454 (s), 1443 (s), 1435 (s), 1387 (m), 1309 (m), 1284 (s), 1242 (m), 1209 (s), 1186 (s), 1149 (s), 1082 (s), 1020 (m), 995 (s), 926 (m), 879 (m), 824 (m), 816 (m), 795 (s), 756 (s), 725 (m), 710 (m), 694 (m), 662 (m), 631 (m), 579 (m), 561 (m), 534 (m).

1,3-Dimethyl-6-(1-naphthylamino)-5-(2,2,3,3,3-pentafluoropropanoyl)pyrimidine-2,4(1*H*,3*H*)-dione (3w). The product was prepared according to the general procedure from 0.341 g of 1,3-dimethyl-6-(1-naphthylamino)pyrimidine-2,4(1*H*,3*H*)-dione, 0.105 g of pyridine and 0.413 g of pentafluoropropionic

anhydride in 3.4 mL of dry dioxane. Yield 0.443 g (86%), yellowish solid, mp 156 °C (dec.). ^{1}H NMR (250.13 MHz, DMSO-d_6): δ = 2.90 (s, 3H, CH_3), 3.26 (s, 3H, CH_3), 7.53-7.63 (m, 2H, CH_{Ar}), 7.64-7.78 (m, 2H, CH_{Ar}), 7.93-8.03 (m, 1H, CH_{Ar}), 8.08 (d, 1H, ^{3}J = 6.94 Hz, CH_{Ar}), 8.15 (d, 1H, ^{3}J = 8.19 Hz, CH_{Ar}), 11.80 (br s, 1H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.8 (CH_3), 36.2 (CH_3), 94.8 (C-5), 123.0 (CH), 123.4 (CH), 126.6 (CH), 128.0 (CH), 128.4 (CH), 128.5 (CH), 128.5, 129.4 (CH), 134.5, 134.8, 151.5, 160.3, 160.7, 181.5 (t, $^{2}J_{(C\text{-}F)}$ = 27.1 Hz, CO). ^{19}F NMR (235.33 MHz, DMSO-d_6): δ = –115.2 (s, CF_2), –78.5 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 428 ($[M+H]^+$, 13), 427 ($[M]^+$, 77), 409 (49), 309 (18), 308 (100), 297 (25), 280 (40), 251 (18), 195 (15), 127 (11), 115 (13). HRMS (ESI): Calcd. for $C_{19}H_{15}F_5N_3O_3$ $[M+H]^+$: 428.10281, found: 428.10233. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3018 (w), 2962 (w), 1728 (m), 1674 (s), 1588 (s), 1574 (s), 1558 (m), 1538 (m), 1515 (s), 1506 (s), 1455 (s), 1435 (s), 1399 (m), 1385 (m), 1368 (m), 1331 (m), 1305 (m), 1283 (m), 1232 (s), 1174 (s), 1139 (s), 1112 (s), 1063 (m), 1032 (m), 1013 (w), 984 (w), 959 (s), 938 (m), 907 (w), 883 (w), 861 (w), 824 (w), 804 (m), 783 (s), 770 (s), 758 (s), 740 (m), 731 (s), 712 (s), 685 (m), 647 (s), 593 (m), 559 (m), 531 (m).

6-(2,3-Dihydro-1*H*-indol-1-yl)-1,3-dimethyl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione (5a). The product was prepared according to the general procedure from 4.085 g of **89a**, 1.507 g of pyridine and 6.669 g of trifluoroacetic anhydride in 41 mL of dry dioxane. Yield 5.428 g (97%), yellow solid, mp 199 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.07-3.33 (m, 2H, CH_2-3'), 3.26 (s, 3H, CH_3), 3.35 (s, 3H, CH_3), 3.72-3.84 (m, 1H, CH_2-2'a), 3.91-4.04 (m, 1H, CH_2-2'b), 6.80 (d, 1H, ^{3}J = 7.75 Hz, H-7'), 6.88-6.97 (m, 1H, CH_{Ar}), 7.05-7.15 (m, 1H, CH_{Ar}), 7.30 (d, 1H, ^{3}J = 6.99 Hz, H-4'). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.6 (CH_3), 29.9 (CH_2-3'), 35.0 (CH_3), 54.8 (CH_2-2'), 99.3 (C-5), 112.6 (CH_{Ar}), 116.2 (q, $^{1}J_{(C\text{-}F)}$ = 290.8 Hz, CF_3), 123.4 (CH_{Ar}), 126.4 (CH_{Ar}), 128.4 (CH_{Ar}), 133.6, 146.0, 152.2, 159.1, 161.6, 181.9 (q, $^{2}J_{(C\text{-}F)}$ = 36.7 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –73.3 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 353 ($[M]^+$, 24), 285 (18), 284 (100), 178 (18), 167 (14), 128 (31), 118 (31), 110 (11). HRMS (ESI): Calcd. for $C_{16}H_{15}F_3N_3O_3$ $[M+H]^+$: 354.10600, found: 354.10633. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3057 (w), 2963 (w), 1722 (w), 1696 (m), 1645 (s), 1549 (m), 1483 (s), 1434 (s), 1401 (s), 1363 (m), 1331 (w), 1303 (w), 1265 (w), 1236 (w), 1229 (w), 1191 (s), 1156 (m), 1141 (s), 1096 (w), 1082 (w), 1045 (w), 1033 (w), 1017 (w), 986 (m), 968 (s), 940 (w), 873 (w), 861 (w), 833 (w), 819 (w), 797 (w), 785 (w), 753 (s), 713 (m), 704 (m), 686 (m), 608 (w), 581 (w), 561 (m), 549 (w), 534 (w).

6-(3,4-Dihydroquinolin-1(2*H*)-yl)-5-(2,2,3,3,4,4,4-heptafluorobutanoyl)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (5b). The product was prepared according to the general procedure from 1.444 g of **89b**, 0.505 g of pyridine and 1.485 g of heptafluorobutyryl chloride in 14 mL of dry dioxane. Yield 82%, yellow solid, mp 131-133 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 1.90-2.19 (m, 2H, CH_2-3'), 2.84 (t, 2H, ^{3}J = 6.42 Hz, CH_2-4'), 3.21 (s, 3H, CH_3), 3.26 (s, 3H, CH_3), 3.36-3.54 (m, 2H, CH_2-2'), 6.83 (d, 1H, ^{3}J = 8.12 Hz, H-8'), 6.84-6.92 (m, 1H, CH_{Ar}), 6.99-7.08 (m, 1H, CH_{Ar}), 7.30 (d, 1H, ^{3}J = 7.36 Hz, H-5'). ^{13}C NMR (75.48 MHz, DMSO-d_6): δ = 21.8 (CH_2), 26.8 (CH_2), 28.6 (CH_3), 34.1 (CH_3), 50.7 (CH_2-2'),

104.2 (C-5), 117.1 (CH_{Ar}), 122.3 (CH_{Ar}), 125.5, 127.8 (CH_{Ar}), 130.7 (CH_{Ar}), 140.8, 152.3, 159.3, 161.6, 185.3 (t, $^{2}J_{(C-F)}$ = 28.5 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –122.2 (s, CF_2), –112.5 (m, CF_2), –80.4 (t, J = 9.20 Hz, CF_3). MS (GC, 70 eV): *m/z* (%) = 467 ($[M]^+$, 38), 299 (18), 298 (99), 278 (13), 271 (17), 270 (100), 185 (40), 169 (11), 132 (22), 130 (18), 128 (11), 117 (12), 86 (14), 82 (11), 81 (15), 69 (14). HRMS (ESI): Calcd. for $C_{16}H_{15}F_3N_3O_3$ $[M+H]^+$: 468.11527, found: 468.11572. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2953 (w), 2867 (w), 1738 (w), 1705 (m), 1657 (s), 1651 (s), 1602 (w), 1591 (w), 1574 (m), 1557 (w), 1538 (w), 1494 (m), 1472 (m), 1428 (s), 1396 (m), 1370 (w), 1344 (m), 1320 (w), 1295 (w), 1275 (w), 1217 (s), 1195 (s), 1179 (s), 1150 (s), 1116 (s), 1079 (m), 1026 (w), 994 (m), 966 (w), 920 (w), 881 (m), 871 (w), 817 (w), 804 (m), 773 (m), 758 (s), 749 (m), 721 (m), 687 (m), 652 (m), 624 (w), 596 (w), 555 (m), 540 (w).

1,3-Dimethyl-6-[methyl(phenyl)amino]-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione (5c). The product was prepared according to the general procedure from 0.35 g of ,3-dimethyl-6-[methyl(phenyl)amino]pyrimidine-2,4(1*H*,3*H*)-dione, 0.135 g of pyridine and 0.599 g of trifluoroacetic anhydride in 3.5 mL of dry dioxane. Yield 0.484 g (99%), yellow solid, mp 137-139 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.16 (s, 3H, CH_3), 3.26 (s, 6H, CH_3), 6.95-7.08 (m, 3H, CH_{Ph}), 7.26-7.34 (m, 2H, CH_{Ph}). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.6 (CH_3), 33.6 (CH_3), 39.5 (CH_3), 103.9 (C-5), 115.9 (q, $^{1}J_{(C-F)}$ = 290.9 Hz, CF_3), 117.5 (CH), 122.8 (CH), 130.2 (CH), 145.6, 152.3, 161.4, 161.7, 182.2 (q, $^{2}J_{(C-F)}$ = 37.2 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –73.9 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 341 ($[M]^+$, 35), 273 (16), 272 (100), 257 (11), 244 (49), 178 (12), 159 (53), 132 (13), 128 (27), 106 (20), 77 (28), 69 (15), 60 (10). HRMS (ESI): Calcd. for $C_{15}H_{15}F_3N_3O_3$ $[M+H]^+$: 342.10600, found: 342.10622. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3051 (w), 3022 (w), 1703 (s), 1651 (s), 1645 (s), 1603 (m), 1587 (m), 1566 (s), 1487 (s), 1441 (s), 1417 (s), 1394 (s), 1331 (m), 1300 (m), 1240 (m), 1230 (m), 1221 (m), 1188 (s), 1159 (s), 1142 (s), 1117 (s), 1105 (s), 1080 (s), 1049 (m), 1026 (m), 974 (s), 932 (m), 903 (m), 825 (s), 812 (m), 787 (m), 754 (s), 710 (s), 698 (s), 650 (s), 617 (m), 582 (m), 548 (s).

6-(Benzylamino)-1,3-dimethyl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione (5d). To a solution of 6-(benzylamino)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (1.825 g, 7.44 mmol, 1 eq) in 9.1 mL of dry dioxane was added trifluoroacetic anhydride (3.125 g, 14.9 mmol, 2 eq). Next day the starting material was still observed on TLC. The solvent was evaporated and the residue was dried in a high vacuum at 100 °C. Then a new portion of dry dioxane (4.5 mL) and trifluoroacetic anhydride (3.125 g, 14.9 mmol, 2 eq) was added and the mixture was allowed to stay at r.t. for one day. After that the formed precipitate was filtered off, washed with diethyl ether and dried in a high vacuum. Yield 2.441 (96%), white solid, mp 177 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.19 (s, 3H, CH_3), 3.53 (s, 3H, CH_3), 4.68 (d, 2H, J = 5.10 Hz, CH_2), 7.34-7.48 (m, 5H, CH_{Ph}), 10.30 (br s, 1H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.6 (CH_3), 36.2 (CH_3), 51.3 (CH_2), 91.6 (C-5), 118.1 (q, $^{1}J_{(C-F)}$ = 288.0 Hz, CF_3), 128.7 (CH_{Ph}), 129.0 (CH_{Ph}), 129.7 (CH_{Ph}), 137.4, 151.6, 160.4, 161.5, 177.4 (q, $^{2}J_{(C-F)}$ = 35.4 Hz, CO). ^{19}F NMR (282.38

MHz, DMSO-d_6): δ = –70.8 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 341 ($[M]^+$, 6.0), 273 (16), 272 ($[M–CF_3]^+$, 100), 243 (16), 242 (49), 226 (25), 157 (13), 122 (31), 105 (11), 91 (73), 82 (27). HRMS (ESI): Calcd. for $C_{15}H_{15}F_3N_3O_3$ $[M+H]^+$: 342.10600, found: 342.10562. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3036 (w), 2142 (w), 2012 (w), 1965 (w), 1720 (w), 1668 (m), 1597 (s), 1582 (s), 1525 (m), 1496 (w), 1485 (w), 1461 (m), 1447 (m), 1439 (m), 1413 (w), 1383 (w), 1357 (m), 1328 (w), 1304 (m), 1268 (w), 1239 (w), 1222 (w), 1208 (s), 1164 (s), 1150 (s), 1099 (m), 1082 (m), 1061 (w), 1033 (w), 1025 (w), 995 (s), 972 (w), 963 (m), 930 (w), 907 (w), 853 (w), 829 (m), 820 (s), 787 (w), 775 (w), 758 (m), 742 (s), 731 (m), 713 (m), 695 (s), 657 (s), 620 (w), 596 (w), 584 (m), 538 (w).

1,3-Dimethyl-6-piperidin-1-yl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione (5e). To a solution of 1,3-dimethyl-6-piperidin-1-ylpyrimidine-2,4(1*H*,3*H*)-dione (2.39 g, 10.7 mmol, 1 eq) in 7.2 mL of dry dioxane was added trifluoroacetic anhydride (4.497 g, 21.4 mmol, 2 eq). Next day the starting material was still observed on TLC. The solvent was evaporated and the residue was dried in a high vacuum at 100 °C. Then a new portion of dry dioxane (3.6 mL) and trifluoroacetic anhydride (2.248 g, 10.7 mmol, 1 eq) was added and the mixture was allowed to stay at r.t. for 3 days. After evaporation and proper drying at 100 °C in a high vacuum the pure title product was obtained. Yield 3.401 g (100%), beige solid, mp 253-255 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 1.60-1.75 (m, 6H, CH_2-3', CH_2-4', CH_2-5'), 2.83-2.92 (m, 4H, CH_2-2', CH_2-6'), 3.19 (s, 3H, CH_3), 3.40 (s, 3H, CH_3). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 24.2 (CH_2), 25.7 (CH_2), 28.3 (CH_3), 35.8 (CH_3), 53.1 (CH_2-2', CH_2-6'), 97.3 (C-5), 116.6 (q, $^1J_{(C\text{-}F)}$ = 290.4 Hz, CF_3), 152.4, 161.7, 163.3, 182.5 (q, $^2J_{(C\text{-}F)}$ = 36.4 Hz, CO). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –73.1 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 319 ($[M]^+$, 0.31), 251 (14), 250 ($[M–CF_3]^+$, 100), 222 (20), 128 (12), 110 (15), 84 (26), 82 (22), 69 (16). HRMS (EI): Calcd. for $C_{13}H_{16}F_3N_3O_3$ $[M]^+$: 353.11383, found: 319.11437. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3006 (w), 2947 (m), 2856 (w), 1780 (w), 1716 (w), 1684 (m), 1650 (s), 1552 (m), 1487 (s), 1436 (s), 1401 (m), 1371 (s), 1336 (w), 1300 (w), 1284 (w), 1259 (w), 1245 (w), 1235 (w), 1217 (m), 1193 (s), 1158 (m), 1139 (s), 1114 (m), 1079 (m), 1067 (w), 1050 (w), 1020 (m), 980 (s), 956 (m), 912 (w), 858 (m), 826 (m), 811 (w), 793 (s), 758 (s), 715 (m), 706 (m), 698 (m), 643 (m), 585 (w), 565 (m).

2.3 Synthesis of 5-polyfluoroalkyl-5-deazaalloxazines

General procedure for the synthesis of 5-polyfluoroalkyl-pyrimido[4,5-b]quinoline-2,4-diones 4a-x. Initial 5-(polyfluoroacyl)-6-amino-1,3-dialkylpyrimidine-2,4(1H,3H)-dione **3** (0.3 g) was dissolved in concentrated H_2SO_4 (1.5 mL) and allowed to stand at r.t. for 3 hours. Then the solution was poured into ice water and formed precipitate was filtered off by suction and recrystallized from methanol giving the pure product.

1,3-Dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4a). The product was

prepared according to the general procedure, starting from 0.474 g of **3a** and 2.4 mL of H_2SO_4. Yield 0.269 g (89%), yellow solid, mp 195 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.52 (s, 3H, CH_3-3), 3.83 (s, 3H, CH_3-1), 7.55-7.62 (m, 1H, H-7), 7.81-7.89 (m, 1H, H-8), 8.01-8.06 (m, 1H, H-9), 8.30-8.36 (m, 1H, H-6). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 29.4 (CH_3-3), 30.6 (CH_3-1), 110.4 (C-4a), 121.7, 123.3 (q, $^1J_{(C\text{-}F)}$ = 278.7 Hz, CF_3), 126.1 (q, $^4J_{(C\text{-}F)}$ = 6.1 Hz, CH-6), 127.2, 129.1 (CH_{Ar}), 133.4 (CH_{Ar}), 138.7 (q, $^2J_{(C\text{-}F)}$ = 33.4 Hz, C-5), 148.2, 150.2, 151.1 (CO-2), 159.3 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –52.5 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 310 ($[M+H]^+$, 13), 309 ($[M]^+$, 77), 197 (100). HRMS (ESI): Calcd. for $C_{14}H_{11}F_3N_3O_2$ $[M+H]^+$: 310.07979, found: 310.07967. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2956 (w), 1713 (s), 1669 (s), 1614 (w), 1583 (s), 1565 (m), 1494 (m), 1464 (s), 1419 (m), 1378 (s), 1332 (m), 1286 (m), 1216 (m), 1194 (m), 1156 (s), 1142 (s), 1124 (s), 1100 (s), 1069 (m), 1030 (m), 989 (s), 929 (w), 877 (w), 856 (w), 812 (m), 775 (s), 756 (s), 745 (s), 712 (w), 624 (s), 592 (m), 550 (m), 532 (w).

5-(Heptafluoropropyl)-1,3-dimethylpyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4b). The product was prepared according to the general procedure, starting from 0.662 g of **3b** and 3.3 mL of H_2SO_4. Yield 0.461 g (73%), yellow solid, mp 183 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.51 (s, 3H, CH_3-3), 3.84 (s, 3H, CH_3-1), 7.54-7.64 (m, 1H, H-7), 7.81-7.90 (m, 1H, H-8), 8.06 (d, 1H, ^3J = 8.50 Hz, H-9), 8.32 (m, 1H, ^3J = 8.88 Hz, H-6). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 29.7 (CH_3-3), 30.8 (CH_3-1), 111.7 (C-4a), 122.7, 127.0 (CH-6), 127.4 (CH_{Ar}), 129.4 (CH_{Ar}), 133.3 (CH_{Ar}), 140.0 (t, $^2J_{(C\text{-}F)}$ = 24.3 Hz, C-5), 148.4, 150.3, 151.1 (CO-2), 159.1 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –116.6 (s, CF_2), –92.0 (br s, CF_2), –80.0 (t, *J* = 9.20 Hz, CF_3). MS (GC, 70 eV): *m/z* (%) = 410 ($[M+H]^+$, 11), 409 ($[M]^+$, 60), 298 (13), 297 (100). HRMS (ESI): Calcd. for $C_{16}H_{11}F_7N_3O_2$ $[M+H]^+$: 410.07340, found: 410.07322. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3154 (w), 1720 (m), 1615 (s), 1614 (w), 1502 (w), 1463 (m), 1424 (m), 1392 (m), 1376 (m), 1347 (w), 1329 (m), 1293 (w), 1271 (w), 1251 (w), 1225 (s), 1202 (s), 1190 (s), 1146 (m), 1128 (m), 1111 (s), 1029 (w), 978 (w), 969 (w), 941 (s), 899 (s), 899 (s), 877 (w), 825 (m), 769 (s), 748 (s), 726 (s), 691 (m), 621 (m), 599 (w), 539 (m).

1,3,7,9-Tetramethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4c). The product was prepared according to the general procedure, starting from 0.429 g of **3c** and 2.1 mL of H_2SO_4. Yield 0.343 g (84%), yellow solid, mp 192 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 2.52 (s, 3H, CH_3), 2.72 (s, 3H, CH_3), 3.51 (s, 3H, CH_3-3), 3.82 (s, 3H, CH_3-1), 7.56s1H (s, 1H, H-8), 7.91s1H (s, 1H, H-8). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 18.5 (CH_3), 22.4 (CH_3), 29.3 (CH_3-3), 30.4 (CH_3-1), 109.6 (C-4a), 121.9, 122.4 (q, $^4J_{(C\text{-}F)}$ = 5.8 Hz, CH-6), 123.4 (q, $^1J_{(C\text{-}F)}$ = 278.2 Hz, CF_3), 135.8 (CH-8), 136.4, 137.2 (q, $^2J_{(C\text{-}F)}$ = 33.1 Hz, C-5), 138.4, 146.6, 148.0, 151.2 (CO-2), 159.5 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –52.4 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 338 ($[M+H]^+$, 19), 337 ($[M]^+$, 100), 309 (10), 268 (14), 226 (10), 225 (83). HRMS (EI): Calcd. for $C_{16}H_{14}F_3N_3O_2$ $[M]^+$: 337.10326, found: 337.10302. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2962 (w), 1713 (m), 1669 (s), 1625 (w), 1570 (s), 1500 (w), 1468 (s), 1435 (m), 1408 (m), 1374 (s), 1348 (m), 1317 (m), 1282 (s), 1239 (s), 1198 (m), 1176 (m), 1150 (s), 1136 (s), 1112 (m), 1101 (s),

1057 (w), 1041 (m), 996 (m), 974 (m), 962 (m), 921 (w), 860 (m), 847 (w), 827 (w), 811 (s), 776 (w), 764 (w), 750 (s), 729 (w), 705 (m), 690 (m), 674 (w), 660 (m), 585 (m), 567 (w), 543 (w).

1,3,7,9-Tetramethyl-5-(pentafluoroethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4d). The product was prepared according to the general procedure, starting from 0.431 g of **3d** and 2.2 mL of H_2SO_4. Yield 0.345 g (84%), yellow solid, mp 225 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 2.52 (s, 3H, CH_3), 2.72 (s, 3H, CH_3), 3.51 (s, 3H, CH_3-3), 3.82 (s, 3H, CH_3-1), 7.56 (s, 1H, H-8), 7.84 (s, 1H, H-8). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 18.7 (CH_3), 22.6 (CH_3), 29.5 (CH_3-3), 30.6 (CH_3-1), 110.6 (C-4a), 122.81 (CH-6), 122.85, 135.8 (CH-8), 136.7, 137.0, 139.4 (t, $^2J_{(C\text{-}F)}$ = 24.1 Hz, C-5), 146.8, 148.0, 151.2 (CO-2), 159.7 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –91.0 (s, CF_2), –74.8 (t, *J* = 2.0 Hz, CF_3). MS (GC, 70 eV): *m/z* (%) = 388 ($[M+H]^+$, 18), 387 ($[M]^+$, 92), 359 (11), 330 (11), 276 (15), 275 (100), 268 (12). HRMS (EI): Calcd. for $C_{17}H_{14}F_5N_3O_2$ $[M]^+$: 387.10007, found: 387.09992. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3369 (w), 2919 (w), 1713 (m), 1668 (s), 1625 (w), 1566 (s), 1504 (w), 1470 (m), 1444 (m), 1435 (m), 1378 (m), 1348 (w), 1292 (m), 1232 (w), 1209 (s), 1192 (s), 1182 (m), 1162 (s), 1133 (s), 1107 (s), 1062 (s), 1037 (m), 1020 (s), 985 (s), 958 (m), 906 (w), 859 (m), 816 (m), 763 (w), 737 (w), 762 (w), 742 (s), 727 (s), 691 (m), 658 (m), 599 (w), 586 (m), 567 (m), 552 (w), 531 (m).

5-(Heptafluoropropyl)-1,3,7,9-tetramethylpyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4e). The product was prepared according to the general procedure, starting from 0.485 g of **3e** and 2.4 mL of H_2SO_4. Yield 0.429 g (92%), yellow solid, mp 198-200 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 2.53 (s, 3H, CH_3), 2.73 (s, 3H, CH_3), 3.51 (s, 3H, CH_3-3), 3.84 (s, 3H, CH_3-1), 7.58 (s, 1H, H-8), 7.93 (s, 1H, H-8). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 18.7 (CH_3), 22.6 (CH_3), 29.6 (CH_3-3), 30.7 (CH_3-1), 111.0 (C-4a), 123.0, 123.3 (CH-6), 135.8 (CH-8), 136.7, 137.0, 139.0 (t, $^2J_{(C\text{-}F)}$ = 23.8 Hz, C-5), 146.9, 148.1, 151.3 (CO-2), 159.4 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –116.5 (s, CF_2), –90.2 (br s, CF_2), –80.0 (t, *J* = 8.7 Hz, CF_3). MS (GC, 70 eV): *m/z* (%) = 438 ($[M+H]^+$, 20), 437 ($[M]^+$, 100), 409 (10), 380 (11), 326 (16), 325 (100), 268 (10), 220 (14), 206 (12). HRMS (EI): Calcd. for $C_{18}H_{14}F_3N_3O_2$ $[M]^+$: 437.09688, found: 437.09679. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2929 (w), 1722 (m), 1678 (s), 1626 (w), 1568 (s), 1494 (w), 1469 (m), 1444 (m), 1376 (s), 1346 (m), 1313 (w), 1289 (w), 1266 (w), 1255 (w), 1228 (s), 1219 (s), 1198 (s), 1176 (s), 1130 (m), 1114 (s), 1055 (w), 1035 (w), 1001 (w), 977 (w), 913 (s), 861 (w), 815 (m), 785 (w), 758 (w), 746 (m), 732 (s), 693 (w), 658 (w), 623 (m), 599 (w), 584 (w), 564 (w), 535 (m).

7-Ethyl-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4f). The product was prepared according to the general procedure, starting from 0.363 g of **3f** and 1.8 mL of H_2SO_4. Yield 0.173 g (50%), yellow solid, mp 164 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 1.30 (t, 3H, ^3J = 7.55 Hz, Et), 2.79 (q, 2H, ^3J = 7.55 Hz, Et), 3.41 (s, 3H, CH_3-3), 3.69 (s, 3H, CH_3-1), 7.61 (dd, 1H, ^3J = 8.69 Hz, ^4J = 1,80 Hz, H-8), 7.80 (d, 1H, ^3J = 8.69 Hz, H-9), 7.96 (s, 1H, H-6). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 15.4 ($CH_{3(Et)}$), 29.4 (CH_3-3), 29.6 ($CH_{2(Et)}$), 30.5 (CH_3-1), 110.2 (C-4a), 121.9 (C-5a), 123.4

(q, $^{1}J_{(C\text{-}F)}$ = 278.7 Hz, CF_3), 123.5 (q, $^{4}J_{(C\text{-}F)}$ = 5.9 Hz, CH-6), 128.9 (CH, C-9), 134.8 (CH, C-8), 137.8 (q, $^{2}J_{(C\text{-}F)}$ = 33.3 Hz, C-5), 143.5 (C-9a), 147.7 (C-10a), 149.2 (C-7), 151.2 (CO-2), 159.5 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –52.5 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 338 ($[M+H]^+$, 19), 337 ($[M]^+$, 100), 322 (27), 309 (10), 268 (16), 265 (16), 226 (11), 225 (77), 224 (11), 210 (12). HRMS (ESI): Calcd. for $C_{16}H_{15}F_3N_3O_2$ $[M+H]^+$: 338.11109, found: 338.11193. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3380 (w), 2970 (w), 1716 (m), 1674 (s), 1620 (w), 1576 (s), 1498 (w), 1457 (s), 1413 (m), 1376 (s), 1356 (m), 1352 (m), 1286 (m), 1251 (w), 1221 (m), 1196 (m), 1147 (s), 1130 (s), 1109 (s), 1071 (m), 1056 (m), 989 (m), 944 (w), 883 (w), 860 (w), 843 (s), 823 (w), 809 (m), 776 (w), 748 (s), 700 (m), 674 (m), 636 (m), 602 (w), 568 (m), 535 (w).

5-[Chloro(difluoro)methyl]-7-ethyl-1,3-dimethylpyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4g). The product was prepared according to the general procedure, starting from 0.369 g of **3g** and 1.8 mL of H_2SO_4. Yield 0.199 g (57%), yellow solid, mp 188 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 1.36 (t, 3H, ^{3}J = 7.56 Hz, Et), 2.87 (q, 2H, ^{3}J = 7.56 Hz, Et), 3.51 (s, 3H, CH_3-3), 3.81 (s, 3H, CH_3-1), 7.71 (d, 1H, ^{3}J = 8.68 Hz, H-8), 7.94 (d, 1H, ^{3}J = 8.68 Hz, H-9), 8.08 (s, 1H, H-6). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 15.4 ($CH_{3(Et)}$), 29.4 (CH_3-3), 29.6 ($CH_{2(Et)}$), 30.6 (CH_3-1), 108.3 (C-4a), 120.7 (C-5a), 123.7 (t, $^{4}J_{(C\text{-}F)}$ = 7.8 Hz, CH-6), 123.9 (t, $^{1}J_{(C\text{-}F)}$ = 290.6 Hz, $CClF_2$), 128.8 (CH, C-9), 134.6 (CH, C-8), 143.1 (C-9a), 143.3 (t, $^{2}J_{(C\text{-}F)}$ = 27.4 Hz, C-5), 147.6 (C-10a), 149.1 (C-7), 151.2 (CO-2), 159.6 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –40.7 (br s, $CClF_2$). MS (GC, 70 eV): *m/z* (%) = 355 ($[M+H]^+$, ^{37}Cl, 35), 354 ($[M+H]^+$, ^{35}Cl, 20), 353 ($[M]^+$, ^{35}Cl, 100), 338 (22), 319 (17), 318 (83), 303 (13), 268 (18), 243 (20), 241 (59). HRMS (ESI): Calcd. for $C_{16}H_{15}ClF_2N_3O_2$ $[M+H, ^{35}Cl]^+$: 354.08154, found: 354.08121. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3370 (w), 2966 (w), 1715 (m), 1667 (s), 1622 (w), 1573 (s), 1503 (w), 1470 (m), 1454 (s), 1414 (m), 1378 (s), 1358 (m), 1322 (m), 1291 (m), 1274 (m), 1253 (w), 1204 (w), 1192m 1152 (m), 1140 (m), 1115 (s), 1095 (m), 1069 (m), 1005 (s), 994 (m), 552 (s), 927 (s), 881 (w), 845 (s), 832 (w), 817 (m), 796 (s), 770 (w), 793 (s), 689 (w), 675 (w), 661 (m), 632 (w), 621 (w), 580 (w), 560 (m).

7-Ethyl-1,3-dimethyl-5-(pentafluoroethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4h). The product was prepared according to the general procedure, starting from 0.466 g of **3h** and 2.3 mL of H_2SO_4. Yield 0.359 g (81%), yellow solid, mp 235 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 1.35 (t, 3H, ^{3}J = 7.55 Hz, Et), 2.86 (q, 2H, ^{3}J = 7.55 Hz, Et), 3.51 (s, 3H, CH_3-3), 3.82 (s, 3H, CH_3-1), 7.72 (d, 1H, ^{3}J = 8.88 Hz, H-8), 7.97 (d, 1H, ^{3}J = 8.88 Hz, H-9), 8.01 (s, 1H, H-6). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 15.3 ($CH_{3(Et)}$), 29.6 (CH_3-3), 29.6 ($CH_{2(Et)}$), 30.7 (CH_3-1), 111.1 (C-4a), 122.7 (C-5a), 123.9 (CH-6), 129.1 (CH, C-9), 134.9 (CH, C-8), 139.4 (t, $^{2}J_{(C\text{-}F)}$ = 24.0 Hz, C-5), 143.4 (C-9a), 147.9 (C-10a), 149.1 (C-7), 151.2 (CO-2), 159.5 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –91.4 (s, CF_2), –75.0 (t, *J* = 2.0 Hz, CF_3). MS (GC, 70 eV): *m/z* (%) = 388 ($[M+H]^+$, 18), 387 ($[M]^+$, 91), 372 (24), 359 (11), 315 (19), 276 (14), 275 (100), 268 (12), 260 (12). HRMS (EI): Calcd. for $C_{17}H_{14}F_5N_3O_2$ $[M]^+$: 387.10007, found: 387.09992. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3381 (w), 2973 (w), 1719 (m), 1675 (s), 1621 (w), 1568 (s), 1504 (w),

1494 (w), 1454 (s), 1410 (m), 1376 (m), 1339 (w), 1313 (w), 1294 (s), 1229 (m), 1176 (s), 1146 (s), 1128 (s), 1107 (s), 1069 (m), 1036 (s), 1006 (w), 969 (s), 939 (m), 895 (w), 846 (s), 822 (w), 805 (m), 758 (w), 746 (s), 736 (m), 725 (s), 683 (m), 672 (m), 635 (w), 598 (w), 578 (w), 557 (m).

9-Methoxy-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4i). The product was prepared according to the general procedure, starting from 0.319 g of **3i** and 1.6 mL of H_2SO_4. Yield 0.147 g (49%), yellow solid, mp 220 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.52 (s, 3H, CH_3-3), 3.87 (s, 3H, CH_3-1), 4.08 (s, 3H, MeO), 7.19 (d, 1H, ^3J = 7.74 Hz, H-8), 7.49 (dd, 1H, $^3J_1$ = 9.06 Hz, $^3J_2$ = 7.74 Hz, H-7), 7.84-7.92 (m, 1H, H-6). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 29.4 (CH_3-3), 30.7 (CH_3-1), 56.7 (MeO), 110.6 (C-4a), 111.3 (CH_{Ar}), 117.6 (q, $^4J_{(C-F)}$ = 6.1 Hz, CH-6), 122.9, 123.2 (q, $^1J_{(C-F)}$ = 278.7 Hz, CF_3), 127.3 (CH_{Ar}), 138.5 (q, $^2J_{(C-F)}$ = 33.5 Hz, C-5), 142.5, 147.4, 151.2 (CO-2), 154.8 (C-9), 159.4 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –52.6 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 340 ($[M+H]^+$, 17), 339 ($[M]^+$, 100), 310 (37), 309 (12), 281 (20), 267 (13), 253 (26), 252 (12), 227 (24). HRMS (EI): Calcd. for $C_{15}H_{12}F_3N_3O_3$ $[M+H]^+$: 339.08253, found: 339.08253. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2953 (w), 2848 (w), 1714 (m), 1667 (s), 1611 (w), 1566 (m), 1504 (w), 1485 (m), 1465 (m), 1444 (w), 1421 (m), 1393 (w), 1376 (m), 1353 (w), 1318 (w), 1287 (s), 1256 (w), 1233 (s), 1207 (m), 1197 (m), 1161 (s), 1147 (s), 1122 (s), 1099 (m), 1059 (m), 1004 (s), 976 (m), 877 (w), 862 (w), 838 (w), 822 (w), 788 (s), 778 (m), 757 (m), 747 (s), 714 (m), 700 (s), 688 (m), 674 (w), 615 (m), 595 (w), 586 (w), 538 (w).

5-[Chloro(difluoro)methyl]-9-methoxy-1,3-dimethylpyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4j). The product was prepared according to the general procedure, starting from 0.344 g of **3j** and 1.7 mL of H_2SO_4. Yield 0.218 g (67%), yellow solid, mp 210 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.52 (s, 3H, CH_3-3), 3.87 (s, 3H, CH_3-1), 4.08 (s, 3H, MeO), 7.18 (d, 1H, ^3J = 7.74 Hz, H-8), 7.50 (dd, 1H, $^3J_1$ = 9.07 Hz, $^3J_2$ = 7.74 Hz, H-7), 7.86-7.93 (m, 1H, H-6). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 29.5 (CH_3-3), 30.7 (CH_3-1), 56.7 (MeO), 108.7 (C-4a), 111.2 (CH_{Ar}), 117.9 (t, $^4J_{(C-F)}$ = 7.9 Hz, CH-6), 121.8, 123.9 (t, $^1J_{(C-F)}$ = 291.2 Hz, CF_3), 127.0 (CH_{Ar}), 142.4, 144.0 (t, $^2J_{(C-F)}$ = 27.5 Hz, C-5), 147.3, 151.2 (CO-2), 154.8 (C-9), 159.5 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –40.1 (br s, $CClF_2$). MS (GC, 70 eV): *m/z* (%) = 357 ($[M]^+$, ^{37}Cl, 34), 356 ($[M+H]^+$, ^{35}Cl, 28), 355 ($[M]^+$, ^{35}Cl, 100), 354 (37), 328 (12), 327 (10), 326 (33), 325 (11), 320 (33), 297 (12), 269 (15), 263 (15), 243 (21). HRMS (EI): Calcd. for $C_{15}H_{12}ClF_2N_3O_3$ [M, ^{35}Cl]$^+$: 355.05298, found: 355.05262; calcd. for $C_{15}H_{12}ClF_2N_3O_3$ [M, ^{37}Cl]$^+$: 357.05003, found: 357.05014. Anal. Calcd for $C_{15}H_{12}ClF_2N_3O_3$: C, 50.65; H, 3.40; N, 11.81. Found: C, 50.87; H, 3.30; N, 11.96. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3377 (w), 2963 (w), 1717 (s), 1667 (s), 1611 (w), 1578 (s), 1564 (s), 1504 (m), 1485 (m), 1463 (m), 1454 (m), 1421 (s), 1392 (m), 1371 (m), 1350 (m), 1317 (w), 1277 (s), 1249 (m), 1214 (s), 1186 (m), 1126 (s), 1101 (m), 1092 (s), 1059 (m), 1013 (s), 980 (m), 952 (s), 926 (s), 880 (m), 862 (w), 825 (w), 782 (s), 773 (s), 756 (m), 746 (s), 706 (w), 680 (m), 662 (m), 629 (w), 610 (m), 587 (w), 563 (w), 534 (w).

8-Methoxy-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4k). The product was prepared according to the general procedures for the synthesis of **3** and **4**, starting from 0.4 g of 6-[(3-methoxyphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione **2e**, 0.145 g of pyridine and 0.643 g of trifluoroacetic anhydride in 4 mL of dioxane; than to isolated crude product were added 2.5 mL of H_2SO_4. Yield 0.062 g (12% after two steps; calculated on **2e**), yellow solid, mp 232-235 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.49 (s, 3H, CH_3-3), 3.80 (s, 3H, CH_3-1), 4.01 (s, 3H, MeO), 7.20 (dd, 1H, ^3J = 9.63 Hz, ^4J = 2.65 Hz, H-7), 7.28 (d, 1H, ^4J = 2.65 Hz, H-9), 8.20 (dq, 1H, ^3J = 9.63 Hz, $^5J_{(H-F)}$ = 2.08 Hz, H-6). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 29.4 (CH_3-3), 30.6 (CH_3-1), 56.2 (MeO), 106.7 (CH_{Ar}), 107.6 (C-4a), 117.3, 121.3 (CH_{Ar}), 123.4 (q, $^1J_{(C-F)}$ = 278.5 Hz, CF_3), 127.5 (q, $^4J_{(C-F)}$ = 6.3 Hz, CH-6), 138.3 (q, $^2J_{(C-F)}$ = 33.8 Hz, C-5), 149.0, 151.3 (CO-2), 153.0, 159.5 (CO-4), 163.8 (CH-8). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –52.4 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 340 ($[M+H]^+$, 11), 339 ($[M]^+$, 66), 311 (12), 270 (21), 228 (13), 227 (100). HRMS (EI): Calcd. for $C_{15}H_{12}F_3N_3O_3$ $[M+H]^+$: 339.08253, found: 339.08256. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3373 (w), 2953 (w), 1716 (m), 1669 (s), 1620 (m), 1569 (m), 1504 (w), 1480 (m), 1471 (m), 1451 (m), 1412 (m), 1381 (m), 1352 (m), 1329 (w), 1289 (m), 1273 (w), 1233 (s), 1215 (s), 1157 (s), 1132 (s), 1019 (m), 992 (m), 976 (m), 959 (w), 895 (w), 853 (s), 832 (m), 803 (s), 749 (s), 733 (w), 698 (m), 673 (w), 639 (s), 571 (w), 544 (w).

5-[Chloro(difluoro)methyl]-8-methoxy-1,3-dimethylpyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4l). The product was prepared according to the general procedures for the synthesis of **3** and **4**, starting from 0.4 g of 6-[(3-methoxyphenyl)amino]-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione **2e**, 0.145 g of pyridine and 0.744 g of chlorodifluoroacetic anhydride in 4 mL of dioxane; than to isolated crude product were added 2.7 mL of H_2SO_4. Yield 0.218 g (40% after two steps; calculated on **2e**), yellow solid, mp 272-274 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.51 (s, 3H, CH_3-3), 3.81 (s, 3H, CH_3-1), 4.01 (s, 3H, MeO), 7.22 (dd, 1H, ^3J = 9.63 Hz, ^4J = 2.83 Hz, H-7), 7.29 (d, 1H, ^4J = 2.83 Hz, H-9), 8.22 (dt, 1H, ^3J = 9.63 Hz, $^5J_{(H-F)}$ = 2.90 Hz, H-6). ^{13}C NMR (75.47 MHz, 12% TFA-*d* in $CDCl_3$): δ = 30.2 (CH_3), 31.7 (CH_3), 56.9 (OMe), 103.3 (CH), 105.8 (C-4a), 116.3, 122.6 (CH), 123.0 (t, $^1J_{(C-F)}$ = 292.1 Hz, $CClF_2$), 129.0 (t, $^4J_{(C-F)}$ = 8.2 Hz, CH-6), 147.9, 148.1, 148.2 (t, $^2J_{(C-F)}$ = 28.6 Hz), 150.7 (CO-2), 158.7 (CO-4), 166.7. ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –40.4 (br s, $CClF_2$). MS (GC, 70 eV): *m/z* (%) = 357 ($[M]^+$, ^{37}Cl, 29), 356 ($[M+H]^+$, ^{35}Cl, 14), 355 ($[M]^+$, ^{35}Cl, 83), 327 (11), 321 (16), 320 (41), 270 (36), 245 (33), 244 (14), 243 (100), 209 (10). HRMS (EI): Calcd. for $C_{15}H_{12}ClF_2N_3O_3$ [M, ^{35}Cl]$^+$: 355.05298, found: 355.05401. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3366 (w), 2952 (w), 1713 (s), 1668 (s), 1619 (m), 1566 (s), 1503 (m), 1482 (s), 1470 (m), 1449 (s), 1411 (m), 1380 (s), 1348 (m), 1326 (w), 1288 (m), 1269 (w), 1232 (s), 1190 (m), 1136 (s), 1114 (s), 1020 (m), 1003 (s), 975 (w), 959 (m), 946 (s), 851 (s), 826 (m), 804 (m), 791 (s), 767 (m), 749 (s), 742 (m), 729 (w), 702 (w), 679 (w), 664 (m), 634 (s), 606 (w), 557 (m), 528 (m).

5-(Heptafluoropropyl)-8-methoxy-1,3-dimethylpyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4m). The product was prepared according to the general procedure, starting from 0.658 g of **3m** and 3.3 mL of

H_2SO_4. Yield 0.204 g (32%), yellow solid, mp 214-216 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.50 (s, 3H, CH_3-3), 3.82 (s, 3H, CH_3-1), 4.02 (s, 3H, MeO), 7.21 (dd, 1H, ^3J = 9.82 Hz, ^4J = 2.79 Hz), H-7, 7.31 (d, 1H, ^4J = 2.79 Hz, H-9), 8.20 (d, 1H, ^3J = 9.82 Hz, H-6). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 29.6 (CH_3-3), 30.7 (CH_3-1), 56.2 (MeO), 106.8 (CH_{Ar}), 108.9 (C-4a), 118.3, 121.3 (CH_{Ar}), 128.4 (CH-6), 139.4 (t, $^2J_{(C-F)}$ = 23.5 Hz, C-5), 149.2, 151.3 (CO-2), 153.0, 159.2 (CO-4), 163.7 (CH-8). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –116.8 (s, CF_2), –90.4 (br s, CF_2), –80.0 (t, J = 8.7 Hz, CF_3). MS (GC, 70 eV): *m/z* (%) = 440 ($[M+H]^+$, 12), 439 ($[M]^+$, 64), 411 (12), 328 (14), 327 (100), 270 (11). HRMS (ESI): Calcd. for $C_{17}H_{13}F_7N_3O_3$ $[M+H]^+$: 440.08397, found: 440.08478. Anal. Calcd for $C_{17}H_{12}F_7N_3O_3$: C, 46.48; H, 2.75; N, 9.57. Found: C, 46.65; H, 2.55; N, 10.06. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3151 (w), 2953 (w), 2848 (w), 1715 (m), 1682 (s), 1620 (m), 1565 (s), 1504 (m), 1485 (s), 1446 (m), 1410 (m), 1380 (s), 1348 (m), 1288 (m), 1271 (w), 1233 (s), 1200 (s), 1185 (s), 1172 (s), 1141 (s), 1132 (s), 1112 (s), 1069 (w), 1041 (w), 1017 (m), 1002 (m), 975 (w), 961 (w), 931 (s), 854 (s), 824 (m), 804 (m), 790 (m), 770 (w), 752 (s), 734 (m), 723 (m), 703 (w), 692 (w), 654 (w), 641 (m), 620 (m), 597 (w), 558 (m), 537 (w).

1,3-Dimethyl-5,8-bis(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4n). The product was prepared according to the general procedure, starting from 0.475 g of **3n** and 2.4 mL of H_2SO_4. Yield 0.233 g (51%), yellow solid, mp 199-201 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.53 (s, 3H, CH_3-3), 3.84 (s, 3H, CH_3-1), 7.75 (dd, 1H, ^3J = 9.16 Hz, ^4J = 1.98 Hz, H-7), 8.33-8.36 (m, 1H, H-9), 8.42-8.50 (dm, 1H, ^3J = 9.16 Hz, H-6). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 29.6 (CH_3-3), 30.9 (CH_3-1), 112.2 (C-4a), 122.7 (CH_{Ar}), 122.9 (q, $^1J_{(C-F)}$ = 278.4 Hz, CF_3), 123.0, 123.5 (q, $^1J_{(C-F)}$ = 273.0 Hz, CF_3), 126.8 (q, $^4J_{(C-F)}$ = 4.4 Hz, CH_{Ar}), 127.8 (q, $^4J_{(C-F)}$ = 6.2 Hz, CH_{Ar}), 134.7 (q, $^2J_{(C-F)}$ = 33.4 Hz), 139.1 (q, $^2J_{(C-F)}$ = 33.9 Hz), 149.3, 149.4, 150.9 (CO-2), 158.9 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –63.7 (s, CF_3-8), –52.7 (s, CF_3-5). MS (GC, 70 eV): *m/z* (%) = 377 ($[M]^+$, 52), 265 (100). HRMS (EI): Calcd. for $C_{15}H_9F_6N_3O_2$ $[M]^+$: 377.05935, found: 377.05920. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3388 (w), 3107 (w), 2966 (w), 1722 (m), 1668 (s), 1585 (m), 1565 (m), 1511 (w), 1464 (m), 1422 (m), 1393 (w), 1378 (m), 1361 (m), 1336 (m), 1300 (m), 1272 (m), 1222 (w), 1172 (s), 1122 (s), 1104 (s), 1072 (s), 966 (m), 945 (m), 910 (s), 885 (m), 831 (m), 804 (s), 780 (w), 760 (w), 745 (s), 710 (m), 700 (s), 679 (m), 673 (m), 657 (w), 630 (m), 581 (w), 553 (w).

1,3-Dimethyl-7-nitro-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4o). The product was prepared according to the general procedure, starting from 0.309 g of **3o** and 1.5 mL of H_2SO_4. Yield 0.242 g (82%), yellow solid, mp 232-234 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.53 (s, 3H, CH_3-3), 3.85 (s, 3H, CH_3-1), 8.17 (d, 1H, ^3J = 9.54 Hz, H-9), 8.61 (d, 1H, ^3J = 9.54 Hz, H-8), 9.32 (s, 1H, H-6). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 29.8 (CH_3-3), 31.1 (CH_3-1), 112.5 (C-4a), 120.2, 122.7 (q, $^1J_{(C-F)}$ = 278.6 Hz, CF_3), 123.6 (q, $^4J_{(C-F)}$ = 6.7 Hz, CH-6), 126.7 (CH_{Ar}), 130.8 (CH_{Ar}), 141.0 (q, $^2J_{(C-F)}$ = 34.1 Hz, C-5), 145.8, 150.7, 150.8, 152.0 (CO-2), 158.5 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –52.6 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 354 ($[M]^+$, 49), 243 (12), 242 (100), 196 (13). HRMS (EI):

Calcd. for $C_{14}H_9F_3N_4O_4$ $[M]^+$: 354.05704, found: 354.05725. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3392 (w), 3133 (w), 2965 (w), 1725 (m), 1680 (s), 1623 (w), 1586 (m), 1574 (s), 1532 (m), 1496 (m), 1471 (s), 1417 (w), 1373 (m), 1363 (w), 1340 (w), 1294 (m), 1280 (s), 1230 (w), 1203 (m), 1180 (m), 1155 (s), 1136 (s), 1110 (s), 1070 (w), 993 (m), 986 (m), 972 (w), 948 (w), 907 (m), 868 (m), 844 (s), 810 (w), 793 (w), 723 (w), 760 (w), 748 (s), 740 (s), 713 (w), 703 (m), 675 (w), 647 (m), 633 (m), 565 (m), 539 (w), 527 (w).

7-Bromo-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4p). The product was prepared according to the general procedure, starting from 1.401 g of **3p** and 7 mL of H_2SO_4. Yield 1.121 g (84%), yellow solid, mp 200 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.49 (s, 3H, CH_3-3), 3.78 (s, 3H, CH_3-1), 7.86 (s, 2H, H-8, H-9), 8.41 (s, 1H, H-6). ^{13}C NMR (75.48 MHz, $CDCl_3$): δ = 29.5 (CH_3-3), 30.7 (CH_3-1), 111.1 (C-4a), 121.5, 122.5, 123.0 (q, $^1J_{(C\text{-}F)}$ = 278.3 Hz, CF_3), 128.2 (q, $^4J_{(C\text{-}F)}$ = 6.6 Hz, CH-6), 130.6 (CH_{Ar}), 136.8 (CH_{Ar}), 137.8 (q, $^2J_{(C\text{-}F)}$ = 33.8 Hz, C-5), 148.5, 148.8, 151.0 (CO-2), 159.0 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –52.7 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 390 ($[M+H]^+$, ^{81}Br, 13), 389 ($[M]^+$, ^{81}Br, 81), 388 ($[M+H]^+$, ^{79}Br, 15), 387 ($[M]^+$, ^{79}Br, 84), 291 (15), 289 (16), 278 (11), 277 (97), 276 (15), 275 (100), 263 (11), 261 (11), 182 (11), 176 (11). HRMS (EI): Calcd. for $C_{14}H_9BrF_3N_3O_2$ [M, ^{79}Br]$^+$: 386.98248, found: 386.9826; calcd. for $C_{14}H_{11}F_3N_3O_2$ [M, ^{81}Br]$^+$: 388.98043, found: 388.98055. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3380 (w), 3116 (w), 2962 (w), 2849 (w), 1719 (m), 1668 (s), 1581 (s), 1564 (s), 1556 (m), 1463 (s), 1447 (s), 1410 (m), 1384 (m), 1372 (s), 1358 (m), 1320 (m), 1295 (m), 1281 (s), 1228 (w), 1205 (m), 1162 (s), 1129 (s), 1103 (s), 1075 (s), 986 (s), 969 (m), 936 (m), 875 (w), 858 (w), 831 (s), 808 (m), 797 (w), 772 (w), 757 (w), 748 (s), 713 (w), 702 (s), 672 (m), 639 (s), 630 (m), 559 (m), 552 (m), 532 (m).

7-Ethoxy-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4q). The product was prepared according to the general procedure, starting from 0.397 g of **3q** and 2 mL of H_2SO_4. Yield 0.276 g (73%), yellow solid, mp 210-212 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 1.44 (t, 3H, ^3J = 7.55 Hz, EtO), 3.44 (s, 3H, CH_3-3), 3.74 (s, 3H, CH_3-1), 4.11 (q, 2H, ^3J = 7.55 Hz, EtO), 7.41-7.48 (m, 2H, H-6, H-8), 7.85 (d, 1H, ^3J = 10,01 Hz, H-9). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 14.9 ($CH_{3(EtO)}$), 29.5 (CH_3-3), 30.6 (CH_3-1), 64.4 ($CH_{2(EtO)}$), 103.9 (q, $^4J_{(C\text{-}F)}$ = 6.3 Hz, CH-6), 110.3 (C-4a), 123.1, 123.6 (q, $^1J_{(C\text{-}F)}$ = 277.29 Hz, CF_3), 127.5 (CH_{Ar}), 130.5 (CH_{Ar}), 136.2 (q, $^2J_{(C\text{-}F)}$ = 33.1 Hz, C-5), 146.8, 146.9, 151.2 (CO-2), 157.6 (C-7), 159.6 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –53.1 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 354 ($[M+H]^+$, 17), 353 ($[M]^+$, 100), 325 (20), 268 (14), 267 (15), 241 (11), 213 (41). HRMS (EI): Calcd. for $C_{16}H_{14}F_3N_3O_3$ $[M]^+$: 353.09818, found: 353.09811. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2991 (w), 1742 (s), 1675 (s), 1623 (m), 1583 (s), 1504 (w), 1471 (m), 1455 (m), 1425 (m), 1414 (s), 1386 (s), 1372 (s), 1324 (w), 1288 (s), 1232 (s), 1209 (s), 1171 (s), 1159 (s), 1123 (s), 1066 (w), 1040 (s), 988 (m), 953 (w), 916 (w), 861 (w), 845 (s), 830 (m), 806 (m), 773 (w), 764 (w), 748 (s), 709 (w), 698 (s), 679 (m), 667 (w), 653 (w), 578 (s), 559 (w), 537 (w).

5-(Difluoromethyl)-7-ethoxy-1,3-dimethylpyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4r). The product was prepared according to the general procedure, starting from 0.469 g of **3r** and 2.3 mL of H_2SO_4. Yield 0.354 g (80%), yellow solid, mp 238 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 1.50 (t, 3H, ^3J = 6.99 Hz, EtO), 3.51 (s, 3H, CH_3-3), 3.81 (s, 3H, CH_3-1), 4.19 (q, 2H, ^3J = 6.99 Hz, EtO), 7.50 (dd, 1H, ^3J = 9.26 Hz, ^4J = 2.64 Hz, H-8), 7.76 (d, 1H, ^4J = 2.64 Hz, H-6), 7.89 (d, 1H, ^3J = 9.26 Hz, H-9), 8.86 (t, 1H, $^2J_{(H-F)}$ = 53.92 Hz, CH_2F). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 14.9 ($CH_{3(EtO)}$), 29.3 (CH_3-3), 30.6 (CH_3-1), 64.3 ($CH_{2(EtO)}$), 105.2 (t, $^4J_{(C-F)}$ = 6.0 Hz, CH-6), 108.6 (C-4a), 112.1 (t, $^1J_{(C-F)}$ = 239.6 Hz, CHF_2), 123.0, 127.6 (CH_{Ar}), 130.3 (CH_{Ar}), 141.9 (t, $^2J_{(C-F)}$ = 23.7 Hz, C-5), 146.5, 146.5, 151.0 (CO-2), 157.2, 161.9. ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –112.5 (s, CHF_2). MS (GC, 70 eV): *m/z* (%) = 336 ($[M+H]^+$, 18), 335 ($[M]^+$, 100), 307 (46), 306 (13), 279 (14), 256 (13), 195 (43). HRMS (EI): Calcd. for $C_{16}H_{15}F_2N_3O_3$ $[M]^+$: 335.10760, found: 335.10773. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3353 (w), 3139 (w), 3078 (w), 2989 (w), 2942 (w), 2918 (w), 2849 (w), 1705 (s), 1659 (s), 1621 (m), 1583 (m), 1538 (w), 1499 (w), 1477 (m), 1462 (m), 1450 (m), 1422 (m), 1412 (m), 1384 (m), 1321 (w), 1290 (m), 1271 (w), 1251 (w), 1223 (m), 1185 (m), 1148 (m), 1116 (m), 1095 (m), 1029 (s), 992 (m), 978 (m), 955 (w), 936 (m), 900 (w), 843 (s), 827 (m), 806 (s), 767 (w), 759 (w), 747 (s), 719 (m), 682 (m), 581 (s), 555 (m).

5-(Difluoromethyl)-7-methoxy-1,3-dipropylpyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4s). The product was prepared according to the general procedures for the synthesis of **3** and **4**, starting from 0.3 g of 6-[(4-methoxyphenyl)amino]-1,3-dipropylpyrimidine-2,4(1*H*,3*H*)-dione **2j**, 0.09 g of pyridine and 0.329 g of difluoroacetic anhydride in 3 mL of dioxane; than to isolated crude product were added 2 mL of H_2SO_4. Yield 0.307 g (86% after two steps; calculated on **2j**), yellow solid, mp 167-168 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 0.94-1.11 (m, 6H, $CH_{3(Pr-1)}$, $CH_{3(Pr-3)}$), 1.66-1.89 (m, 4H, $CH_{2(Pr-1)}$, $CH_{2(Pr-3)}$), 3.95 (s, 3H, MeO), 4.06 (t, 2H, ^3J = 7.55 Hz, NCH_2-3), 4.41 (t, 2H, ^3J = 7.46 Hz, NCH_2-1), 7.48 (d, 1H, H-8), 7.77 (s, 1H, H-6), 7.88 (d, 1H, ^3J = 9.15 Hz, H-9), 8.86 (t, 1H, $^2J_{(H-F)}$ = 54.01 Hz, CH_2F). ^{13}C NMR (75.48 MHz, $CDCl_3$): δ = 11.6 ($CH_{3(Pr)}$), 11.7 ($CH_{3(Pr)}$), 21.3 ($CH_{2(Pr)}$), 21.4 ($CH_{2(Pr)}$), 44.3 ($CH_{2(Pr)}$), 45.0 ($CH_{2(Pr)}$), 55.9 (MeO), 104.5 (t, $^4J_{(C-F)}$ = 6.0 Hz, CH-6), 108.8 (C-4a), 112.2 (t, $^1J_{(C-F)}$ = 239.11 Hz, CHF_2), 122.9, 127.2 (CH_{Ar}), 130.4 (CH_{Ar}), 142.0 (t, $^2J_{(C-F)}$ = 23.7 Hz, C-5), 146.3, 146.7, 150.5 (CO-2), 157.7, 161.6. ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –112.4 (s, CHF_2). MS (GC, 70 eV): *m/z* (%) = 378 ($[M+H]^+$, 17), 377 ($[M]^+$, 76), 336 (18), 335 (100), 307 (17), 294 (21), 293 (100), 277 (26), 265 (15), 263 (23), 250 (14), 249 (18), 236 (12), 208 (14), 188 (16). HRMS (EI): Calcd. for $C_{19}H_{21}F_3N_3O_3$ $[M]^+$: 377.15455, found: 377.15478. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3356 (w), 3093 (w), 3004 (w), 2963 (w), 2936 (w), 2876 (w), 2834 (w), 1703 (m), 1655 (s), 1622 (m), 1589 (s), 1572 (s), 1505 (w), 1457 (m), 1442 (s), 1423 (w), 1411 (s), 1396 (s), 1370 (m), 1348 (w), 1322 (m), 1302 (w), 1282 (w), 1271 (m), 1253 (w), 1226 (s), 1187 (w), 1175 (w), 1142 (m), 1112 (m), 1049 (m), 1031 (w), 1015 (s), 966 (w), 920 (w), 903 (w), 872 (w), 837 (s), 807 (m), 772 (w), 759 (w), 749 (m), 729 (w), 707 (m), 696 (w), 674 (m), 622 (w), 570 (m), 560 (m), 530 (m).

7-Methoxy-5-(pentafluoroethyl)-1,3-dipropylpyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (4t). The product was prepared according to the general procedure, starting from 0.342 g of **3t** and 1.7 mL of H_2SO_4. Yield 0.265 (81%), yellow solid, mp 115 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 0.98 (t, 3H, ^3J = 7.55 Hz, $CH_{3(Pr)}$), 1.03 (t, 3H, ^3J = 7.36 Hz, $CH_{3(Pr)}$), 1.66-1.89 (m, 4H, $CH_{2(Pr\text{-}1)}$, $CH_{2(Pr\text{-}3)}$), 3.93 (s, 3H, MeO), 4.05 (t, 2H, ^3J = 7.55 Hz, NCH_2-3), 4.40 (t, 2H, ^3J = 7.55 Hz, NCH_2-1), 7.44-7.53 (m, 2H, H-6, H-8), 7.91 (d, 1H, ^3J = 9.07 Hz, H-9). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 11.58 ($CH_{3(Pr)}$), 11.64 ($CH_{3(Pr)}$), 21.37 ($CH_{2(Pr)}$), 21.43 ($CH_{2(Pr)}$), 44.4 ($CH_{2(Pr)}$), 45.0 ($CH_{2(Pr)}$), 55.8 (MeO), 103.6 (CH-6), 111.5 (C-4a), 123.7, 127.0 (CH_{Ar}), 130.7 (CH_{Ar}), 137.7 (t, $^2J_{(C\text{-}F)}$ = 23.8 Hz, C-5), 146.7, 146.9, 150.7 (CO-2), 158.0 (C-7), 159.4 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –92.6 (s, CF_2), –74.9 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 446 ($[M–F]^+$, 18), 445 (80), 404 (20), 403 (100), 375 (12), 361 (18), 346 (11), 345 (28), 334 (38), 333 (26), 331 (38), 319 (18), 318 (64), 317 (33), 304 (16), 277 (12), 274 (10), 206 (10), 41 (14). HRMS (EI): Calcd. for $C_{20}H_{20}F_5N_3O_3$ $[M]^+$: 455.14193, found: 455.14179. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3371 (w), 2969 (w), 2940 (w), 2882 (w), 2833 (w), 1712 (m), 1668 (s), 1622 (m), 1565 (m), 1504 (m), 1449 (s), 1442 (s), 1407 (m), 1390 (s), 1368 (m), 1325 (m), 1301 (m), 1272 (w), 1255 (w), 1226 (s), 1181 (s), 1157 (s), 1140 (s), 1120 (s), 1047 (s), 1030 (m), 1011 (s), 975 (m), 959 (m), 902 (w), 895 (w), 872 (w), 845 (s), 828 (m), 802 (m), 755 (m), 742 (m), 724 (s), 691 (m), 685 (m), 676 (m), 642 (w), 635 (w), 600 (m), 564 (s), 529 (m).

1,1',3,3'-Tetramethyl-5,5'-bis(trifluoromethyl)-7,7'-bipyrimido[4,5-*b*]quinoline-2,2',4,4'(1*H*,1'*H*,3*H*,3'*H*)-tetrone (4u). The product was prepared according to the general procedure, starting from 0.329 g of **3u** and 1.6 mL of H_2SO_4. Yield 0.143 (46%), yellow solid, mp > 375 °C. ^{1}H NMR (300.13 MHz, 12% TFA-*d* in $CDCl_3$): δ = 3.60 (s, 6H, CH_3-3, CH_3-3'), 3.96 (s, 6H, CH_3-1, CH_3-1'), 8,30 (s, 4H, H-8, H-9, H-8', H-9'), 8.66 (s, 2H, H-6, H-6'). ^{13}C NMR (75.47 MHz, TFA-*d*): δ = 31.5 (CH_3), 33.0 (CH_3), 114.3 (C-4a, C-4a'), 124.0, 124.1 (q, $^1J_{(C\text{-}F)}$ = 278.9 Hz, CF_3), 127.1 (CH), 127.8 (q, $^4J_{(C\text{-}F)}$ = 5.7 Hz, CH-6, CH-6'), 138.1 (CH), 142.0, 145.5, 147.1 (q, $^2J_{(C\text{-}F)}$ = 35.4 Hz), 150.0, 152.6 (CO-2, CO-2'), 160.9 (CO-4, CO-4'). ^{19}F NMR (282.38 MHz, 12% TFA-*d* in $CDCl_3$): δ = –52.7 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 617 ($[M+H]^+$, 26), 616 ($[M]^+$, 100), 504 (39), 406 (10), 196 (22), 69 (11). HRMS (EI): Calcd. for $C_{28}H_{18}F_6N_6O_4$ $[M]^+$: 616.12882, found: 616.12925. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3070 (w), 2960 (w), 1716 (s), 1680 (s), 1619 (w), 1567 (s), 1499 (w), 1468 (m), 1434 (s), 1399 (m), 1384 (m), 1370 (m), 1357 (m), 1331 (s), 1288 (m), 1271 (m), 1205 (m), 1168 (s), 1145 (s), 1106 (s), 1062 (m), 1044 (w), 986 (m), 926 (w), 868 (w), 835 (s), 808 (m), 788 (w), 771 (w), 760 (w), 747 (s), 727 (w), 712 (w), 699 (m), 677 (w), 643 (m), 602 (m), 555 (m), 535 (w).

7,7'-Methylenebis[1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione] (4v). The product was prepared according to the general procedure, starting from 0.46 g of **3v** and 2.3 mL of H_2SO_4. Yield 0.224 (51%), yellow solid, mp 368-370 °C. ^{1}H NMR (300.13 MHz, 12% TFA-*d* in $CDCl_3$): δ = 3.60 (s, 6H, CH_3-3, CH_3-3'), 3.96 (s, 6H, CH_3-1, CH_3-1'), 4.46 (s, 2H, CH_2), 7.80 (d, 2H, ^3J =

8.87 Hz, H-8, H-8'), 8.14 (d, 2H, ^{3}J = 8.87 Hz, H-9, H-9'), 8.24 (s, 2H, H-6, H-6'). ^{13}C NMR (62.90 MHz, 12% TFA-*d* in $CDCl_3$): δ = 30.1 (CH_3), 31.3 (CH_3), 42.8 (CH_2), 110.2, 122.4, 123.0 (q, $^{1}J_{(C-F)}$ = 278.4 Hz, CF_3), 125.6 (q, $^{4}J_{(C-F)}$ = 5.9 Hz, CH-6, CH-6'), 129.4 (CH), 136.0 (CH), 139.5 (q, $^{2}J_{(C-F)}$ = 35.7 Hz), 139.8, 147.7, 149.2, 152.2 (CO-2, CO-2'), 160.2 (CO-4, CO-4'). ^{19}F NMR (282.38 MHz, 12% TFA-*d* in $CDCl_3$): δ = –52.8 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 631 ($[M+H]^+$, 30), 630 ($[M]^+$, 100), 561 (13), 518 (19), 498 (32), 429 (16), 203 (30), 69 (29), 44 (16), 40 (21). HRMS (EI): Calcd. for $C_{29}H_{20}F_6N_6O_4$ $[M]^+$: 630.14447, found: 630.14403. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3372 (w), 3078 (w), 2952 (w), 1719 (m), 1667 (s), 1621 (w), 1580 (s), 1564 (m), 1495 (w), 1470 (s), 1462 (s), 1456 (s), 1414 (m), 1292 (m), 1272 (m), 1215 (m), 1192 (m), 1163 (s), 1127 (s), 1108 (s), 1064 (m), 987 (m), 920 (w), 897 (w), 860 (w), 847 (w), 837 (m), 820 (w), 811 (m), 770 (w), 747 (s), 721 (w), 708 (m), 696 (m), 677 (w), 667 (w), 638 (m), 574 (m), 564 (w), 542 (w).

9,11-Dimethyl-7-(pentafluoroethyl)benzo[*h*]pyrimido[4,5-*b*]quinoline-8,10(9*H*,11*H*)-dione (4w). The product was prepared according to the general procedure, starting from 0.393 g of **3w** and 2 mL of H_2SO_4. Yield 0.307 (54%), yellow solid, mp 313-315 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.55 (s, 3H, CH_3-9), 3.98 (s, 3H, CH_3-11), 7.73-7.86 (m, 3H, CH_{Ar}), 7.91 (d, 1H, ^{3}J = 7.55 Hz, CH_{Ar}), 8.02-8.11 (m, 1H, CH_{Ar}), 9.20 (d, 1H, ^{3}J = 7.74 Hz, CH_{Ar}). ^{13}C NMR (62.90 MHz, 12% TFA-*d* in $CDCl_3$): δ = 30.1 (CH_3), 31.2 (CH_3), 109.4 (C-7a), 122.0 (CH-6), 122.2, 126.5 (CH), 128.2 (CH), 128.5 (CH), 129.7 (CH), 130.1, 131.7 (CH), 134.7, 139.4 (t, $^{2}J_{(C-F)}$ = 24.2 Hz), 147.6, 150.6, 152.5, 160.3 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –90.9 (s, CF_2), –74.9 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 410 ($[M+H]^+$, 23), 409 ($[M]^+$, 100), 352 (11), 311 (12), 298 (12), 297 (72). HRMS (EI): Calcd. for $C_{19}H_{12}F_5N_3O_2$ $[M]^+$: 409.08442, found: 409.08417. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3377 (w), 3056 (w), 2959 (w), 1719 (m), 1673 (s), 1620 (w), 1573 (m), 1562 (s), 1513 (w), 1503 (m), 1470 (m), 1450 (m), 1435 (w), 1422 (m), 1387 (w), 1367 (s), 1336 (m), 1295 (m), 1239 (w), 1226 (m), 1189 (s), 1159 (m), 1138 (s), 1113 (m), 1101 (m), 1074 (w), 1047 (m), 1028 (m), 997 (m), 969 (s), 934 (w), 885 (w), 878 (w), 834 (w), 810 (m), 796 (w), 787 (m), 761 (m), 747 (m), 735 (s), 726 (m), 708 (m), 682 (m), 663 (w), 628 (w), 594 (w), 566 (w), 558 (w), 543 (w).

3,6,8-Trimethyl-1-phenyl-4-(trifluoromethyl)-1*H*-pyrazolo[4',3':5,6]pyrido[2,3-*d*]pyrimidine-5,7(6*H*,8*H*)-dione (4x). The product was prepared according to the general procedure for the synthesis of compounds **3** from 0.477 g of **2n**, 0.136 g of pyridine and 0.603 g of trifluoroacetic anhydride in 4.5 mL of dry dioxane. Yield 0.42 g (75%, calculated on 1,3-dimethyl-6-[(3-methyl-1-phenyl-1*H*-pyrazol-5-yl)amino]pyrimidine-2,4(1*H*,3*H*)-dione **2n**, which cyclizes immediately while acylated by TFAA; non-cyclized intermediate product hasn't been obtained), yellow solid, mp 254 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 2.73 (q, 3H, $^{6}J_{(H-F)}$ = 3.07 Hz, CH_3-3) 3.51 (s, 3H, CH_3-6), 3.78 (s, 3H, CH_3-8), 7.36 (t, 1H, ^{3}J = 7.46 Hz, CH_{Ph}), 7.50-7.59 (m, 2H, CH_{Ph}), 8.12-8.20 (m, 2H, CH_{Ph}). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 17.5 (q, $^{5}J_{(C-F)}$ = 7.4 Hz, CH_3-3), 29.3 (CH_3-6), 31.1 (CH_3-8), 104.5, 111.8, 121.3 (CH_{Ph}), 122.3 (q,

$^{1}J_{(C\text{-}F)}$ = 278.8 Hz, CF_3), 127.0 (CH_{Ph}), 129.4 (CH_{Ph}), 136.7 (q, $^{2}J_{(C\text{-}F)}$ = 37.3 Hz, C-4), 138.4, 144.5, 151.00, 151.04, 151.06, 159.1 (CO-5). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –54.6 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 390 ($[M+H]^+$, 20), 389 ($[M]^+$, 100), 277 (33), 276 (17), 77 (21). HRMS (EI): Calcd. for $C_{18}H_{14}F_3N_5O_2$ $[M]^+$: 389.10941, found: 389.10929. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3114 (w), 2996 (w), 2956 (w), 1715 (s), 1669 (s), 1593 (m), 1575 (s), 1532 (m), 1504 (m), 1489 (s), 1470 (m), 1462 (m), 1456 (m), 1421 (s), 1411 (s), 1385 (m), 1367 (s), 1336 (s), 1272 (m), 1227 (s), 1210 (m), 1179 (m), 1152 (s), 1135 (s), 1117 (s), 1062 (m), 1043 (m), 1025 (m), 1000 (w), 987 (m), 970 (w), 911 (w), 864 (m), 845 (w), 805 (m), 774 (w), 763 (s), 754 (m), 746 (s), 700 (m), 691 (s), 661 (m), 645 (w), 632 (w), 601 (m), 539 (w).

2.4 Synthesis of 5-hydroxy-1,3-dimethyl-5-perfluoroalkyl-5,10-dihydro-5-deazaalloxazines

General procedure for the synthesis of 5-hydroxy-1,3-dimethyl-5-perfluoroalkyl-5,10-dihydro-1*H*-pyrimido[4,5-*b*]quinoline-2,4-diones 6a-c. Initial 5-(perfluoroacyl)-6-amino-1,3-dimethylrimidine-2,4(1*H*,3*H*)-dione **5** (1 g) was dissolved in concentrated H_2SO_4 (5 mL) and allowed to stand at r.t. for 2 hours. Then the solution was poured into ice water and extracted with chloroform, extracts were died over Na_2SO_4 and evaporated by rotovap. The crude product was purified via short-part column chromatography (silica gel / $CHCl_3$), followed by recrystallization from methanol to give pure product.

6-Hydroxy-8,10-dimethyl-6-(trifluoromethyl)-1,2-dihydro-6*H*-pyrimido[4,5-*b*]pyrrolo[3,2,1-*ij*]quinoline-7,9(8*H*,10*H*)-dione (6a). The product was prepared following the general procedure, starting from 0.336 g of **5a** and 1.7 mL of H_2SO_4. Yield 0.299 g (89%), white solid, mp 253-255 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.25 (s, 3H, CH_3), 3.26-3.49 (m, 2H, CH_2-2), 3.67 (s, 3H, CH_3), 4.22-4.35 (m, 1H, CH_2-1a), 4.80-4.92 (m, 1H, CH_2-1b), 7.25 (dd, 1H, $^{3}J_1$ = 7.74 Hz, $^{3}J_2$ = 7.36 Hz, H-4), 7.39 (d, 1H, ^{3}J = 7.36 Hz, CH_{Ar}), 7.45 (d, 1H, ^{3}J = 7.74 Hz, CH_{Ar}), 8.69 (s, 1H, OH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.5 (CH_3), 29.1 (CH_2), 37.7 (CH_3), 54.1 (CH_2), 72.7 (q, $^{2}J_{(C\text{-}F)}$ = 30.7 Hz, C-6), 80.6 (C-6a), 116.7 125.0 (CH_{Ar}), 125.9 (CH_{Ar}), 126.3 (CH_{Ar}), 126.7 (q, $^{1}J_{(C\text{-}F)}$ = 291.2 Hz, CF_3), 130.3, 140.8, 152.0, 152.7, 164.7. ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –82.5 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 285 ($[M+H–CF_3]^+$, 17), 284 ($[M–CF_3]^+$, 100), . HRMS (ESI): Calcd. for $C_{16}H_{14}F_3N_3NaO_3$ $[M+Na]^+$: 376.08795, found: 376.08866. Anal. Calcd for $C_{16}H_{14}F_3N_3O_3$: C, 54.39; H, 3.99; N, 11.89. Found: C, 54.30; H, 4.05; N, 11.52. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3029 (m), 2967 (m), 1695 (s), 1639 (w), 1606 (m), 1544 (m), 1494 (s), 1462 (s), 1455 (s), 1443 (s), 1430 (s), 1401 (m), 1379 (m), 1360 (m), 1344 (m), 1301 (w), 1259 (m), 1242 (s), 1233 (s), 1220 (m), 1184 (w), 1156 (s), 1129 (s), 1157 (s), 1035 (m), 1005 (w), 991 (m), 964 (s), 936 (m), 866 (m), 832 (w), 783 (s), 773 (m), 764 (m), 753 (s), 745 (m), 716 (m), 704 (s), 679 (m), 616 (w), 574 (w), 534 (w).

7-(Heptafluoropropyl)-7-hydroxy-9,11-dimethyl-2,3-dihydro-1*H*,7*H*-pyrido[3,2,1-*ij*]pyrimido[4,5-*b*]quinoline-8,10(9*H*,11*H*)-dione (6b). The product was prepared following the general procedure,

starting from 0.2 g of **5b** and 1 mL of H_2SO_4. Yield 0.188 g (94%), white solid, mp 177 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 2.09-2.23 (m, 1H, CH_2-2a), 2.24-2.43 (m, 1H, CH_2-2b), 2.94-3.05 (m, 2H, CH_2-3), 3.25-3.35 (m, 1H, CH_2-1a), 3.35 (s, 3H, CH_3), 3.50 (s, 3H, CH_3),3.92-4.02 (m, 1H, CH_2-1b), 7.12-7.21 (m, 2H, CH_{Ar}), 7.60-7.67 (m, 1H, CH_{Ar}), 8.41 (s, 1H, OH). ^{13}C NMR (75.48 MHz, $CDCl_3$): δ = 22.8 (CH_2), 25.4 (CH_2), 28.3 (CH_3), 37.5 (CH_3), 47.3 (CH_2-1), 74.4 (t, $^2J_{(C\text{-}F)}$ = 25.2 Hz, C-7), 88.9 (C-7a), 123.1, 124.6 (CH_{Ar}), 125.3 (CH_{Ar}), 126.7, 129.7, 136.5 (CH_{Ar}), 150.5, 152.8, 165.1. ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –125.3 (dd, ^2J = 289.17 Hz, ^3J = 9.19 Hz, CF_2-1a), –123.6 (dd, ^2J = 289.17 Hz, ^3J = 7,16 Hz, CF_2-1b), 121.6 (m, CF_2-2), –80.8 (t, J = 12.27 Hz, CF_3). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3216 (m), 2956 (w), 2849 (w), 1693 (m), 1622 (m), 1601 (m), 1575 (m), 1504 (m), 1462 (s), 1455 (s), 1428 (s), 1407 (m), 1389 (w), 1371 (m), 1345 (m), 1286 (w), 1250 (w), 1206 (s), 1184 (s), 1116 (s), 1091 (m), 1061 (m), 1045 (m), 1032 (m), 1003 (w), 984 (w), 942 (w), 907 (w), 878 (w), 856 (m), 827 (w), 807 (w), 782 (m), 769 (m), 746 (s), 733 (w), 701 (m), 676 (w), 667 (m), 646 (s), 589 (w), 575 (w), 568 (w), 550 (w), 530 (w).

5-Hydroxy-1,3,10-trimethyl-5-(trifluoromethyl)-5,10-dihydropyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (6c). The product was prepared following the general procedure, starting from 0.25 g of **5c** and 1.3 mL of H_2SO_4. Yield 0.18 g (72%), white solid, mp 216-218 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.26 (s, 3H, CH_3), 3.48 (s, 3H, CH_3), 3.51 (s, 3H, CH_3), 7.32 (dd, 1H, $^3J_1$ = 7.74 Hz, $^3J_2$ = 7.17 Hz, H-7), 7.46 (d, 1H, ^3J = 8.31 Hz, H-9), 7.55 (dd, 1H, $^3J_1$ = 8.31 Hz, $^3J_2$ = 7.17 Hz, H-8), 7.67 (d, 1H, ^3J = 7.74 Hz, H-6), 8.45 (br s, 1H, OH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 28.5 (CH_3), 37.3 (CH_3), 41.8 (CH_3), 71.8 (q, $^2J_{(C\text{-}F)}$ = 30.5 Hz), 88.1 (C-4a), 119.3 (CH), 125.2 (CH), 126.2 (q, $^1J_{(C\text{-}F)}$ = 290.5 Hz, CF_3), 126.7 (CH), 130.8 (CH), 141.7, 152.4, 153.3, 165.0. ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –83.1 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 273 (41), 272 (100), 257 (10). HRMS (ESI): Calcd. for $C_{15}H_{15}F_3N_3O_3$ $[M+H]^+$: 342.10600, found: 342.10635. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3271 (w), 3190 (w), 2980 (w), 1703 (s), 1687 (m), 1622 (s), 1608 (s), 1574 (m), 1504 (s), 1487 (s), 1470 (s), 1464 (s), 1456 (s), 1423 (s), 1396 (m), 1381 (m), 1323 (m), 1254 (s), 1207 (m), 1161 (s), 1119 (s), 1090 (m), 1070 (s), 1049 (s), 972 (m), 955 (w), 937 (m), 922 (s), 866 (w), 833 (m), 779 (s), 768 (s), 760 (s), 746 (s), 710 (s), 662 (s), 642 (s), 602 (m), 565 (m), 550 (m), 538 (m).

2.5 Synthesis of 9-(ω-chloroalkyl)-1,3-dimethyl-5-trifluoromethyl-5-deazaalloxazines

Synthesis of 9-(2-Chloroethyl)-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione 7a and 9-(3-Chloropropyl)-5-(heptafluoropropyl)-1,3-dimethylpyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione 7b. General procedure. A starting material (6-hydroxy-8,10-dimethyl-6-(trifluoromethyl)-1,2-dihydro-6*H*-pyrimido[4,5-*b*]pyrrolo[3,2,1-*ij*]quinoline-7,9(8*H*,10*H*)-dione **6a** or 7-(heptafluoropropyl)-7-hydroxy-9,11-dimethyl-2,3-dihydro-1*H*,7*H*-pyrido[3,2,1-*ij*]pyrimido[4,5-*b*]quinoline-8,10(9*H*,11*H*)-dione **6b**) was dissolved in chloroform and then refluxed with thionyl chloride

(2 eq) for 3 hours till the solid phase disappeared. Afterwards the solvent was evaporated and the crude product was purified via short-part column chromatography (silica gel / $CHCl_3$), followed by recrystallization from methanol.

9-(2-Chloroethyl)-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (7a). The product was prepared following the general procedure, starting from 0.4 g of **6a**, 0.269 g of thionyl chloride and 8 mL of chloroform. Yield 100%, yellow solid, mp 151-153 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.52 (s, 3H, CH_3-3), 3.67 (t, 2H, ^3J = 7.55 Hz, Ar-CH_2-), 3.83 (s, 3H, CH_3-1), 3.94 (t, 2H, ^3J = 7.55 Hz, CH_2Cl), 7.55 (dd, 1H, $^3J_1$ = 8.97 Hz, $^3J_2$ = 6.99 Hz, H-7), 7.78 (d, 1H, ^3J = 6.99 Hz, H-8), 8.23-8.30 (dm, 1H, ^3J = 8.97 Hz, H-6). ^{13}C NMR (75.48 MHz, $CDCl_3$): δ = 29.5 (CH_3-3), 30.7 (CH_3-1), 36.1 (Ar-CH_2-), 44.2 (CH_2Cl), 110.4 (C-4a), 122.1, 123.2 (q, $^1J_{(C-F)}$ = 278.3 Hz, CF_3), 125.4 (q, $^4J_{(C-F)}$ = 6.0 Hz, CH-6), 126.9 (CH_{Ar}), 134.4 (CH_{Ar}), 136.1, 139.3 (q, $^2J_{(C-F)}$ = 33.5 Hz, C-5), 147.6, 148.6, 151.2 (CO-2), 159.3 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –52.4 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 371 ($[M]^+$, ^{35}Cl, 7.9), 337 ($[M+H–Cl]^+$, 20), 336 ($[M–Cl]^+$, 100), 279 (29). HRMS (ESI): Calcd. for $C_{16}H_{13}F_3N_3O_2$ $[M-Cl]^+$: 336.09544, found: 336.09572. Anal. Calcd for $C_{16}H_{13}ClF_3N_3O_2$: C, 51.69; H, 3.52; N, 11.30. Found: C, 47.85; H, 3.52; N, 10.05. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2953 (w), 1718 (m), 1669 (s), 1607 (w), 1574 (s), 1494 (w), 1479 (m), 1464 (m), 1467 (m), 1445 (m), 1421 (m), 1391 (m), 1375 (m), 1352 (m), 1327 (m), 1290 (m), 1277 (m), 1224 (s), 1195 (m), 1158 (s), 1134 (s), 1116 (s), 1079 (m), 1032 (m), 977 (m), 928 (w), 875 (m), 845 (w), 828 (w), 794 (m), 780 (m), 770 (s), 746 (s), 723 (m), 711 (m), 700 (s), 682 (m), 605 (w), 579 (m), 564 (m), 551 (m), 541 (m).

9-(3-Chloropropyl)-5-(heptafluoropropyl)-1,3-dimethylpyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (7b). The product was prepared following the general procedure, starting from 1.2 g of **6b**, 0.611 g of thionyl chloride and 24 mL of chloroform. Yield 1.121 g (90%), yellow solid, mp 113-114 °C. ^{1}H NMR (250.13 MHz, $CDCl_3$): δ = 2.19-2.34 (m, 2H, CH_2), 3.40 (t, 2H, ^3J = 7.41 Hz, Ar-CH_2-), 3.51 (s, 3H, CH_3-3), 3.60 (t, 2H, ^3J = 6.31 Hz, CH_2Cl), 3.85 (s, 3H, CH_3-1), 7.52 (dd, 1H, $^3J_1$ = 8.99 Hz, $^3J_2$ = 6.94 Hz, H-7), 7.76 (d, 1H, ^3J = 6.94 Hz, H-8), 8.22 (d, 1H, ^3J = 8.99 Hz, H-5). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 29.7 (CH_3-3), 30.0 (CH_2), 30.9 (CH_3-1), 33.1 (CH_2), 45.0 (CH_2), 111.5 (C-4a), 123.1 (C-5a), 125.5 (m, CH-6), 127.1 (CH), 133.4 (CH), 139.4, 140.4 (t, $^2J_{(C-F)}$ = 24.0 Hz, C-5), 147.7, 148.7, 151.1 (CO-2), 159.1 (CO-4). ^{19}F NMR (235.33 MHz, $CDCl_3$): δ = –116.5 (s, CF_2), –90.4 (br s, CF_2), –80.0 (t, *J* = 9.54 Hz, CF_3). MS (GC, 70 eV): *m/z* (%) = 485 ($[M]^+$, ^{35}Cl, 15), 451 (21), 450 (100), 436 (36), 423 (28), 393 (16), 311 (10). HRMS (ESI): Calcd. for $C_{19}H_{16}ClF_7N_3O_2$ $[M+H, ^{35}Cl]^+$: 486.08138, found: 486.08130. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2958 (w), 2929 (w), 1722 (s), 1678 (s), 1612 (w), 1568 (s), 1504 (m), 1479 (m), 1462 (m), 1423 (s), 1392 (m), 1371 (m), 1344 (m), 1319 (m), 1311 (m), 1288 (m), 1269 (m), 1255 (m), 1227 (s), 1211 (s), 1188 (s), 1171 (s), 1132 (s), 1113 (s), 1078 (s), 1047 (m), 1020 (m), 980 (m), 949 (m), 910 (s), 878 (m), 825 (m), 798 (m), 785 (s), 777 (s), 760 (s), 743 (s), 731 (s), 721 (s), 700 (s), 692 (s), 623 (s), 617 (s), 590 (m), 565 (m), 550 (s), 536 (m).

2.6 Suzuki–Miyaura cross-coupling with 7-bromo-1,3-dimethyl-5-(trifluoromethyl)-5-deazaalloxazine

1,3-Dimethyl-7-phenyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (10). A sealed ACE pressure tube was charged with 0.05 g of 7-bromo-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione **4p** (0.13 mmol, 1 eq), 0.019 g of phenylboronic acid (0.15 mmol, 1.2 eq), 0.053 g of K_2CO_3 (0.039 mmol, 3 eq), 0.003 g of $Pd(PPh_3)_4$ (0.0026 mmol, 0.02 eq), 2.5 mL of dioxane and 0.5 mL of water. The reaction mixture was stirred under argon at 100 °C for half an hour. After cooling to r.t. formed precipitate was filtered off by suction, washed twice with methanol and dried in high vacuum to give the pure product. Yield 0.047 g (95%), green solid, mp 230 °C. ^{1}H NMR (300.13 MHz, 12% TFA-*d* in $CDCl_3$): δ = 3.58 (s, 3H, CH_3-3), 3.94 (s, 3H, CH_3-1), 7.44-7.59 (m, 3H, CH_{Ph}), 7.68-7.74 (m, 2H, CH_{Ph}), 8.23 (s, 2H, H-8, H-9), 8.53 (s, 1H, H-6). ^{13}C NMR (62.90 MHz, 12% TFA-*d* in $CDCl_3$): δ = 30.1 (CH_3-3), 31.3 (CH_3-1), 110.3 (C-4a), 122.6, 122.7 (q, $^1J_{(C\text{-}F)}$ = 278.4 Hz, CF_3), 123.8 (q, $^4J_{(C\text{-}F)}$ = 6.0 Hz, CH-6), 128.1 (CH_{Ar}), 129.0 (CH_{Ar}), 129.1 (CH_{Ar}), 129.7 (CH_{Ar}), 134.9 (CH_{Ar}), 139.5, 140.1 (q, $^2J_{(C\text{-}F)}$ = 33.8 Hz, C-5), 141.4, 147.4, 149.2, 152.2 (CO-2), 160.3 (CO-4). ^{19}F NMR (282.38 MHz, 12% TFA-*d* in $CDCl_3$): δ = –52.8 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 386 ($[M+H]^+$, 23), 385 ($[M]^+$, 100), 316 (10), 287 (16), 274 (14), 273 (78), 259 (13). HRMS (EI): Calcd. for $C_{20}H_{14}F_3N_3O_2$ $[M]^+$: 385.10326, found: 385.10314. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3379 (w), 3054 (w), 2958 (w), 1720 (m), 1668 (s), 1651 (m), 1621 (w), 1574 (s), 1516 (w), 1469 (s), 1433 (s), 1328 (m), 1293 (m), 1281 (m), 1212 (m), 1165 (s), 1152 (s), 1131 (s), 1074 (m), 1027 (w), 994 (m), 942 (w), 918 (w), 894 (w), 883 (w), 860 (w), 843 (m), 807 (m), 765 (m), 756 (s), 744 (s), 706 (m), 694 (s), 674 (m), 639 (m), 617 (w), 607 (w), 594 (w), 557 (m), 540 (w).

2.7 Sonogashira cross-coupling with 7-bromo-1,3-dimethyl-5-(trifluoromethyl)-5-deazaalloxazine

Sonogashira coupling with 7-bromo-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione 4p. General procedure. Into a flask were placed 7-bromo-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione **4p** (1 eq), terminal acetylene (1.2 eq), $Pd(PPh_3)_2Cl_2$ (0.02 eq), CuI (0.01 eq), diisopropylamine (10 eq) and THF (1 mL per 0.05 g of starting aryl bromide). The mixture was stirred for 3 hours and then allowed to stay at r.t. for two days. After that the reaction mixture was diluted with water, the formed precipitate was filtered off by suction, washed with methanol and heptane and dried in high vacuum.

1,3-Dimethyl-7-(phenylethynyl)-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (11a). The product was prepared following the general procedure, starting from 0.05 g of 8-bromo derivative **4p**, 0.016 g of phenylacetylene, 0.9 mg of $Pd(PPh_3)_2Cl_2$, 0.12 mg of CuI, 0.13 g of

diisopropylamine and 1 mL of THF. Yield 0.047 g (89%), yellow solid, mp 269 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.51 (s, 3H, CH_3-3), 3.82 (s, 3H, CH_3-1), 7.35-7.44 (m, 3H, CH_{Ph}), 7.55-7.62 (m, 2H, CH_{Ph}), 7.90 (d, 1H, ^{3}J = 8.88 Hz, H-8), 7.99 (d, 1H, ^{3}J = 8.88 Hz, H-9), 8.46 (s, 1H, H-6). ^{13}C NMR (75.48 MHz, $CDCl_3$): δ = 29.6 (CH_3-3), 30.8 (CH_3-1), 88.8 (C-sp), 92.4 (C-sp), 111.0 (C-4a), 121.6, 122.7, 122.8, 123.2 (q, $^{1}J_{(C-F)}$ = 278.4 Hz, CF_3), 128.8 (CH_{Ar}), 129.19 (q, $^{4}J_{(C-F)}$ = 6.1 Hz, CH-6), 129.26 (CH_{Ph}), 129.29 (CH_{Ph}), 132.1 (CH_{Ph}), 136.0 (CH_{Ar}), 138.2 (q, $^{2}J_{(C-F)}$ = 33.6 Hz, C-5), 148.7, 149.7, 151.1 (CO-2), 159.2 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –52.6 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 410 ($[M+H]^+$, 25), 409 ($[M]^+$, 100), 311 (15), 298 (11), 297 (54), 283 (16). HRMS (ESI): Calcd. for $C_{22}H_{15}F_3N_3O_2$ $[M+H]^+$: 410.11109, found: 410.11143. Anal. Calcd for $C_{22}H_{14}F_3N_3O_2$: C, 50.22; H, 3.58; N, 11.71. Found: C, 49.43; H, 3.21; N, 10.13. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3375 (w), 3061 (w), 2952 (w), 2213 (w), 1714 (s), 1674 (s), 1652 (m), 1616 (w), 1574 (s), 1558 (m), 1512 (w), 1505 (w), 1490 (w), 1470 (m), 1440 (s), 1418 (m), 1405 (m), 1386 (m), 1373 (s), 1324 (m), 1303 (m), 1290 (m), 1275 (m), 1207 (m), 1162 (s), 1143 (s), 1128 (s), 1070 (m), 1027 (w), 996 (m), 985 (m), 919 (w), 884 (w), 864 (w), 835 (s), 807 (w), 783 (w), 755 (m), 744 (s), 704 (m), 689 (s), 674 (w), 662 (m), 641 (w), 578 (m), 538 (w), 529 (m).

7-Hex-1-yn-1-yl-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (11b). The product was prepared following the general procedure, starting from 0.25 g of 8-bromo derivative **4p**, 0.063 g of phenylacetylene, 4.52 mg of $Pd(PPh_3)_2Cl_2$, 0.61 mg of CuI, 0.652 g of diisopropylamine and 5 mL of THF. Yield 0.234 (89%), yellow solid, mp 180 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 0.97 (t, 3H, ^{3}J = 7.27 Hz, Bu), 1.43-1.70 (m, 4H, Bu), 2.47 (t, 2H, Bu, ^{3}J = 7.08 Hz), 3.49 (s, 3H, CH_3-3), 3.78 (s, 3H, CH_3-1), 7.74 (d, 1H, ^{3}J = 8.87 Hz, H-8), 7.87 (d, 1H, ^{3}J = 8.87 Hz, H-9), 8.28 (s, 1H, H-6). ^{13}C NMR (75.48 MHz, $CDCl_3$): δ = 13.9 ($CH_{3(Bu)}$), 19.5 ($CH_{2(Bu)}$), 22.4 ($CH_{2(Bu)}$), 29.5 (CH_3-3), 30.7 (CH_3-1), 30.9 ($CH_{2(Bu)}$), 80.1 (C-sp), 94.0 (C-sp), 110.8 (C-4a), 121.5, 123.1 (q, $^{1}J_{(C-F)}$ = 278.5 Hz, CF_3), 123.4, 128.7 (q, $^{4}J_{(C-F)}$ = 6.1 Hz, CH-6), 128.9 (CH_{Ar}), 136.3 (CH_{Ar}), 137.8 (q, $^{2}J_{(C-F)}$ = 33.5 Hz, C-5), 148.3, 149.2, 151.0 (CO-2), 159.2 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –52.7 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 390 ($[M+H]^+$, 21), 389 ($[M]^+$, 100), 388 (12), 360 (23), 346 (30), 317 (14), 289 (21), 277 (27), 261 (10), 234 (23), 220 (15). HRMS (ESI): Calcd. for $C_{20}H_{19}F_3N_3O_2$ $[M+H]^+$: 390.14239, found: 390.14253. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3379 (w), 3089 (w), 2960 (w), 2934 (w), 2862 (w), 2228 (w), 1726 (m), 1671 (s), 1614 (w), 1581 (s), 1468 (s), 1451 (s), 1411 (m), 1386 (m), 1370 (s), 1322 (w), 1287 (m), 1240 (w), 1205 (m), 1173 (s), 1159 (s), 1145 (s), 1132 (s), 1108 (s), 1071 (m), 1019 (w), 989 (m), 956 (w), 933 (w), 887 (m), 858 (w), 854 (s), 807 (m), 775 (w), 761 (w), 748 (s), 728 (w), 704 (s), 689 (w), 672 (m), 659 (w), 641 (m), 589 (w), 575 (m), 538 (w).

2.8 Reduction of 5-(trifluoromethyl)-5-deazaalloxazines

Reduction of 5-polyfluoroalkyl-pyrimido[4,5-b]quinoline-2,4-diones 4. General procedure.

Method A. Into a 50-mL flask were placed 5-polyfluoroalkyl-pyrimido[4,5-b]quinoline-2,4-dione **4** (1.48 mmol, 1 eq), sodium cyanoborohydride (5.93 mmol, 4 eq) and THF (10 mL). Then the mixture was cooled to 0 °C and acetic acid (11.9 mmol, 8 eq) was added. Afterwards the reaction mixture was allowed to warm to r.t.. Three days later the reaction was monitored by TLC and stirred 8 hours at 45 °C, if the starting material still was detected. After that mixture was diluted with water. Precipitate was filtered off to give a pure product.

Method B. A sealed ACE pressure tube was charged with 0.1 g of 1,3,7,9-tetramethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione **4c** (0.30 mmol, 1 eq), 0.451 g of diethyl 1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylate (1.78 mmol, 6 eq), 0.0056 g of TsOH (0.03 mmol, 0.1 eq) and 3 mL of xylene. The reaction mixture was stirred under argon at 155 °C for 5 hours. Then the solution was cooled to r.t. and formed precipitate was filtered off, washed twice with xylene and dried in high vacuum to give the desired product.

1,3,7,9-Tetramethyl-5-(trifluoromethyl)-5,10-dihydropyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (8a). Yield 99% (**Method A**; starting from 0.5 g of **4c**, 0.373 g of sodium cyanoborohydride, 0.712 g of acetic acid and 10 mL of THF) and 41% (**Method B**), white solid, mp 263-265 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 2.32 (s, 6H, CH_3-7, CH_3-9), 3.40 (s, 3H, CH_3), 3.60 (s, 3H, CH_3), 4.88 (q, 1H, $^{3}J_{(H\text{-}F)}$ = 8.22 Hz, CH-5), 6.40 (br s, 1H, NH), 7.01 (s, 1H, CH_{Ar}), 7.04 (s, 1H, CH_{Ar}). ^{13}C NMR (75.47 MHz, DMSO-d_6): δ = 17.9 (Ar-CH_3), 21.1 (Ar-CH_3), 28.7 (N-CH_3), 30.4 (N-CH_3), 40.2 (q, $^{2}J_{(C\text{-}F)}$ = 29.2 Hz, CH-5), 79.6, 117.5, 126.4, 129.0 (CH), 127.4 (q, $^{1}J_{(C\text{-}F)}$ = 284.3 Hz, CF_3), 132.3 (CH), 133.6, 134.1, 148.7, 151.8, 161.7. ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –73.7 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 339 ($[M]^+$, 5.0), 271 (17), 270 ($[M–CF_3]^+$, 100), 213 (11). HRMS (ESI): Calcd. for $C_{16}H_{17}F_3N_3O_2$ $[M+H]^+$: 340.12674, found: 340.12665. Anal. Calcd for $C_{16}H_{16}F_3N_3O_2$: C, 56.64; H, 4.75; N, 12.38. Found: C, 56.72; H, 4.73; N, 12.10. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3457 (m), 3322 (w), 2914 (w), 1693 (m), 1633 (s), 1611 (m), 1520 (s), 1489 (m), 1475 (s), 1445 (m), 1418 (w), 1382 (w), 1354 (w), 1336 (m), 1326 (m), 1275 (w), 1240 (s), 1218 (m), 1180 (w), 1146 (s), 1107 (s), 1057 (w), 1042 (w), 991 (w), 968 (w), 951 (w), 936 (w), 900 (w), 870 (w), 844 (m), 820 (w), 777 (w), 768 (m), 751 (s), 710 (w), 696 (w), 681 (w), 667 (m), 580 (w), 568 (w).

7-Ethyl-1,3-dimethyl-5-(trifluoromethyl)-5,10-dihydropyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (8b). The product was prepared according to the **Method A**, starting from 0.15 g of **4f**, 0.112 g of sodium cyanoborohydride, 0.214 g of acetic acid and 3 mL of THF. Yield 0.144 g (95%), white solid, mp 241 °C. ^{1}H NMR (250.13 MHz, DMSO-d_6): δ = 1.20 (t, 3H, ^{3}J = 7.57 Hz, Et), 2.61 (q, 2H, ^{3}J = 7.57 Hz, Et), 3.24 (s, 3H, CH_3), 3.51 (s, 3H, CH_3), 4.91 (q, 1H, $^{3}J_{(H\text{-}F)}$ = 8.51 Hz, CH-5), 7.23 (dd, 1H, ^{3}J = 8.20 Hz, ^{4}J = 1.82 Hz, H-8), 7.28 (s, 1H, H-6), 7.35 (d, 1H, ^{3}J = 8.20 Hz, H-9), 9.57 (br s, 1H, NH). ^{13}C NMR (62.90

MHz, DMSO-d_6): δ = 16.5 (CH_3), 28.4 (CH_2), 28.7 (CH_3), 30.9 (CH_3), 40.0 (q, $^2J_{(C-F)}$ = 28.9 Hz, CH-5), 77.3 (C-4a), 115.6, 117.6 (CH_{Ar}), 127.4 (q, $^1J_{(C-F)}$ = 284.3 Hz, CF_3), 129.3 (CH_{Ar}), 130.0 (CH_{Ar}), 136.4, 140.0, 148.5, 151.6, 161.6. ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –72.7 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 339 ($[M]^+$, 3.7), 271 (18), 270 ($[M–CF_3]^+$, 100), 213 (13). HRMS (EI): Calcd. for $C_{16}H_{16}F_3N_3O_2$ $[M]^+$: 339.11891, found: 339.11894. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3275 (m), 3206 (w), 3139 (w), 2973 (w), 2893 (w), 1701 (s), 1633 (m), 1607 (s), 1557 (s), 1497 (s), 1476 (s), 1460 (m), 1429 (m), 1394 (w), 1368 (w), 1328 (m), 1312 (m), 1292 (w), 1282 (w), 1258 (m), 1237 (s), 1217 (m), 1189 (m), 1157 (s), 1148 (m), 1141 (m), 1121 (m), 1113 (s), 1049 (w), 981 (m), 952 (w), 929 (w), 895 (w), 846 (m), 833 (m), 813 (w), 803n (w), 773 (m), 750 (m), 727 (w), 713 (m), 676 (m), 667 (m), 642 (m), 577 (w), 555 (w), 545 (w).

2.9 Alkylation of 1,3,7,9-tetramethyl-5-(trifluoromethyl)-5,10-dihydro-5-deazaalloxazine

(4a*R*,5*R*)- and (4a*S*,5*S*)-4a-Benzyl-1,3,7,9-tetramethyl-5-(trifluoromethyl)-4a,5-dihydropyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (9), racemic mixture of enantiomers. A mixture of 1,3,7,9-tetramethyl-5-(trifluoromethyl)-5,10-dihydropyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione **8a** (0.1 g, 0.29 mmol, 1 eq), benzyl bromide (0.055 g, 0.32 mmol, 1.1 eq), K_2CO_3 (0.081 g, 0.59 mmol, 2 eq) and DMF (2 mL) was stirred overnight under argon. The next day the reaction mixture was diluted with water and heptane. The formed precipitate was filtered off by suction, washed twice with water and heptanes and dried in high vacuum to give the pure product. Yield 104 g (82%), white solid, mp 159-161 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 2.39 (s, 3H, Ar-CH_3), 2.51 (s, 3H, Ar-CH_3), 3.00 (d, 1H, ^2J = 12.56 Hz, CH_2-a), 3.09 (d, 1H, ^2J = 12.56 Hz, CH_2-b), 3.15 (s, 3H, N-CH_3), 3.28 (s, 3H, N-CH_3), 4.00 (q, 1H, $^3J_{(H-F)}$ = 8.25 Hz, H-5), 6.82-6.91 (m, 2H, $CH_{o\text{-}Ph}$), 6.99 (s, 1H, H-6), 7.17 (s, 1H, H-8), 7.20-7.32 (m, 3H, CH_{Ph}). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 17.9 (CH_3), 21.4 (CH_3), 28.4 (CH_3), 29.8 (CH_3), 42.9 (CH_2), 47.8 (C-4a), 48.8 (q, $^2J_{(C-F)}$ = 26.8 Hz, CH), 118.7, 125.4 (q, $^1J_{(C-F)}$ = 283.4 Hz, CF_3), 128.7 (CH), 128.7 (CH), 128.7 (CH), 129.4 (CH), 133.0 (CH), 133.5, 134.4, 136.0, 139.2, 150.2, 151.6, 168.8. ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –65.5 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 430 ($[M+H]^+$, 14), 429 ($[M]^+$, 51), 91 (100). HRMS (EI): Calcd. for $C_{23}H_{22}O_2N_3F_3$ $[M]^+$: 429.16586, found: 429.16570. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2933 (w), 2920 (w), 1726 (m), 1682 (s), 1622 (s), 1597 (s), 1471 (m), 1443 (s), 1427 (s), 1381 (s), 1344 (m), 1325 (s), 1315 (s), 1294 (s), 1273 (s), 1255 (s), 1238 (s), 1215 (m), 1196 (m), 1151 (s), 1119 (s), 1068 (m), 1051 (m), 1032 (m), 995 (m), 982 (m), 959 (m), 939 (m), 916 (m), 893 (m), 870 (w), 858 (m), 851 (m), 831 (m), 804 (m), 791 (m), 770 (m), 764 (m), 743 (s), 702 (s), 671 (m), 648 (m), 582 (m), 571 (m), 548 (m).

2.10 Nucleophilic additions to position 5 of 5-polyfluoroalkyl-5-deazaalloxazines

2.10.1 Addition of acetophenone

Addition of acetophenone to 1,3-dialkyl-5-polyfluoroalkyl-pyrimido[4,5-b]quinoline-2,4-diones. General procedure. Into a flask were placed 1,3-dialkyl-5-polyfluoroalkyl-pyrimido[4,5-b]quinoline-2,4-dione (1 eq), acetophenone (1.5 eq), dry THF (20 mL per 1 g of starting material) and sodium hydride (60% in mineral oil, 2 eq). The reaction mixture was stirred for half an hour at r.t. and then allowed to stay overnight. Afterwards 2.5 eq of acetic acid was added and the mixture was diluted with water. The formed precipitate was filtered off by suction, washed with heptane and recrystallized from methanol/water giving the pure product.

7-Ethyl-1,3-dimethyl-5-(2-oxo-2-phenylethyl)-5-(trifluoromethyl)-5,10-dihydropyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (12a). The product was prepared according to the general method, starting from 0.2 g of **4f**, 0.107 g of acetophenone, 0.047 g of sodium hydride (60% in mineral oil) and 4 mL of THF. Yield 0.219 g (81%), white solid, mp 233 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 1.09 (t, 3H, ^{3}J = 7.55 Hz, Et), 2.53 (q, 2H, ^{3}J = 7.55 Hz, Et), 3.09 (s, 3H, CH_3), 3.59 (s, 3H, CH_3), 4.33 (d, 1H, ^{2}J = 18.70 Hz, CH_2CO-a), 5.50 (d, 1H, ^{2}J = 18.70 Hz, CH_2CO-b), 7.18 (d, 1H, ^{3}J = 8.12 Hz, H-8), 7.36 (d, 1H, ^{3}J = 8.12 Hz, H-9), 7.41 (s, 1H, H-6), 7.50-7.60 (m, 2H, $CH_{m\text{-Ph}}$), 7.62-7.70 (m, 1H, $CH_{p\text{-Ph}}$), 7.95-8.04 (m, 2H, $CH_{o\text{-Ph}}$) 9.38 (br s, 1H, NH). ^{13}C NMR (75.48 MHz, DMSO-d_6): δ = 16.6 (CH_3), 28.5 (CH_2), 28.6 (CH_3), 31.2 (CH_3), 38.5 (CH_2CO), 47.5 (q, $^{2}J_{(C\text{-}F)}$ = 25.7 Hz, C-5), 79.9 (C-4a), 117.6 (CH_{Ar}), 119.9, 127.0 (CH_{Ar}), 128.6 (q, $^{1}J_{(C\text{-}F)}$ = 287.3 Hz, CF_3), 128.7 (CH_{Ar}), 128.9 (CH_{Ar}), 129.5 (CH_{Ar}), 133.9 (CH_{Ar}), 135.0, 137.6, 139.6, 148.1, 151.1, 161.6, 195.8. ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –75.8 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 457 ($[M]^+$, 1.7), 338 ($[M–CF_3]^+$, 42), 337 (28), 225 (35), 105 (100), 77 (33). HRMS (ESI): Calcd. for $C_{24}H_{23}F_3N_3O_3$ $[M+H]^+$: 458.16860, found: 458.16921. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3375 (w), 3340 (m), 2959 (w), 2873 (w), 1707 (w), 1694 (m), 1681 (s), 1634 (s), 1615 (m), 1598 (s), 1531 (s), 1504 (s), 1477 (m), 1447 (m), 1404 (m), 1387 (m), 1367 (m), 1319 (w), 1261 (m), 1234 (s), 1218 (s), 1184 (m), 1157 (s), 1144 (s), 1094 (w), 1056 (w), 1043 (w), 1030 (w), 1003 (m), 963 (w), 948 (w), 928 (w), 896 (w), 879 (w), 828 (m), 795 (w), 772 (m), 752 (s), 730 (w), 706 (w), 687 (m), 675 (m), 643 (w), 628 (w), 599 (w), 576 (m), 551 (m), 534 (m).

8,10-Dimethyl-6-(2-oxo-2-phenylethyl)-6-(trifluoromethyl)-1,2-dihydro-6*H*-pyrimido[4,5-*b*]pyrrolo[3,2,1-*ij*]quinoline-7,9(8*H*,10*H*)-dione (13a). The product was prepared according to the general method, starting from 0.15 g of **7a**, 0.073 g of acetophenone, 0.032 g of sodium hydride (60% in mineral oil) and 3 mL of THF. Yield 0.171 g (93%), white solid, mp 304-305 °C. ^{1}H NMR (250.13 MHz, $CDCl_3$): δ = 3.18 (s, 3H, CH_3), 3.20-3.44 (m, 2H, CH_2-2), 3.64 (s, 3H, CH_3), 3.85 (d, 1H, ^{2}J = 18.36 Hz, CH_2CO-a), 4.00-4.14 (m, 1H, CH_2-1a), 4.54-4.65 (m, 1H, CH_2-1b), 5.63 (d, 1H, ^{2}J = 18.36 Hz, CH_2CO-b), 7.00 (dd, 1H, $^{3}J_1$ = 7.18 Hz, $^{3}J_2$ = 8.12 Hz, H-4), 7.11-7.19 (m, 2H, CH_{Ar}), 7.39-7.49 (m, 2H, CH_{Ar}), 7.54 (t, 1H, ^{3}J = 7.25 Hz, $CH_{p\text{-Ph}}$), 7.91-7.98 (m, 2H, CH_{Ar}). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 28.5 (CH_3), 28.9 (CH_2), 38.4 (CH_2), 38.6 (CH_3), 47.8 (q, $^{2}J_{(C\text{-}F)}$ = 26.7 Hz), 53.4 (CH_2), 84.7 (C-6a), 117.6, 124.4 (CH), 124.8 (CH), 125.0 (CH), 127.5 (q, $^{1}J_{(C\text{-}F)}$ = 286.6 Hz, CF_3), 128.2 (CH), 128.8, 128.9 (CH),

133.3, 137.2, 141.8, 152.9, 152.9, 162.0, 195.7. ^{19}F NMR (235.33 MHz, $CDCl_3$): δ = –76.8 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 455 ($[M]^+$, 5.8), 387 (26), 386 (100), 336 (15), 105 (38), 77 (14). HRMS (ESI): Calcd. for $C_{24}H_{21}F_3N_3O_3$ $[M+H]^+$: 456.15295, found: 456.15399. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3043 (w), 3016 (w), 2929 (w), 1691 (s), 1633 (s), 1626 (s), 1539 (s), 1498 (s), 1464 (s), 1446 (s), 1435 (s), 1408 (s), 1375 (s), 1360 (s), 1342 (m), 1302 (m), 1242 (s), 1227 (s), 1201 (m), 1186 (m), 1176 (m), 1155 (s), 1120 (s), 1078 (m), 1057 (m), 1041 (m), 1028 (m), 1001 (m), 976 (m), 964 (m), 939 (m), 912 (m), 897 (w), 860 (w), 847 (w), 779 (s), 770 (m), 756 (s), 748 (s), 737 (s), 714 (m), 694 (s), 658 (m), 617 (s), 581 (m), 569 (m), 528 (m).

2.10.2 Addition of nitromethane

Addition of nitromethane to 1,3-dialkyl-5-polyfluoroalkyl-pyrimido[4,5-*b*]quinoline-2,4-diones. General procedure. Into a flask were placed 1,3-dialkyl-5-polyfluoroalkyl-pyrimido[4,5-b]quinoline-2,4-dione (1 eq), nitromethane (10 eq), dry THF (20 mL per 1 g of starting material), dry methanol (20 mL per 1 g of starting material) and sodium methylate (2 eq). The reaction mixture was allowed to stay at r.t. overnight. Afterwards 2.5 eq of acetic acid was added and the mixture was diluted with water. The formed precipitate was filtered off by suction and recrystallized from methanol/water giving the pure product.

7-Ethyl-1,3-dimethyl-5-(nitromethyl)-5-(trifluoromethyl)-5,10-dihydropyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (12b). The product was prepared according to the general method, starting from 0.45 g of **4f**, 0.814 g of nitromethane, 0.144 g of sodium methylate, 9 mL of methanol and 9 mL of THF. Yield 0.457 g (86%), white solid, mp 351-353 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 1.19 (t, 3H, ^3J = 7.55 Hz, Et), 2.62 (q, 2H, ^3J = 7.55 Hz, Et), 3.22 (s, 3H, CH_3), 3.57 (s, 3H, CH_3), 5.93 (d, 1H, ^2J = 14.78 Hz, CH_2NO_2-a), 6.90 (d, 1H, ^2J = 14.78 Hz, CH_2NO_2-b), 7.27 (d, 1H, ^3J = 8.31 Hz, H-8), 7.41 (d, 1H, ^3J = 8.31 Hz, H-9), 7.62 (s, 1H, H-6), 9.54 (br s, 1H, NH). ^{13}C NMR (75.48 MHz, DMSO-d_6): δ = 16.5 (CH_3), 28.6 (CH_2), 28.7 (CH_3), 31.4 (CH_3), 49.8 (q, $^2J_{(C\text{-}F)}$ = 26.6 Hz, C-5), 72.8 (CH_2NO_2), 77.4 (C-4a), 116.3, 118.2 (CH_{Ar}), 127.0 (q, $^1J_{(C\text{-}F)}$ = 288.9 Hz, CF_3), 127.3 (CH_{Ar}), 130.1 (CH_{Ar}), 134.9, 140.1, 148.6, 151.0, 162.0. ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –73.8 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 398 ($[M]^+$, 8.6), 338 (22), 337 ($[M–CH_3NO_2]^+$, 77), 329 (60), 322 (18), 284 (30), 283 (100), 282 (37), 268 (15), 265 (12), 225 (77), 224 (11), 210 (11). HRMS (ESI): Calcd. for $C_{17}H_{18}F_3N_4O_4$ $[M+H]^+$: 399.12747, found: 399.12780. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3362 (m), 3034 (w), 2967 (w), 2879 (w), 1688 (m), 1614 (s), 1552 (s), 1530 (s), 1511 (s), 1479 (s), 1435 (s), 1438 (m), 1392 (m), 1375 (s), 1338 (w), 1318 (m), 1302 (w), 1289 (w), 1264 (m), 1229 (s), 1208 (m), 1183 (s), 1170 (s), 1163 (s), 1147 (s), 1103 (m), 1062 (w), 1017 (m), 986 (w), 969 (m), 949 (w), 900 (w), 831 (s), 787 (w), 773 (m), 752 (m), 738 (w), 692 (w), 668 (s), 592 (m), 568 (m), 538 (w).

8,10-Dimethyl-6-(nitromethyl)-6-(trifluoromethyl)-1,2-dihydro-6*H*-pyrimido[4,5-*b*]pyrrolo[3,2,1-*ij*]quinoline-7,9(8*H*,10*H*)-dione (13b). The product was prepared according to the general method, starting from 0.05 g of **7a**, 0.082 g of nitromethane, 0.015 g of sodium methylate, 1 mL of methanol and 1 mL of THF. Yield 0.049 g (92%), white solid, mp 285-286 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.19-3.45 (m, 2H, CH_2-2), 3.32 (s, 3H, CH_3), 3.64 (s, 3H, CH_3), 3.95-4.70 (m, 1H, CH_2-1a), 4.55-4.65 (m, 1H, CH_2-1b), 5.22 (d, 1H, ^{2}J = 14.17 Hz, CH_2NO_2-a), 7.11 (dd, 1H, $^{3}J_1$ = 7.36 Hz, $^{3}J_2$ = 8.12 Hz, H-4), 7.16 (d, 1H, ^{2}J = 14.17 Hz, CH_2NO_2-b), 7.22 (d, 1H, ^{3}J = 7.36 Hz, H-3), 7.29 (d, 1H, ^{3}J = 8.12 Hz, H-5). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ = 28.7 (CH_3), 28.8 (CH_2), 38.6 (CH_3), 50.2 (q, $^{2}J_{(C-F)}$ = 27.8 Hz), 53.6 (CH_2), 72.1 (CH_2), 82.5 (C-6a), 113.6, 124.8 (CH), 125.5 (CH), 125.9 (q, $^{1}J_{(C-F)}$ = 288.0 Hz, CF_3), 126.0 (CH), 129.5, 141.7, 152.6, 153.0, 162.3. ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –74.4 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 396 ($[M]^+$, 8.2), 327 (33), 282 (18), 281 (100), HRMS (ESI): Calcd. for $C_{17}H_{16}F_3N_4O_4$ $[M+H]^+$: 397.11182, found: 397.11096. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3034 (w), 2974 (w), 1697 (s), 1626 (s), 1545 (s), 1497 (s), 1471 (s), 1446 (s), 1417 (s), 1404 (s), 1381 (s), 1371 (s), 1304 (m), 1267 (m), 1255 (s), 1227 (s), 1184 (s), 1159 (s), 1134 (s), 1124 (s), 1078 (m), 1065 (m), 1047 (m), 1030 (m), 1011 (s), 968 (s), 943 (m), 933 (m), 864 (m), 849 (m), 779 (s), 768 (s), 748 (s), 731 (s), 714 (m), 677 (s), 654 (m), 606 (m), 581 (m), 571 (m), 546 (m), 532 (m).

2.10.3 Addition of hydrogen cyanide

Addition of hydrogen cyanide to 1,3-dialkyl-5-polyfluoroalkyl-pyrimido[4,5-b]quinoline-2,4-diones. General procedure. Initial 1,3-dialkyl-5-polyfluoroalkyl-pyrimido[4,5-b]quinoline-2,4-dione (1 eq) was suspended in DMSO. Then KCN (2 eq) was added. Reaction mixture was stirred overnight and afterwards acetic acid (2 eq) was carefully added under fume hood. Then mixture was diluted with water. The formed precipitate was filtered off by suction and recrystallized from methanol/water giving the pure product.

7-Ethyl-1,3-dimethyl-2,4-dioxo-5-(trifluoromethyl)-1,2,3,4,5,10-hexahydropyrimido[4,5-*b*]quinoline-5-carbonitrile (12c). The product was prepared according to the general method, starting from 0.2 g of **4f**, 0.077 g of KCN and 4 mL of DMSO. Yield 0.203 g (94%), white solid, mp 179 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 1.22 (t, 3H, ^{3}J = 7.56 Hz, Et), 2.70 (q, 2H, ^{3}J = 7.56 Hz, Et), 3.26 (s, 3H, CH_3), 3.54 (s, 3H, CH_3), 7.43 (dd, 1H, ^{3}J = 8.39 Hz, ^{4}J = 1.79 Hz, H-8), 7.51 (d, 1H, ^{3}J = 8.39 Hz, H-9), 7.53 (s, 1H, H-6), 9.96 (br s, 1H, NH). ^{13}C NMR (75.48 MHz, DMSO-d_6): δ = 16.4 (CH_3), 28.3 (CH_2), 28.8 (CH_3), 31.4 (CH_3), 46.3 (q, $^{2}J_{(C-F)}$ = 31.9 Hz, C-5), 74.5 (C-4a), 112.6, 115.9, 118.7 (CH_{Ar}), 124.8 (q, $^{1}J_{(C-F)}$ = 289.3 Hz, CF_3), 128.4 (CH_{Ar}), 131.7 (CH_{Ar}), 134.6, 141.0, 148.3, 151.0, 160.4. ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –75.1 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 364 ($[M]^+$, 1.03), 338 (17), 337 ($[M–HCN]^+$, 97), 322 (27), 309 (11), 296 (10), 295 (53), 280 (11), 268 (19), 265 (23), 239 (10), 238 (16), 237 (11), 226 (12), 225 (100), 224 (13), 210 (17), 196 (11). HRMS (ESI): Calcd. for $C_{17}H_{16}F_3N_4O_2$ $[M+H]^+$:

365.12199, found: 365.12186. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3526 (w), 3326 (m), 2977 (w), 1688 (m), 1633 (m), 1613 (s), 1601 (m), 1531 (s), 1502 (s), 1472 (s), 1435 (s), 1414 (m), 1392 (w), 1368 (w), 1338 (w), 1300 (w), 1260 (w), 1232 (w), 1218 (m), 1180 (s), 1159 (m), 1145 (m), 1101 (w), 1068 (w), 1035 (m), 1002 (w), 965 (m), 940 (w), 894 (w), 866 (w), 835 (s), 771 (m), 759 (m), 733 (w), 706 (w), 692 (w), 661 (w), 577 (m), 565 (m), 545 (m), 531 (w).

8,10-Dimethyl-7,9-dioxo-6-(trifluoromethyl)-1,2,7,8,9,10-hexahydro-6*H*-pyrimido[4,5-*b*]pyrrolo[3,2,1-*ij*]quinoline-6-carbonitrile (13c). The product was prepared according to the general method, starting from 0.2 g of **7a**, 0.105 g of KCN and 4 mL of DMSO. Yield 0.136 g (70%), white solid, mp 242 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.26-3.54 (m, 2H, CH_2-2), 3.34 (s, 1H, CH_3), 3.68 (s, 1H, CH_3), 4.03-4.16 (m, 1H, CH_2-1a), 4.65-4.77 (m, 1H, (m, 1H, CH_2-1b), 7.23 (dd, 1H, $^{3}J_1$ = 7.74 Hz, $^{3}J_2$ = 7.37 Hz, CH-4), 7.32 (d, 1H, ^{3}J = 7.37 Hz, CH_{Ar}), 7.62 (d, 1H, ^{3}J = 7.74 Hz, CH_{Ar}). ^{13}C NMR (75.48 MHz, $CDCl_3$): δ = 28.7 (CH_3), 29.0 (CH_2), 38.0 (CH_3), 46.2 (q, $^{2}J_{(C-F)}$ = 33.0 Hz, C-6), 53.8 (CH_2), 79.5 (C-6a), 110.8, 115.0, 124.0 (q, $^{1}J_{(C-F)}$ = 288.7 Hz, CF_3), 126.3 (CH_{Ar}), 126.8 (CH_{Ar}), 127.3 (CH_{Ar}), 129.5, 140.9, 152.2, 152.2, 160.3. ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –75.8 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 362 ($[M]^+$, 2.0), 294 (18), 293 ($[M–CF_3]^+$, 100), 236 (23). HRMS (EI): Calcd. for $C_{17}H_{13}F_3N_4O_2$ $[M]^+$: 362.09851, found: 362,09826. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3071 (w), 2951 (w), 2858 (w), 1716 (m), 1640 (m), 1633 (m), 1545 (m), 1498 (m), 1449 (s), 1435 (s), 1403 (m), 1363 (m), 1342 (w), 1300 (w), 1285 (w), 1266 (w), 1224 (w), 1208 (m), 1185 (s), 1174 (s), 1161 (s), 1107 (m), 1054 (w), 1025 (w), 1001 (w), 987 (m), 964 (m), 939 (m), 867 (w), 826 (w), 796 (s), 768 (s), 746 (s), 712 (m), 679 (w), 666 (w), 611 (w), 571 (w), 539 (w).

2.10.4 Addition of indole

7-Ethyl-5-(1*H*-indol-1-yl)-1,3-dimethyl-5-(trifluoromethyl)-5,10-dihydropyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (12d). Initial 7-ethyl-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione **4f** (0.25 g, 0.74 mmol, 1 eq) was added to a mixture of indole (0.13 g, 1.11 mmol, 1,5 eq) and sodium hydride (60% in mineral oil, 0.044g, 1.11 mmol, 1.5 eq) in dry THF (2.5 mL). The reaction mixture was stirred for 5 min at r.t., followed by addition of acetic acid (0.1 g, 1.67 mmol, 2.25 eq) and dilution with water. The formed precipitate was filtered off by suction, washed with water, recrystallized from DMSO containing one drop of acetic acid (just to stabilize the product) and dried in high vacuum at 60 °C (avoid overheating). Yield 0.194 g (58%), white solid, mp 212 °C (dec.). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 0.89 (t, 3H, ^{3}J = 7.56 Hz, Et), 2.33 (q, 2H, ^{3}J = 7.56 Hz, Et), 2.97 (s, 3H, CH_3), 3.65 (s, 3H, CH_3), 6.42 (s, 1H, CH_{Ar}), 6.61 (d, 1H, ^{3}J = 3.21 Hz, CH_{Ar}), 6.69 (d, 1H, ^{3}J = 8.31 Hz, CH_{Ar}), 6.74-6.82 (m, 1H, CH_{Ar}), 6.89-6.98 (m, 1H, CH_{Ar}), 7.28 (d, 1H, ^{3}J = 7.93 Hz, H-8), 7.55 (m, 2H, CH_{Ar}), 7.71 (s, 1H, H-5), 9.92 (br s, 1H, NH). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 16.2 (CH_3), 28.2 (CH_2), 28.3 (CH_3), 31.5 (CH_3), 65.3 (q, $^{2}J_{(C-F)}$ = 29.7 Hz), 78.7 (C-4a), 101.9 (CH), 112.9 (CH), 117.7,

117.8 (CH), 120.1 (CH), 121.4 (CH), 121.7 (CH), 126.4 (q, $^{1}J_{(C\text{-}F)}$ = 290.5 Hz, CF_3), 127.2 (CH), 129.6, 130.2 (CH), 130.7 (CH), 134.1, 135.7, 139.8, 147.9, 151.2, 159. ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –72.2 (s, CF_3). MS (EI, 70 eV): *m/z* (%) = 338 (25), 337 (100), 322 (40), 309 (11), 280 (11), 268 (17), 265 (23), 239 (10), 226 (14), 225 (95), 224 (13), 210 (15), 117 (92), 90 (30), 89 (18). HRMS (ESI): Calcd. for $C_{24}H_{22}F_3N_4O_2$ $[M+H]^+$: 455.16894, found: 455.16903. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3273 (w), 3207 (w), 1713 (s), 1626 (s), 1614 (s), 1599 (m), 1527 (s), 1504 (s), 1479 (s), 1456 (s), 1444 (m), 1390 (m), 1369 (w), 1315 (w), 1298 (m), 1259 (m), 1238 (s), 1211 (m), 1203 (m), 1173 (s), 1161 (s), 1153 (s), 1140 (m), 1126 (w), 1059 (m), 1016 (w), 984 (m), 939 (w), 916 (w), 891 (s), 879 (w), 847 (w), 827 (m), 770 (m), 739 (s), 708 (s), 692 (m), 679 (m), 658 (m), 625 (w), 596 (w), 582 (m), 563 (m), 542 (w).

7-Ethyl-5-(1*H*-indol-3-yl)-1,3-dimethyl-5-(trifluoromethyl)-5,10-dihydropyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (12e). Initial 7-ethyl-1,3-dimethyl-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione **4f** (0.15 g, 0.44 mmol, 1 eq) was added to a mixture of indole (0.078 g, 0.67 mmol, 1,5 eq) and sodium hydride (60% in mineral oil, 0.036 g, 0.89 mmol, 2 eq) in dry DMF (3 mL). The reaction mixture was stirred for 5 hours at 60 °C under argon. After cooling to r.t. 0.134 g of acetic acid (2.22 mmol, 3.75 eq) and water were added. The formed precipitate was filtered off by suction and recrystallized from methanol giving the pure product. Yield 0.115 g (57%), pinkish solid, mp 295-297 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 0.92 (t, 3H, ^{3}J = 7.55 Hz, Et), 2.31 (q, 2H, ^{3}J = 7.55 Hz, Et), 2.96 (s, 3H, CH_3), 3.63 (s, 3H, CH_3), 6.64-6.72 (m, 2H, CH_{Ar}, NH-1'), 6.91-7.01 (m, 2H, CH_{Ar}), 7.13 (dd, 1H, ^{3}J = 8.22 Hz, ^{4}J = 2.00 Hz, CH_{Ar}), 7.33-7.42 (m, 3H, CH_{Ar}), 9.47 (s, 1H, H-2'), 11.00 (s, 1H, NH-10). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 16.4 (CH_3), 28.3 (CH_2), 28.3 (CH_3), 31.2 (CH_3), 49.1 (q, $^{2}J_{(C\text{-}F)}$ = 27.0 Hz), 81.1 (C-4a), 112.3 (CH), 114.4, 117.2 (CH), 118.9 (CH), 120.1 (CH), 120.4, 121.4 (CH), 121.7 (q, $^{1}J_{(C\text{-}F)}$ = 288.4 Hz, CF_3), 123.9 (CH), 126.8, 129.1 (CH), 130.1 (CH), 134.7, 137.0, 138.7, 148.0, 151.4, 159.7. MS (EI, 70 eV): *m/z* (%) = 454 ($[M]^+$, 3.0), 385 (16), 338 (28), 337 (100), 322 (42.92), 309 (12), 280 (13), 268 (20), 265 (26), 239 (11), 237 (10), 226 (16), 225 (96), 224 (14), 210 (15), 196 (10), 117 (34), 90 (11), 60 (10). HRMS (EI): Calcd. for $C_{24}H_{21}F_3N_4O_2$ $[M]^+$: 454.16111, found: 454.16137. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3271 (w), 3207 (w), 2914 (w), 1713 (s), 1626 (s), 1614 (s), 1599 (s), 1525 (s), 1504 (s), 1479 (s), 1454 (s), 1444 (s), 1390 (m), 1369 (m), 1315 (m), 1298 (m), 1288 (m), 1259 (m), 1238 (s), 1211 (m), 1173 (s), 1153 (s), 1126 (m), 1099 (m), 1057 (s), 1016 (m), 982 (m), 941 (w), 916 (w), 891 (s), 879 (m), 847 (m), 827 (m), 770 (s), 739 (s), 708 (s), 692 (m), 679 (m), 658 (m), 625 (m), 596 (m), 582 (m), 563 (m), 542 (m).

2.11 Synthesis of 1,3-dimethyl-9-{2-[(4-methylphenyl)thio]ethyl}-5-(trifluoromethyl)-5-deazaalloxazine

1,3-Dimethyl-9-{2-[(4-methylphenyl)thio]ethyl}-5-(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione (13d). In a 10-mL flask were placed 0.5 g of 9-(2-chloroethyl)-1,3-dimethyl-5-

(trifluoromethyl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-dione **7a** (0.13 mmol, 1 eq), 0.33 g of 4-methylthiophenol (0.27 mmol, 2 eq), 0.013 g of sodium methylate (0.24 mmol, 1.8 eq) and 1 mL of DMF. The reaction mixture was stirred for 4 hours and then diluted with water. The formed precipitate was filtered off by suction, washed with water and recrystallized from methanol giving the pure product. Yield 0.059 g (95%), yellow solid, mp 142-143 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 2.31 (s, 3H, CH_3), 3.28 (t, 2H, CH_2-Ar), 3.45-3.55 (m, 5H, CH_3, CH_2-S), 3.66 (s, 1H, CH_3), 7.06 (d, 2H, ^{3}J = 7.93 Hz, H-2', H-6'), 7.25 (d, 2H, ^{3}J = 7.93 Hz, H-3', H-5'), 7.50 (dd, 1H, $^{3}J_1$ = 7.11 Hz, $^{3}J_2$ = 8.62 Hz, H-7), 7.70 (d, 1H, ^{3}J = 7.11 Hz, H-8), 8.19 (d, 1H, ^{3}J = 8.62 Hz, H-6). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 21.3 (Ar-CH_3), 29.5 (CH_3-3), 30.5 (CH_3-1), 33.1 (CH_2), 35.4 (CH_2), 110.1 (C-4a), 122.0, 123.6 (q, $^{1}J_{(C-F)}$ = 278.3 Hz, CF_3), 124.9 (q, $^{4}J_{(C-F)}$ = 5.9 Hz, CH-6), 127.0 (CH), 129.9 (CH), 131.3 (CH), 132.5, 133.8 (CH), 137.0, 138.4, 139.1 (q, $^{2}J_{(C-F)}$ = 33.2 Hz, C-5), 147.4, 148.6, 151.2 (CO-2), 159.3 (CO-4). ^{19}F NMR (282.38 MHz, $CDCl_3$): δ = –52.4 (s, CF_3). MS (GC, 70 eV): *m/z* (%) = 459 ($[M]^+$, 35), 337 (19), 336 (100), 279 (29), 137 (68). HRMS (EI): Calcd. for $C_{23}H_{20}O_2N_3F_3S$ $[M+H]^+$: 459.12228, found: 459.122964. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2955 (w), 2929 (w), 1728 (s), 1666 (s), 1608 (w), 1585 (s), 1574 (s), 1485 (s), 1470 (s), 1421 (s), 1394 (m), 1379 (s), 1356 (s), 1333 (m), 1286 (s), 1261 (m), 1227 (s), 1198 (m), 1169 (s), 1134 (s), 1115 (s), 1082 (m), 1039 (m), 1014 (m), 982 (m), 930 (m), 883 (w), 856 (w), 820 (m), 804 (s), 789 (s), 779 (s), 762 (s), 748 (s), 739 (m), 702 (s), 685 (m), 675 (m), 667 (m), 590 (w), 555 (m), 542 (w).

2.12 Cyclisation of 6-(benzylamino)-1,3-dimethyl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione

6,8-Dimethyl-2-phenyl-4-(trifluoromethyl)-4,8-dihydro-2*H*-pyrimido[4,5-*d*][1,3]oxazine-5,7(1*H*,6*H*)-dione (14). A sealed ACE pressure tube was charged with 1 g of 6-(benzylamino)-1,3-dimethyl-5-(trifluoroacetyl)pyrimidine-2,4(1*H*,3*H*)-dione **5e** (2.93 mmol, 1 eq), 1.186 g of dry triethylamine (11.7 mmol, 4 eq) and 10 mL of dry DMF. The reaction mixture was stirred for 10 hours at 125 °C under argon. Then the solvent was evaporated and the crude product was purified via short-part column chromatography (silica gel / EtOAc), following by washing with ether. Yield 0.798 g (80%), white solid, mp 220-222 °C. ^{1}H NMR (300.13 MHz, DMSO-d_6): δ = 3.31 (s, 3H, CH_3-6-a), 3.32 (s, 0.15H, CH_3-6-b), 3.32 (s, 0.15H, CH_3-8-b), 3.36 (s, 3H, CH_3-8-a), 5.27 (q, 1H, $^{4}J_{(H-F)}$ = 7.18 Hz, H-4-a), 5.49.(q, 0.15H, $^{4}J_{(H-F)}$ = 5.29 Hz, H-4-b), 5.55 (d, 0.15H, *J* = 3.11 Hz, H-2-b), 5.91 (br s, 1H, H-2-a), 7.48-7.64 (m, 5.75H, CH_{Ph}-a, CH_{Ph}-b), 8.11 (d, 0.15H, *J* = 3.11 Hz, NH-b), 8.15 (br s, 1H, NH-a). ^{13}C NMR (62.90 MHz, $CDCl_3$): δ = 28.2 (CH_3-6-a,b), 30.1 (CH_3-8-b), 30.4 (CH_3-8-a), 69.6 (q, $^{2}J_{(C-F)}$ = 31.6 Hz, CH-4-a), 70.5 (q, $^{2}J_{(C-F)}$ = 31.9 Hz, CH-4-b), 77.2 (4a-a), 81.9 (CH-2-a), 82.2 (4a-b), 83.0 (CH-2-b), 125.7 (q, $^{1}J_{(C-F)}$ = 287.6 Hz, CF_3-a), 128.5 ($CH_{o\text{-}Ph}$-b), 128.6 ($CH_{o\text{-}Ph}$-a), 129.3 ($CH_{m\text{-}Ph}$-b), 129.4 ($CH_{m\text{-}Ph}$-a), 130.4 ($CH_{p\text{-}Ph}$-b), 130.8 ($CH_{p\text{-}Ph}$-a), 137.0 (C_{Ph}-b), 137.6 (C_{Ph}-a), 150.5 (C-8-a), 151.5 (CO-7-b), 151.6 (CO-7-a), 154.0 (C-8-b), 160.2 (CO-5-a), 160.4 (CO-5-b). ^{19}F NMR (282.38 MHz, DMSO-d_6): δ = –75.5 (s, CF_3-b), –71.3 (s, CF_3-a). MS (EI, 70 eV): *m/z* (%) = 341 ($[M]^+$, 16), 273 (32), 272 (100), 258 (17), 110 (11), 105 (15), 82 (12), 77 (12). HRMS (ESI): Calcd. for $C_{15}H_{15}F_3N_3O_3$ $[M+H]^+$: 342.10600, found: 340.10654.

Anal. Calcd for $C_{15}H_{14}F_3N_3O_3$: C, 52.79; H, 4.13; N, 12.31. Found: C, 52.95; H, 3.87; N, 11.79. IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3243 (s), 3097 (w), 3040 (w), 2952 (w), 1707 (s), 1616 (s), 1556 (s), 1482 (s), 1459 (m), 1439 (m), 1395 (w), 1383 (m), 1360 (m), 1335 (w), 1321 (m), 1307 (w), 1290 (w), 1258 (s), 1248 (s), 1234 (m), 1167 (s), 1123 (s), 1076 (m), 1053 (m), 1028 (w), 1005 (m), 998 (m), 982 (w), 967 (m), 670 (s), 650 (w), 634 (s), 617 (w), 582 (m), 531 (m).

2.13 Detection of 5-deazaalloxazine-10-ium cation

8,10-Dimethyl-7,9-dioxo-6-(trifluoromethyl)-1,2,7,8,9,10-hexahydropyrimido[4,5-*b*]pyrrolo[3,2,1-*ij*]quinolin-11-ium trifluoromethanesulfonate (6'a). The solution of title salt was prepared inside a NMR tube by addition of triflic anhydride to 6-hydroxy-8,10-dimethyl-6-(trifluoromethyl)-1,2-dihydro-6*H*-pyrimido[4,5-*b*]pyrrolo[3,2,1-*ij*]quinoline-7,9(8*H*,10*H*)-dione **6a** dissolved in pure $CDCl_3$ or $CDCl_3/CD_2Cl_2$ mixture. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 3.42 (s, 3H, CH_3-3), 3.80 (t, 2H, ^3J = 7.27 Hz, Ar-CH_2-), 3.96 (s, 3H, CH_3-1), 5.48 (t, 2H, ^3J = 7.27 Hz, -CH_2-N_{Ar}^+), 7.89 (dd, 1H, $^3J_1$ = 8.59 Hz, $^3J_2$ = 7,27 Hz, H-4), 8.03 (d, 1H, ^3J = 7.27 Hz, H-3), 8.24-8.32 (dm, 1H, ^3J = 8.59 Hz, H-5), 13.99 (s, 1.67H, TfOH). ^{13}C NMR (75.47 MHz, $CD_2Cl_2/CDCl_3$): δ = 27.8 (CH_2-2), 30.0 (CH_3-8), 36.6 (CH_3-10), 60.0 (CH_2-1), 115.6 (C-6a), 118.8 (q, $^1J_{(C-F)}$ = 317.6 Hz, TfOH/TfO^-), 120.5, 121.6 (q, $^1J_{(C-F)}$ = 279.6 Hz, CF_3), 124.6 (q, $^4J_{(C-F)}$ = 5.9 Hz, CH-5), 131.9 (CH_{Ar}), 133.1 (CH_{Ar}), 134.5, 143.3, 145.2 (q, $^2J_{(C-F)}$ = 35.9 Hz, C-6), 149.2, 149.3, 155.9.

3 X-Ray structures

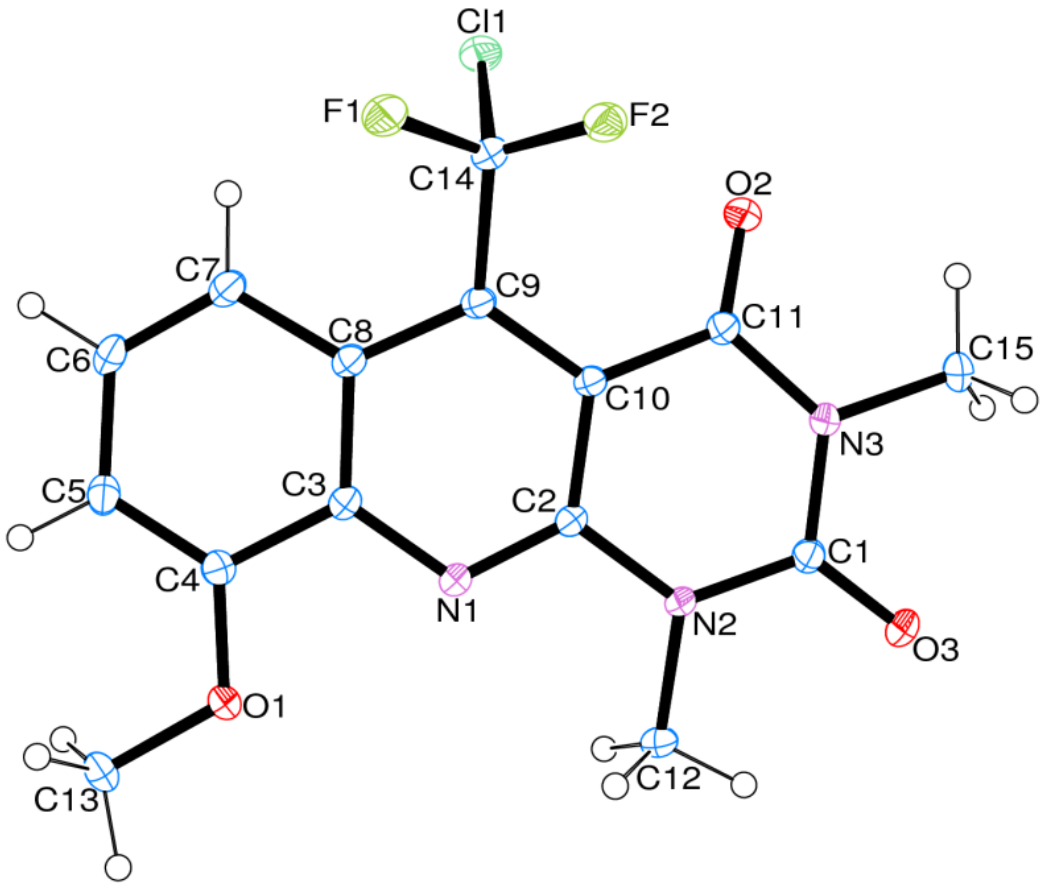


Figure 1. Molecular structure of compound **4j** (35% probability level).

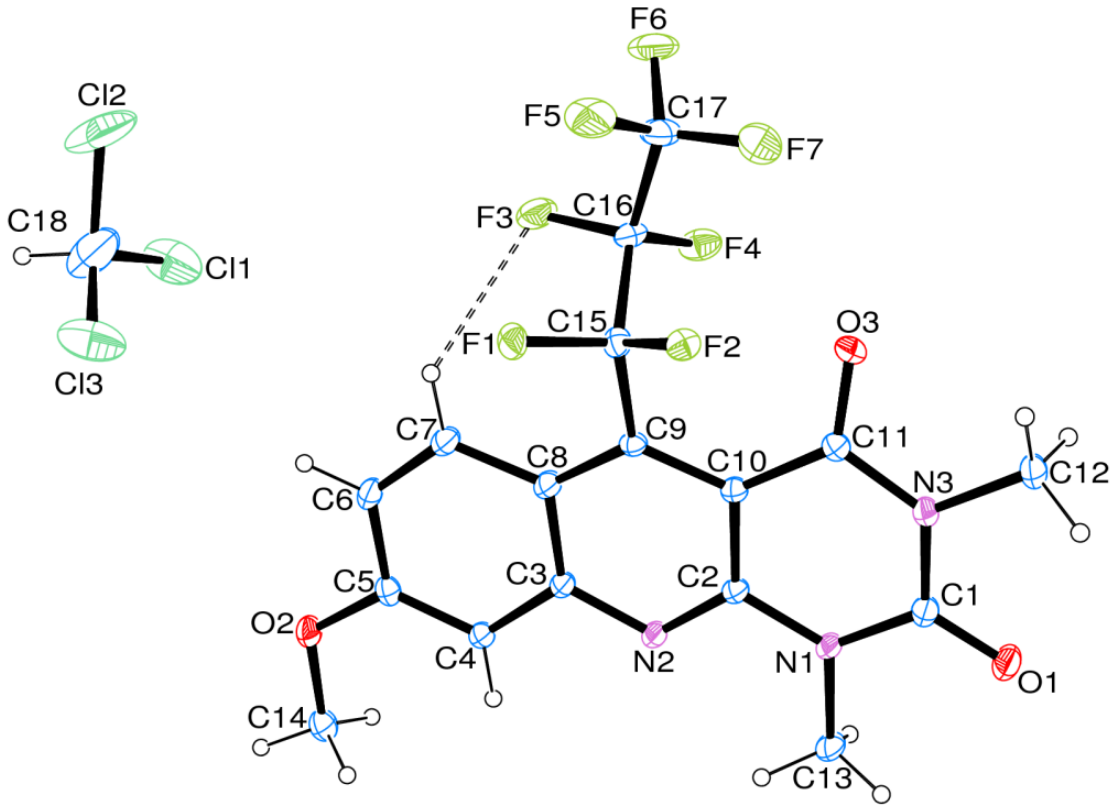


Figure 2. Molecular structure of compound **4m** (25% probability level).

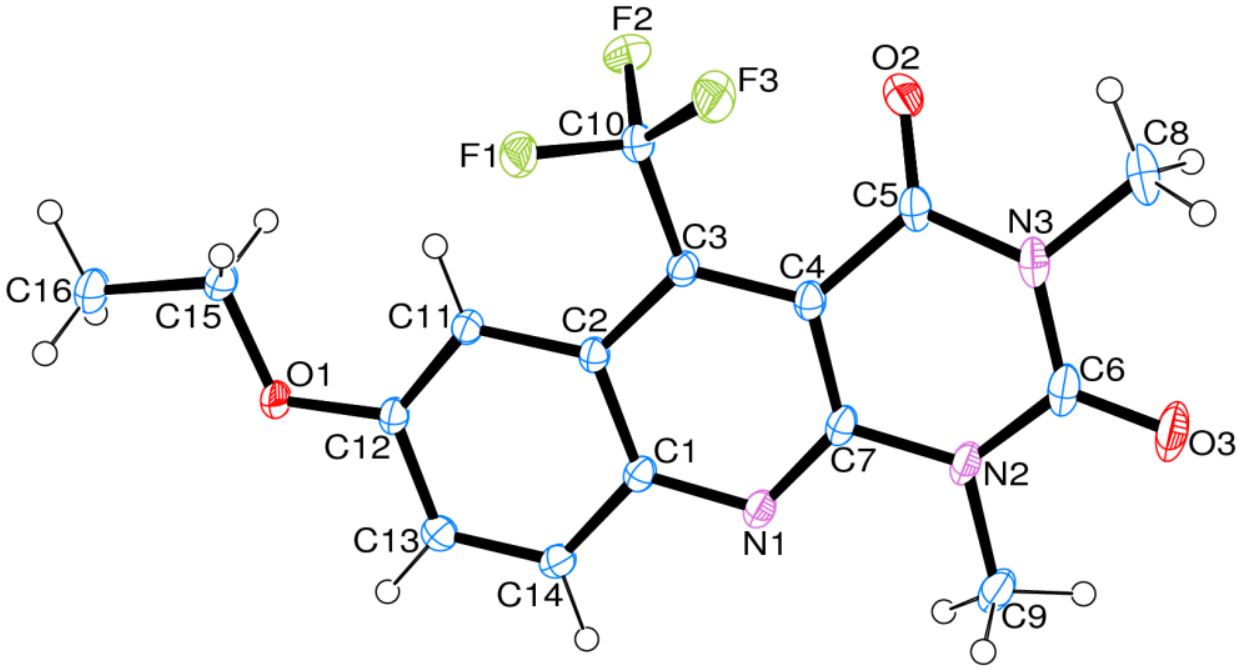


Figure 3. Molecular structure of compound **4q** (35% probability level).

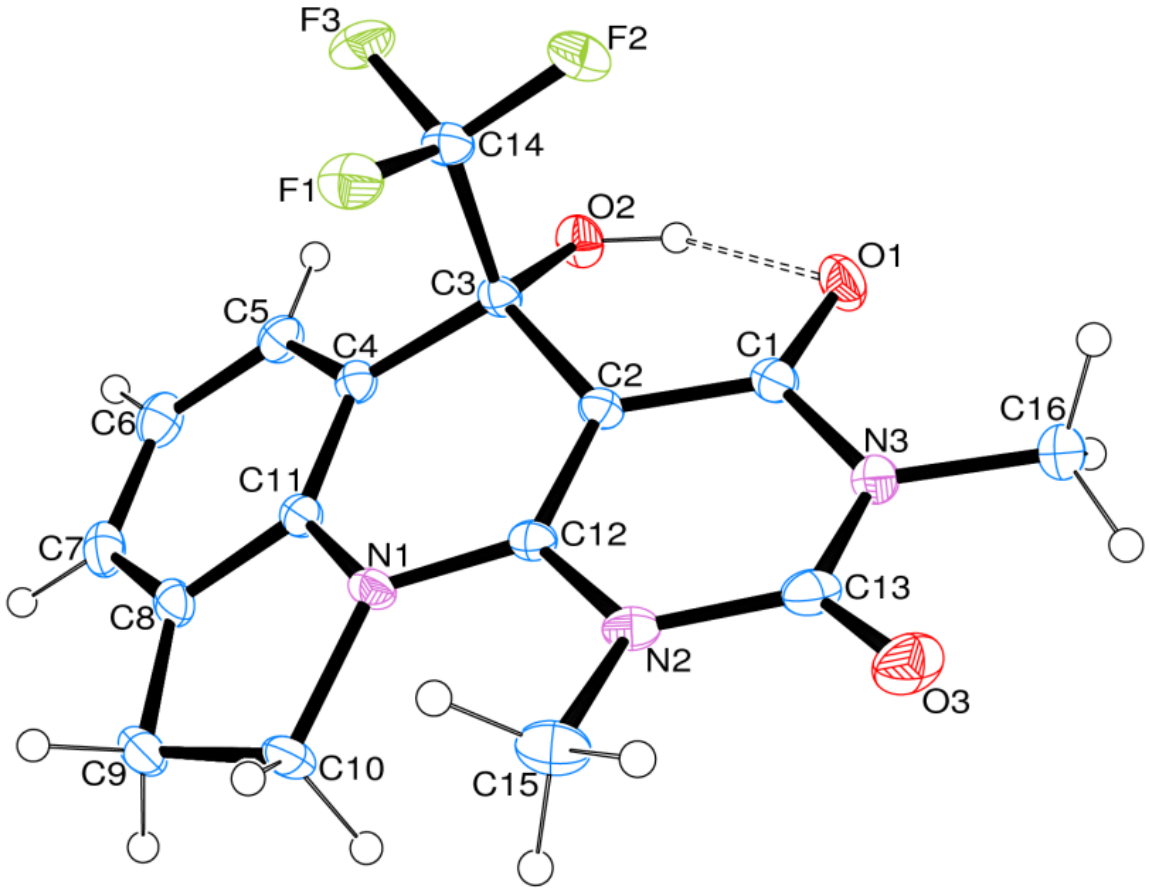


Figure 4. Molecular structure of compound **6a** (35% probability level).

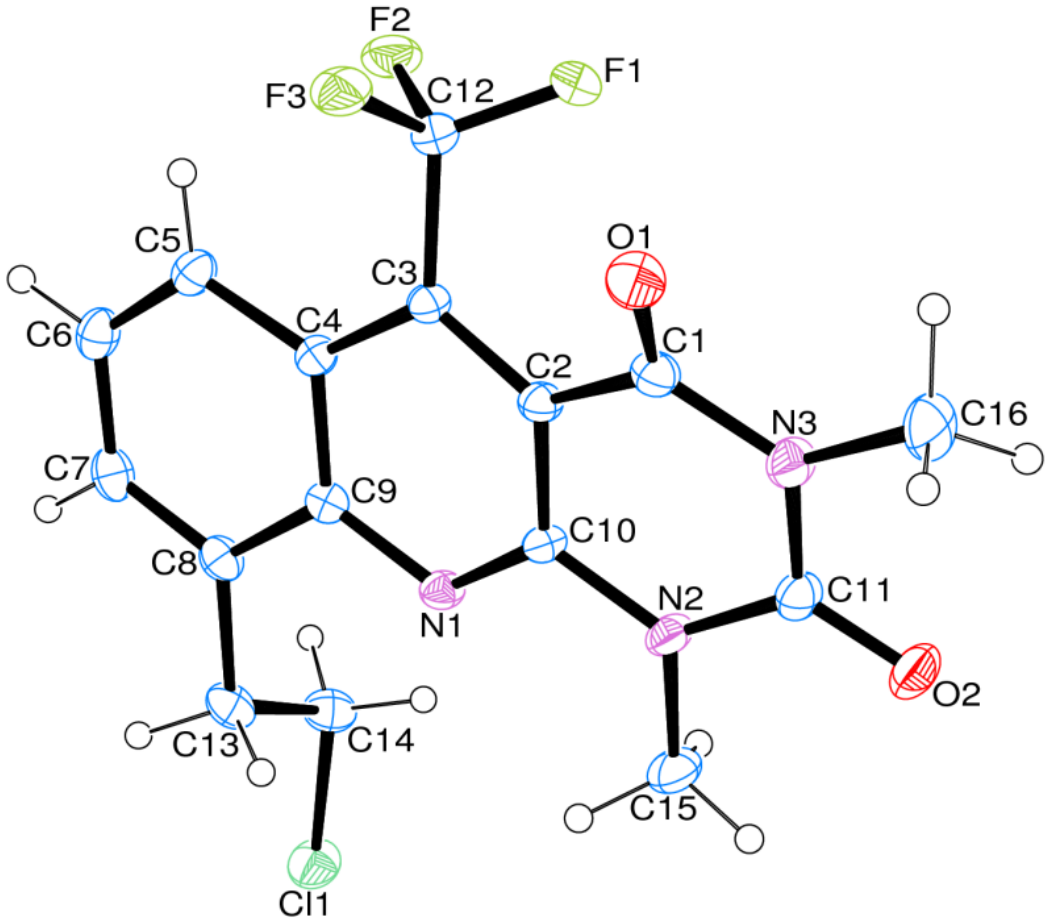


Figure 5. Molecular structure of compound **7a** (35% probability level).

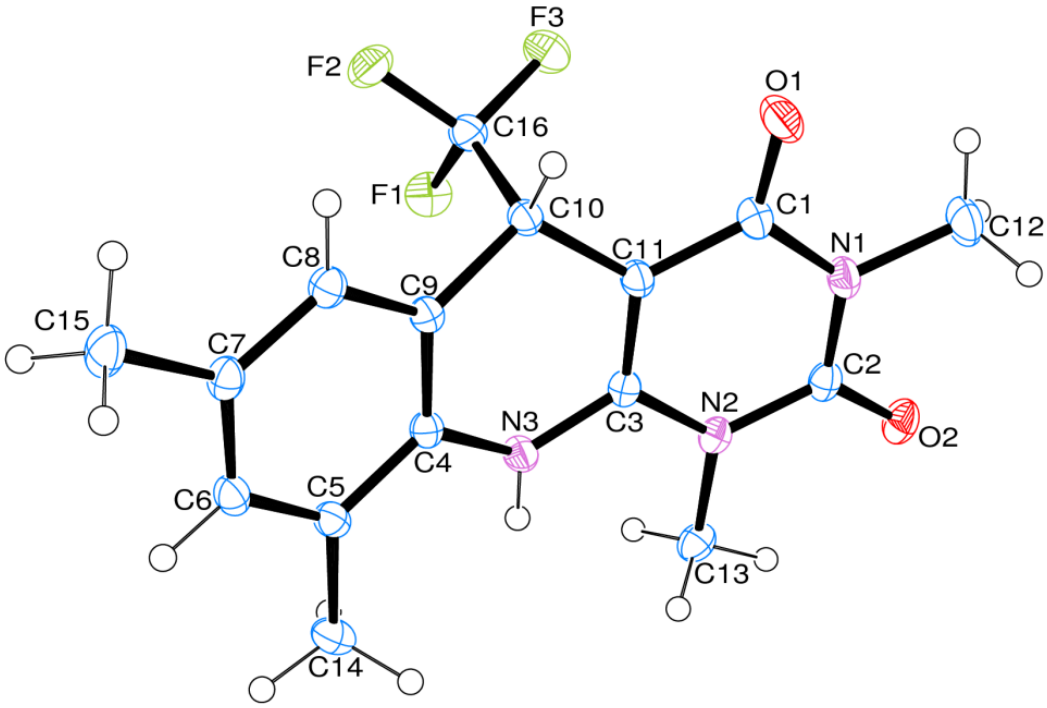


Figure 6. Molecular structure of compound **8a** (40% probability level).

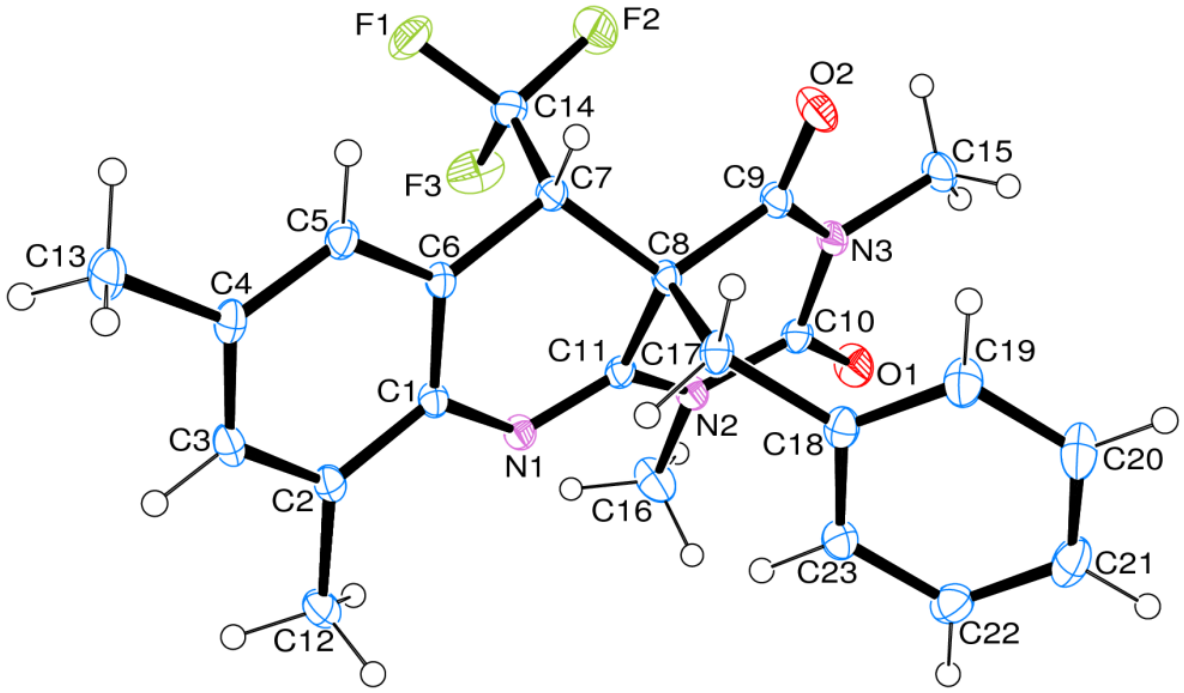


Figure 7. Molecular structure of compound **9** (40% probability level).

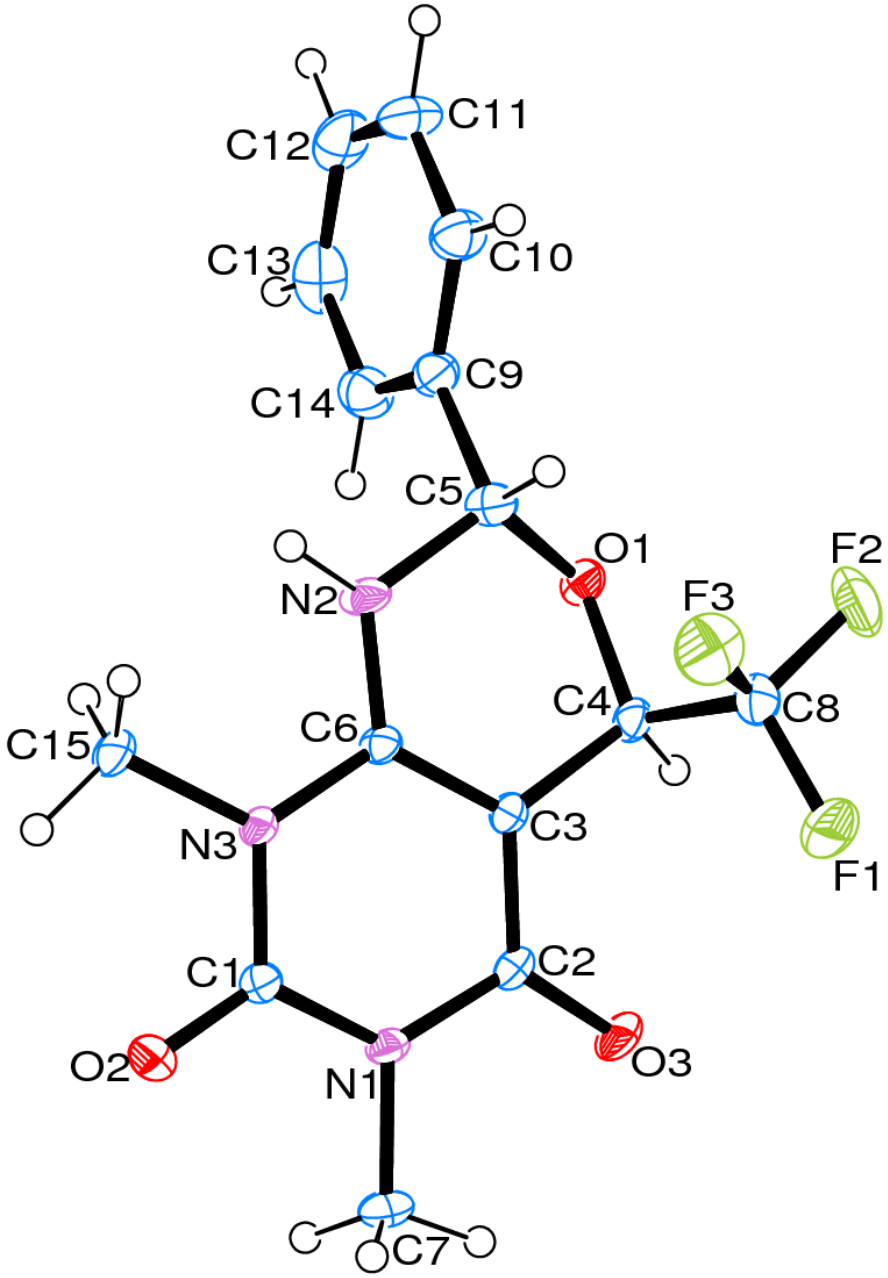


Figure 8. Molecular structure of compound **14** (40% probability level).

4 Photophysical properties of some 5-polyfluoroalkyl-5-deazaalloxazines

Table 1.Photophysical properties of 5-deazaalloxazines in chloroform: molar absorption coefficients ε at absorption maxima λ_a, fluorescence band maxima λ_f, and Stokes shift $\Delta\nu_{St}$.

Compd	λ_a,nm	ε,$M^{-1}\cdot cm^{-1}$	λ_f,nm	$\Delta\nu_{St}$, cm^{-1}
4w	405	9500	460	2950
4x	353	12400	516	8950
4f	397	5200	468	3820
4u	410	17500	480	3560
11a	417	9800	494	3740
7b	395	5400	466	3860

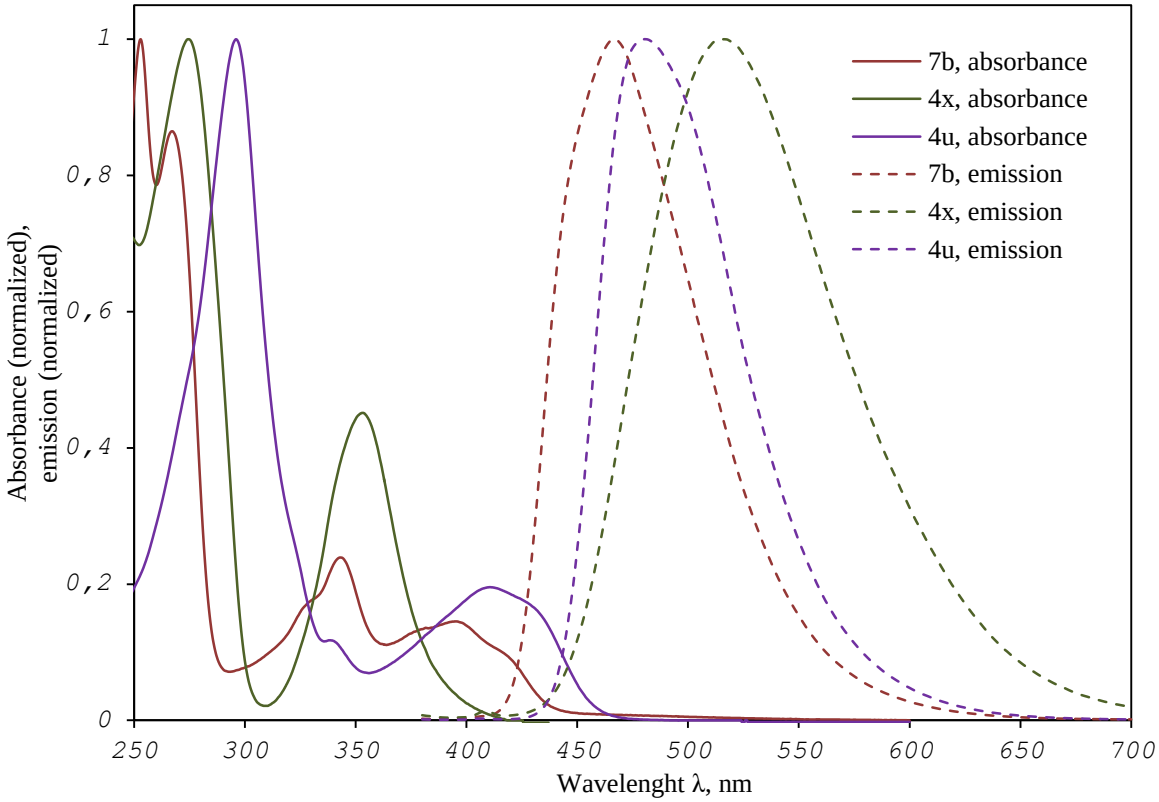


Figure 16. Normalized absorption and uncorrected emission spectra of compounds **7b**, **4x** and **4u** in chloroform.

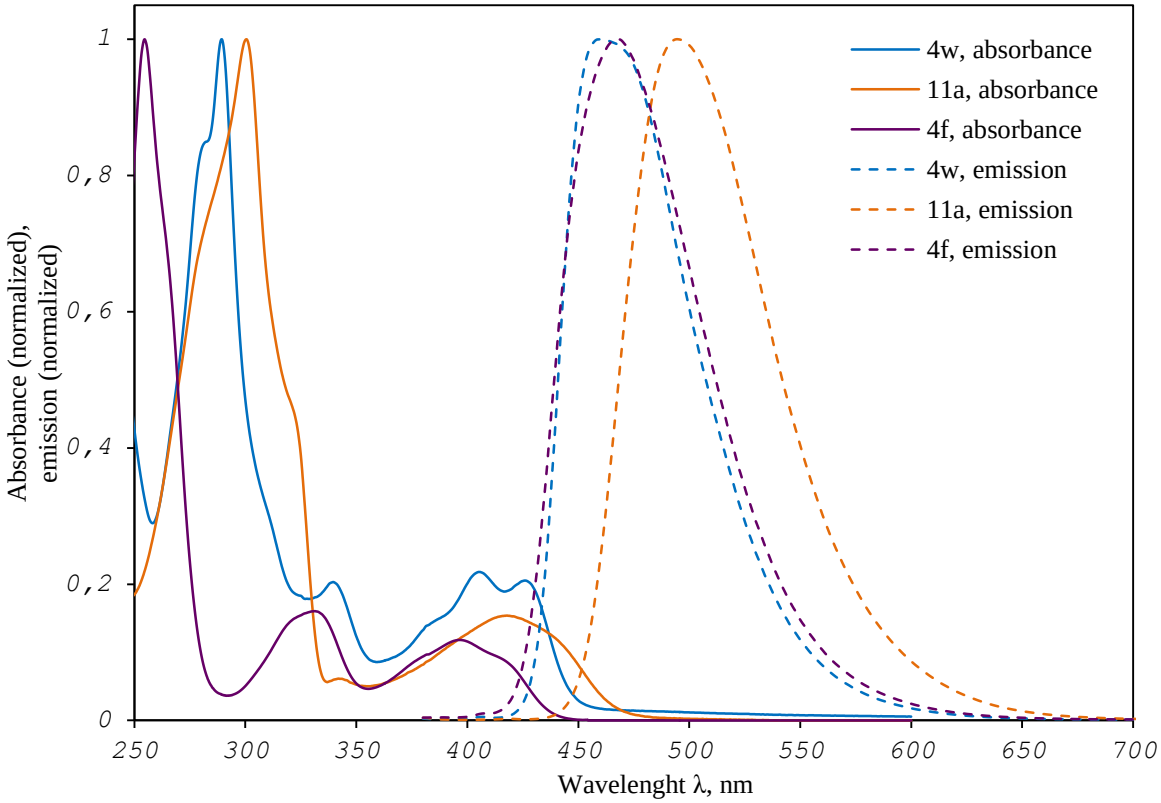
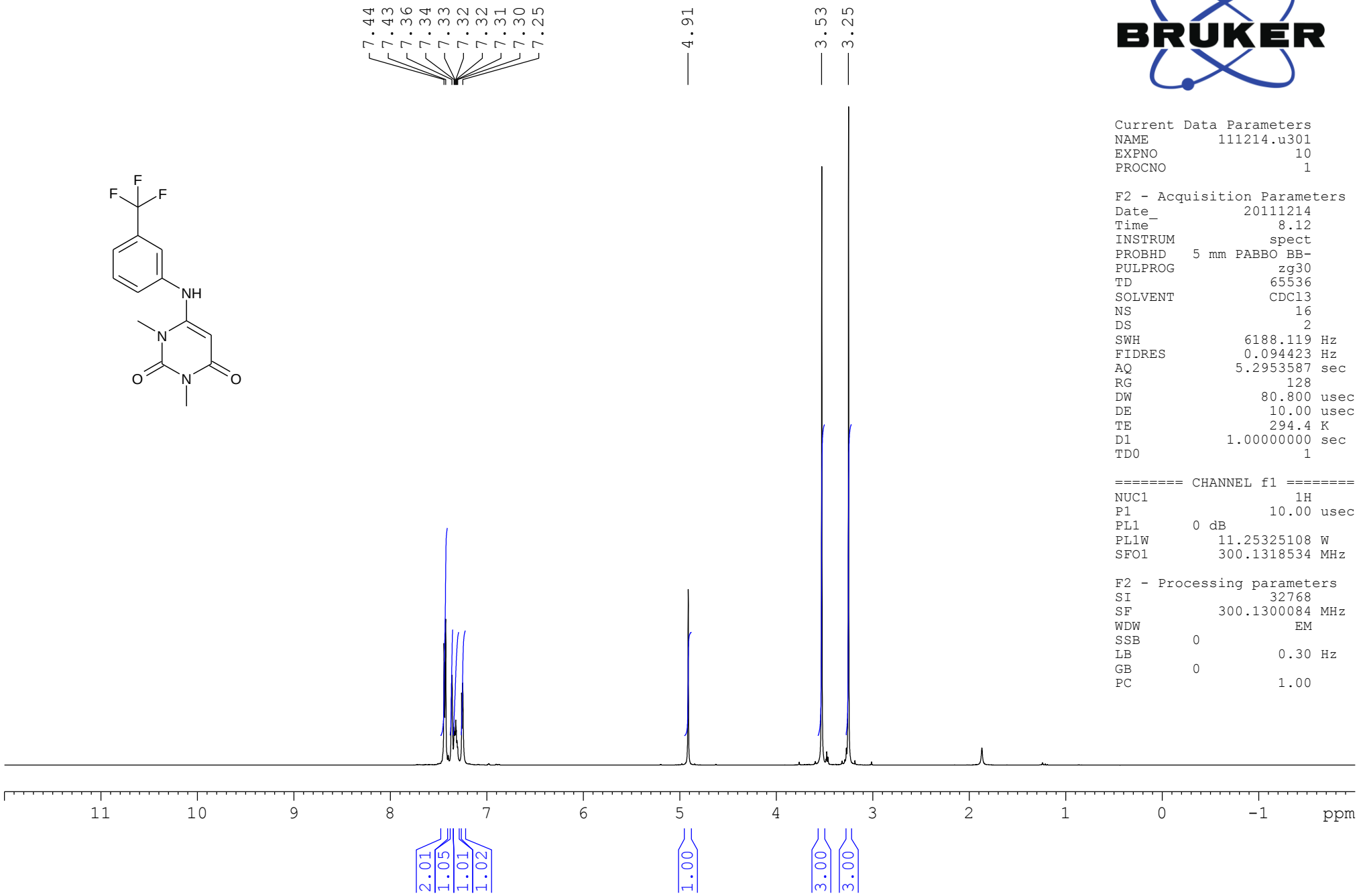


Figure 17. Normalized absorption and uncorrected emission spectra of compounds **4w**, **11a** and **4f** in chloroform.

5 Copies of ^{1}H and ^{13}C NMR spectra

Dudkin sd343 1H CDCl3



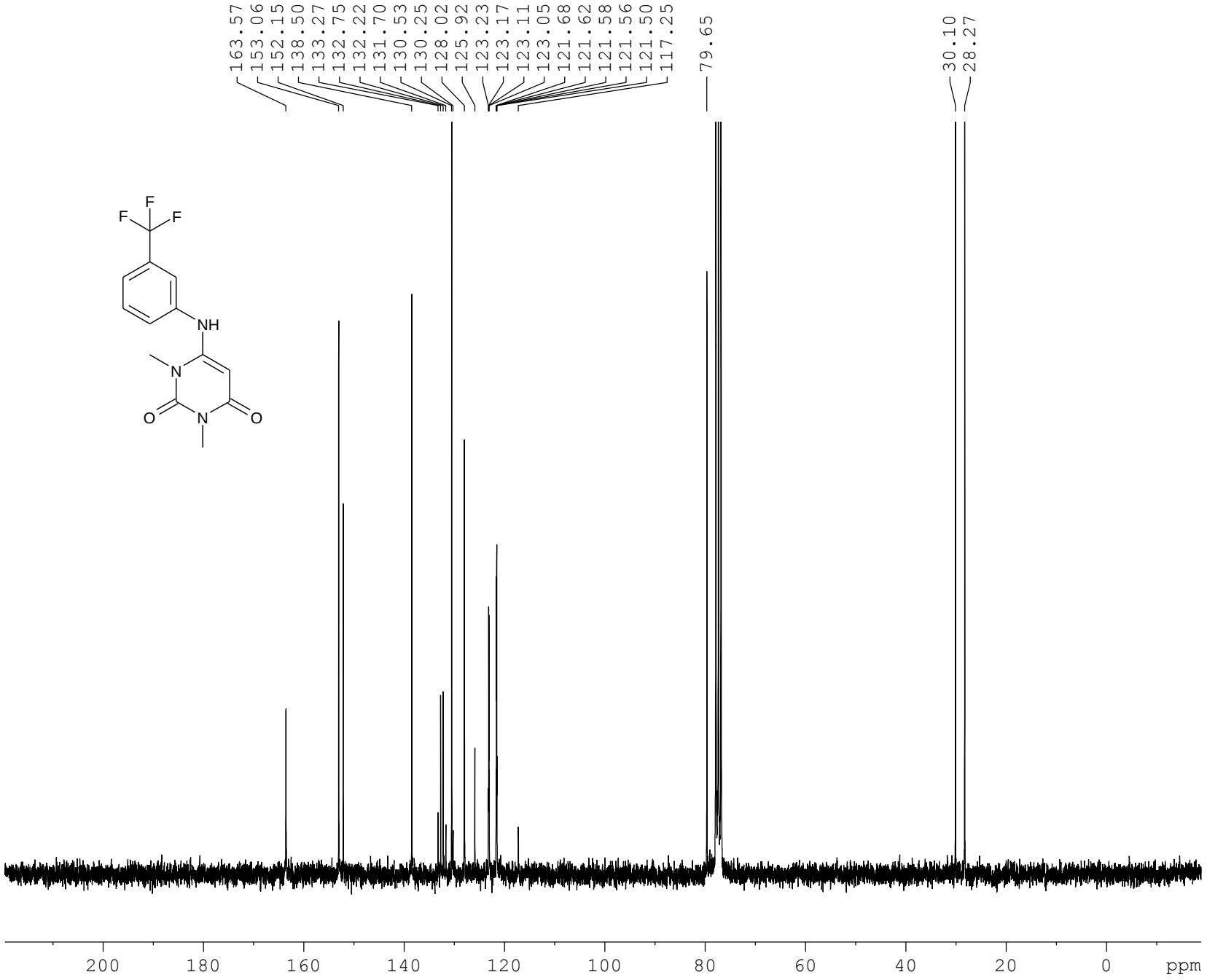

```
Current Data Parameters
NAME         111214.u301
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20111214
Time                8.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   128
DW                80.800 usec
DE                10.00 usec
TE                294.4 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300084 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd343 13C CDCl3

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Current Data Parameters
NAME          111214.208
EXPNO                 10
PROCNO                 1

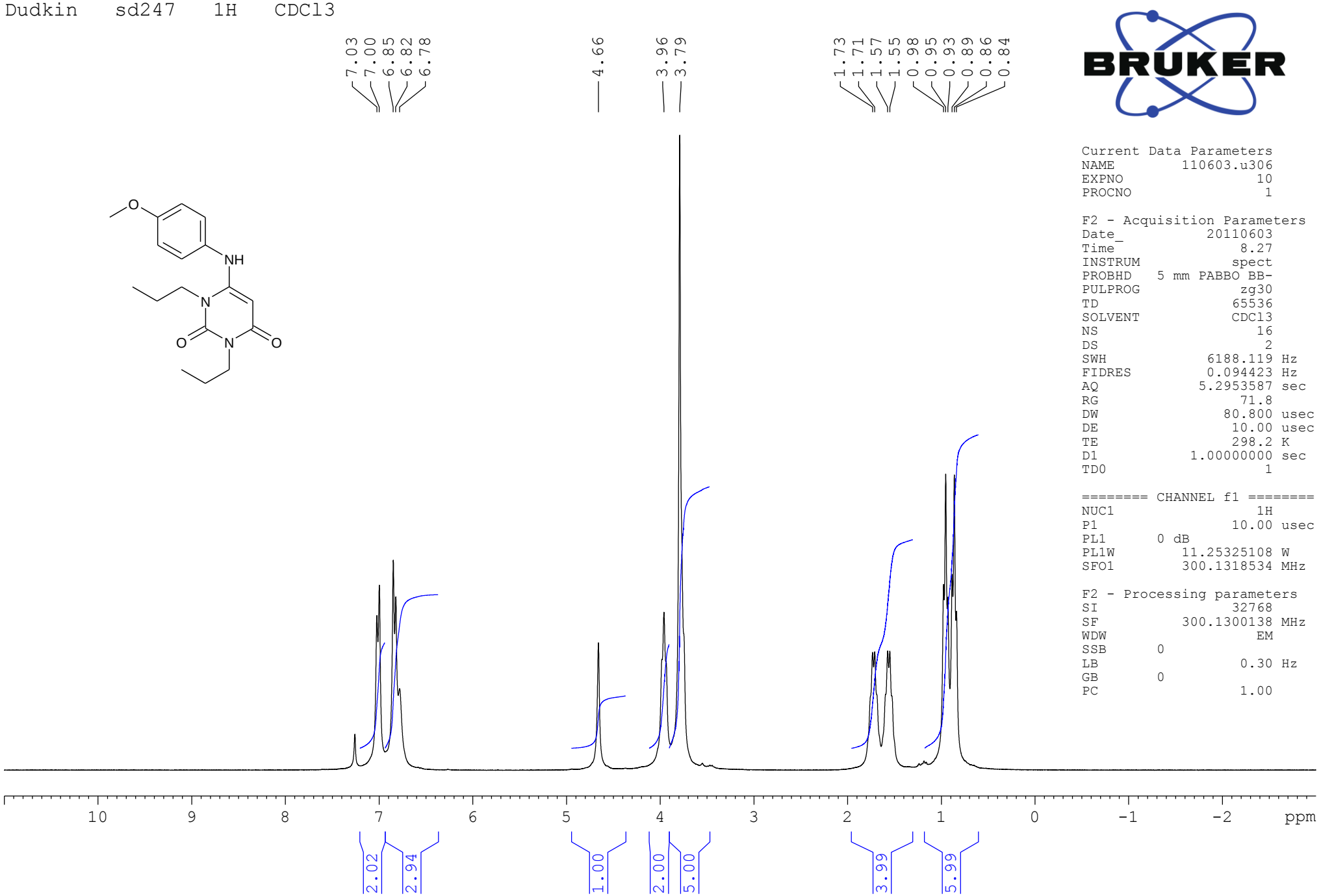
F2 - Acquisition Parameters
Date_           20111215
Time                7.56
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3132
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                673.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1       0 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              14.00 dB
PL13              14.00 dB
PL2               -3.00 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952175 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd247 1H CDCl3



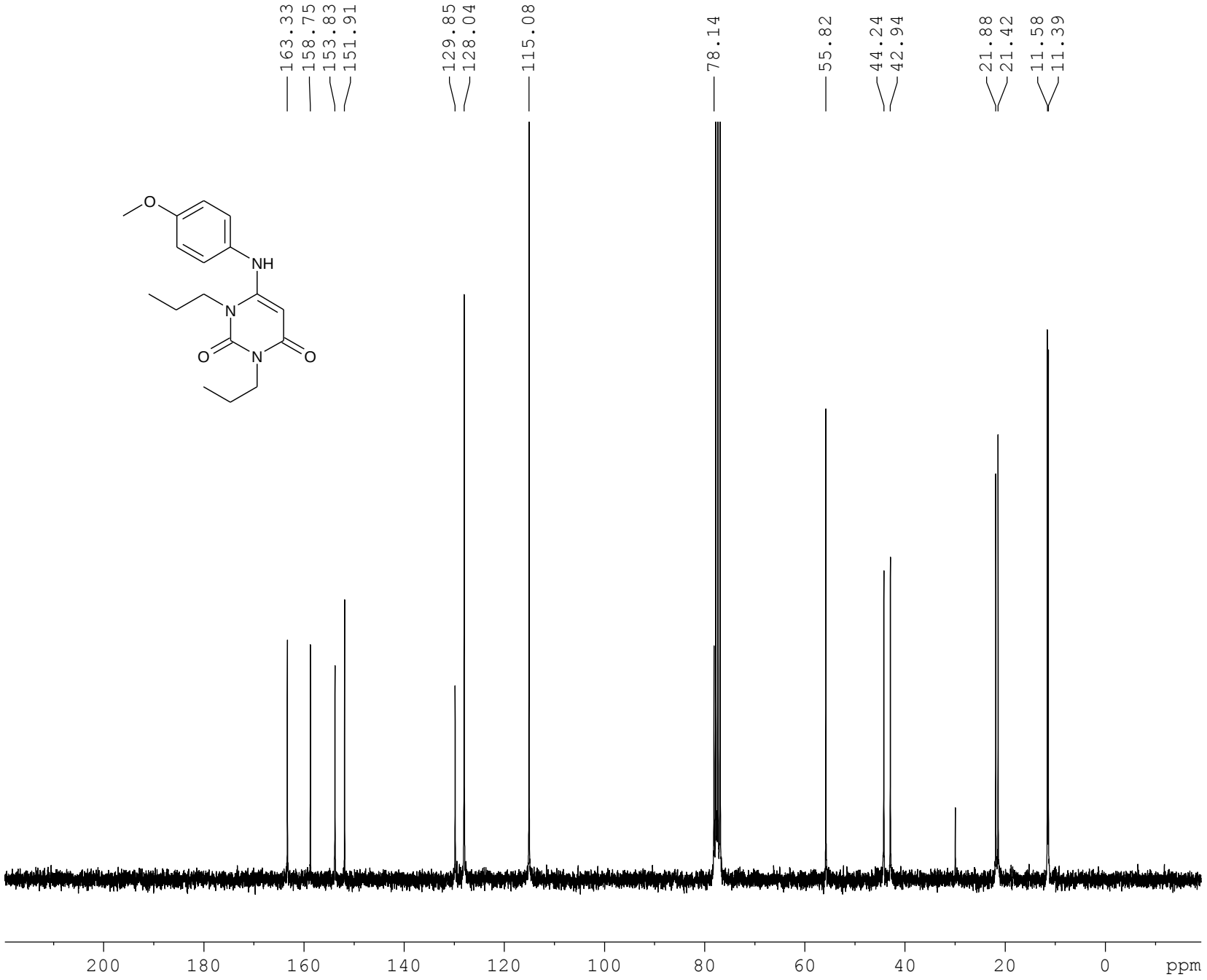
Current Data Parameters
NAME 110603.u306
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110603
Time 8.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 71.8
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd247 13C CDCl3



Current Data Parameters
NAME 110603.u306
EXPNO 11
PROCNO 1

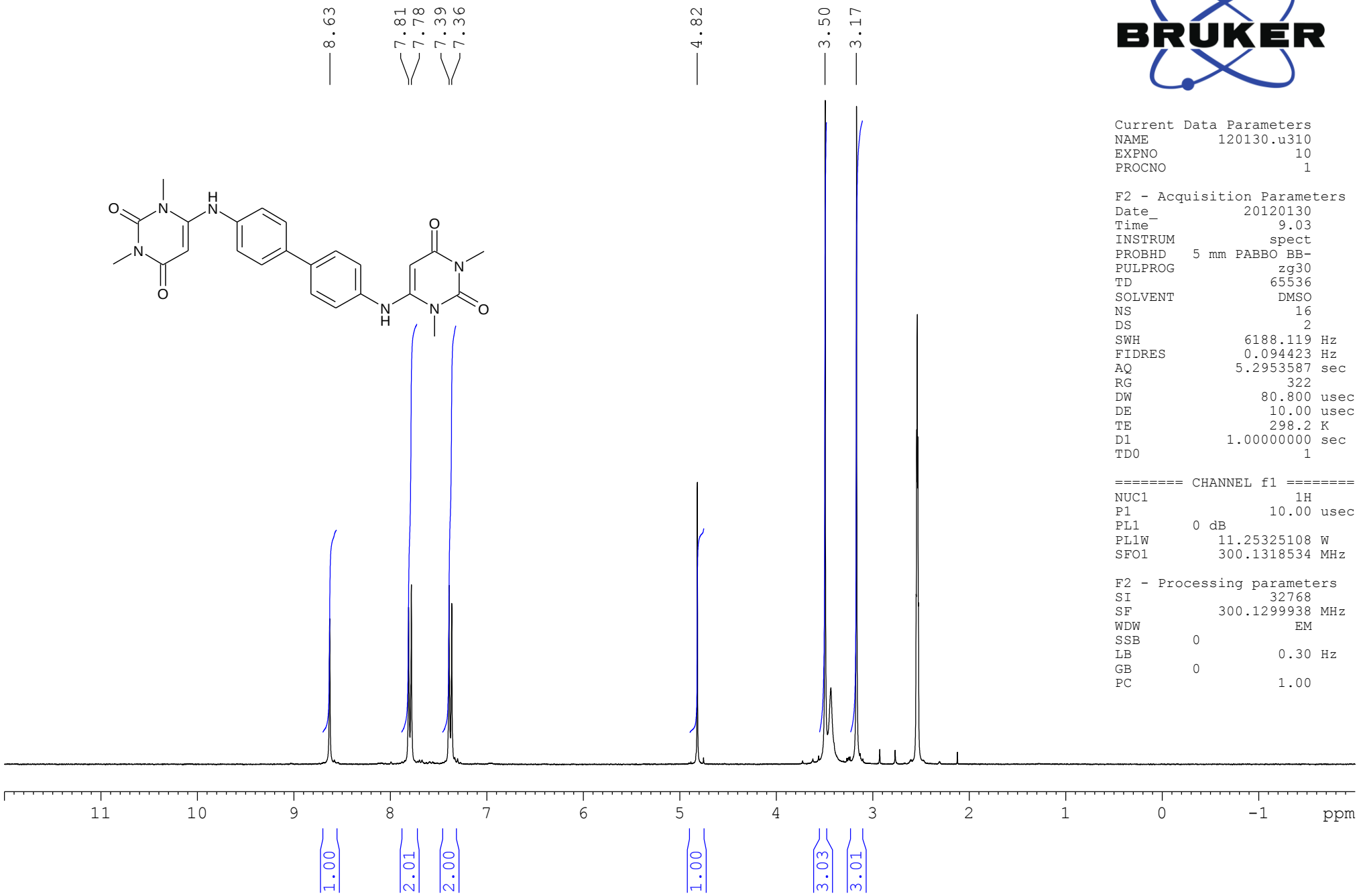
F2 - Acquisition Parameters
Date_ 20110603
Time 17.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677276 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd357 1H DMSO



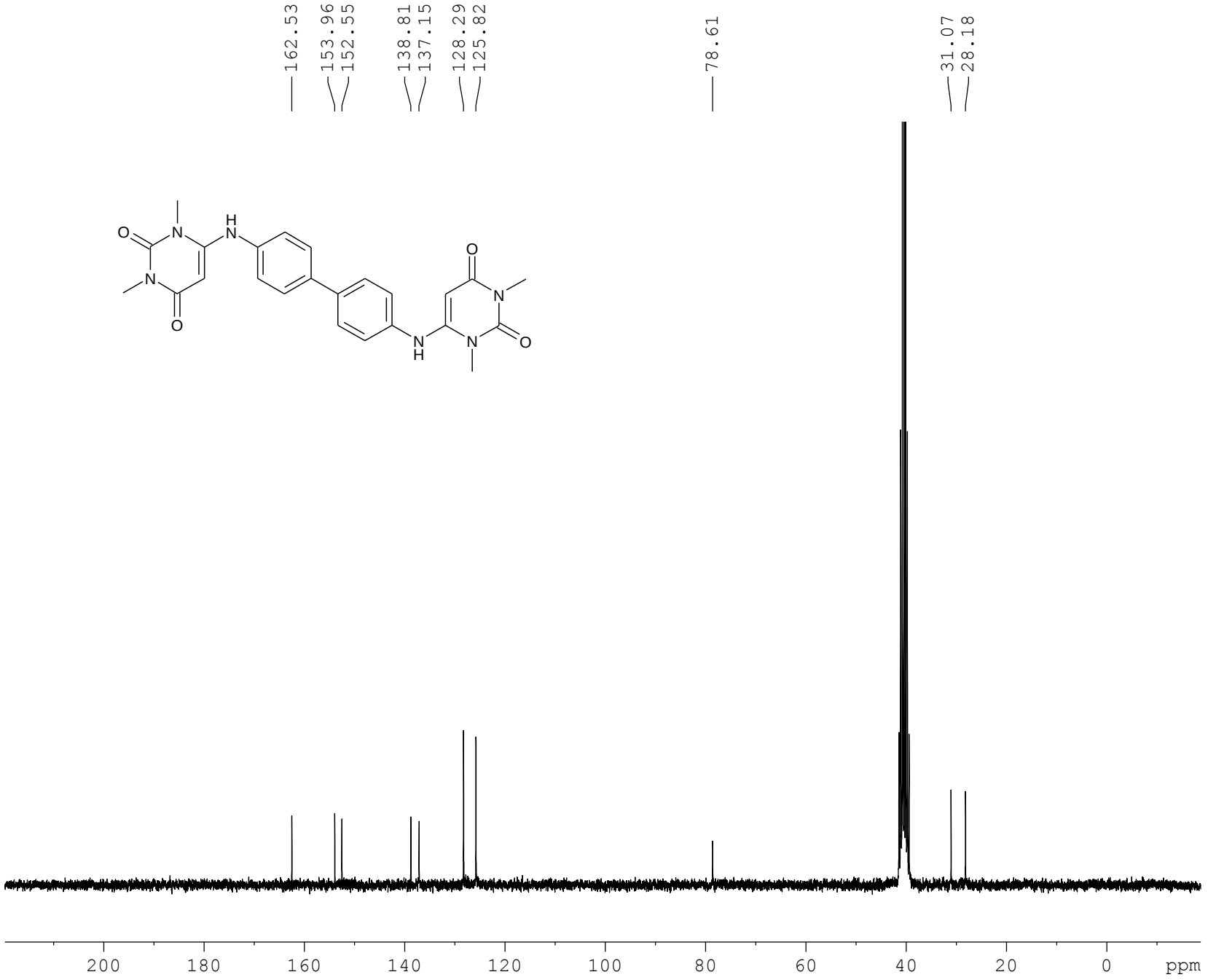

```
Current Data Parameters
NAME         120130.u310
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120130
Time                9.03
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   322
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1299938 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd357 13C DMSO




```
Current Data Parameters
NAME          120202.213
EXPNO                 10
PROCNO                 1

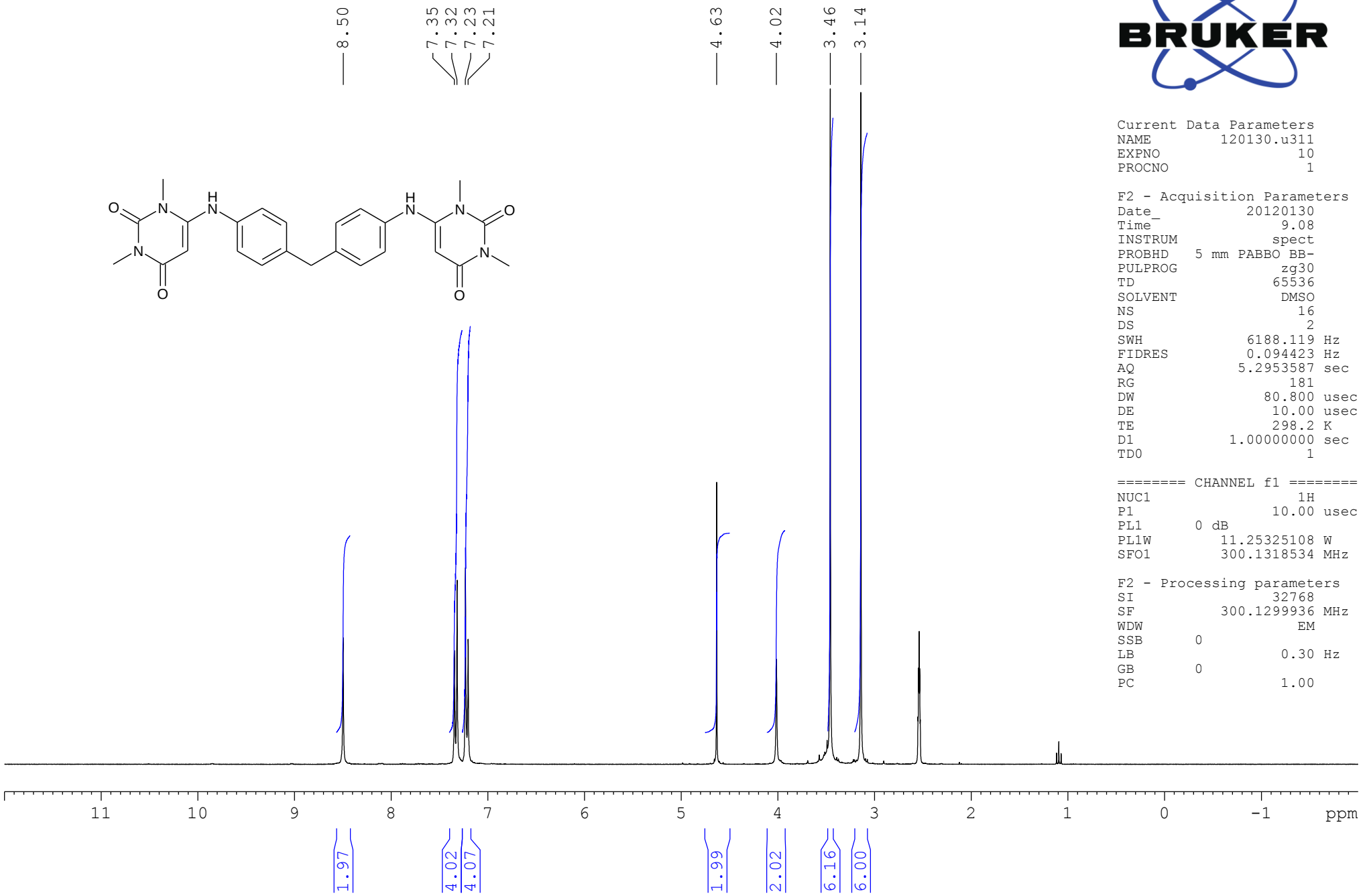
F2 - Acquisition Parameters
Date_           20120203
Time                0.17
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 1024
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1       0 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              14.00 dB
PL13              14.00 dB
PL2               -3.00 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                 32768
SF           62.8952078 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd358 1H DMSO



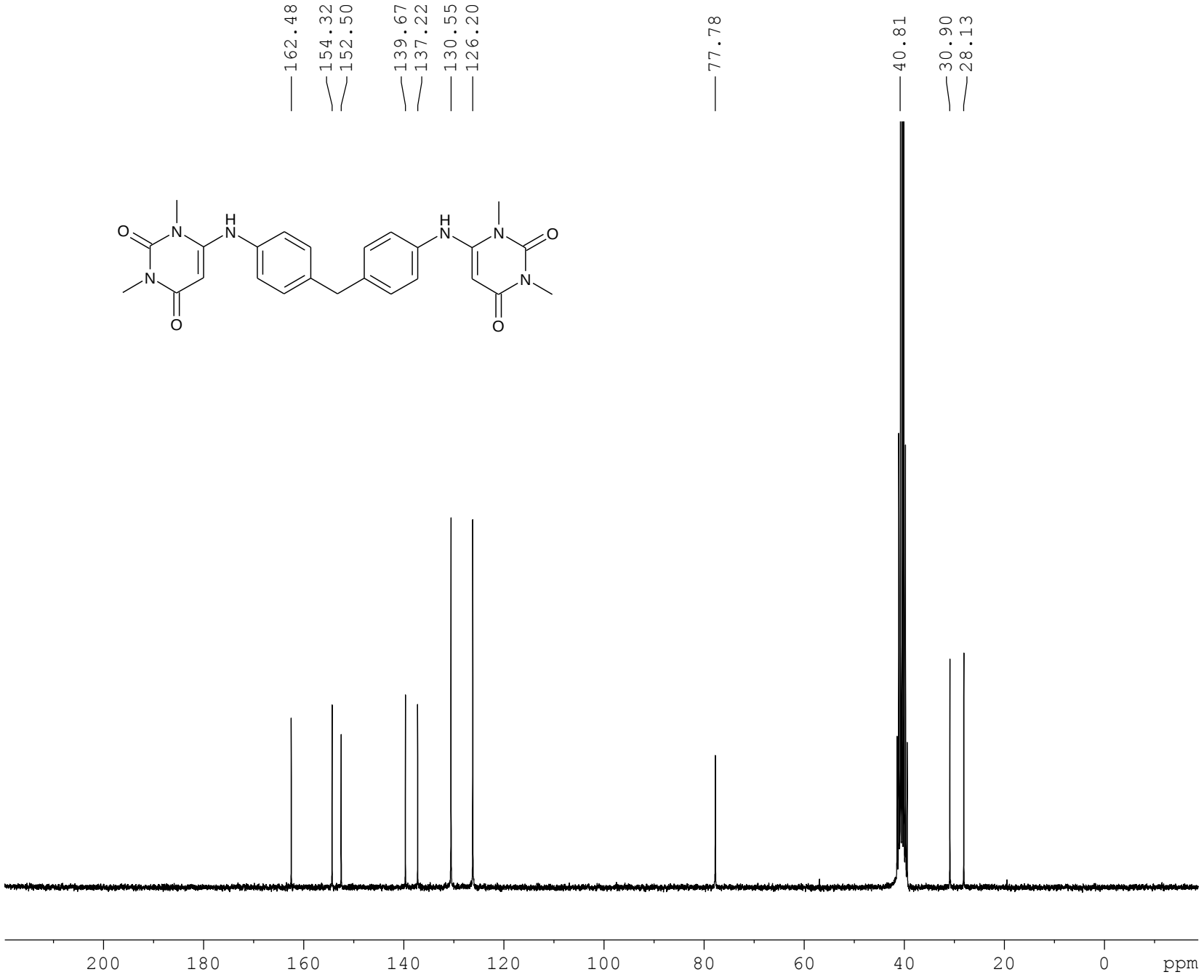

```
Current Data Parameters
NAME          120130.u311
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120130
Time                9.08
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   181
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1299936 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd358 13C DMSO



Current Data Parameters
NAME 120203.206
EXPNO 11
PROCNO 1

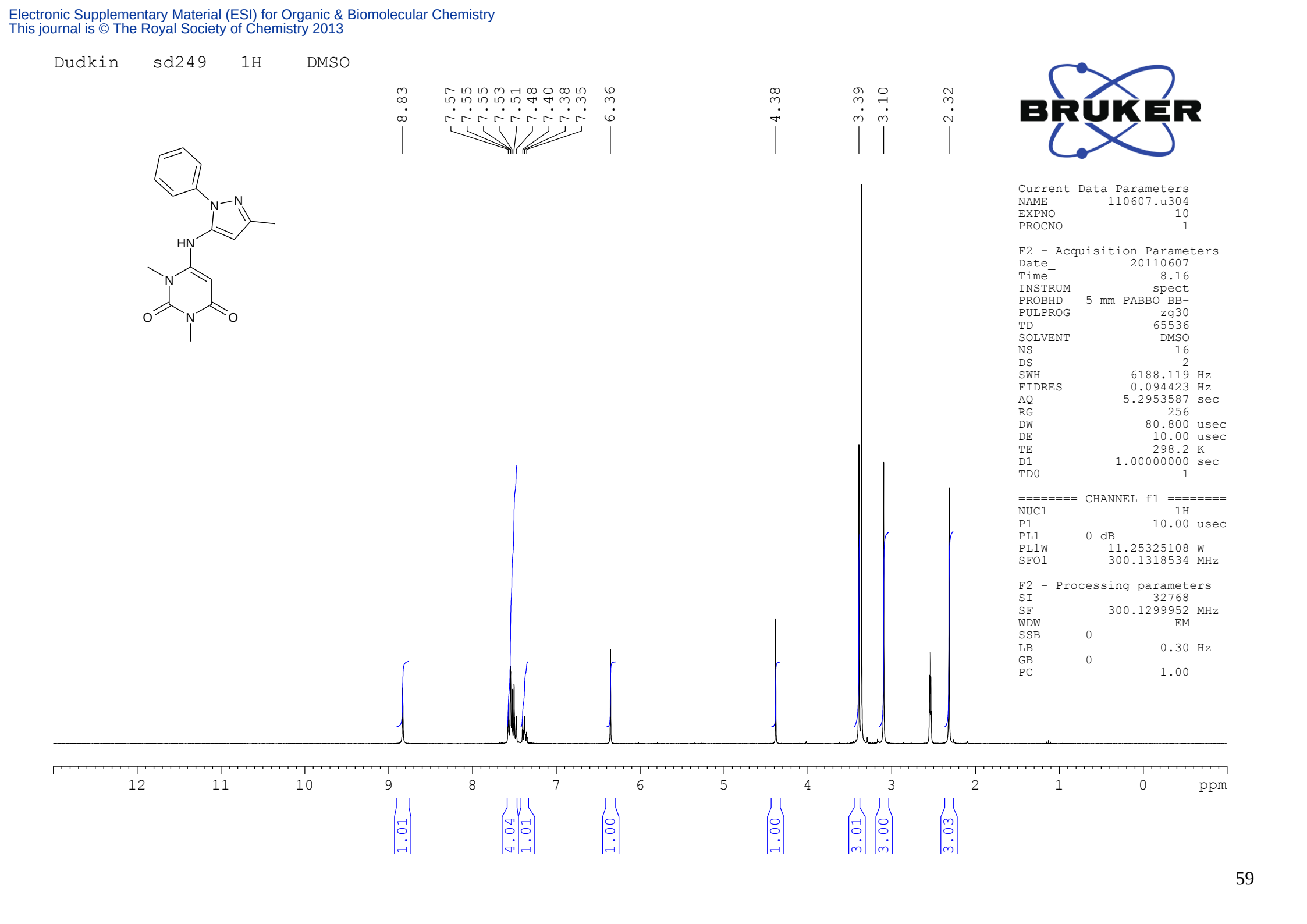
F2 - Acquisition Parameters
Date_ 20120203
Time 21.34
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.20 usec
PL1 0 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 14.00 dB
PL13 14.00 dB
PL2 -3.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952077 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd249 1H DMSO



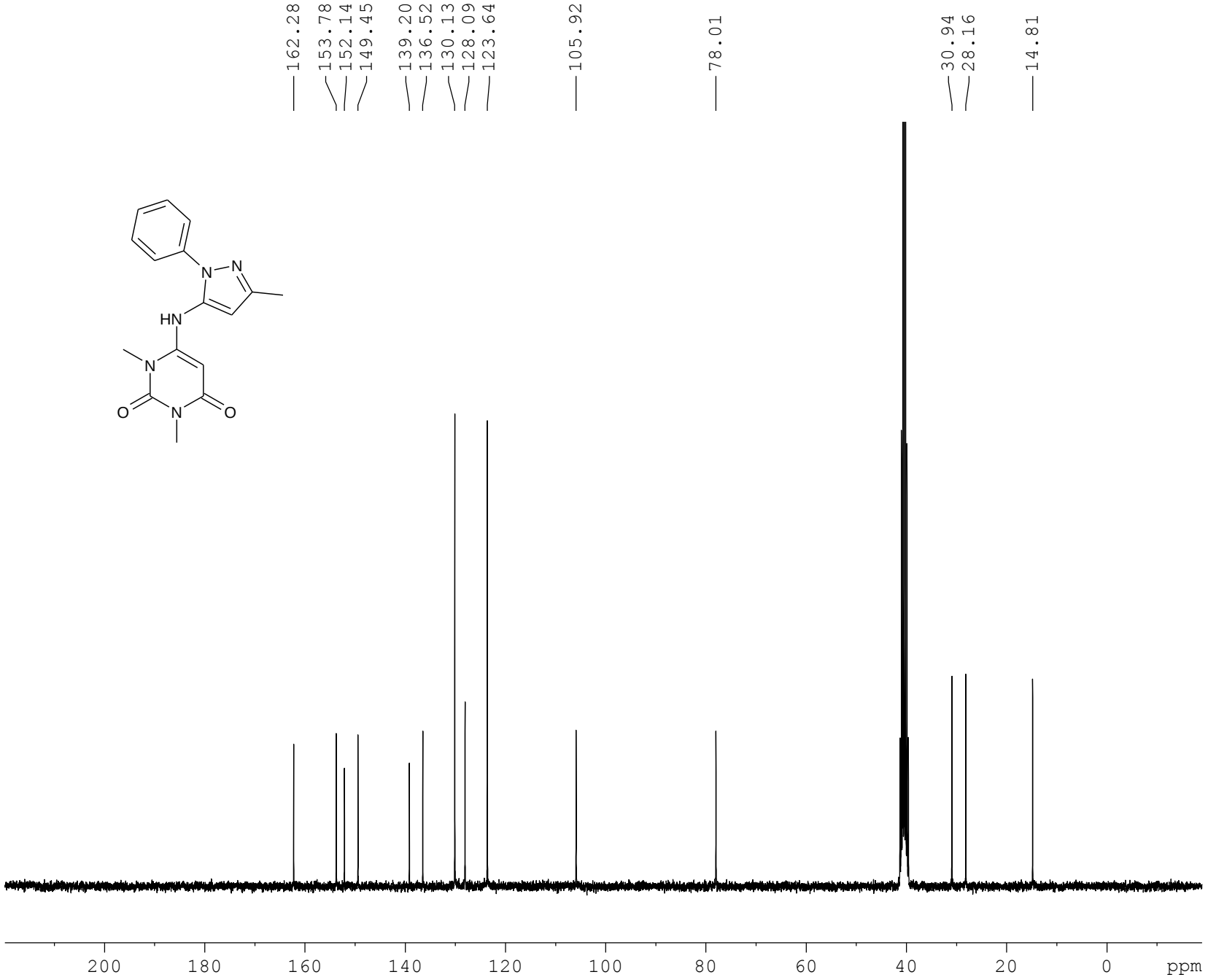
Current Data Parameters
NAME 110607.u304
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110607
Time 8.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 256
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299952 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin, sd 249, DMSO, 13C




```
Current Data Parameters
NAME         110623.u325
EXPNO                 10
PROCNO                 1

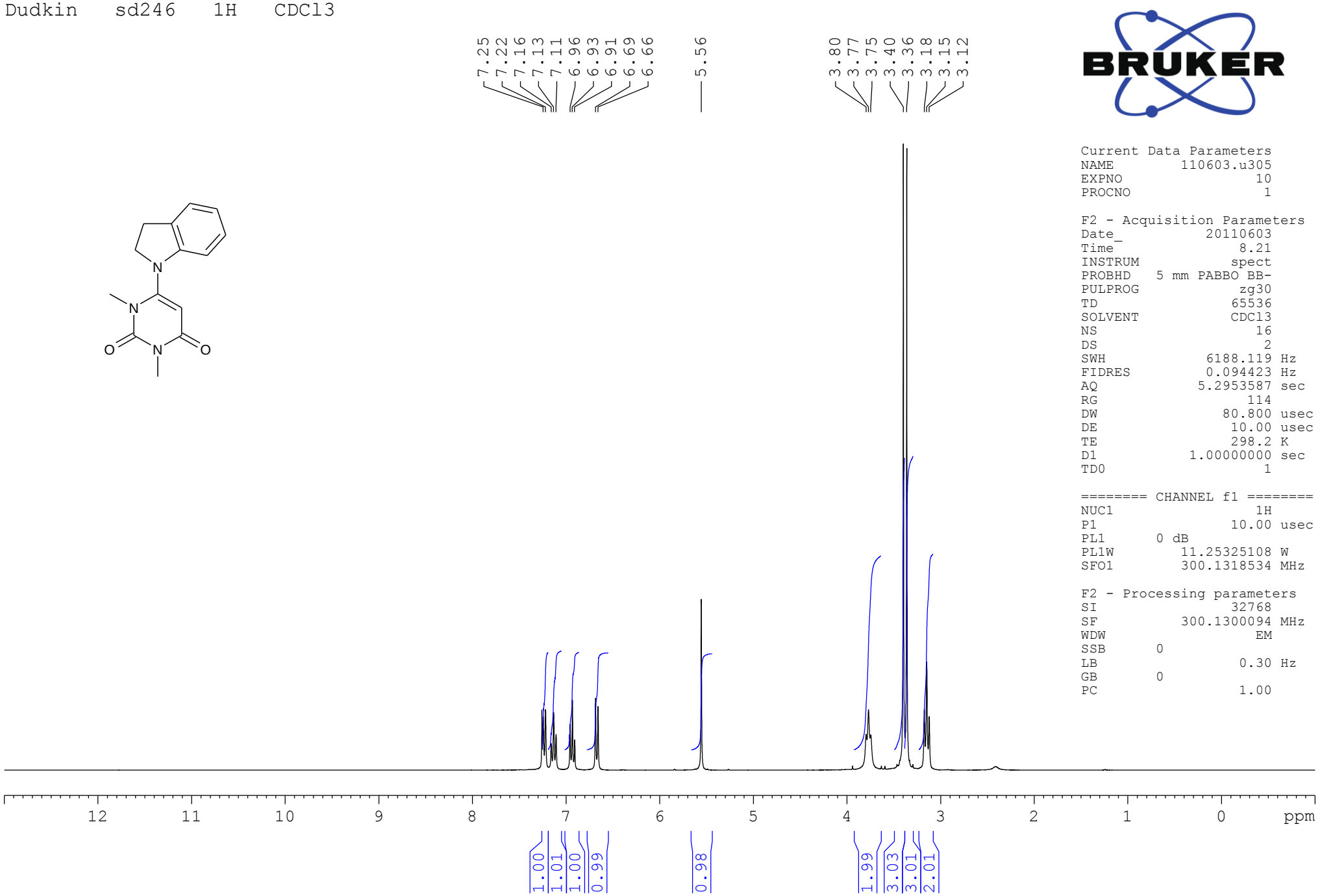
F2 - Acquisition Parameters
Date_           20110624
Time                2.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 1024
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                 2050
DW               27.733 usec
DE               10.00 usec
TE               298.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1               10.00 usec
PL1              -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

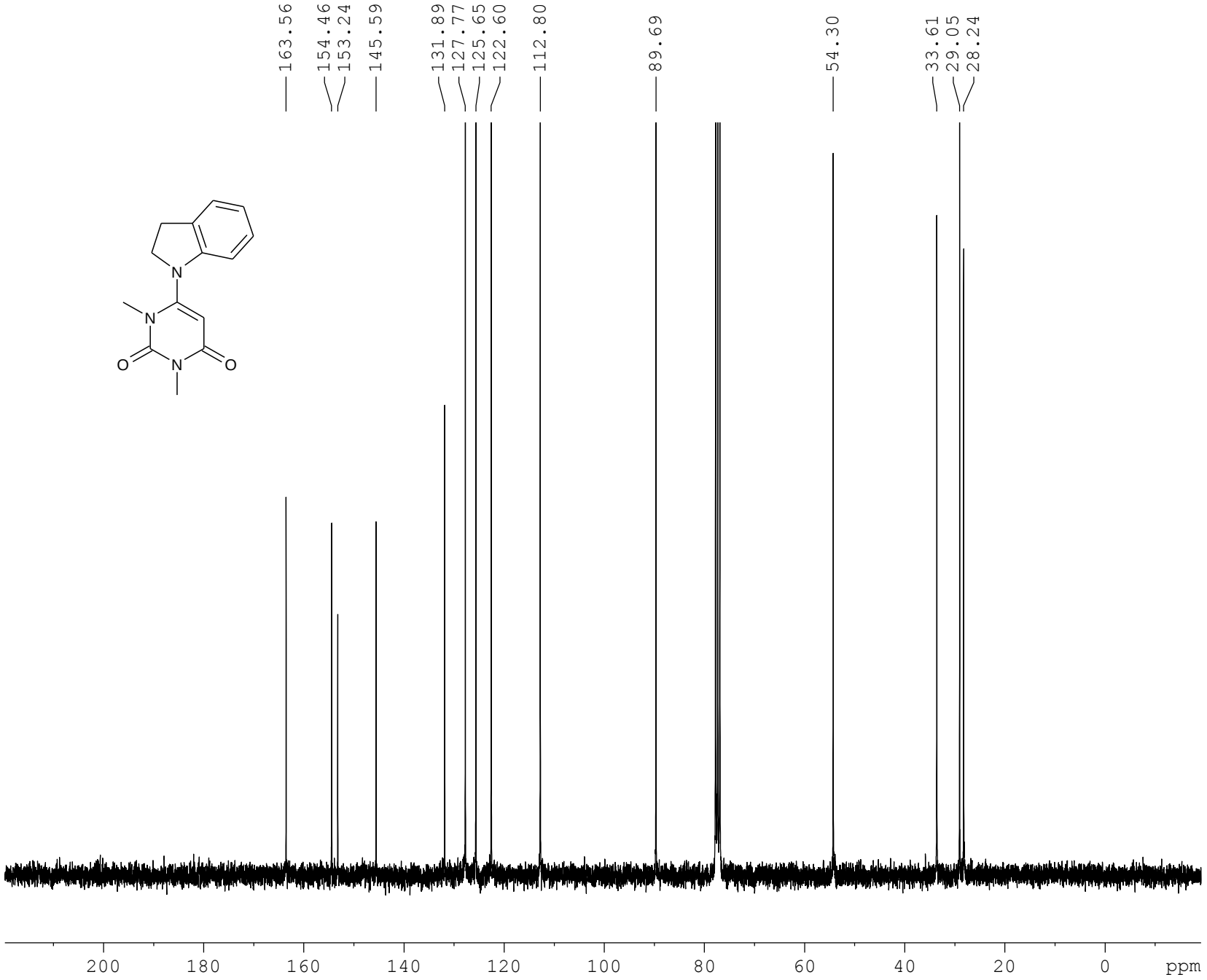
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            72.00 usec
PL2       0 dB
PL12             17.00 dB
PL13             17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677153 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

Dudkin sd246 1H CDCl3



Dudkin sd246 13C CDCl3




```
Current Data Parameters
NAME          110603.u305
EXPNO                  11
PROCNO                  1

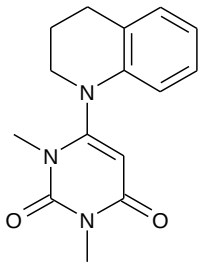
F2 - Acquisition Parameters
Date_            20110603
Time                15.58
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                  2050
DW                27.733 usec
DE                10.00 usec
TE                298.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              72.00 usec
PL2       0 dB
PL12               17.00 dB
PL13               17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677292 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Dudkin, sd 294, CDCl3, 1H



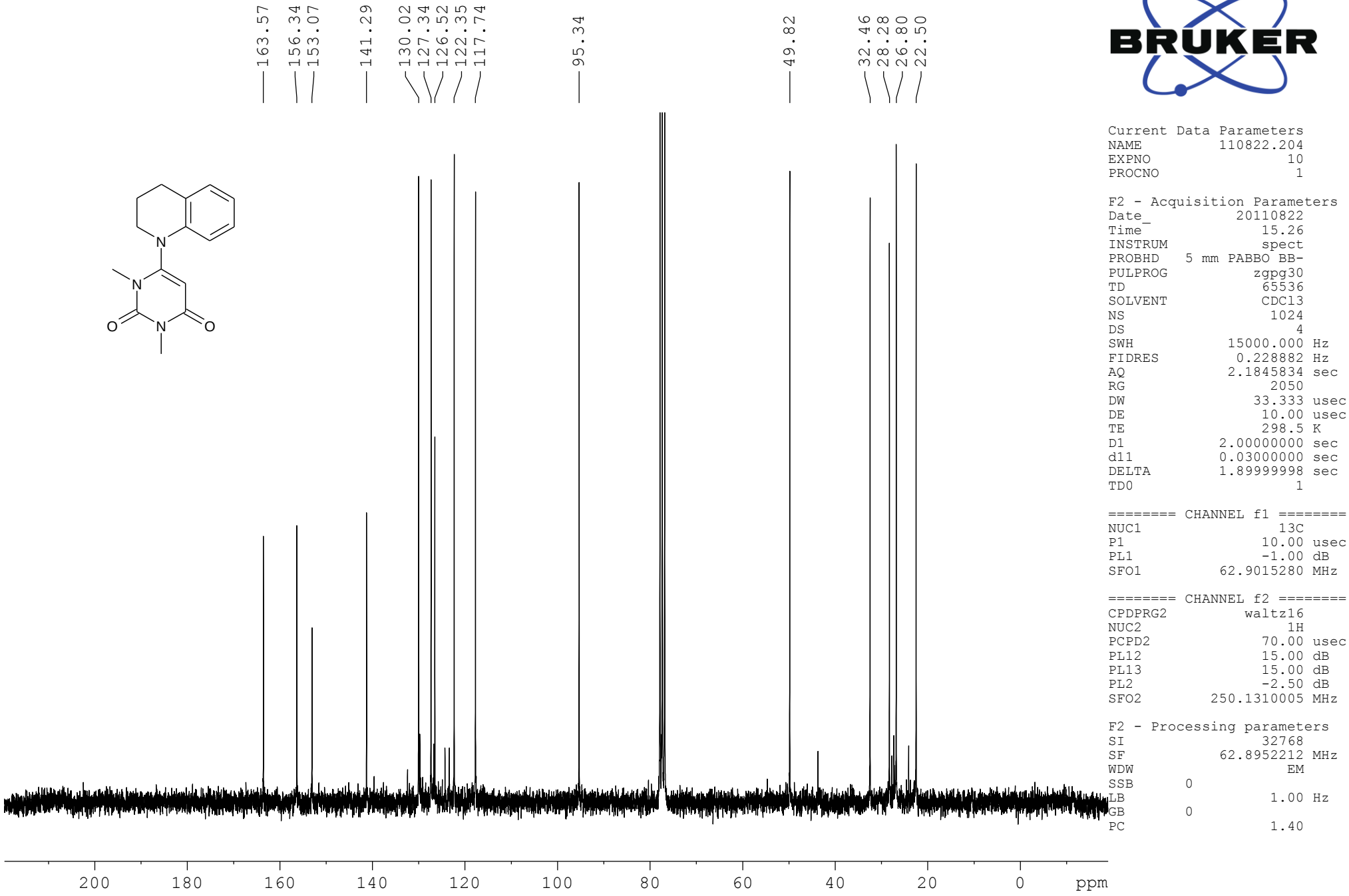
Current Data Parameters
NAME 110819.u303
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110819
Time 8.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300013 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin, sd 294, CDCl3, 13C




```
Current Data Parameters
NAME          110822.204
EXPNO                 10
PROCNO                 1

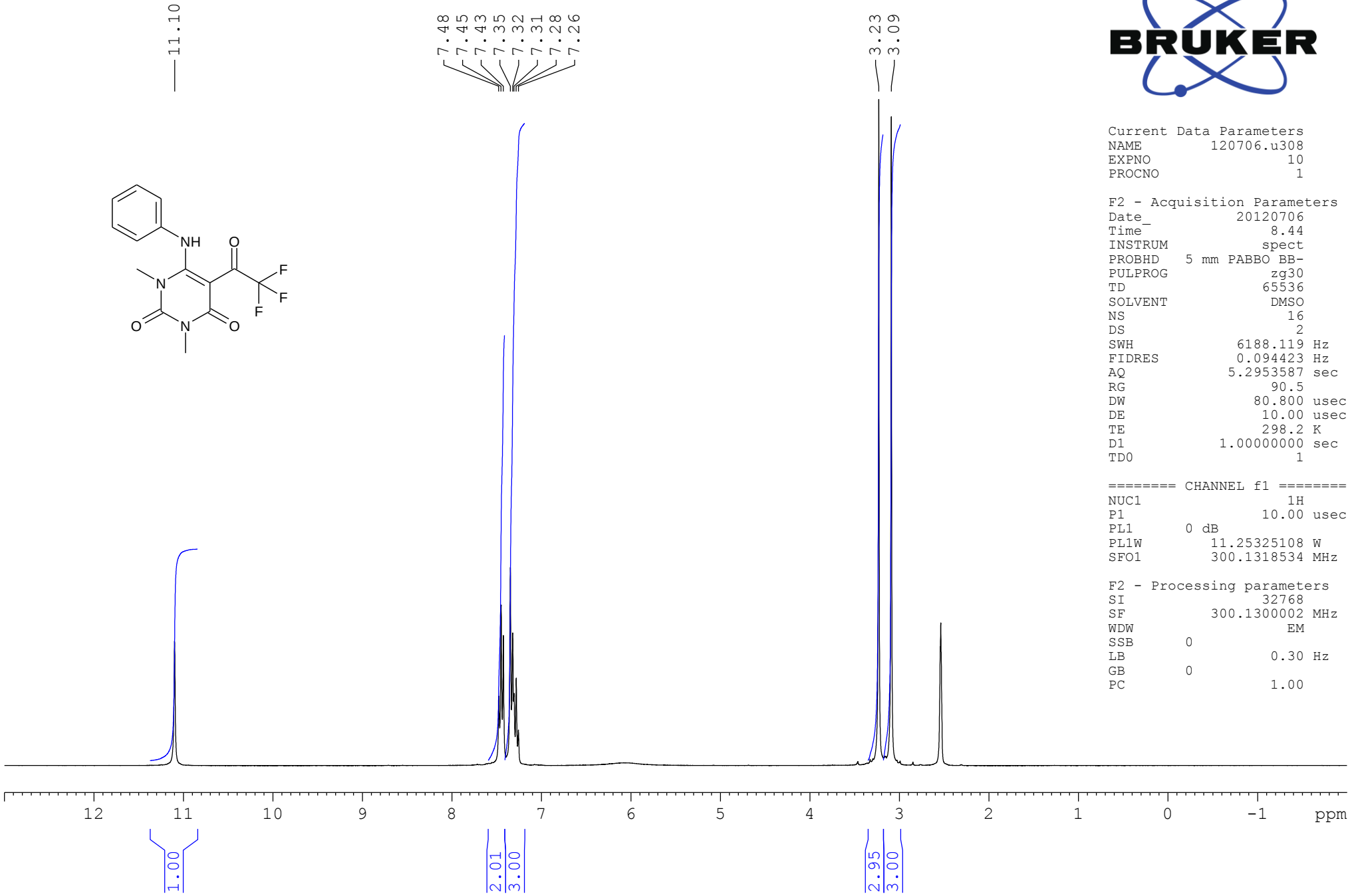
F2 - Acquisition Parameters
Date_           20110822
Time               15.26
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.5 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952212 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin, sd 439, DMSO, 1H



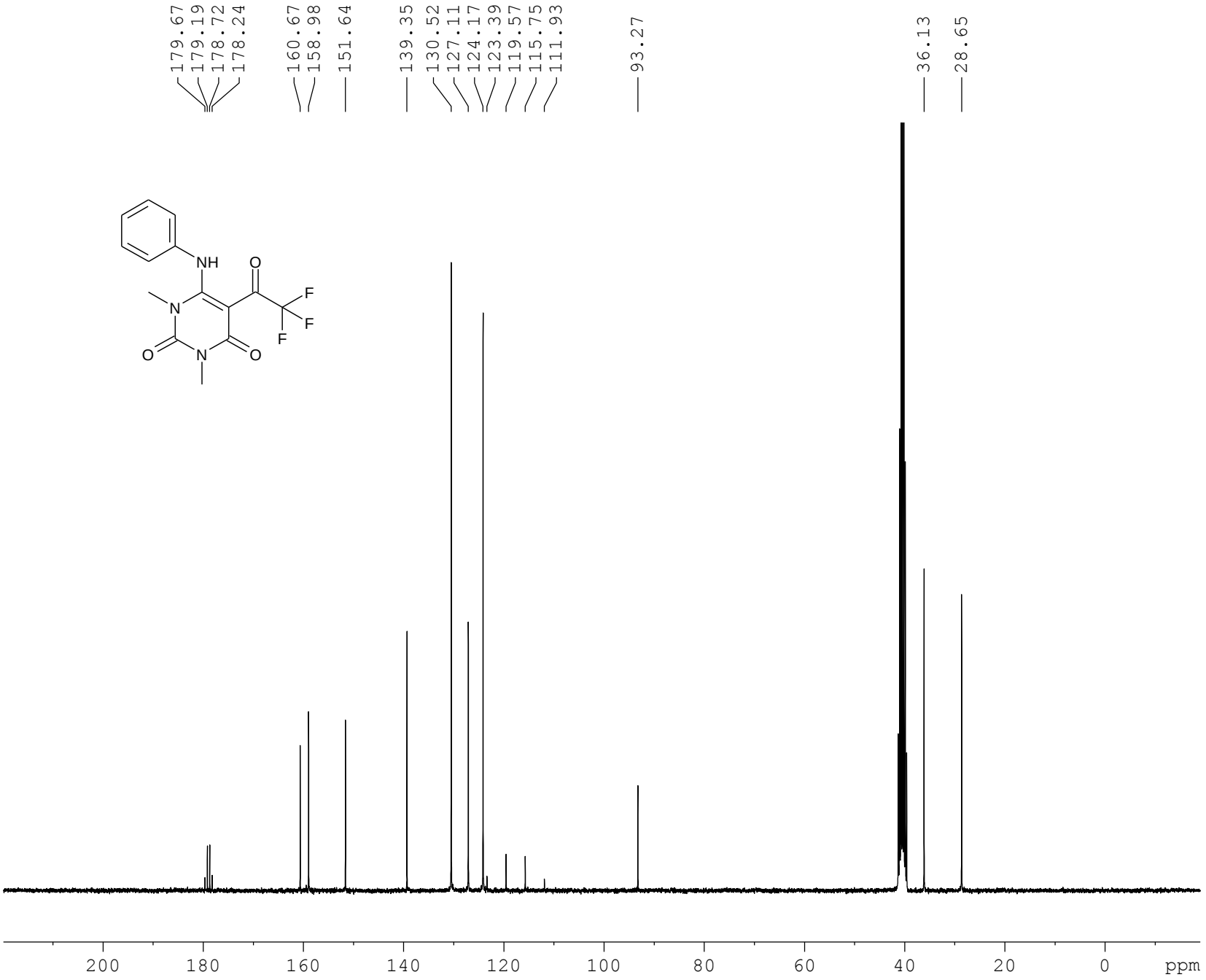

```
Current Data Parameters
NAME          120706.u308
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120706
Time                8.44
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                  90.5
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300002 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin, sd 439, DMSO, 13C




```
Current Data Parameters
NAME         120706.u308
EXPNO                 12
PROCNO                 1

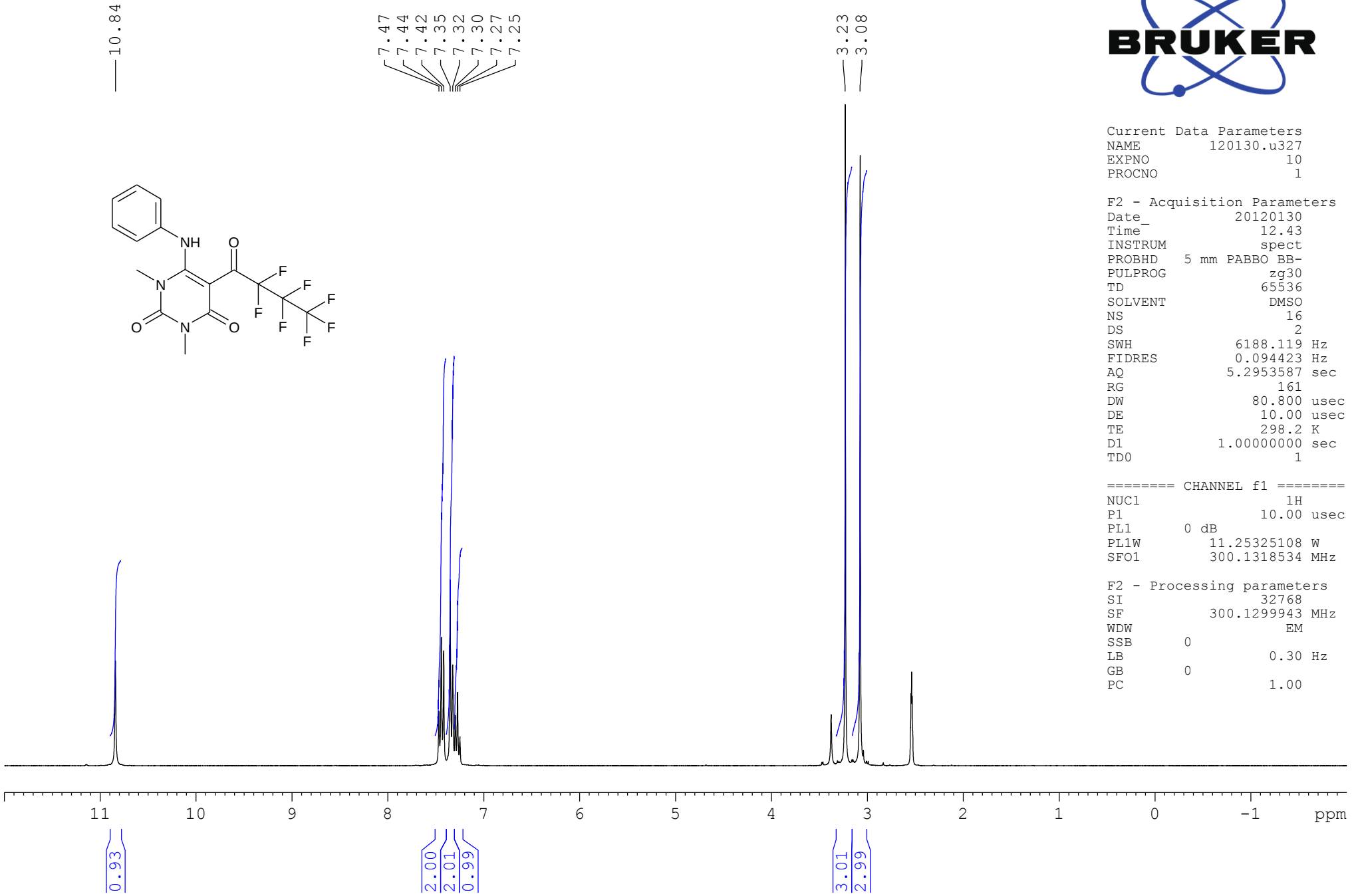
F2 - Acquisition Parameters
Date_           20120708
Time                7.43
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 4096
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                 2050
DW               27.733 usec
DE               10.00 usec
TE               298.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             72.00 usec
PL2       0 dB
PL12              17.00 dB
PL13              17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677159 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd360 1H DMSO



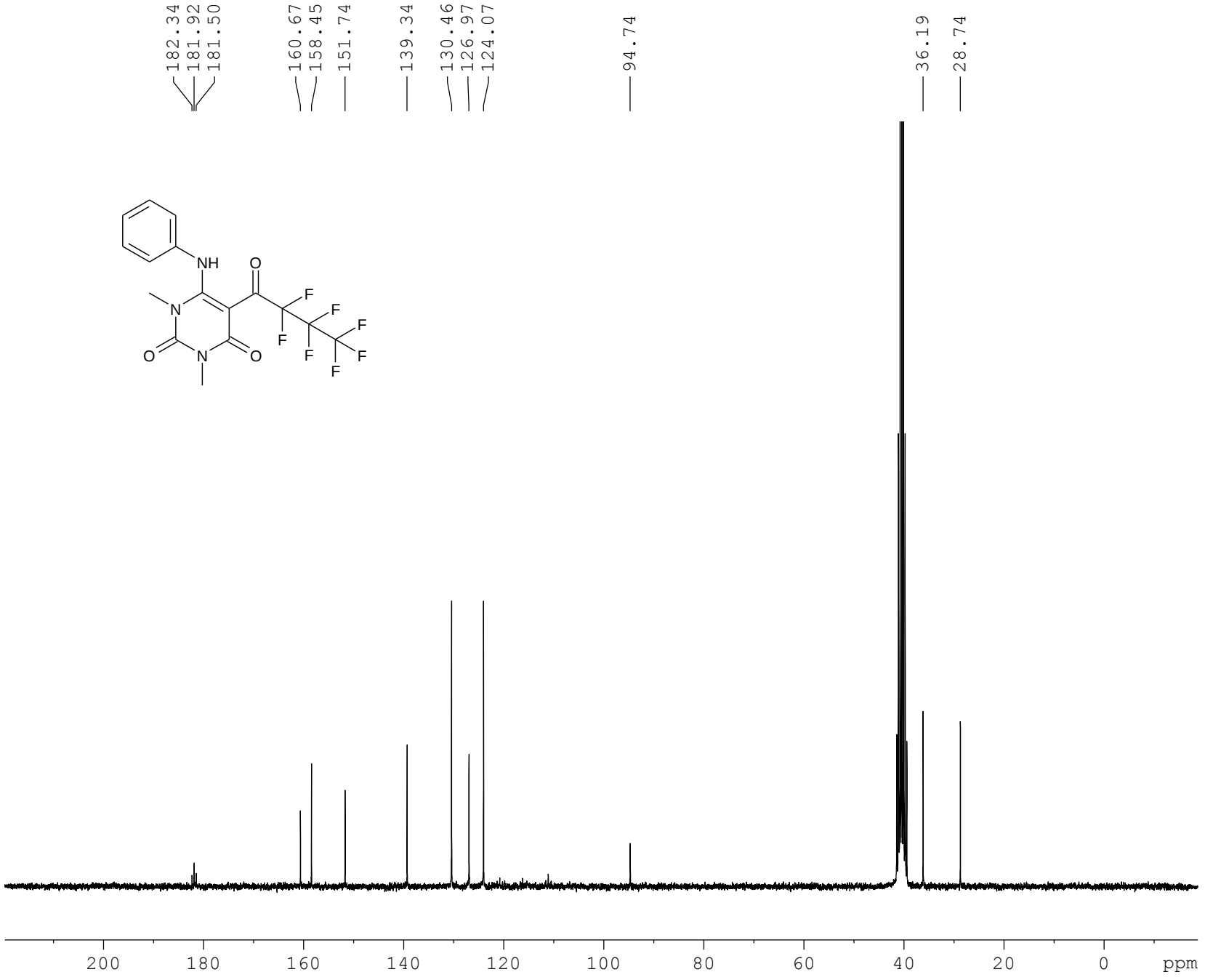

```
Current Data Parameters
NAME          120130.u327
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120130
Time                12.43
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.094423 Hz
AQ               5.2953587 sec
RG                    161
DW                 80.800 usec
DE                 10.00 usec
TE                 298.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1       0 dB
PL1W         11.25325108 W
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF           300.1299943 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

Dudkin sd360 13C DMSO



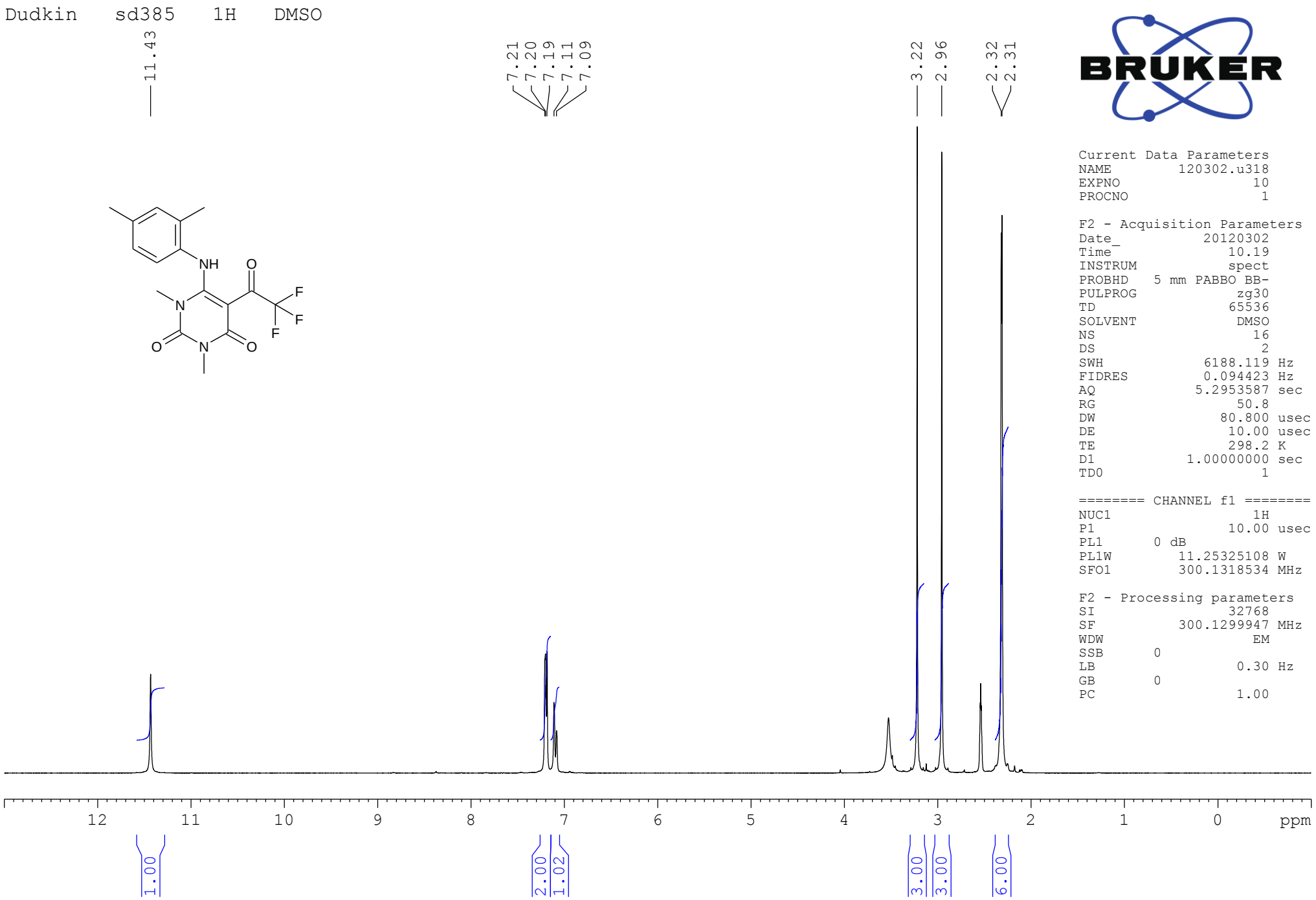

```
Current Data Parameters
NAME          120203.211
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120205
Time                1.16
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  3072
DS                     4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                  2050
DW                33.333 usec
DE                10.00 usec
TE                298.1 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

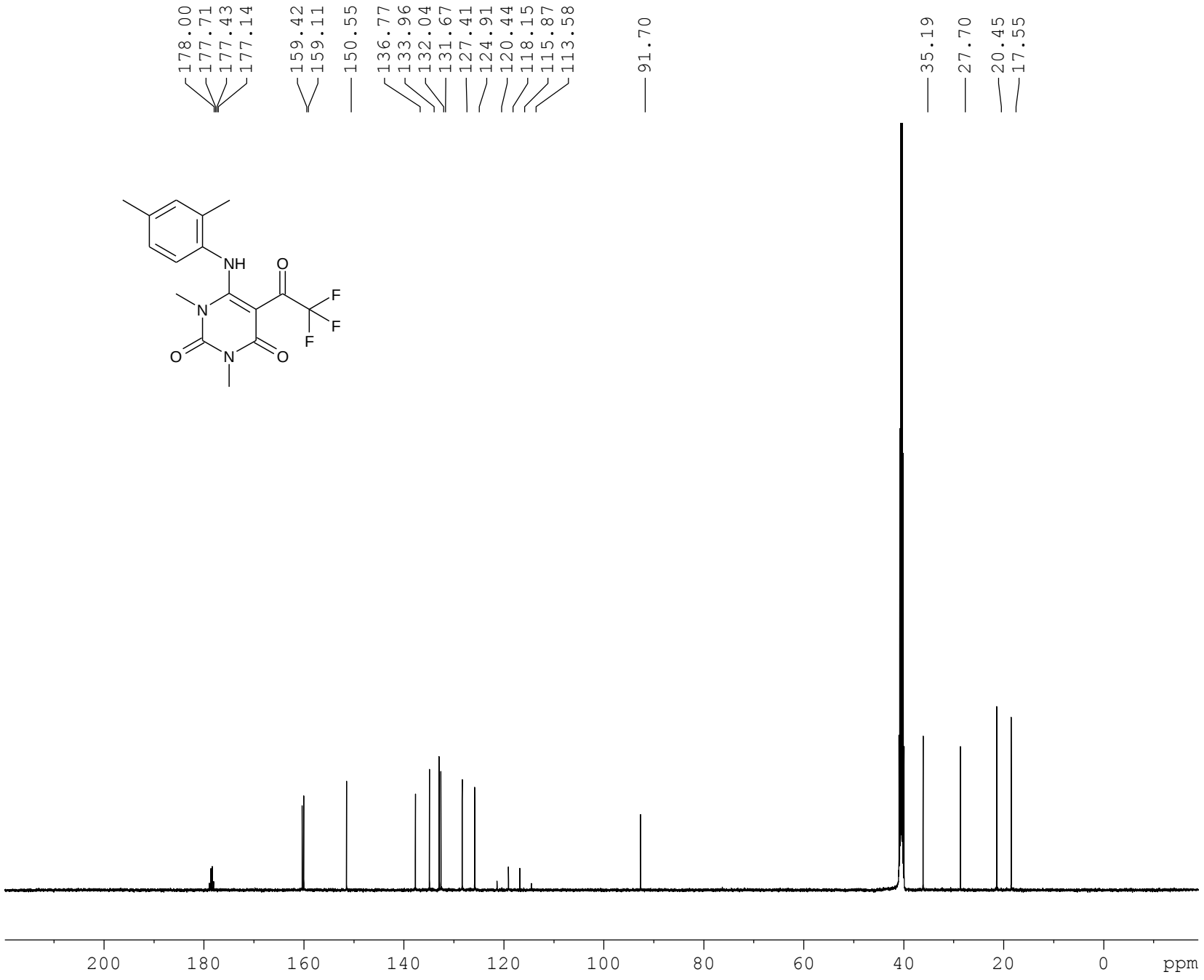
======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1       0 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             70.00 usec
PL12              14.00 dB
PL13              14.00 dB
PL2               -3.00 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                 32768
SF           62.8952076 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



S. Dudkin, sd 385, 13C in DMSO




```
Current Data Parameters
NAME          120305.502
EXPNO                 12
PROCNO                 1

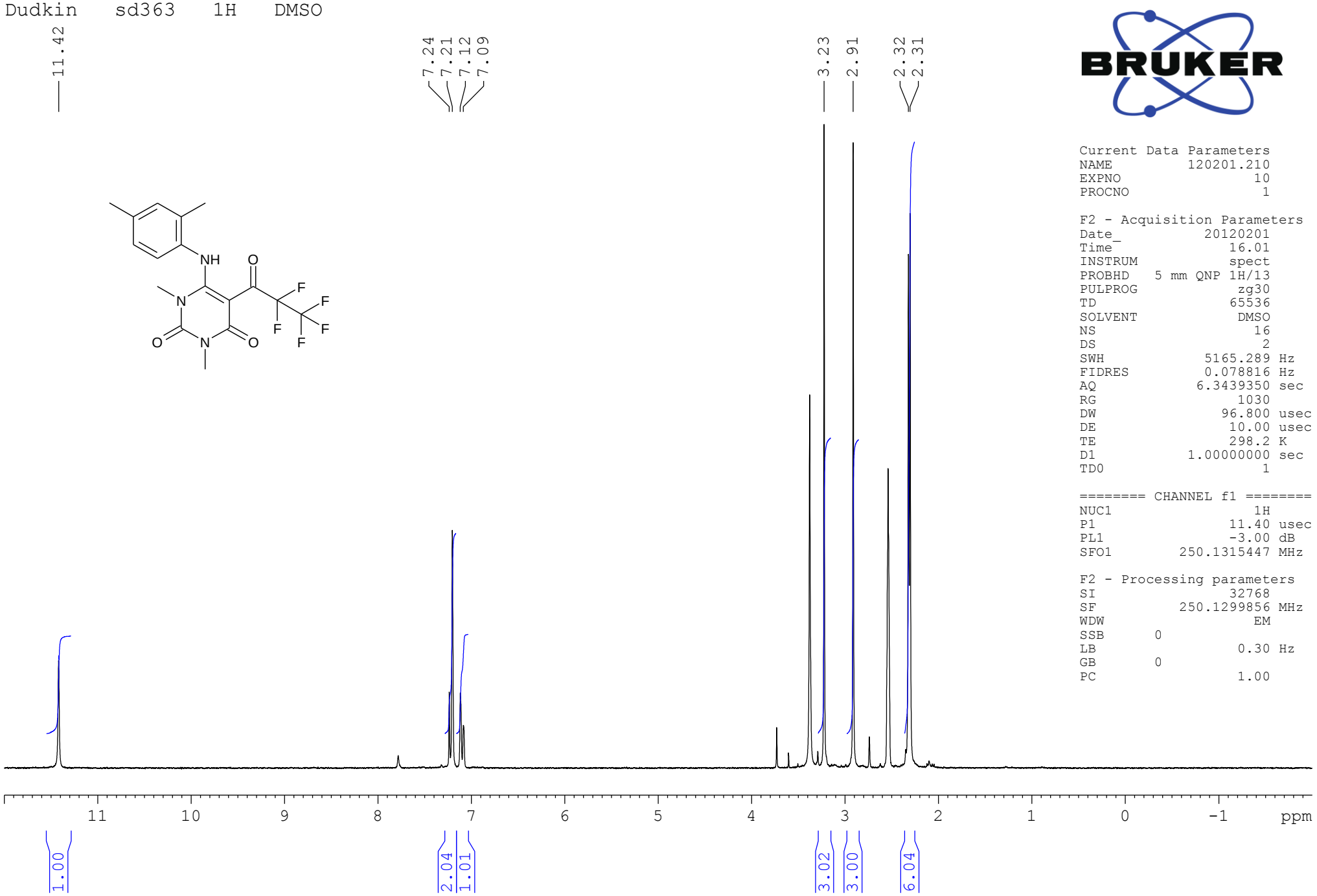
F2 - Acquisition Parameters
Date_           20120305
Time               20.19
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG                1149.4
DW               16.650 usec
DE                6.50 usec
TE               300.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                9.00 usec
PL1               4.50 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            70.00 usec
PL2              -3.00 dB
PL12             14.08 dB
PL13            120.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577328 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd363 1H DMSO



Current Data Parameters
NAME 120201.210
EXPNO 10
PROCNO 1

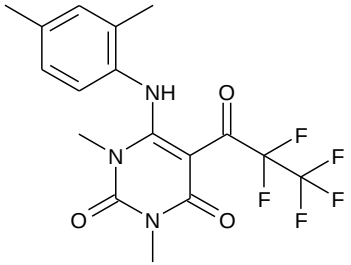
F2 - Acquisition Parameters
Date_ 20120201
Time 16.01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 1030
DW 96.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.40 usec
PL1 -3.00 dB
SFO1 250.1315447 MHz

F2 - Processing parameters
SI 32768
SF 250.1299856 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd363 13C DMSO

181.45 181.01 180.59 160.28 160.18 151.54 137.82 134.76 132.97 132.60 128.36 125.96 94.06 36.44 28.77 21.42 18.53



Current Data Parameters
NAME 120203.208
EXPNO 11
PROCNO 1

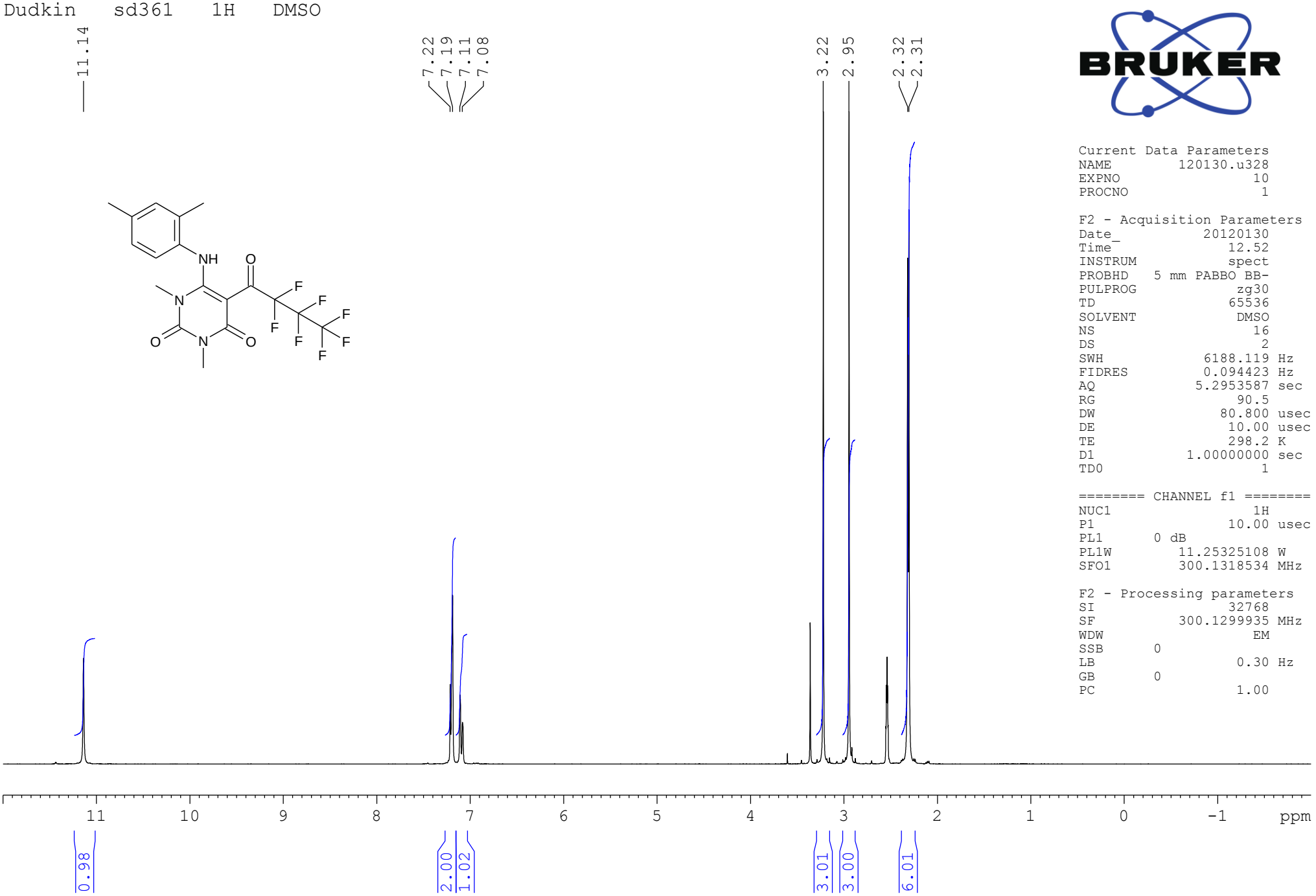
F2 - Acquisition Parameters
Date_ 20120204
Time 6.55
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.20 usec
PL1 0 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 14.00 dB
PL13 14.00 dB
PL2 -3.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952083 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd361 1H DMSO



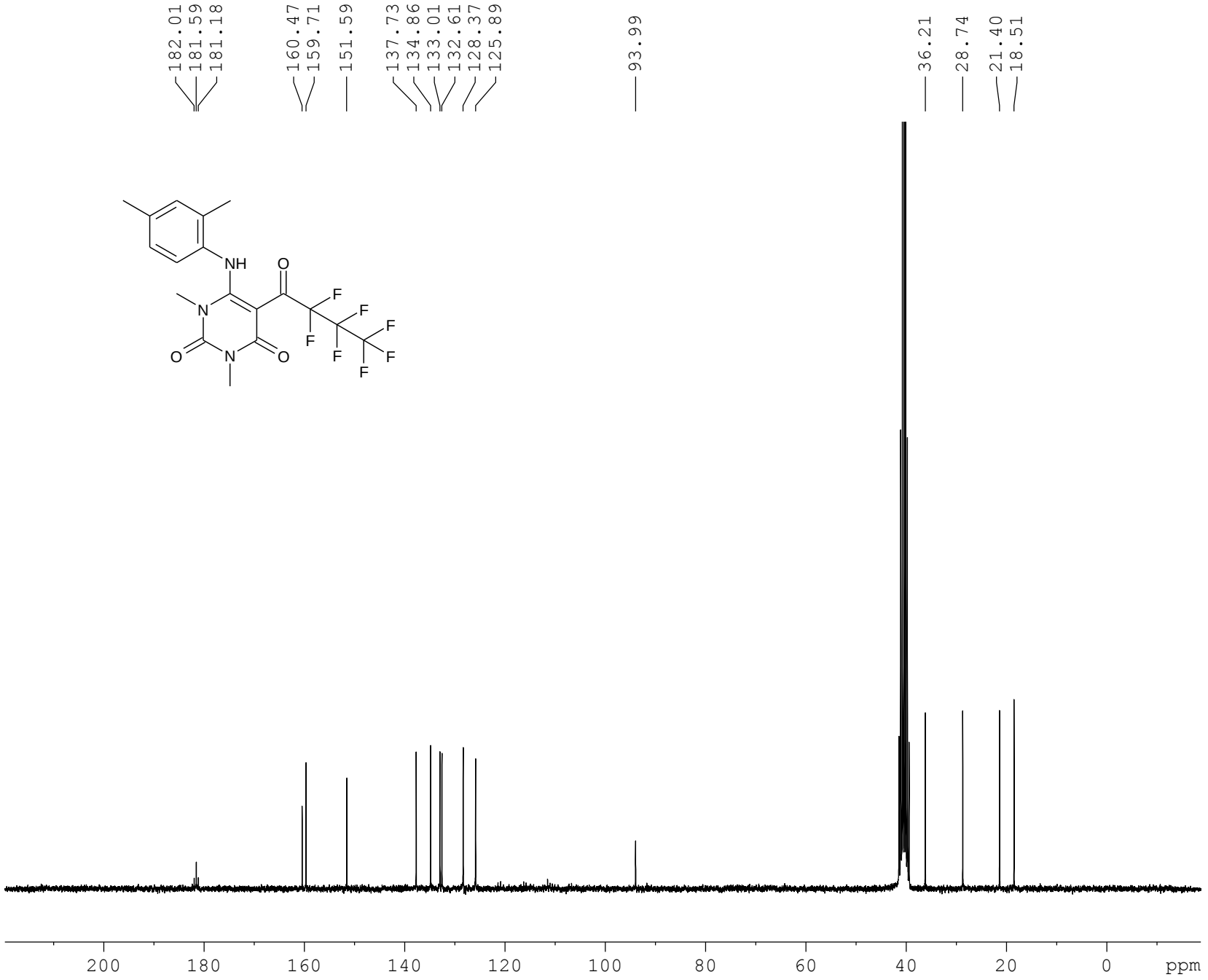
Current Data Parameters
NAME 120130.u328
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120130
Time 12.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 90.5
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299935 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd361 13C DMSO




```
Current Data Parameters
NAME          120203.212
EXPNO                 10
PROCNO                 1

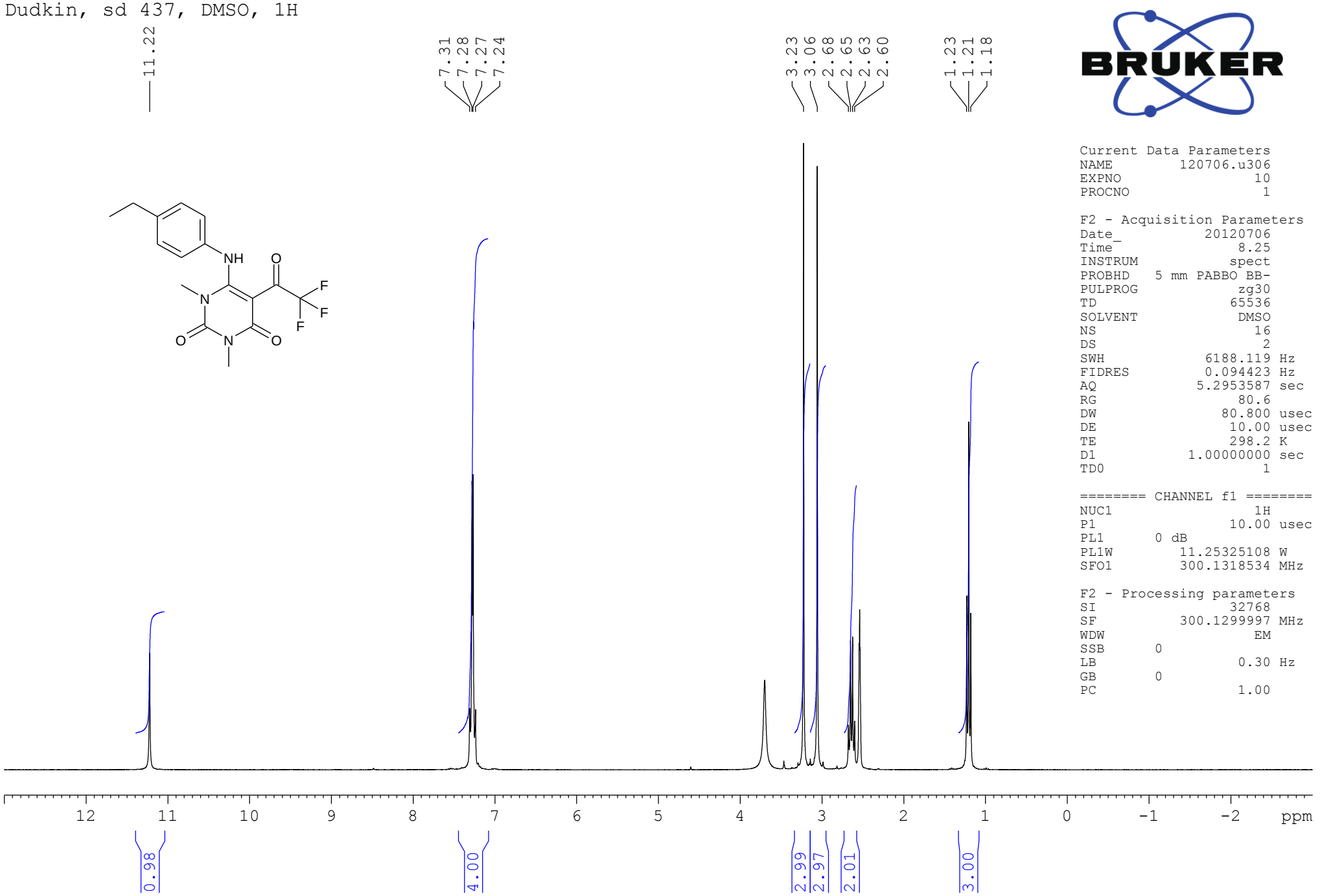
F2 - Acquisition Parameters
Date_           20120205
Time                5.55
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1       0 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              14.00 dB
PL13              14.00 dB
PL2               -3.00 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952077 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin, sd 437, DMSO, 1H



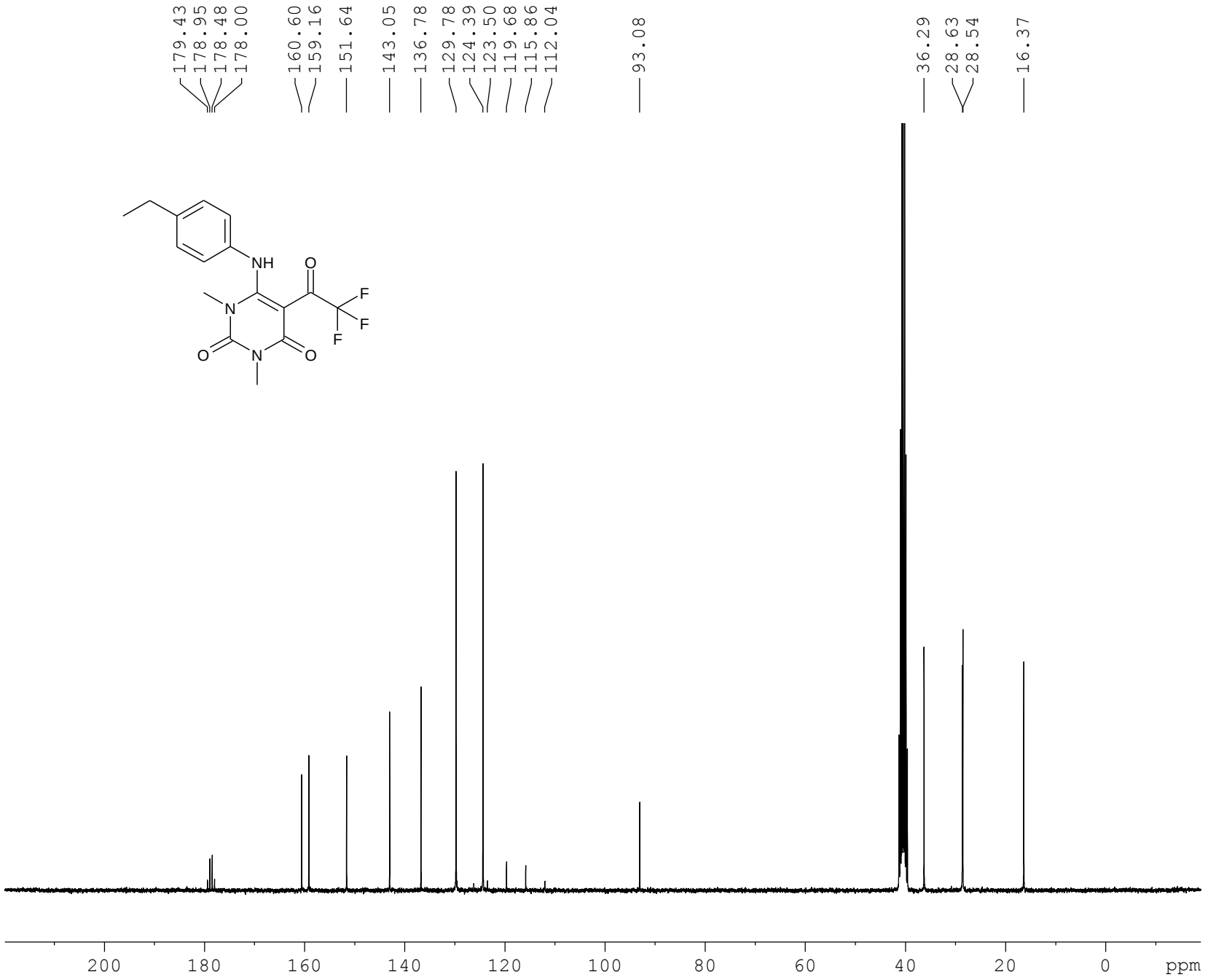

```
Current Data Parameters
NAME          120706.u306
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120706
Time                 8.25
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   80.6
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF          300.1299997 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

Dudkin, sd 437, DMSO, 13C




```
Current Data Parameters
NAME         120706.u306
EXPNO                 12
PROCNO                 1

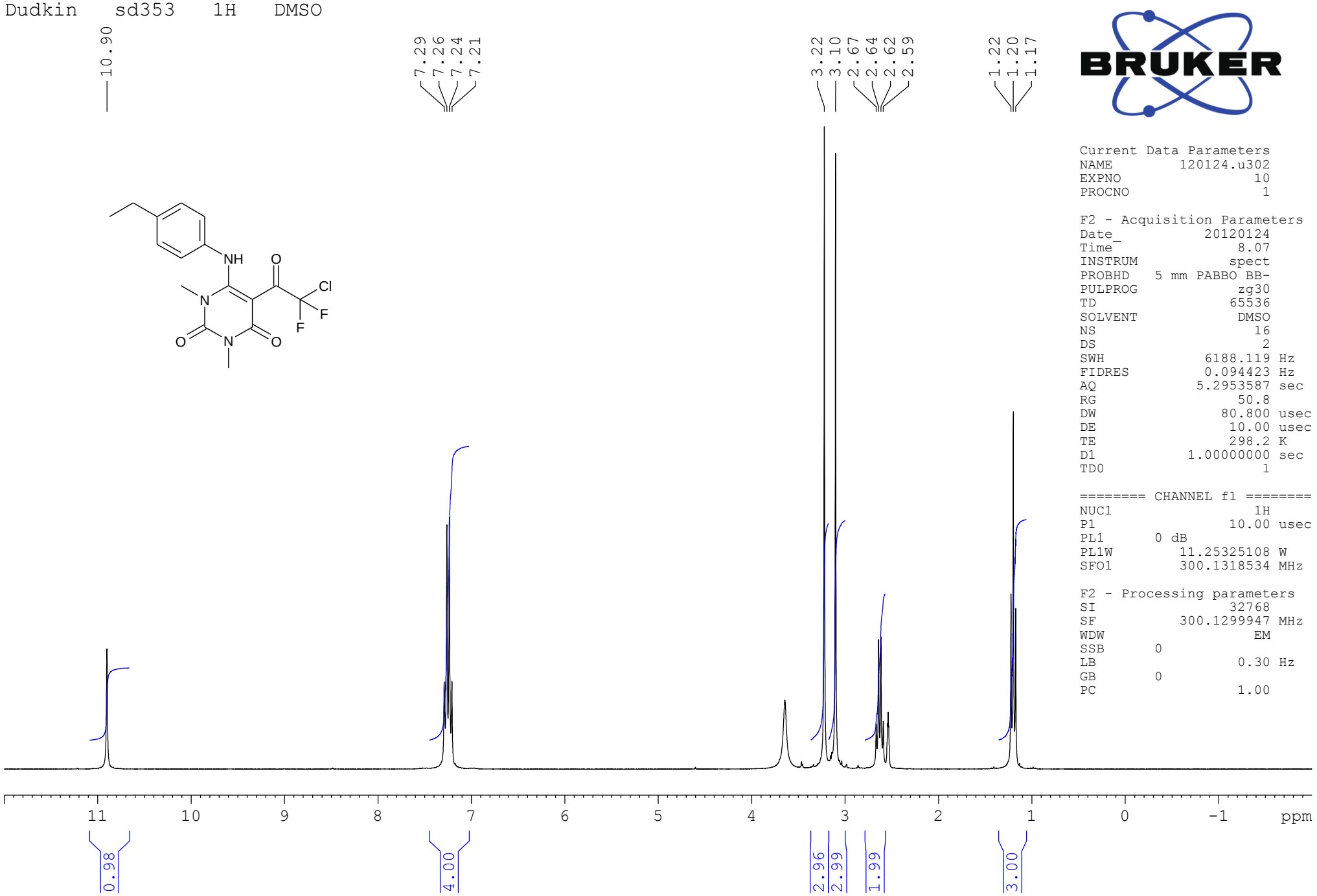
F2 - Acquisition Parameters
Date_           20120707
Time               21.21
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT            DMSO
NS                 4096
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ             1.8175818 sec
RG                 2050
DW               27.733 usec
DE                10.00 usec
TE                299.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -0.50 dB
PL1W         33.25691986 W
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             72.00 usec
PL2       0 dB
PL12              17.00 dB
PL13              17.00 dB
PL2W         11.25325108 W
PL12W         0.22453187 W
PL13W         0.22453187 W
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677164 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd353 1H DMSO



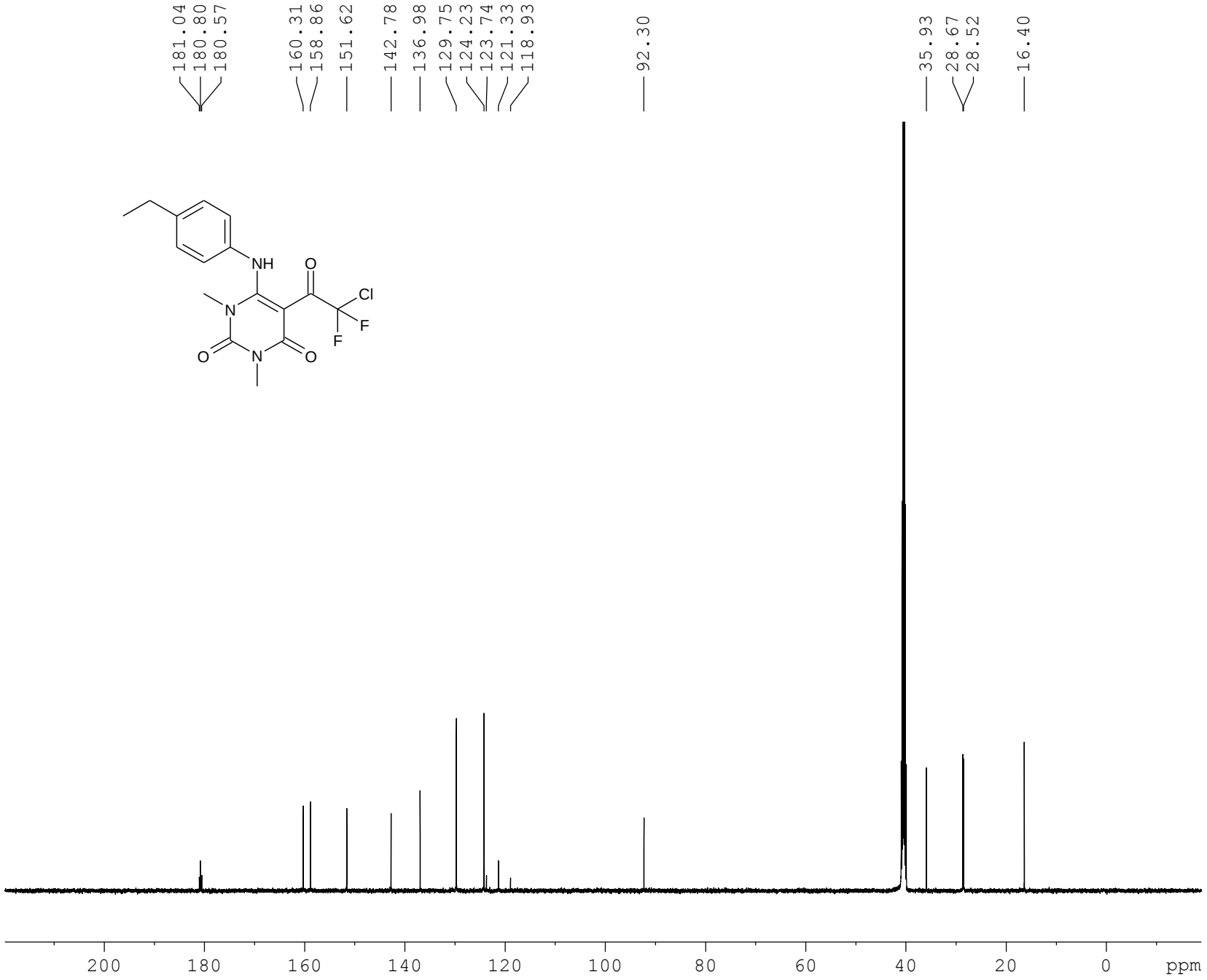
Current Data Parameters
NAME 120124.u302
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120124
Time 8.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 50.8
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299947 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Sergii Dudkin, sd 353, 13C in DMSO




```
Current Data Parameters
NAME          120124.507
EXPNO                 12
PROCNO                 1

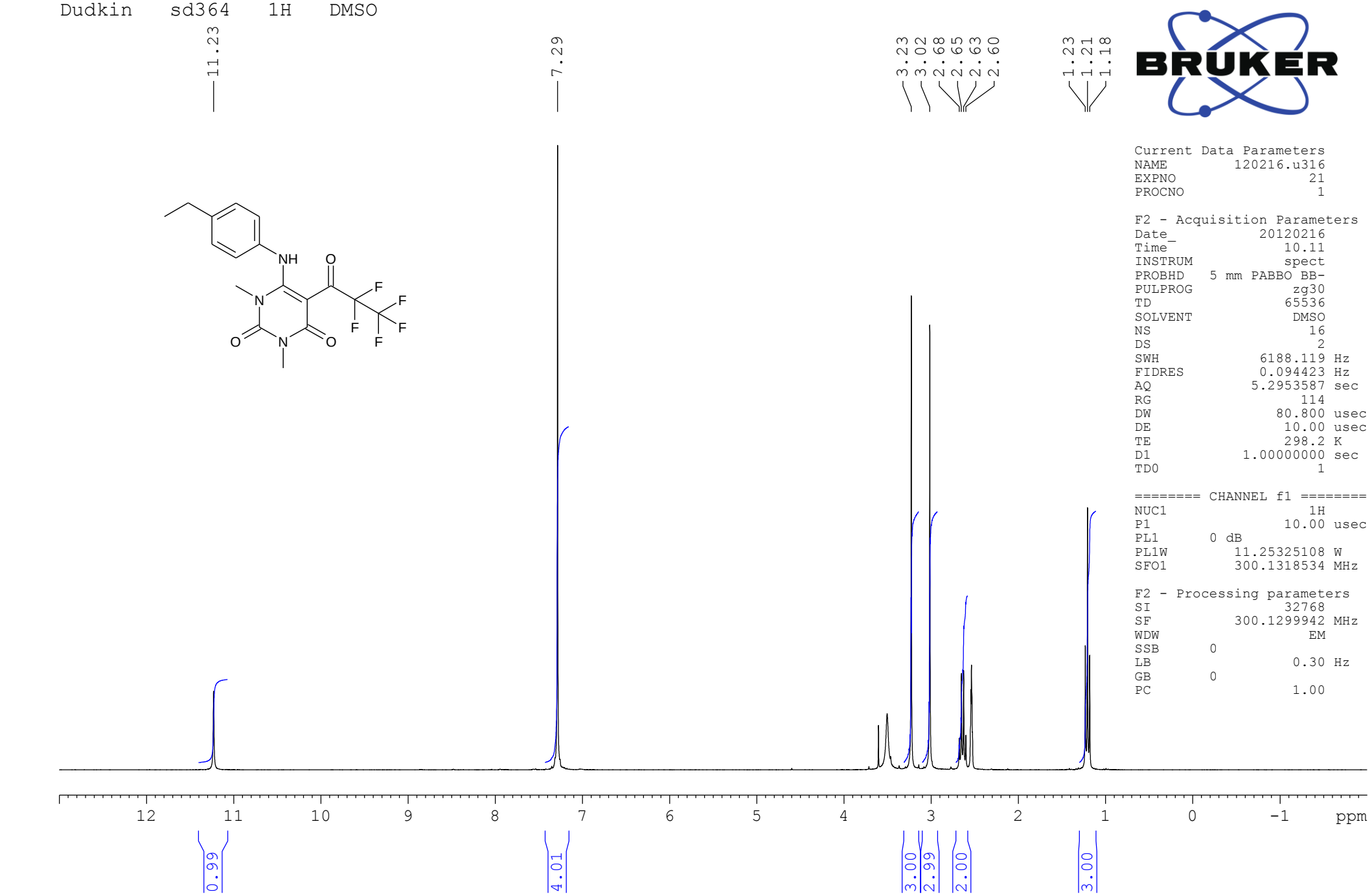
F2 - Acquisition Parameters
Date_           20120125
Time               9.24
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                   988
DS                     4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG               3649.1
DW              16.650 usec
DE               6.50 usec
TE              300.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                9.00 usec
PL1               4.50 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            70.00 usec
PL2              -3.00 dB
PL12              14.08 dB
PL13             120.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577337 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd364 1H DMSO



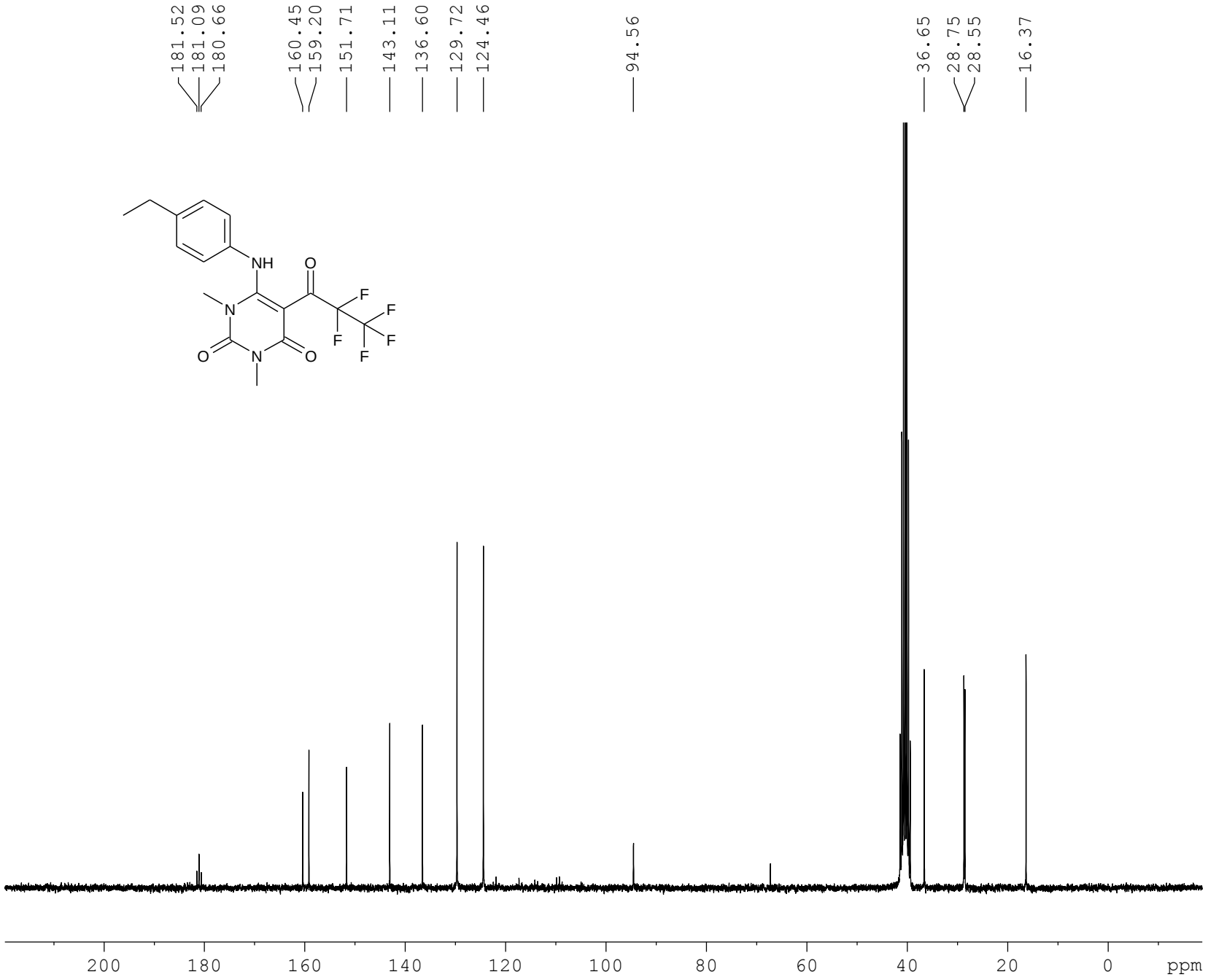
Current Data Parameters
NAME 120216.u316
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120216
Time 10.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 114
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299942 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd364 13C DMSO




```
Current Data Parameters
NAME          120217.213
EXPNO                 10
PROCNO                 1

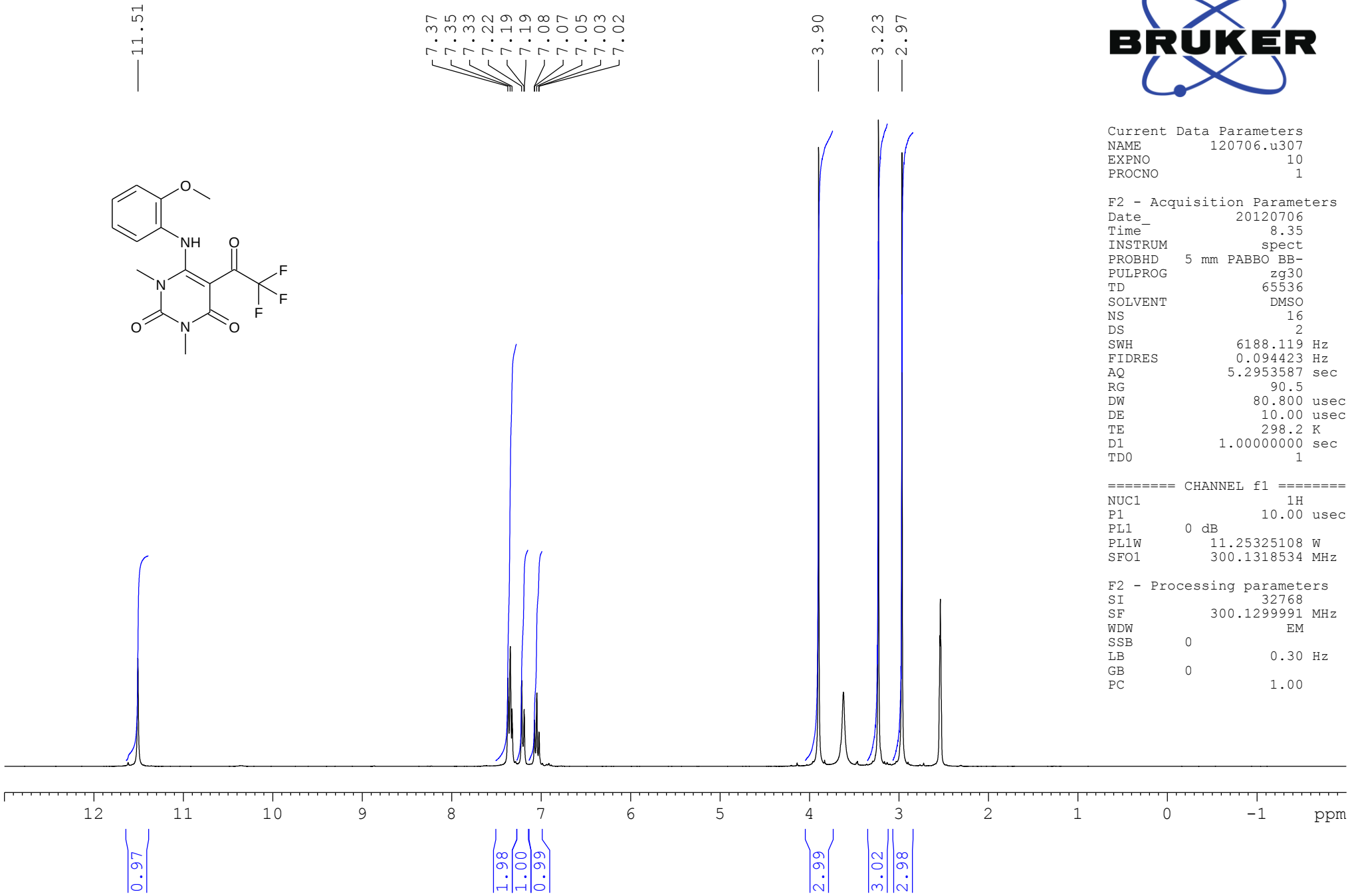
F2 - Acquisition Parameters
Date_           20120218
Time                4.47
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1       0 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              14.00 dB
PL13              14.00 dB
PL2               -3.00 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952072 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin, sd 438, DMSO, 1H



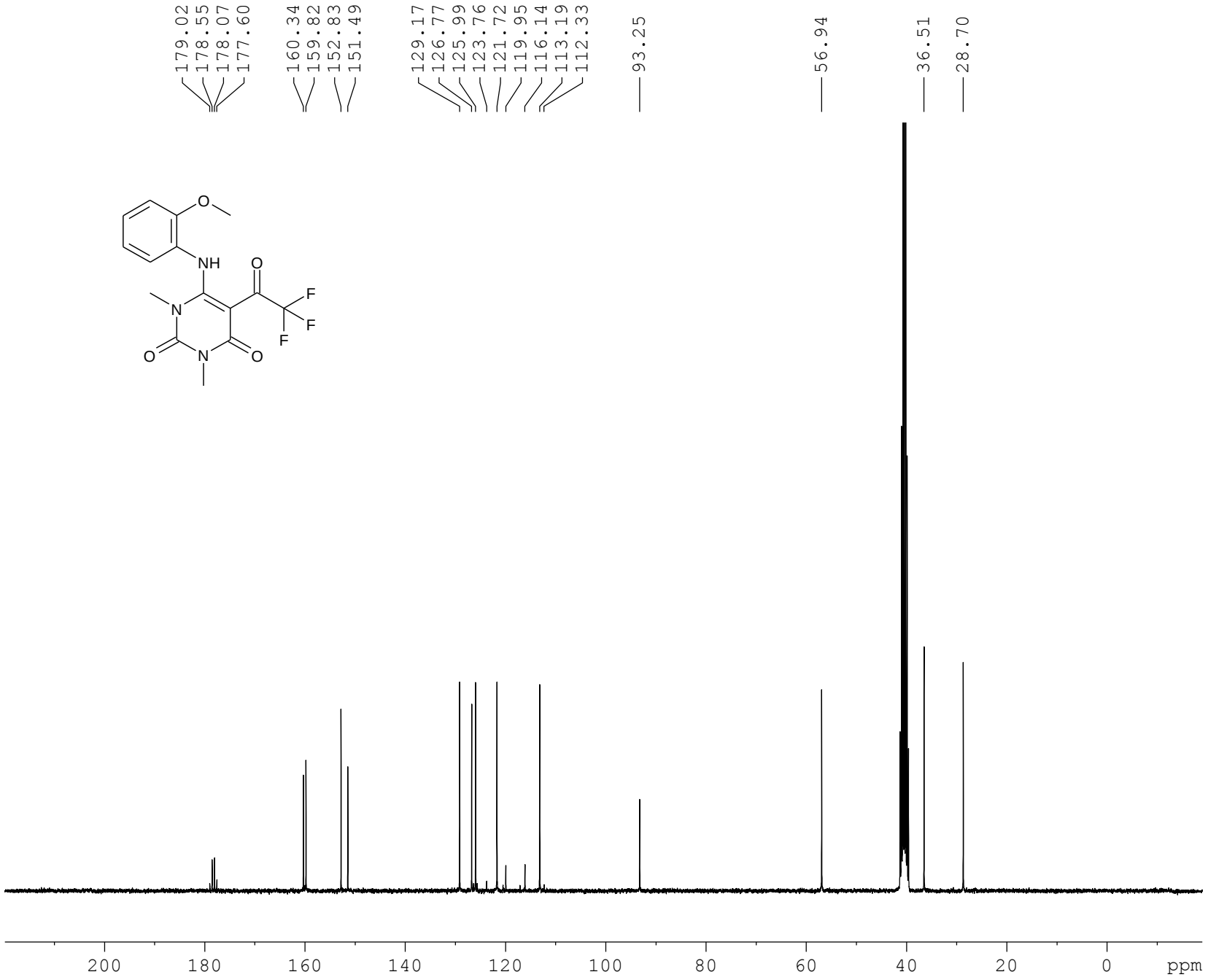

```
Current Data Parameters
NAME          120706.u307
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120706
Time                8.35
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                  90.5
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1299991 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin, sd 438, DMSO, 13C




```
Current Data Parameters
NAME         120706.u307
EXPNO                 12
PROCNO                 1

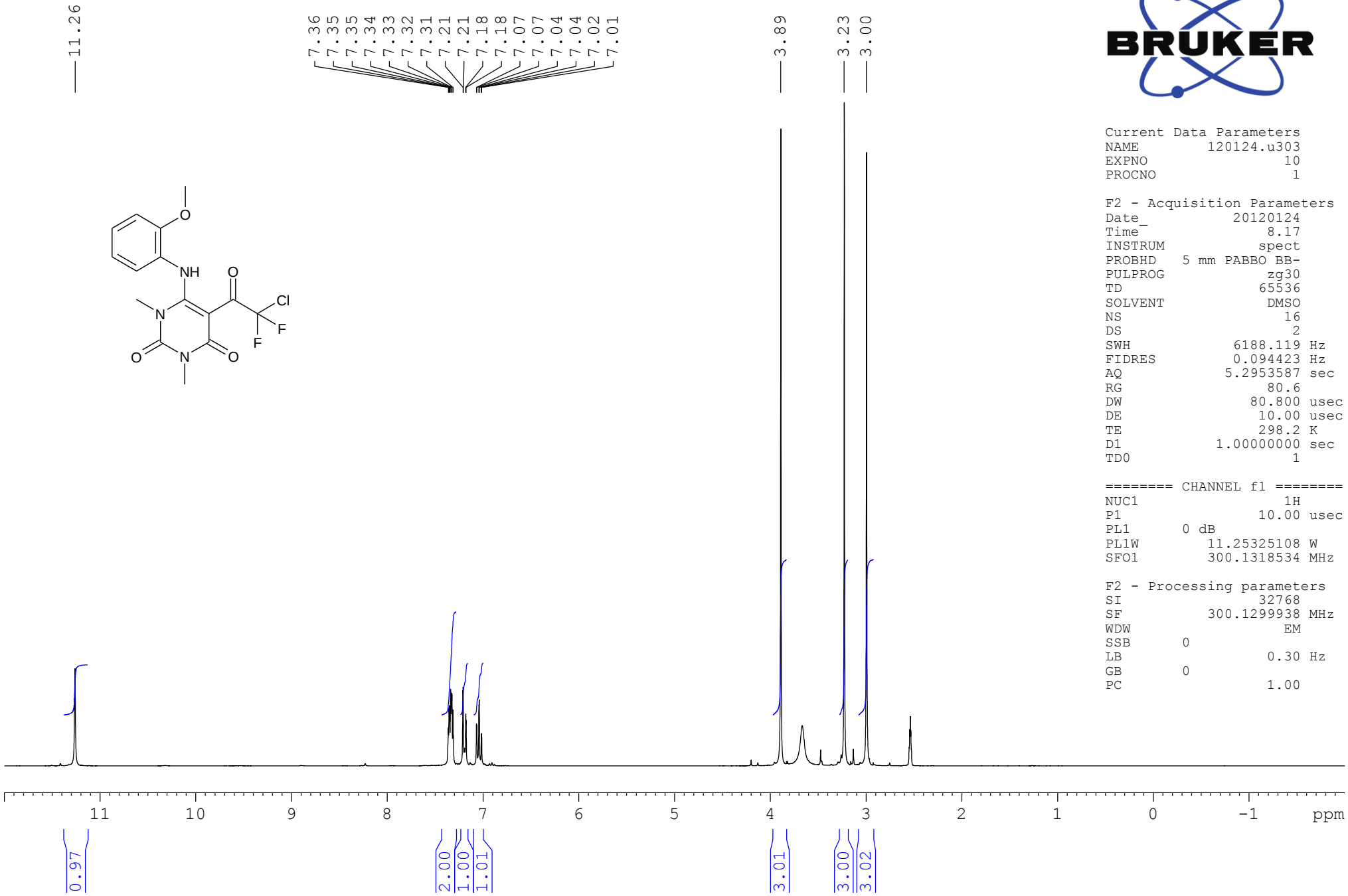
F2 - Acquisition Parameters
Date_           20120708
Time                2.08
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 4096
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                 2050
DW               27.733 usec
DE               10.00 usec
TE               298.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             72.00 usec
PL2       0 dB
PL12              17.00 dB
PL13              17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677164 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Dudkin sd354 1H DMSO



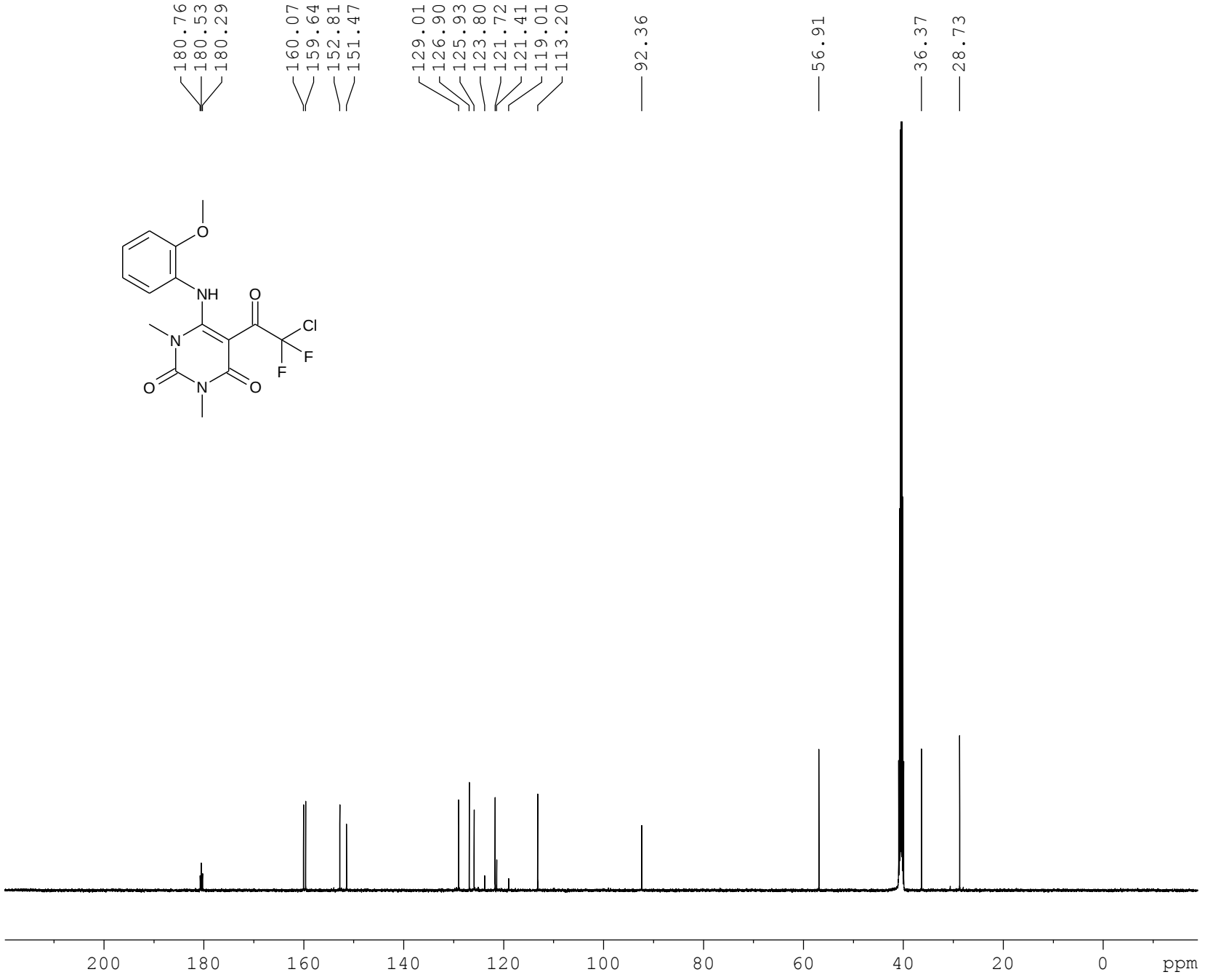
Current Data Parameters
NAME 120124.u303
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120124
Time 8.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 80.6
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299938 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Sergii Dudkin, sd 354, 13C in DMSO




```
Current Data Parameters
NAME          120124.508
EXPNO                 12
PROCNO                 1

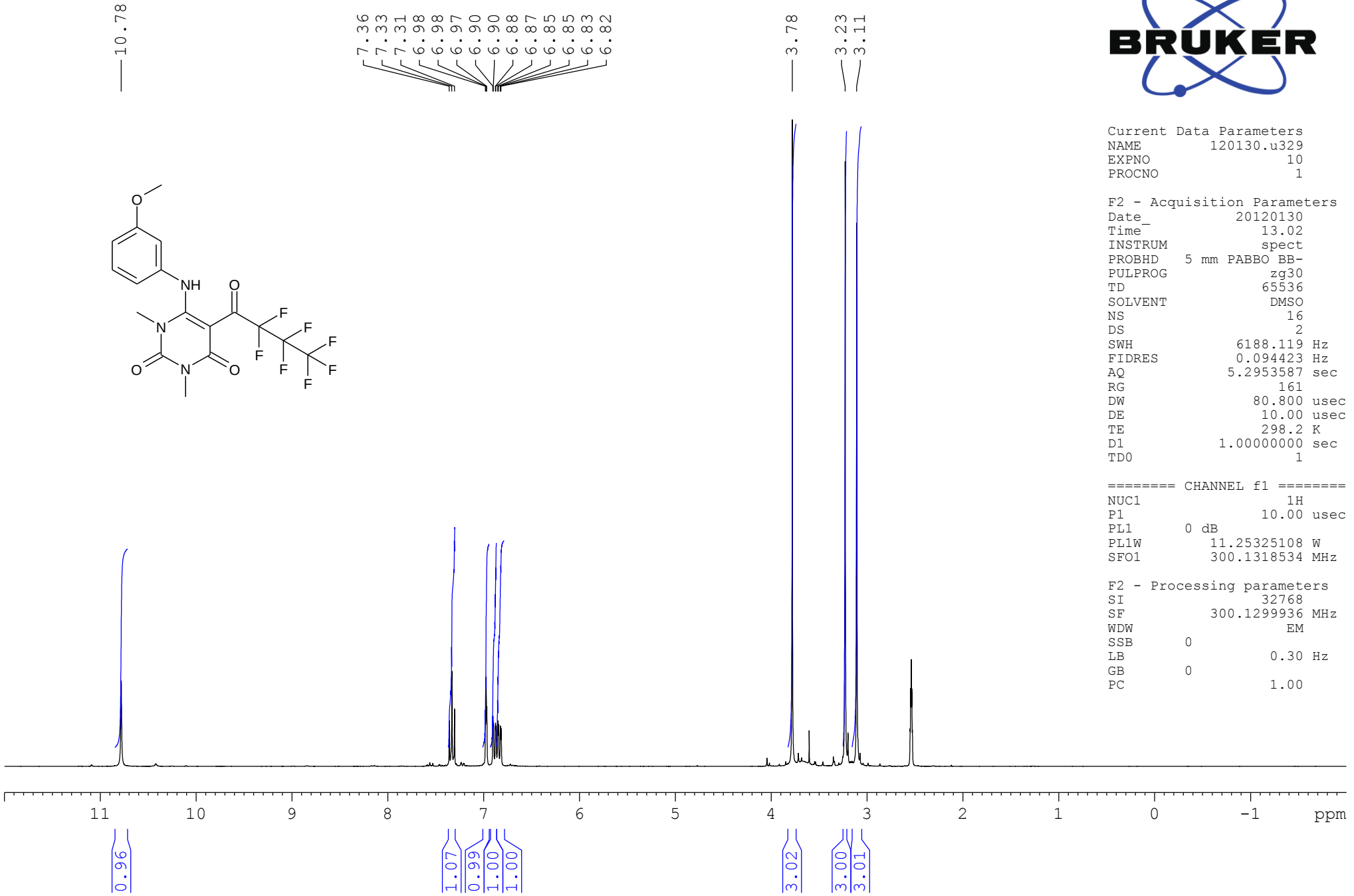
F2 - Acquisition Parameters
Date_           20120125
Time               10.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 2048
DS                    4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG                 2048
DW               16.650 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.00 usec
PL1                4.50 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             70.00 usec
PL2               -3.00 dB
PL12              14.08 dB
PL13             120.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577337 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Dudkin sd362 1H DMSO




```
Current Data Parameters
NAME          120130.u329
EXPNO                  10
PROCNO                  1

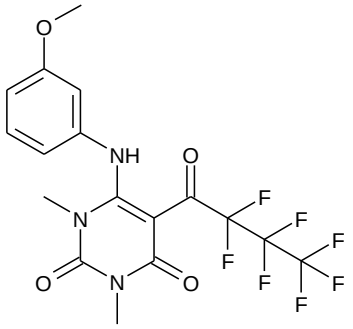
F2 - Acquisition Parameters
Date_            20120130
Time                13.02
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.094423 Hz
AQ               5.2953587 sec
RG                    161
DW                 80.800 usec
DE                 10.00 usec
TE                 298.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1       0 dB
PL1W         11.25325108 W
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF           300.1299936 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

Dudkin sd362 13C DMSO

182.37 181.95 181.53 161.11 160.69 158.34 151.73 140.45 131.23 116.13 112.86 109.53 94.80 56.23 35.99 28.72



Current Data Parameters
NAME 120203.213
EXPNO 10
PROCNO 1

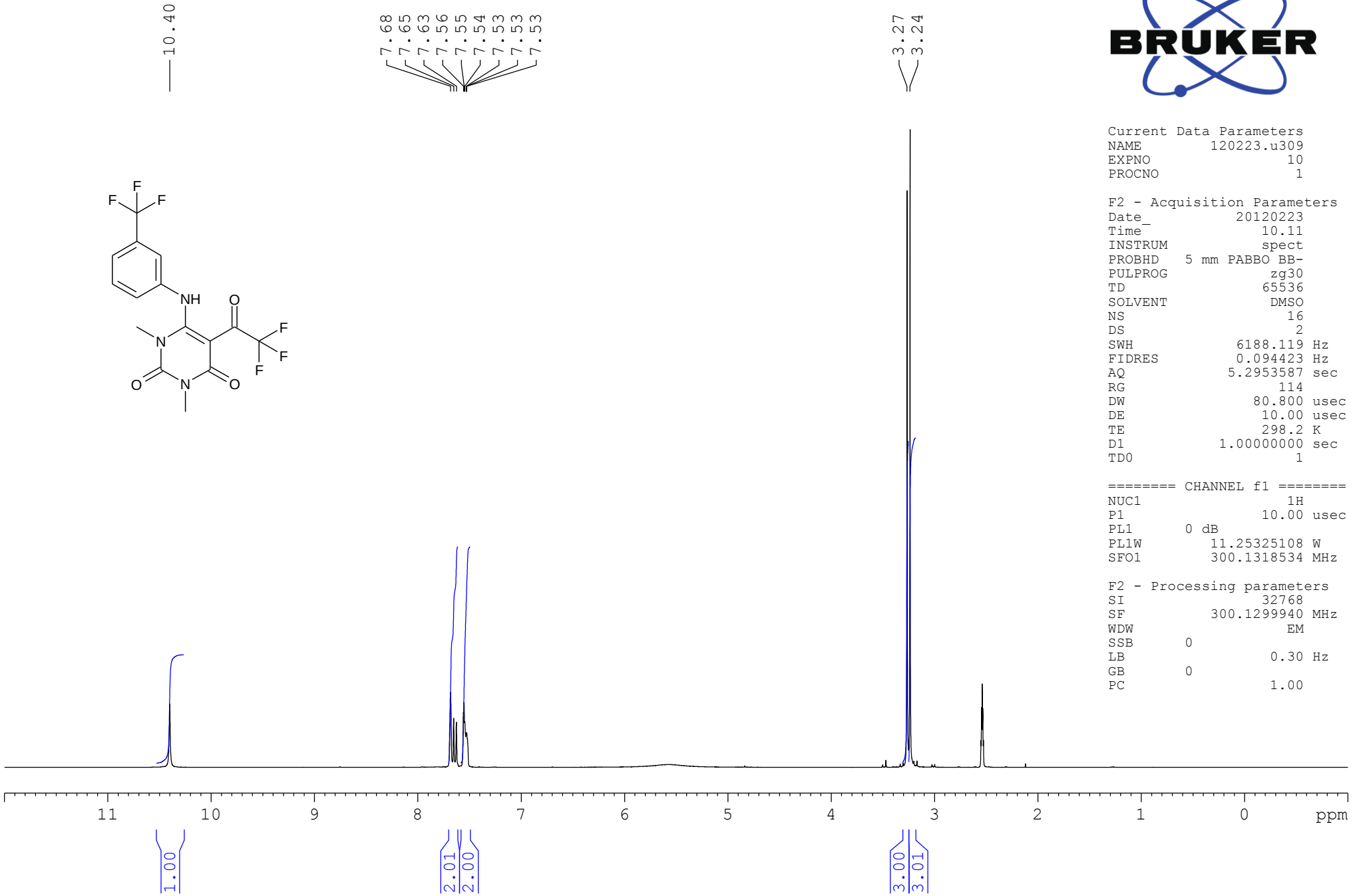
F2 - Acquisition Parameters
Date_ 20120205
Time 10.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.20 usec
PL1 0 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 14.00 dB
PL13 14.00 dB
PL2 -3.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952076 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd376 1H DMSO



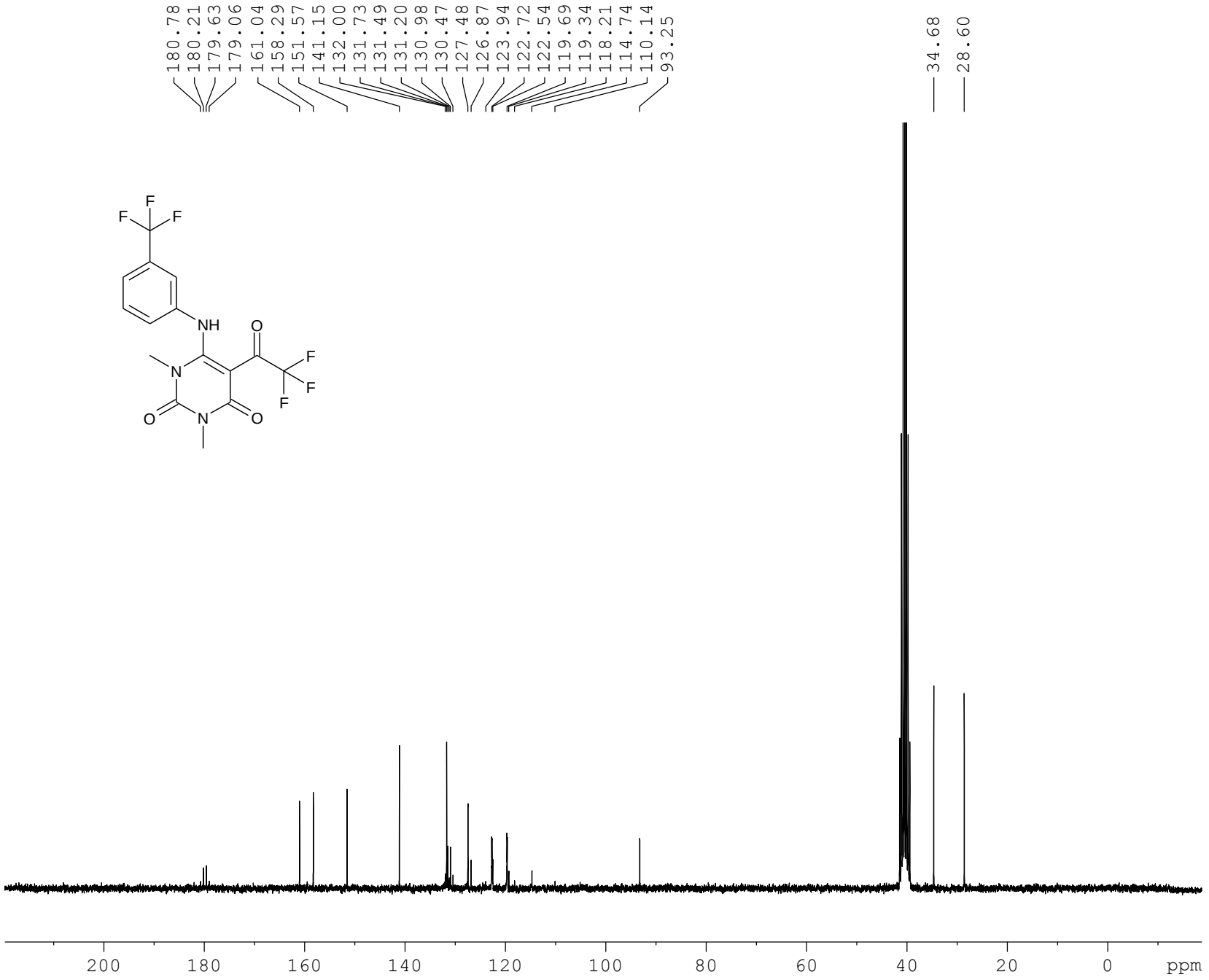
Current Data Parameters
NAME 120223.u309
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120223
Time 10.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 114
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd376 13C DMSO



Current Data Parameters
NAME 120301.206
EXPNO 10
PROCNO 1

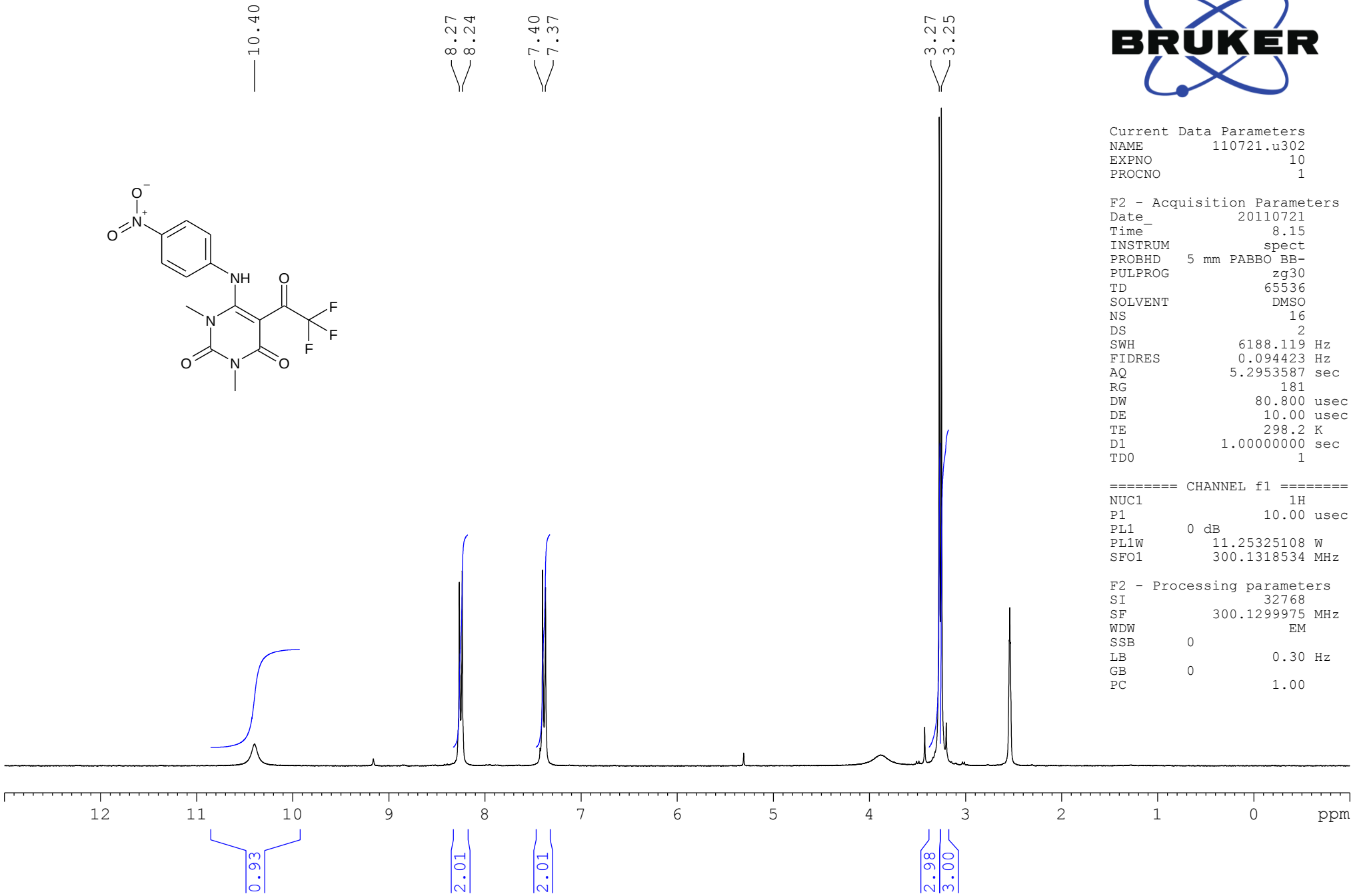
F2 - Acquisition Parameters
Date_ 20120302
Time 0.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952079 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd254 1H DMSO




```
Current Data Parameters
NAME          110721.u302
EXPNO                  10
PROCNO                  1

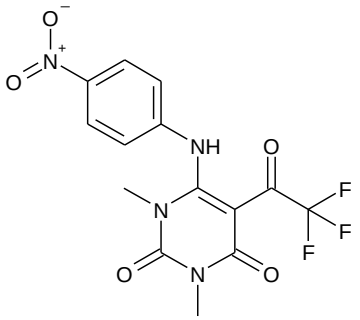
F2 - Acquisition Parameters
Date_            20110721
Time                8.15
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   181
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1299975 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd254 13C DMSO

180.97 180.49 180.01 179.53 160.91 157.10 151.60 147.43 143.85 126.34 122.62 121.40 118.78 114.94 111.10 96.46 34.62 28.70



Current Data Parameters
NAME 110722.u322
EXPNO 10
PROCNO 1

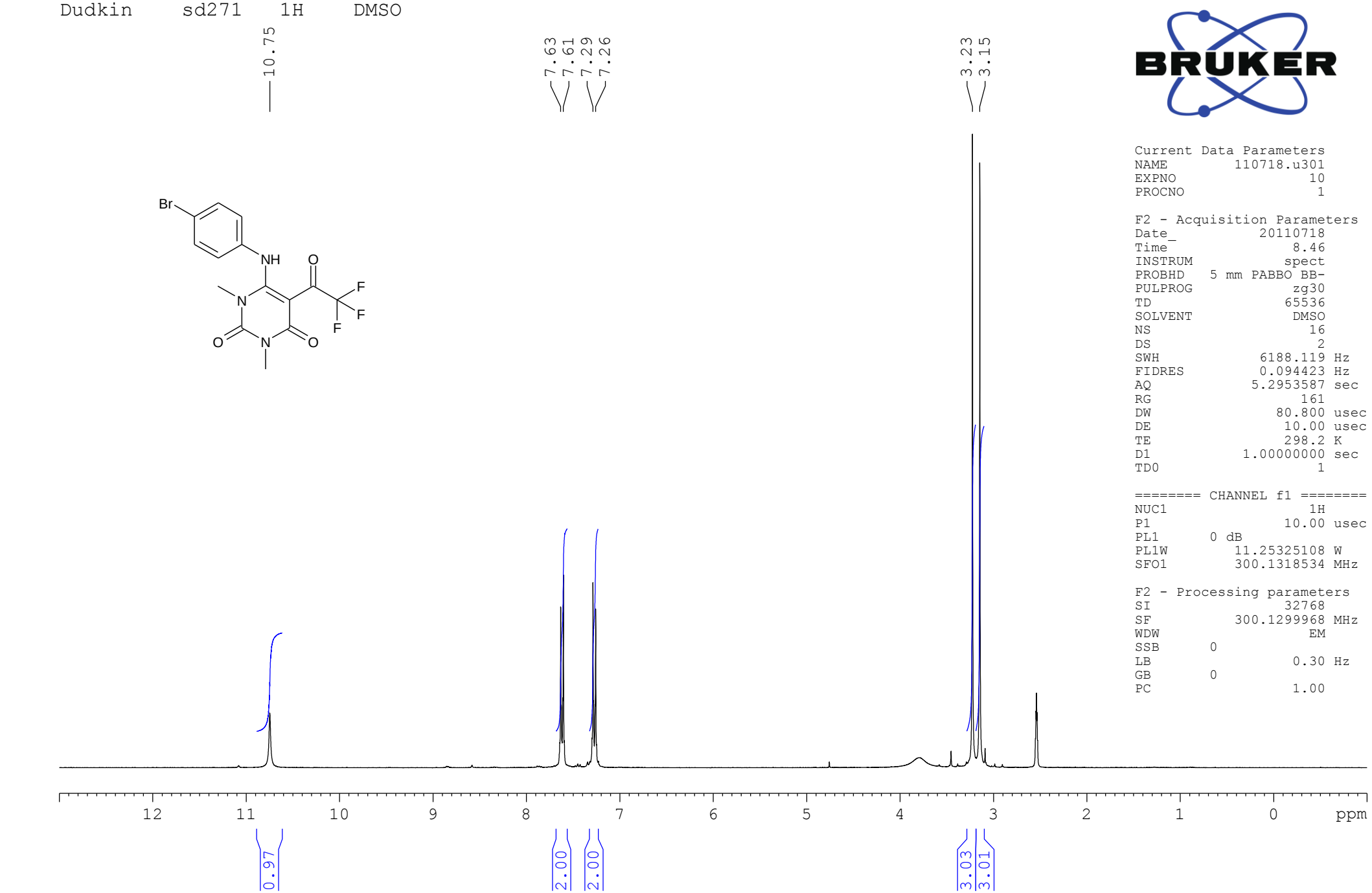
F2 - Acquisition Parameters
Date_ 20110723
Time 18.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677179 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd271 1H DMSO



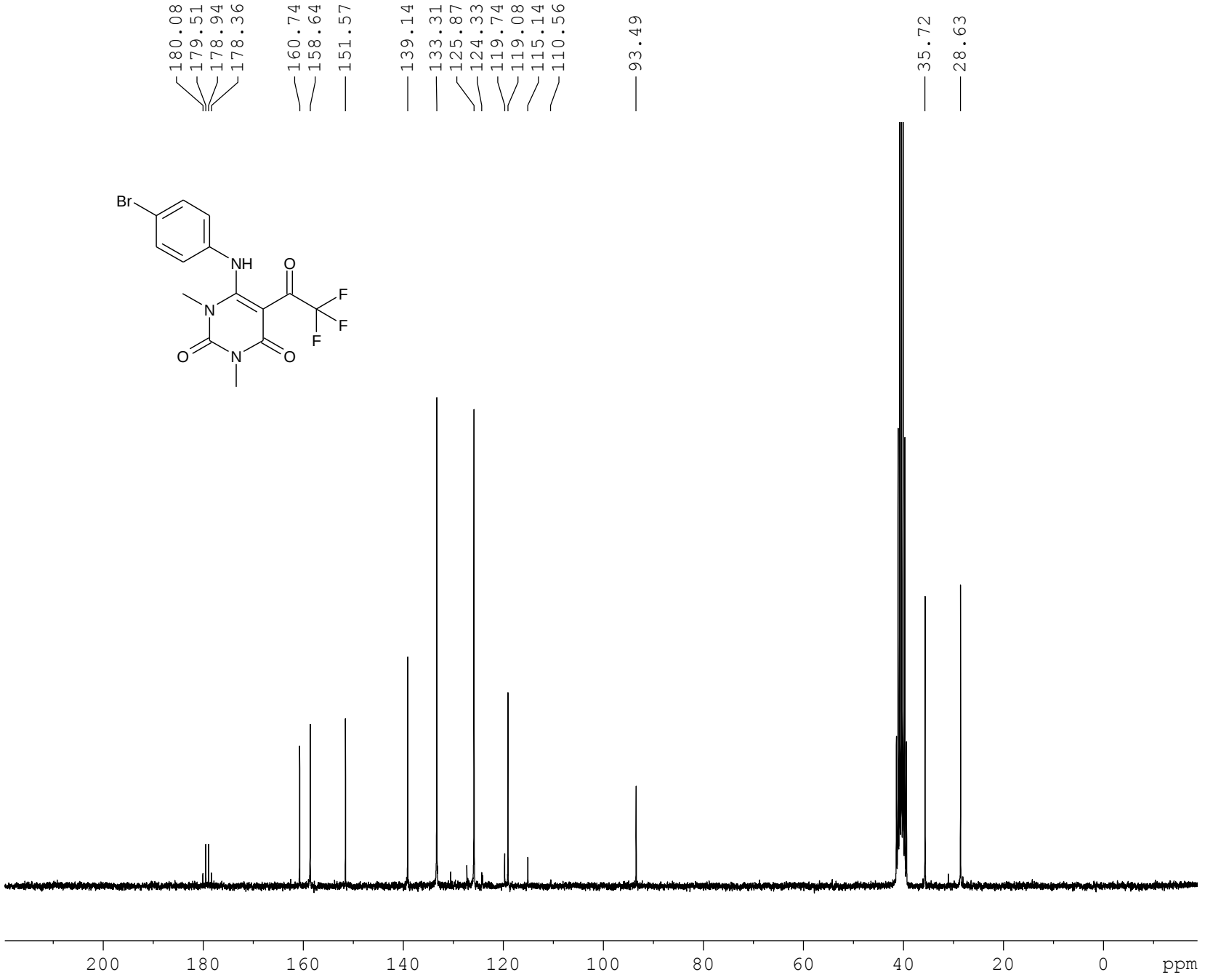
Current Data Parameters
NAME 110718.u301
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110718
Time 8.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 161
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299968 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd271 13C DMSO




```
Current Data Parameters
NAME          110719.210
EXPNO                 10
PROCNO                 1

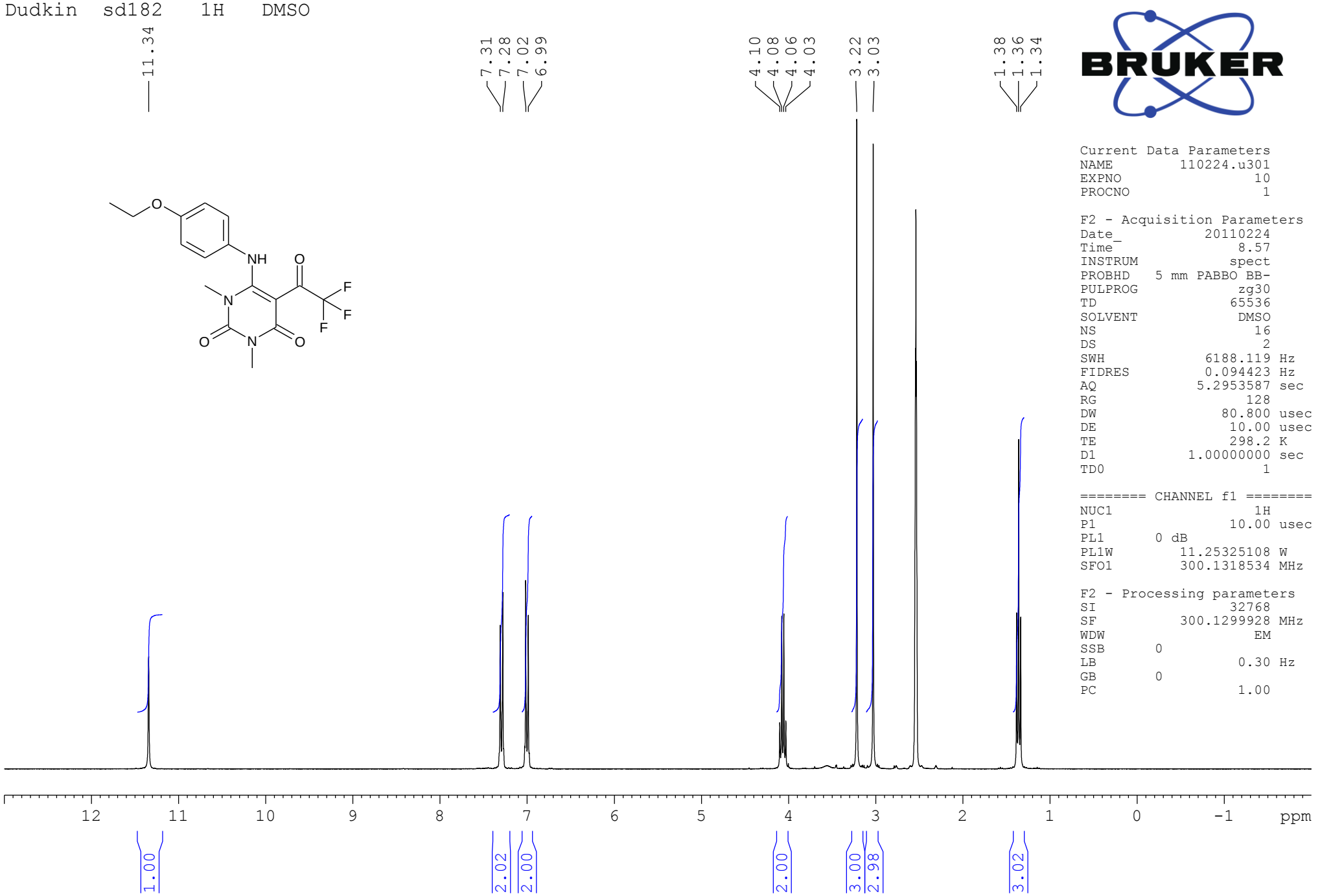
F2 - Acquisition Parameters
Date_           20110720
Time                2.56
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  3072
DS                     4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                  2050
DW                33.333 usec
DE                10.00 usec
TE                299.3 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                 32768
SF           62.8952090 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Dudkin sd182 1H DMSO



Current Data Parameters
NAME 110224.u301
EXPNO 10
PROCNO 1

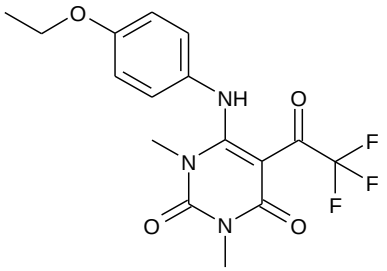
F2 - Acquisition Parameters
Date_ 20110224
Time 8.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299928 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S. Dudkin, sd 386, 13C in DMSO

178.82 178.54 178.25 177.97 160.56 159.36 157.91 151.66 131.50 126.28 121.33 119.04 116.75 116.12 114.46 92.73 64.27 36.35 28.62 15.45




```
Current Data Parameters
NAME          120305.503
EXPNO                 12
PROCNO                 1

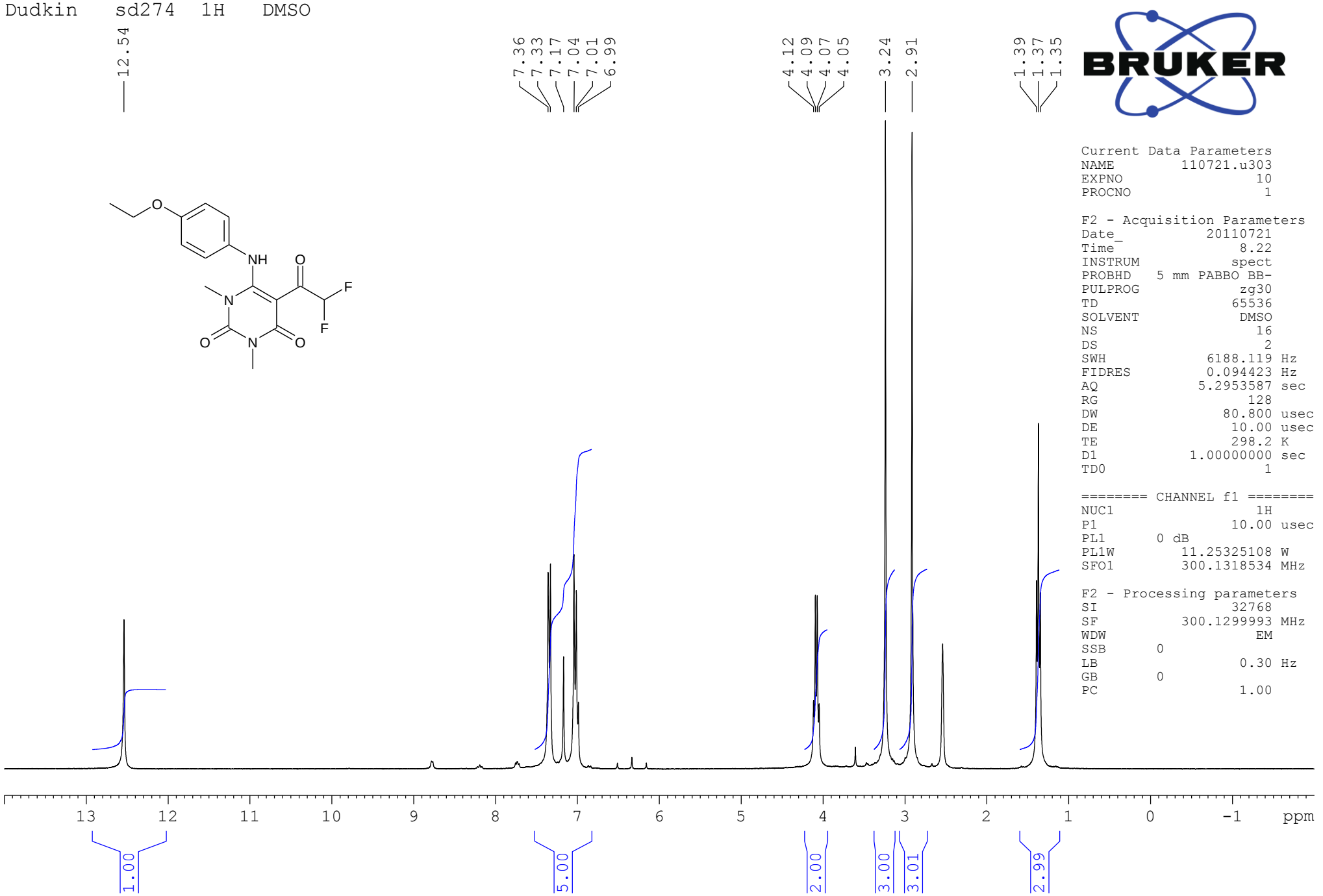
F2 - Acquisition Parameters
Date_           20120305
Time               23.38
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG                1149.4
DW               16.650 usec
DE                6.50 usec
TE               300.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                9.00 usec
PL1               4.50 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            70.00 usec
PL2              -3.00 dB
PL12             14.08 dB
PL13            120.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577328 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd274 1H DMSO



Current Data Parameters
NAME 110721.u303
EXPNO 10
PROCNO 1

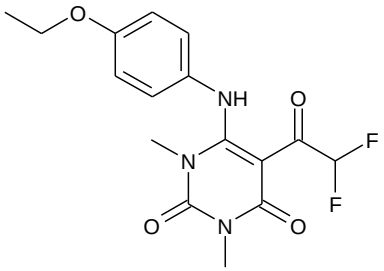
F2 - Acquisition Parameters
Date_ 20110721
Time 8.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299993 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd274 13C DMSO

185.82 185.50 185.19 162.01 159.82 158.13 151.63 130.99 126.59 116.10 112.45 109.23 106.02 94.04 64.31 37.13 28.70 15.48




```
Current Data Parameters
NAME          110722.u323
EXPNO                  10
PROCNO                  1

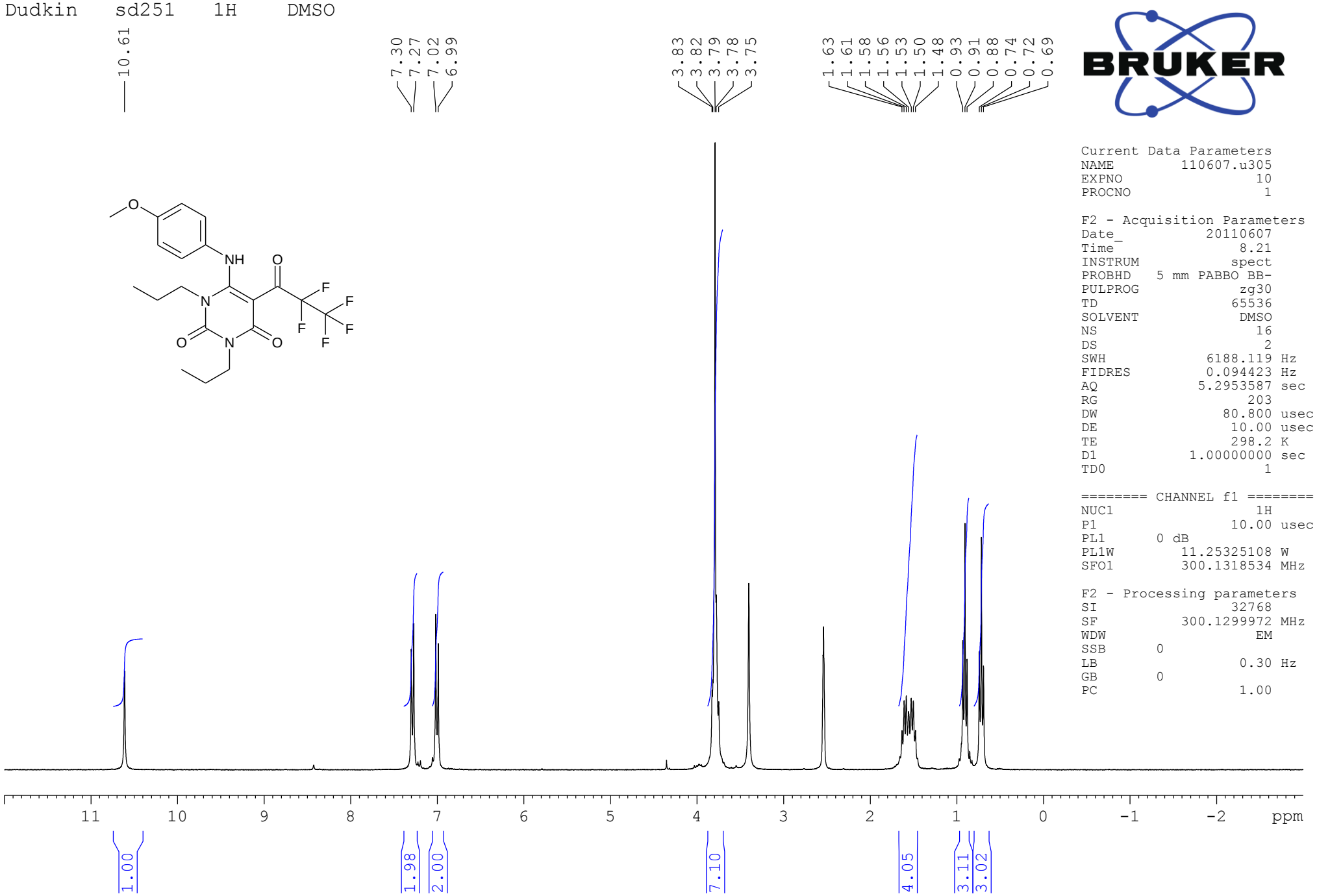
F2 - Acquisition Parameters
Date_            20110723
Time                22.25
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  3072
DS                     4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                  2050
DW                27.733 usec
DE                10.00 usec
TE                298.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              72.00 usec
PL2       0 dB
PL12               17.00 dB
PL13               17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677159 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Dudkin sd251 1H DMSO




```
Current Data Parameters
NAME          110607.u305
EXPNO                  10
PROCNO                  1

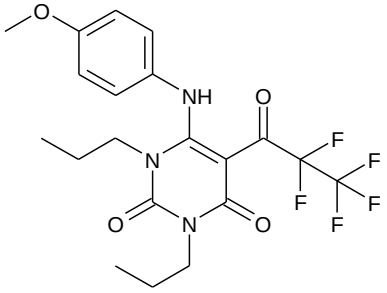
F2 - Acquisition Parameters
Date_            20110607
Time                8.21
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   203
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1299972 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd251 13C DMSO

181.99 181.56 181.14 160.22 158.80 158.03 151.18 131.78 126.42 115.70 93.32 56.32 47.18 43.32 21.44 21.26 12.00 11.46




```
Current Data Parameters
NAME          110608.212
EXPNO                 10
PROCNO                 1

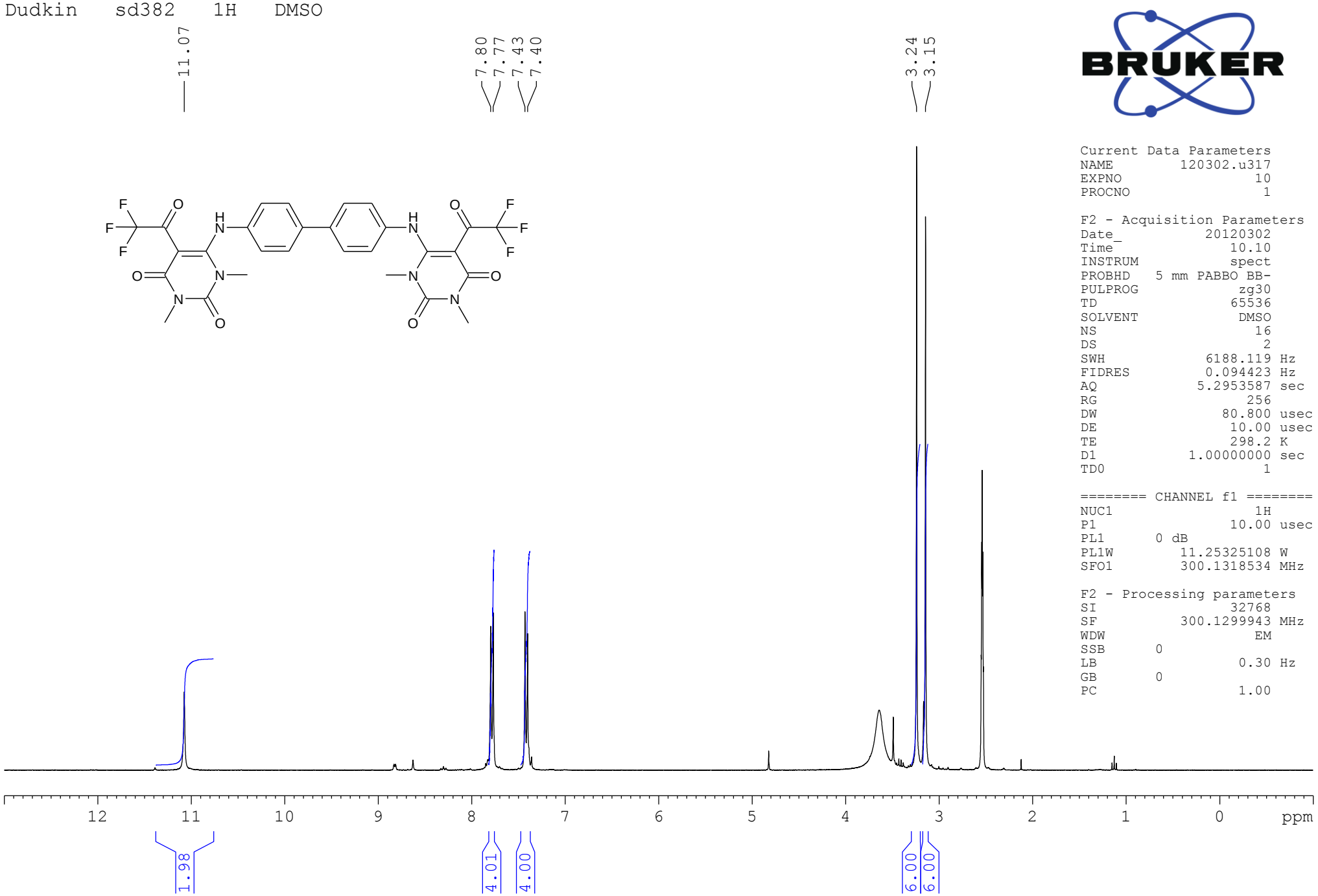
F2 - Acquisition Parameters
Date_           20110609
Time               8.34
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                297.9 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952083 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd382 1H DMSO



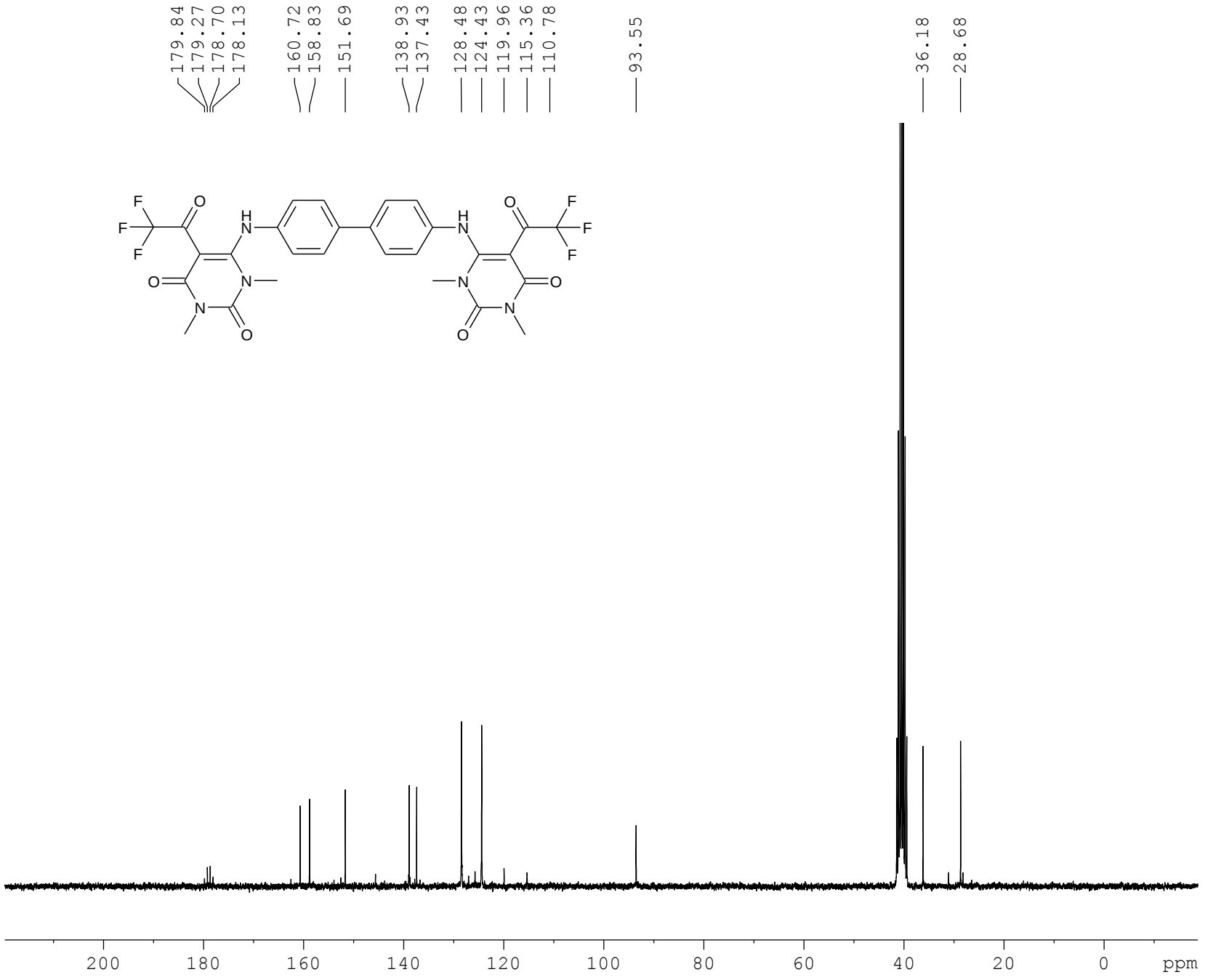

```
Current Data Parameters
NAME          120302.u317
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120302
Time                10.10
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.094423 Hz
AQ               5.2953587 sec
RG                    256
DW                 80.800 usec
DE                 10.00 usec
TE                 298.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1       0 dB
PL1W         11.25325108 W
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF           300.1299943 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

Dudkin sd382 13C DMSO




```
Current Data Parameters
NAME          120305.211
EXPNO                 10
PROCNO                 1

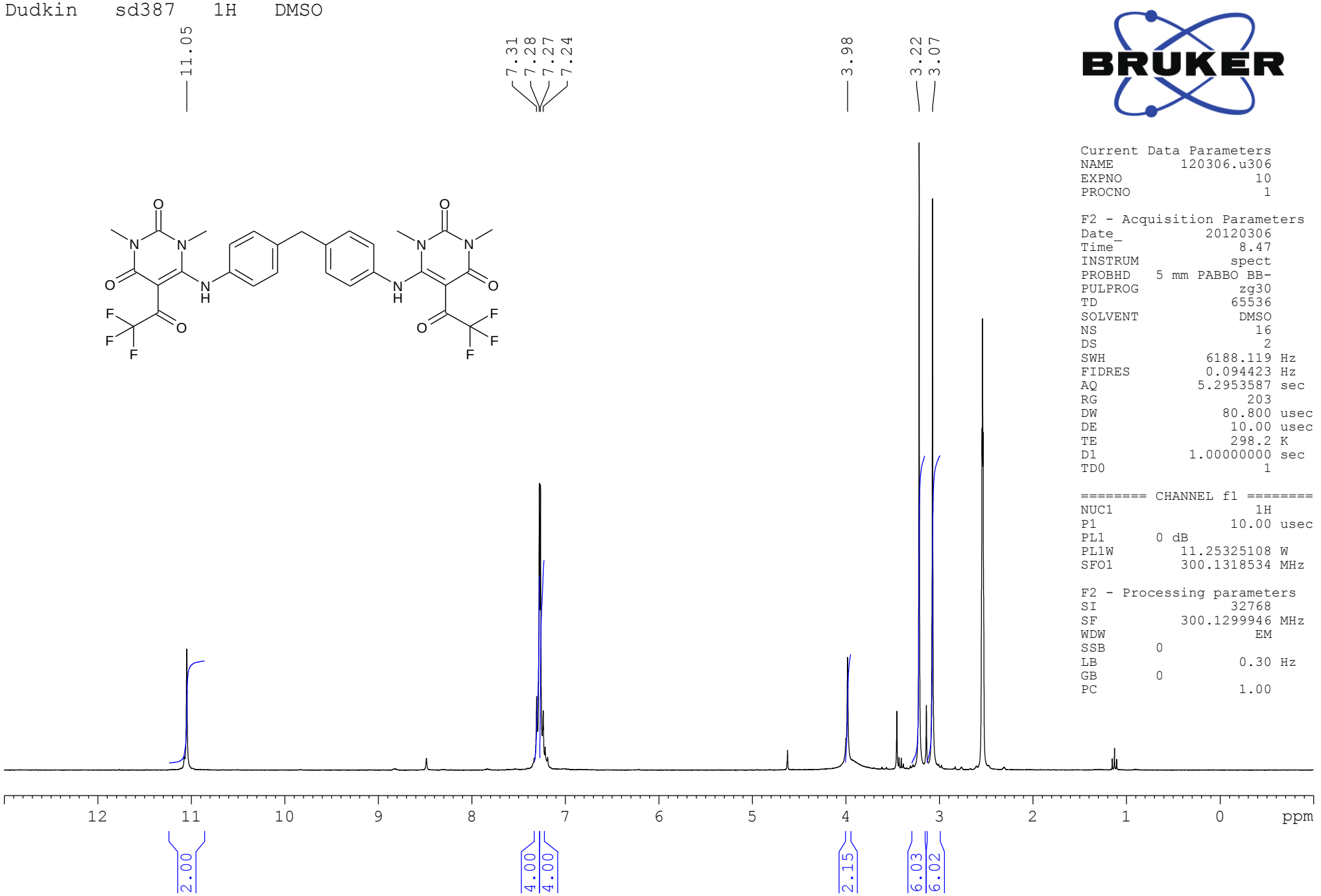
F2 - Acquisition Parameters
Date_           20120306
Time                4.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  3072
DS                     4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                  2050
DW                33.333 usec
DE                10.00 usec
TE                297.9 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                 32768
SF           62.8952083 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Dudkin sd387 1H DMSO



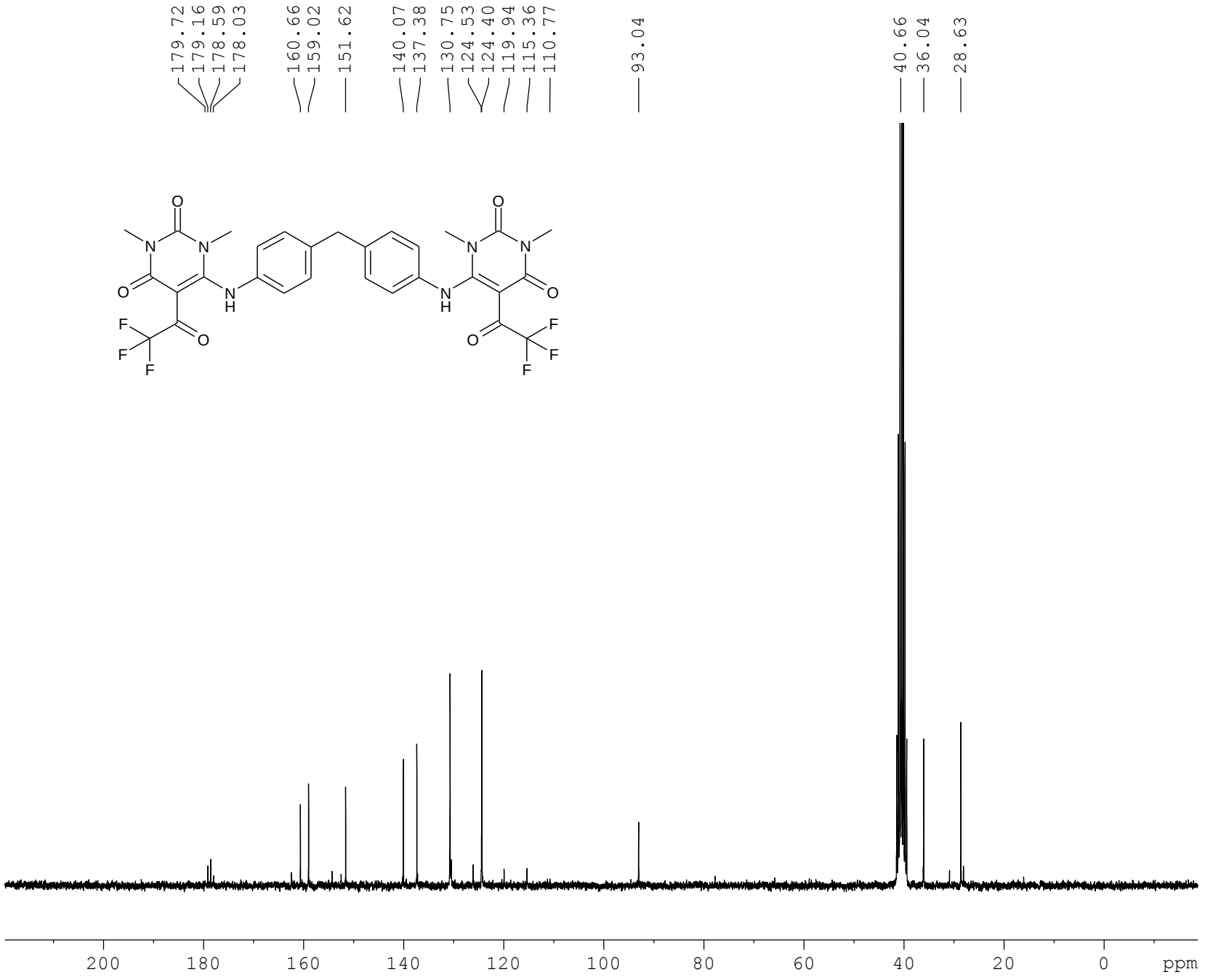

```
Current Data Parameters
NAME         120306.u306
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120306
Time               8.47
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH            6188.119 Hz
FIDRES        0.094423 Hz
AQ            5.2953587 sec
RG                  203
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1299946 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd387 13C DMSO



Current Data Parameters
NAME 120308.208
EXPNO 10
PROCNO 1

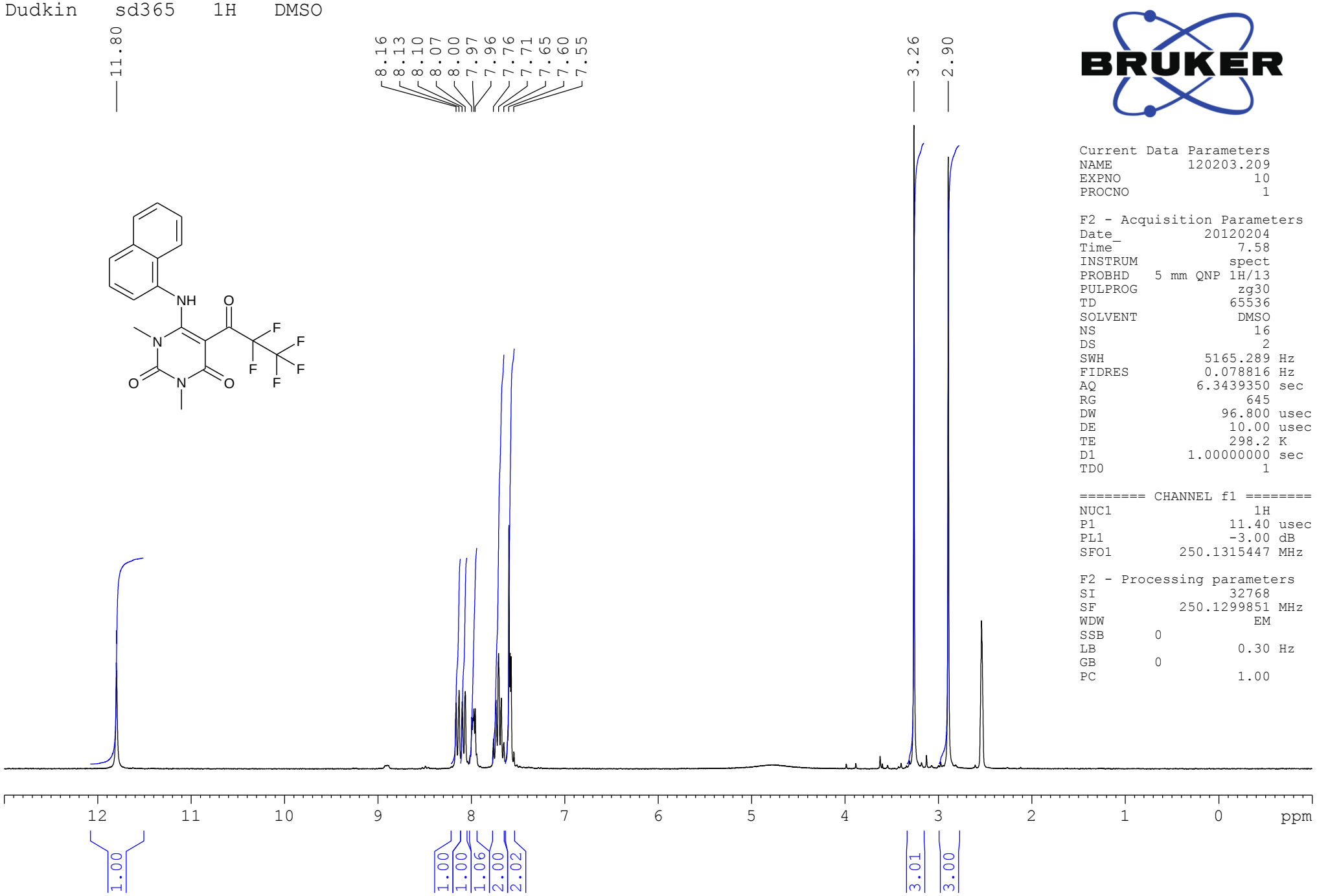
F2 - Acquisition Parameters
Date_ 20120308
Time 21.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952087 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd365 1H DMSO



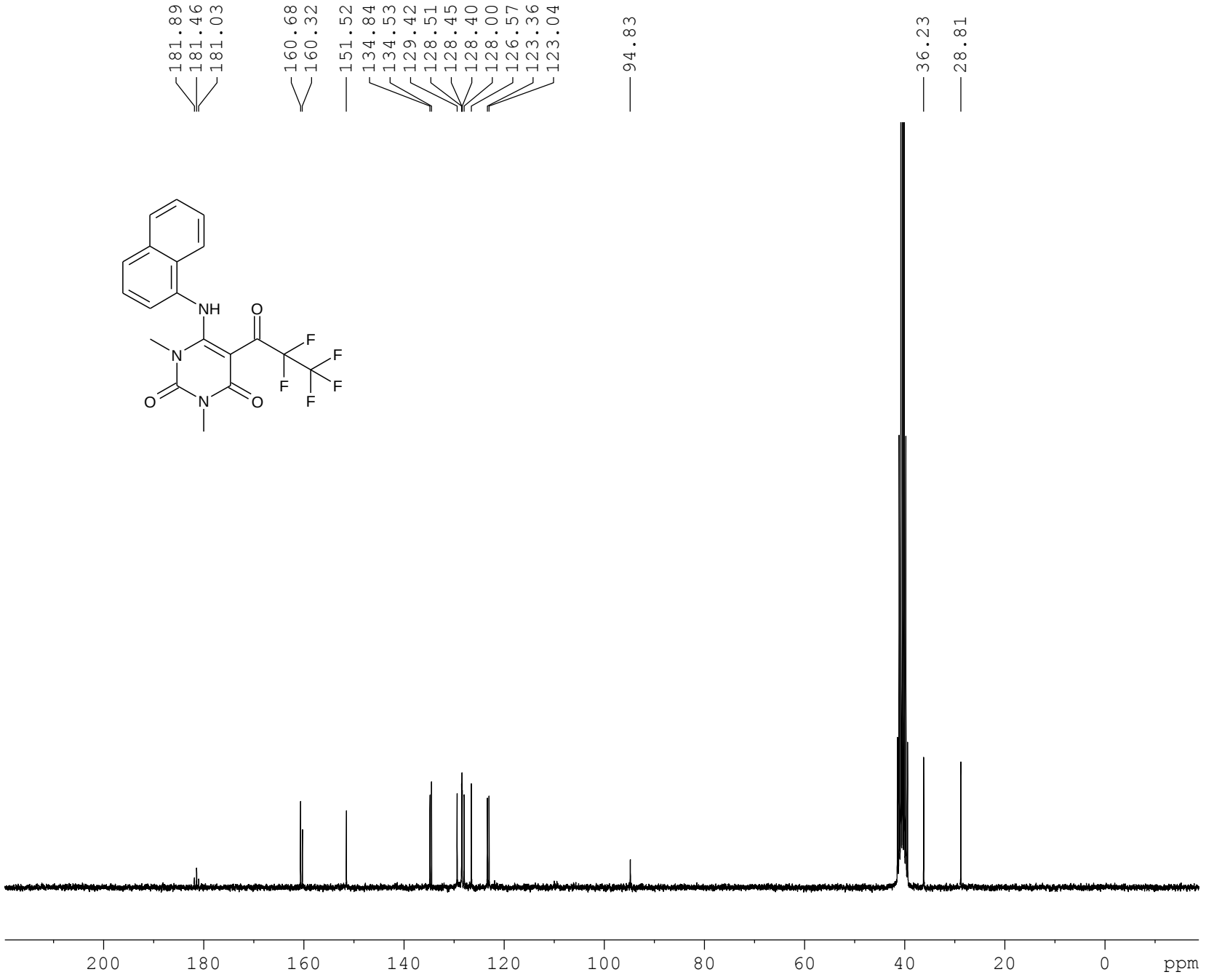
Current Data Parameters
NAME 120203.209
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120204
Time 7.58
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 645
DW 96.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.40 usec
PL1 -3.00 dB
SFO1 250.1315447 MHz

F2 - Processing parameters
SI 32768
SF 250.1299851 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd365 13C DMSO




```
Current Data Parameters
NAME          120203.209
EXPNO                 11
PROCNO                 1

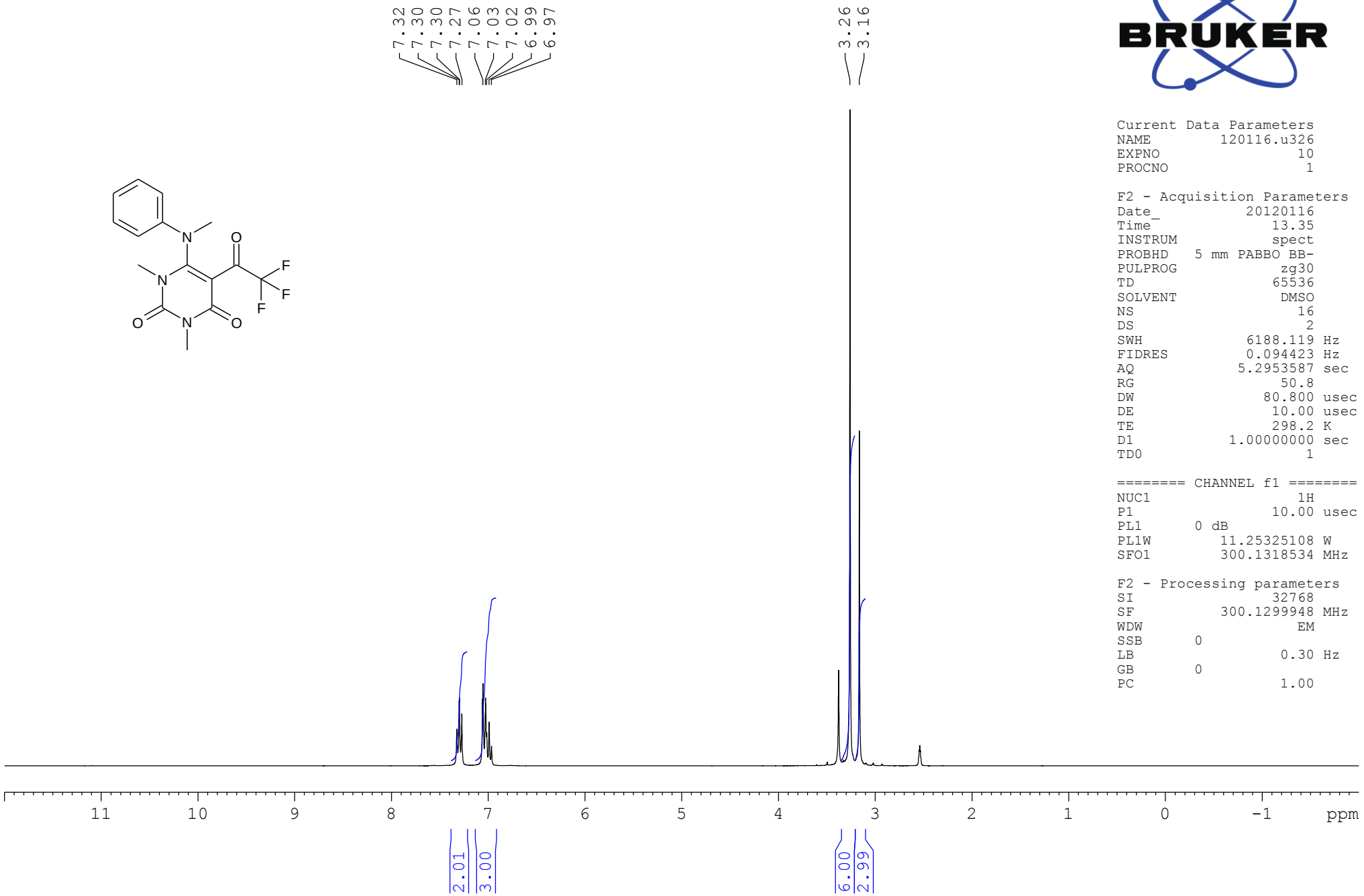
F2 - Acquisition Parameters
Date_           20120204
Time               11.36
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1       0 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              14.00 dB
PL13              14.00 dB
PL2               -3.00 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952081 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin, sd 350, DMSO, 1H



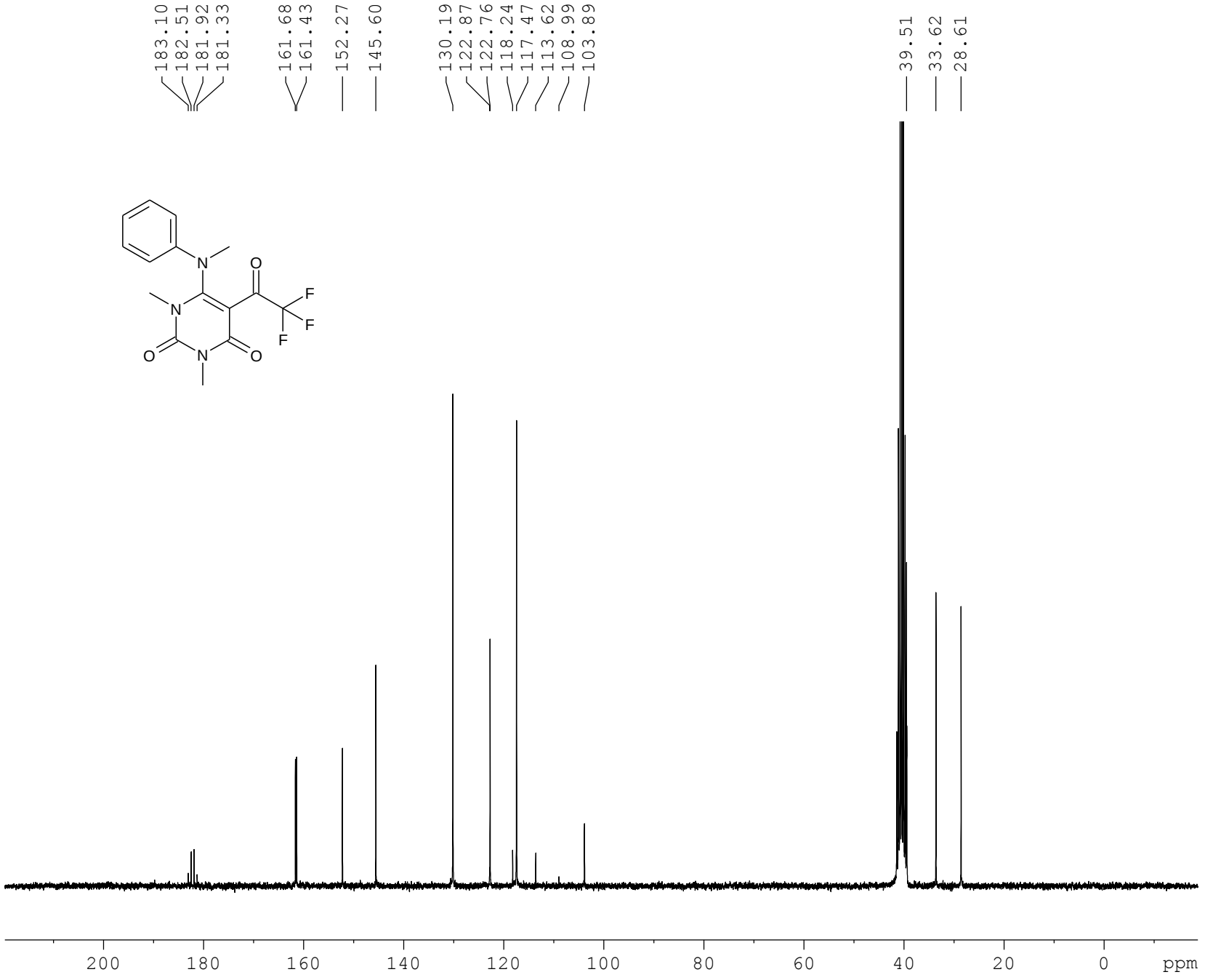

```
Current Data Parameters
NAME         120116.u326
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120116
Time                13.35
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.094423 Hz
AQ               5.2953587 sec
RG                   50.8
DW                 80.800 usec
DE                 10.00 usec
TE                 298.2 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1       0 dB
PL1W         11.25325108 W
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF           300.1299948 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

Dudkin sd350 13C DMSO




```
Current Data Parameters
NAME          120120.201
EXPNO                 10
PROCNO                 1

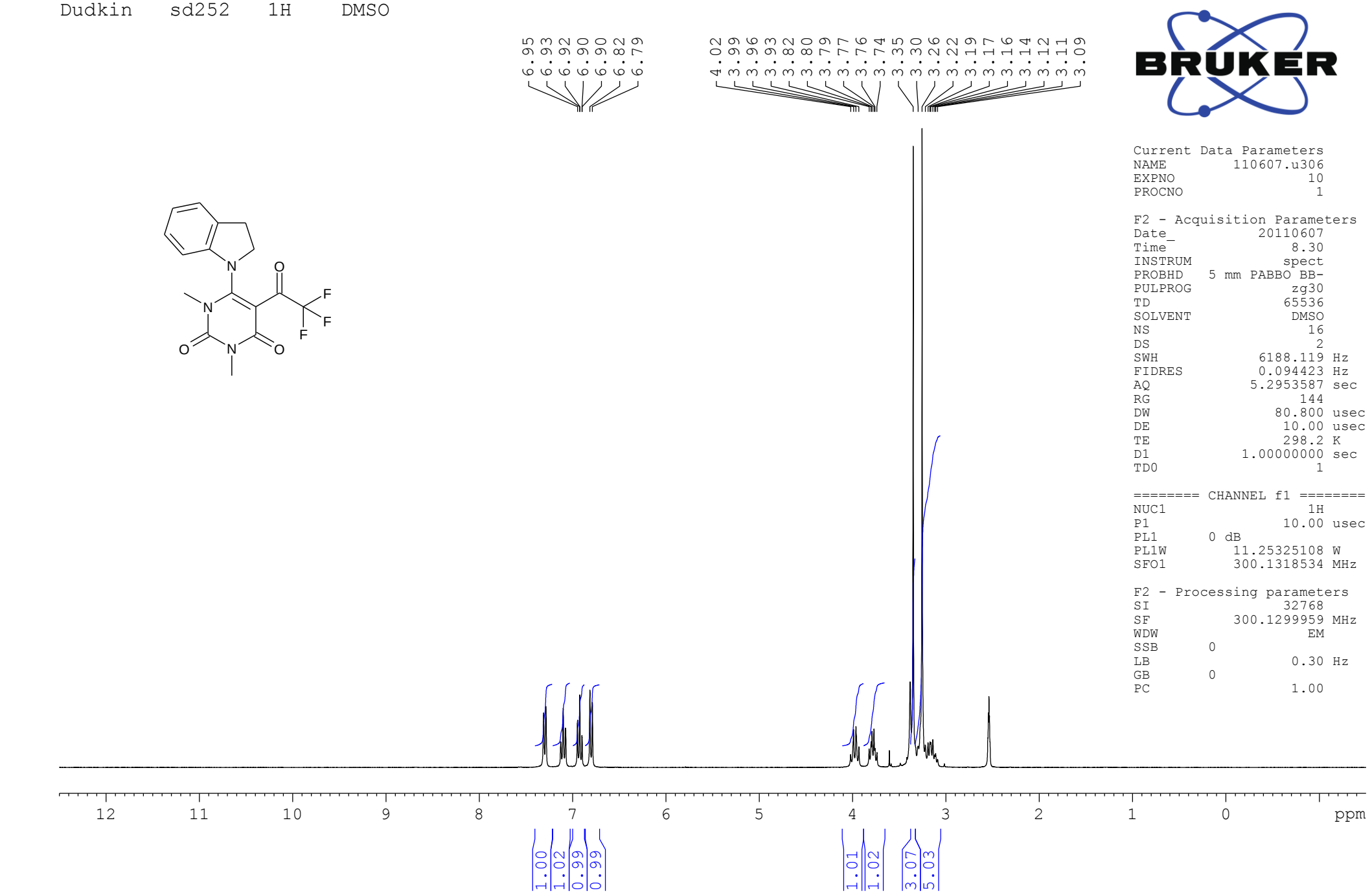
F2 - Acquisition Parameters
Date_           20120120
Time               12.45
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ             2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1       0 dB
SFO1          62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             70.00 usec
PL12              14.00 dB
PL13              14.00 dB
PL2               -3.00 dB
SFO2         250.1310005 MHz

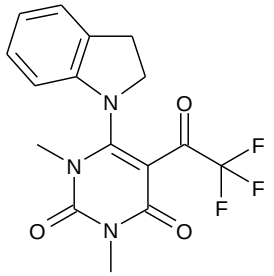
F2 - Processing parameters
SI                32768
SF            62.8952077 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd252 1H DMSO



Dudkin sd252 13C DMSO

182.81 182.22 181.64 181.05 161.60 159.15 152.19 146.02 133.63 128.40 126.44 123.40 123.15 118.53 113.91 112.56 109.29 99.29 54.77 35.00 29.89 28.56



Current Data Parameters
NAME 110610.212
EXPNO 10
PROCNO 1

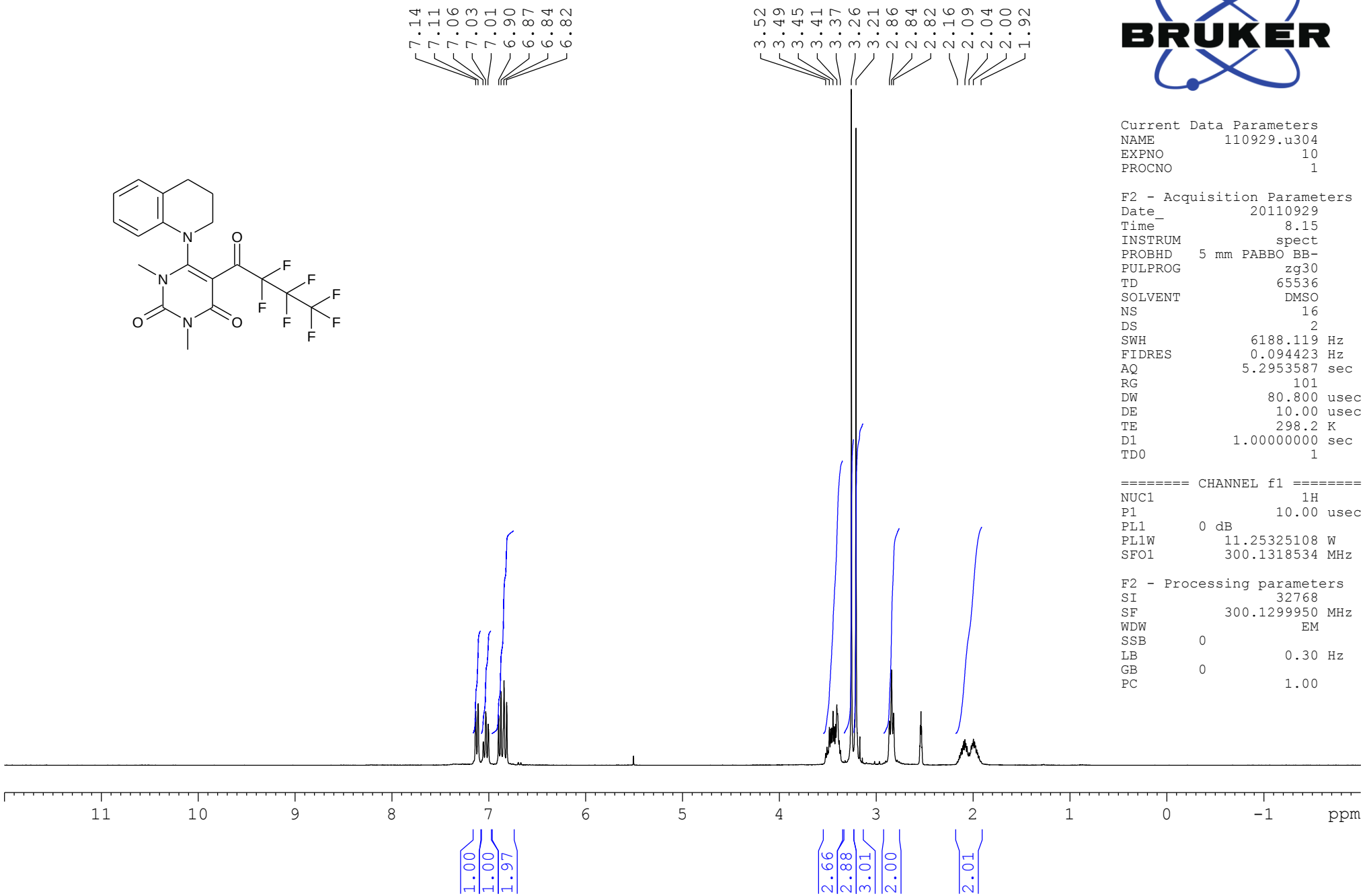
F2 - Acquisition Parameters
Date_ 20110611
Time 9.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2500
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 299.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952099 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd319 1H DMSO



Current Data Parameters
NAME 110929.u304
EXPNO 10
PROCNO 1

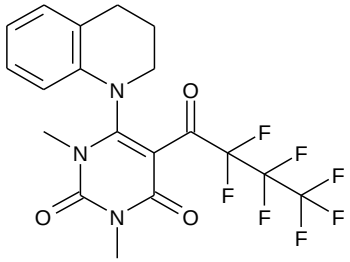
F2 - Acquisition Parameters
Date_ 20110929
Time 8.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 101
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299950 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd319 13C DMSO

185.65 185.28 184.90 161.62 159.35 152.30 140.83 130.74 127.79 125.47 122.33 117.12 104.17 50.67 34.12 28.64 26.80 21.77




```
Current Data Parameters
NAME         110929.u304
EXPNO                 12
PROCNO                 1

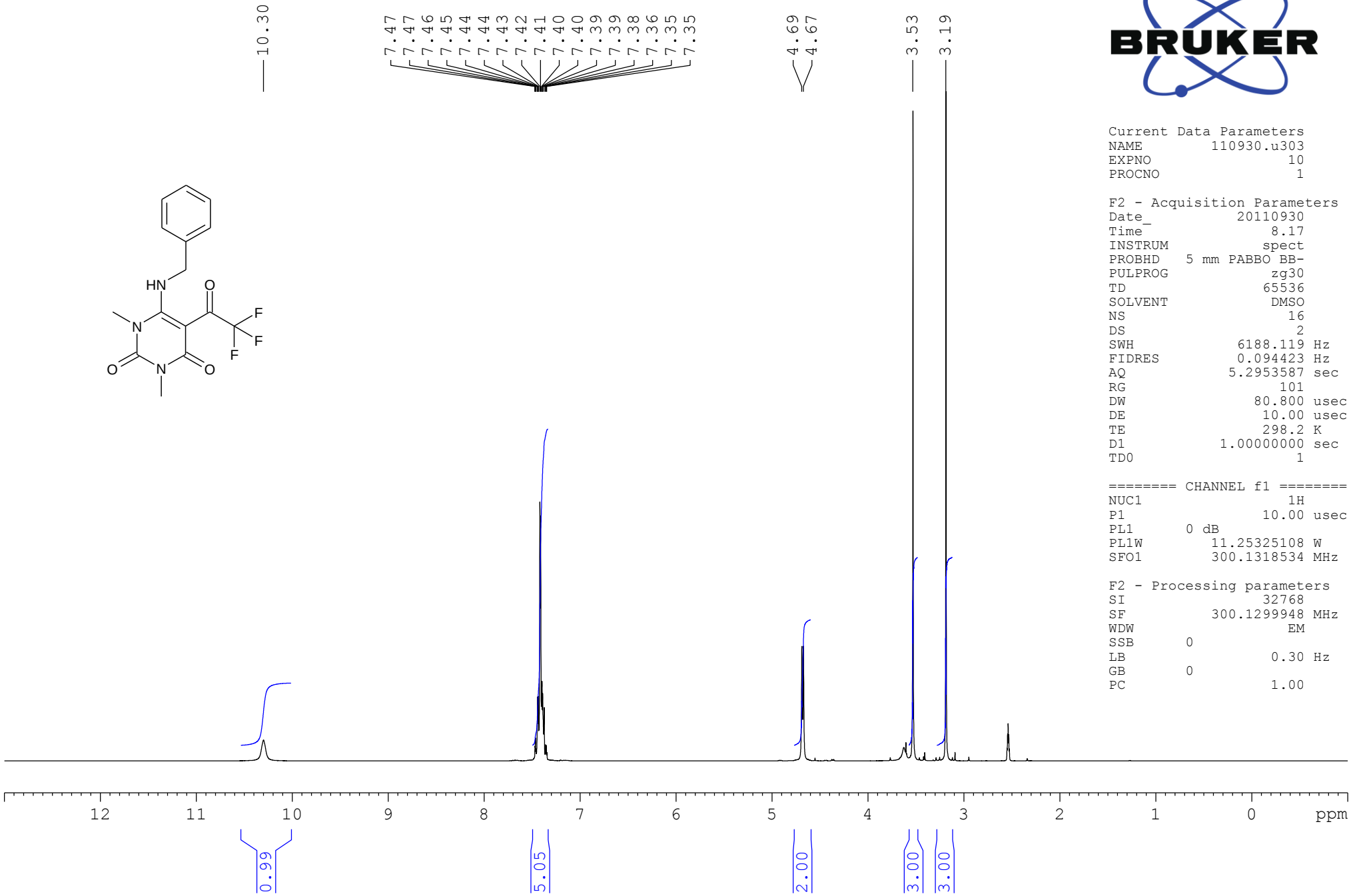
F2 - Acquisition Parameters
Date_           20110929
Time              22.08
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                 2050
DW               27.733 usec
DE               10.00 usec
TE               298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             72.00 usec
PL2       0 dB
PL12              17.00 dB
PL13              17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677157 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin, sd 322, DMSO, 1H



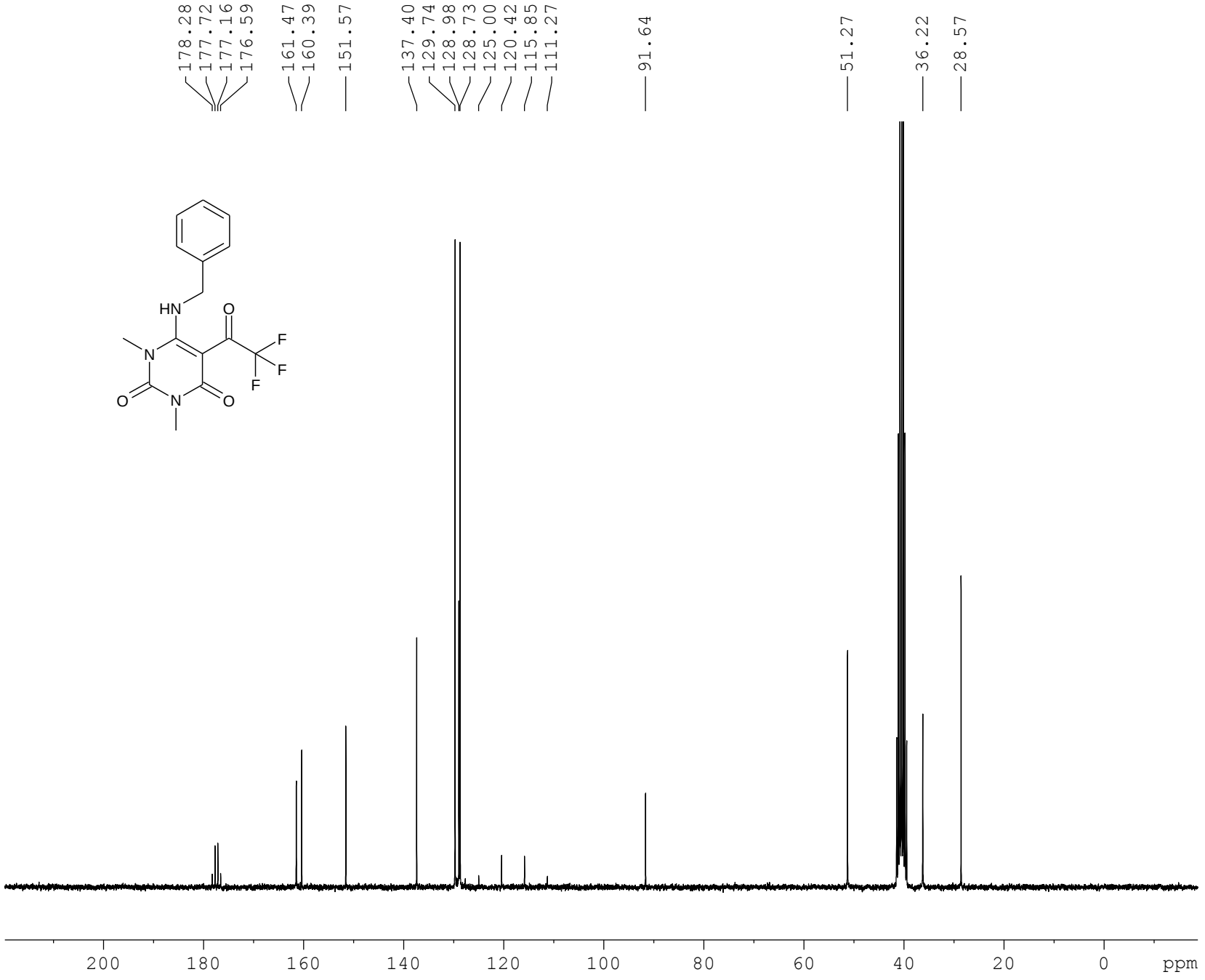

```
Current Data Parameters
NAME          110930.u303
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20110930
Time                8.17
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   101
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1299948 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin, sd 322, DMSO, 13C




```
Current Data Parameters
NAME          110930.205
EXPNO                 10
PROCNO                 1

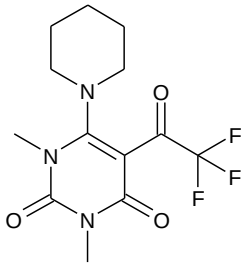
F2 - Acquisition Parameters
Date_           20110930
Time               22.23
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 4096
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.4 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952094 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd312 1H DMSO



Current Data Parameters
NAME 110913.u302
EXPNO 10
PROCNO 1

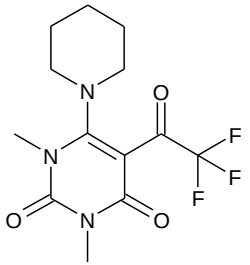
F2 - Acquisition Parameters
Date_ 20110913
Time 7.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 71.8
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1314218 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd312 13C DMSO

183.40 182.82 182.24 181.66 163.34 161.69 152.44 123.54 118.92 114.31 109.69 97.32 53.11 35.76 28.30 25.69 24.15



Current Data Parameters
NAME 110913.208
EXPNO 11
PROCNO 1

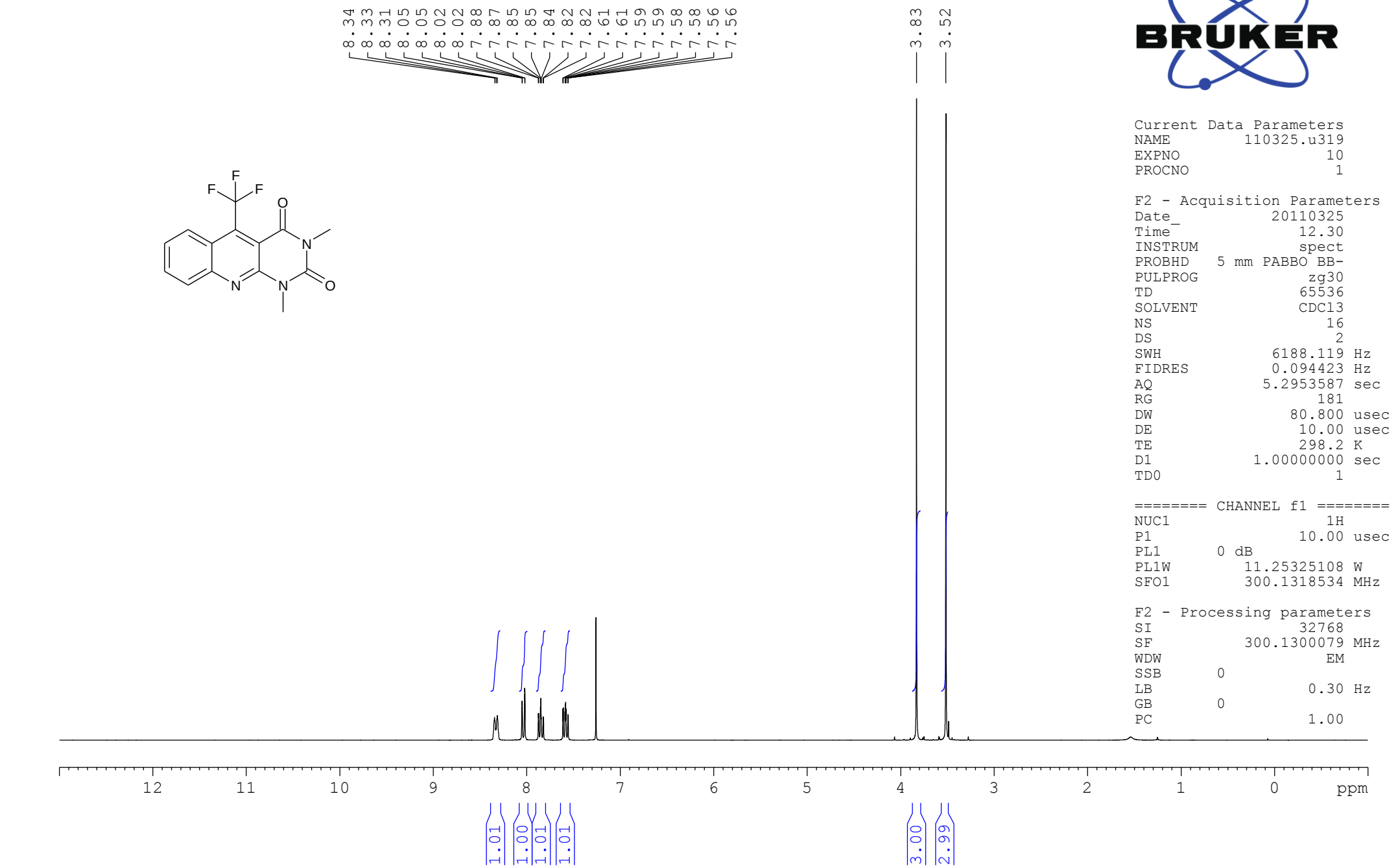
F2 - Acquisition Parameters
Date_ 20110914
Time 6.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 1290
DW 33.333 usec
DE 10.00 usec
TE 297.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952083 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd202 1H CDCl3




```
Current Data Parameters
NAME         110325.u319
EXPNO                 10
PROCNO                 1

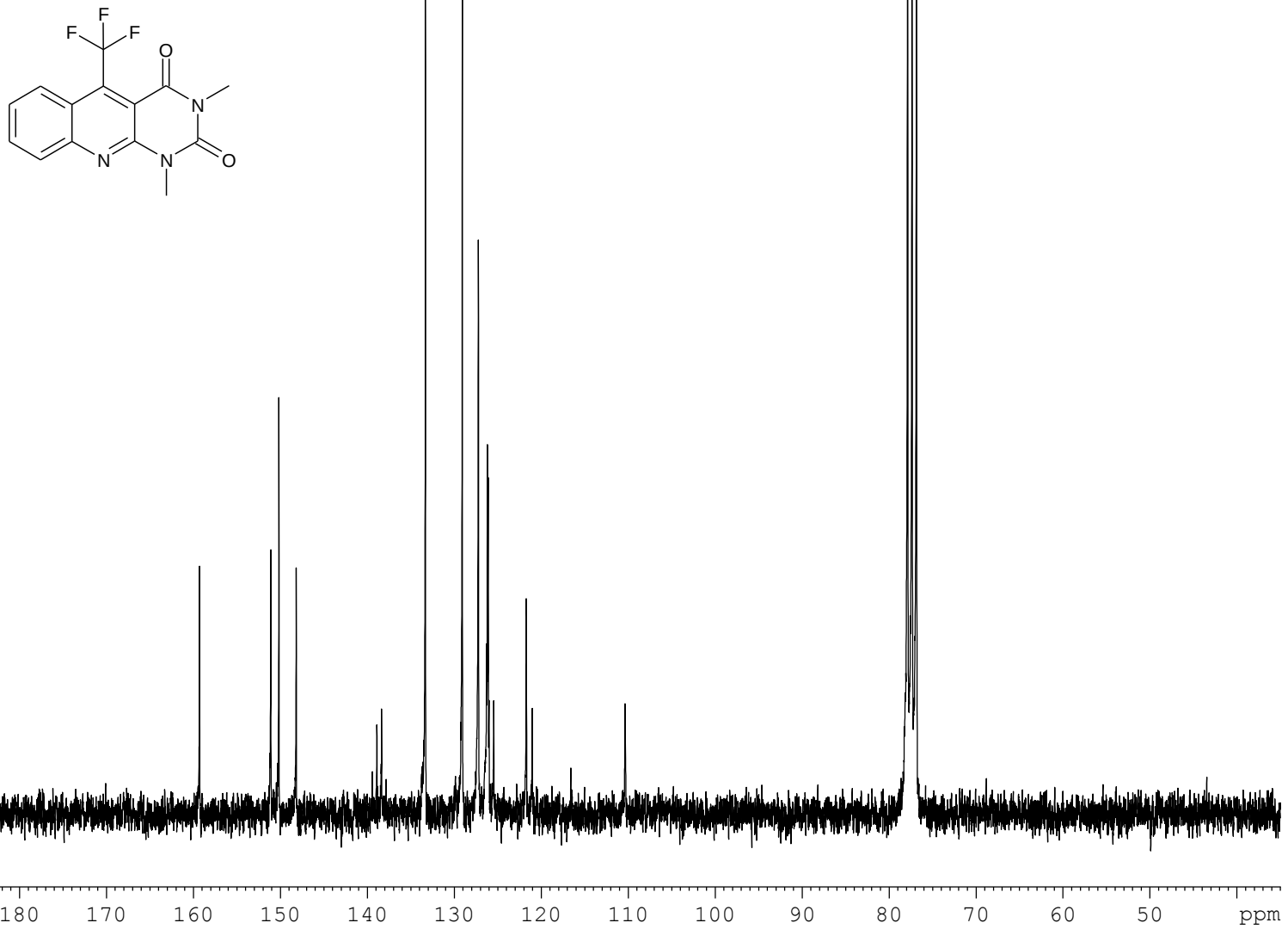
F2 - Acquisition Parameters
Date_           20110325
Time               12.30
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   181
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300079 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd202 13C CDCl3

159.33
151.14
150.20
148.21
139.47
138.94
138.40
137.88
133.36
129.90
129.11
127.24
126.28
126.19
126.09
126.00
125.46
121.72
121.03
116.61
110.35




```
Current Data Parameters
NAME          110401.238
EXPNO                 10
PROCNO                 1

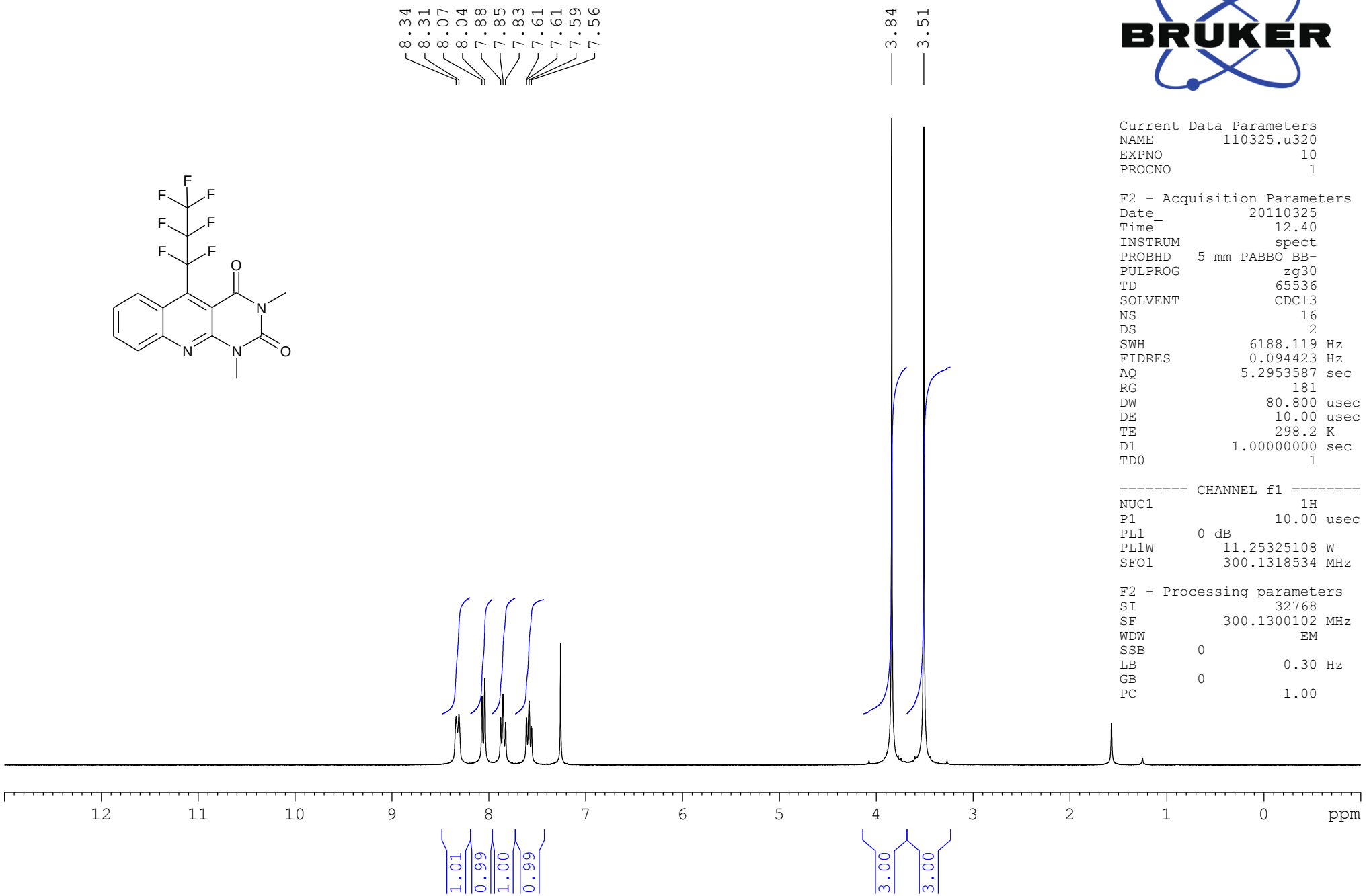
F2 - Acquisition Parameters
Date_           20110404
Time                5.18
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE               10.00 usec
TE               298.2 K
D1            4.00000000 sec
d11           0.03000000 sec
DELTA         3.90000010 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952178 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd203 1H CDCl3



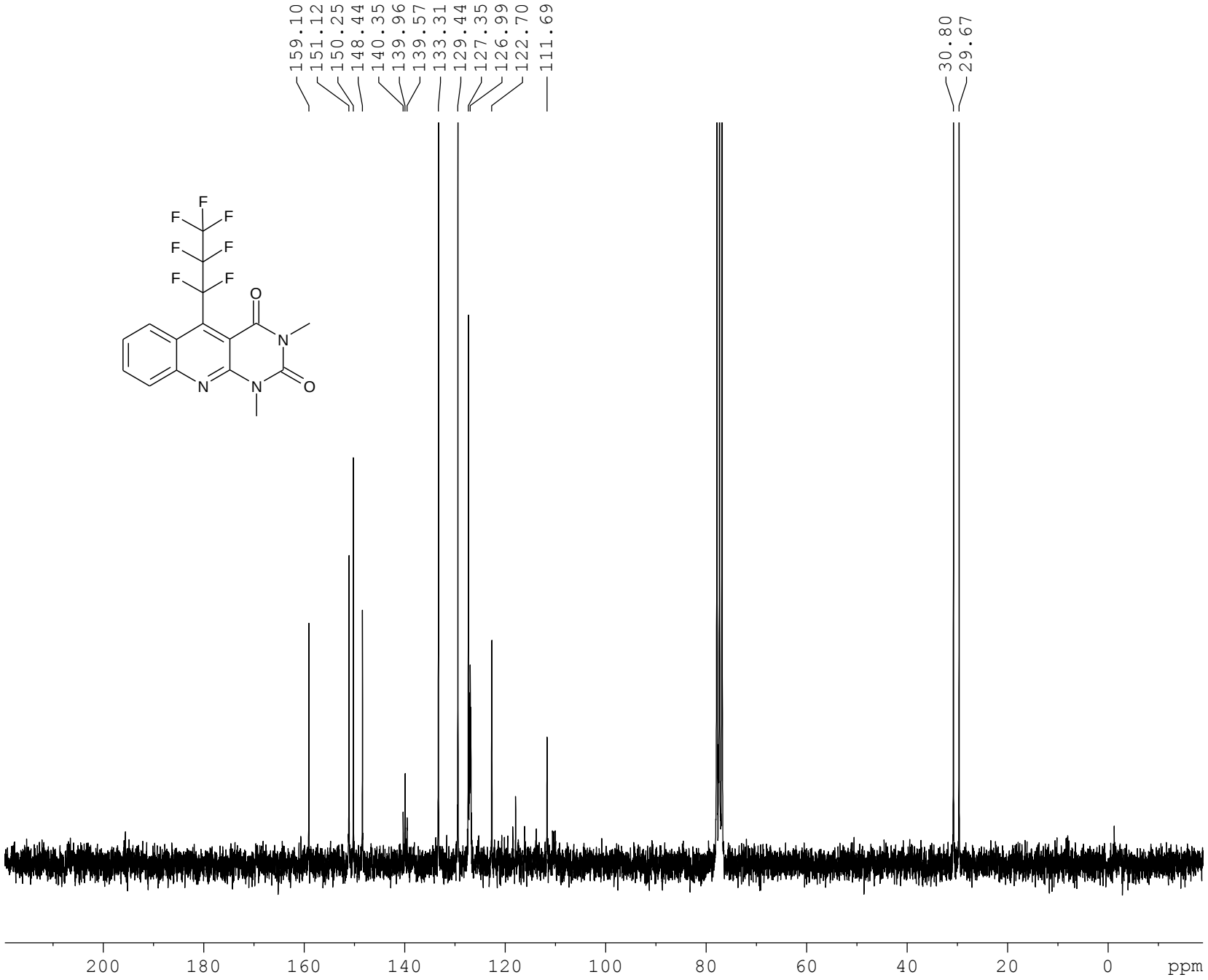
Current Data Parameters
NAME 110325.u320
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110325
Time 12.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 181
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd203 13C CDCl3




```
Current Data Parameters
NAME          110401.239
EXPNO                 10
PROCNO                 1

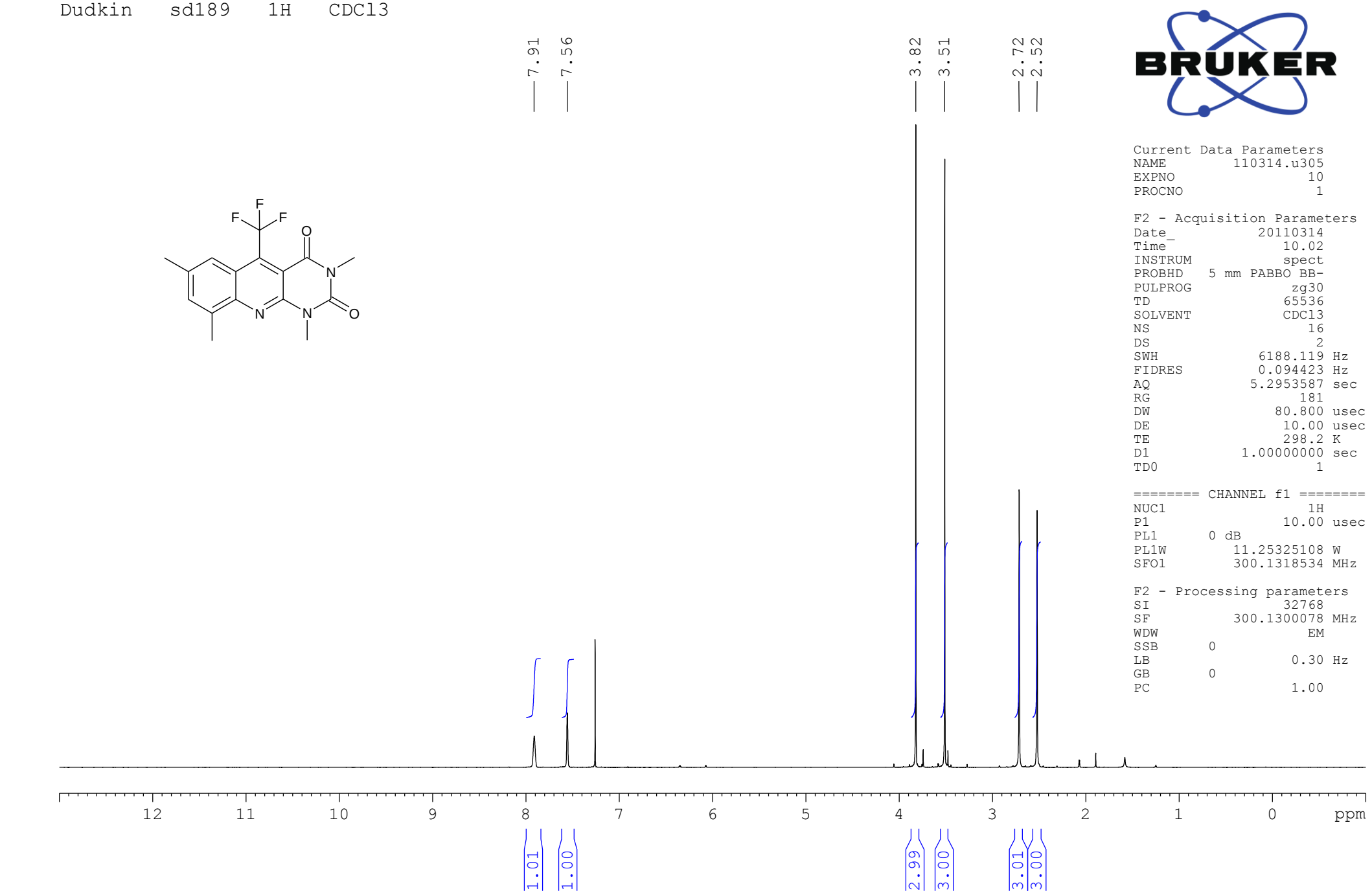
F2 - Acquisition Parameters
Date_           20110404
Time                7.31
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           15000.000 Hz
FIDRES            0.228882 Hz
AQ             2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.0 K
D1            4.00000000 sec
d11           0.03000000 sec
DELTA         3.90000010 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952162 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd189 1H CDCl3



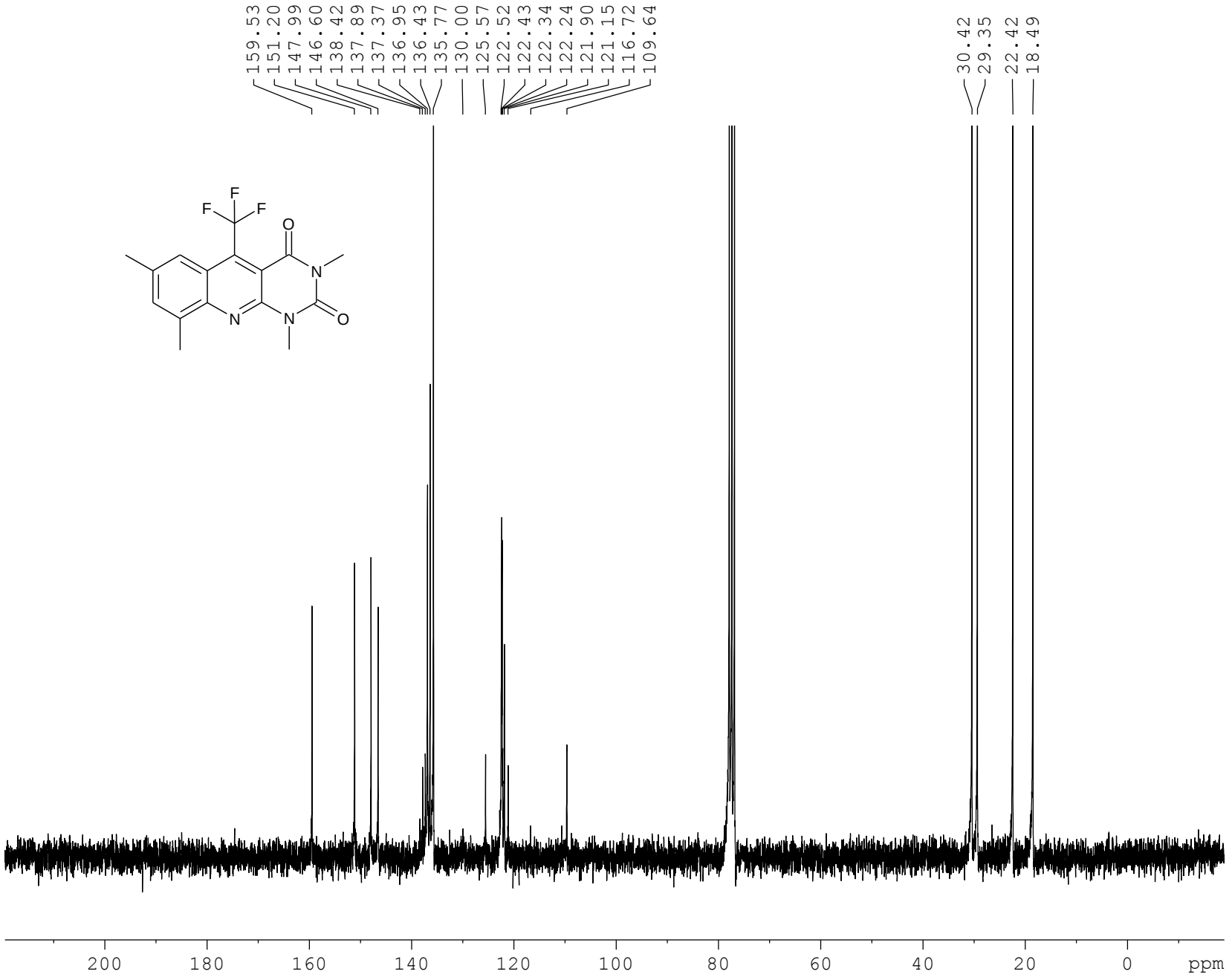
Current Data Parameters
NAME 110314.u305
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110314
Time 10.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 181
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd189 13C CDCl3



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```
Current Data Parameters
NAME          110318.214
EXPNO                 10
PROCNO                 1

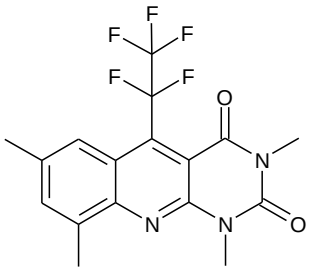
F2 - Acquisition Parameters
Date_           20110319
Time                2.54
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE               10.00 usec
TE               298.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952185 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd225 1H CDCl3



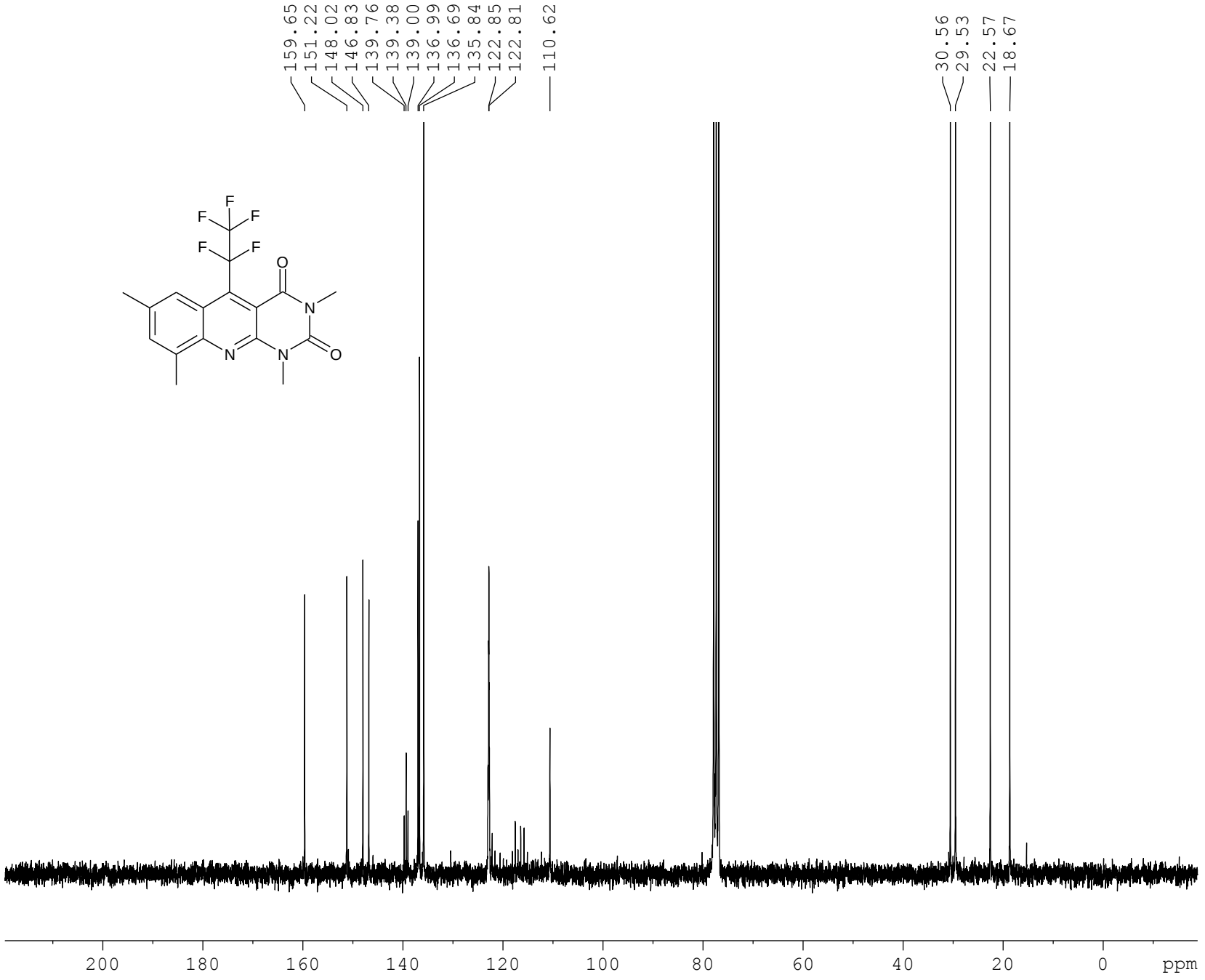
Current Data Parameters
NAME 110413.u302
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110413
Time 8.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 101
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd225 13C CDCl3



Current Data Parameters
NAME 110509.211
EXPNO 10
PROCNO 1

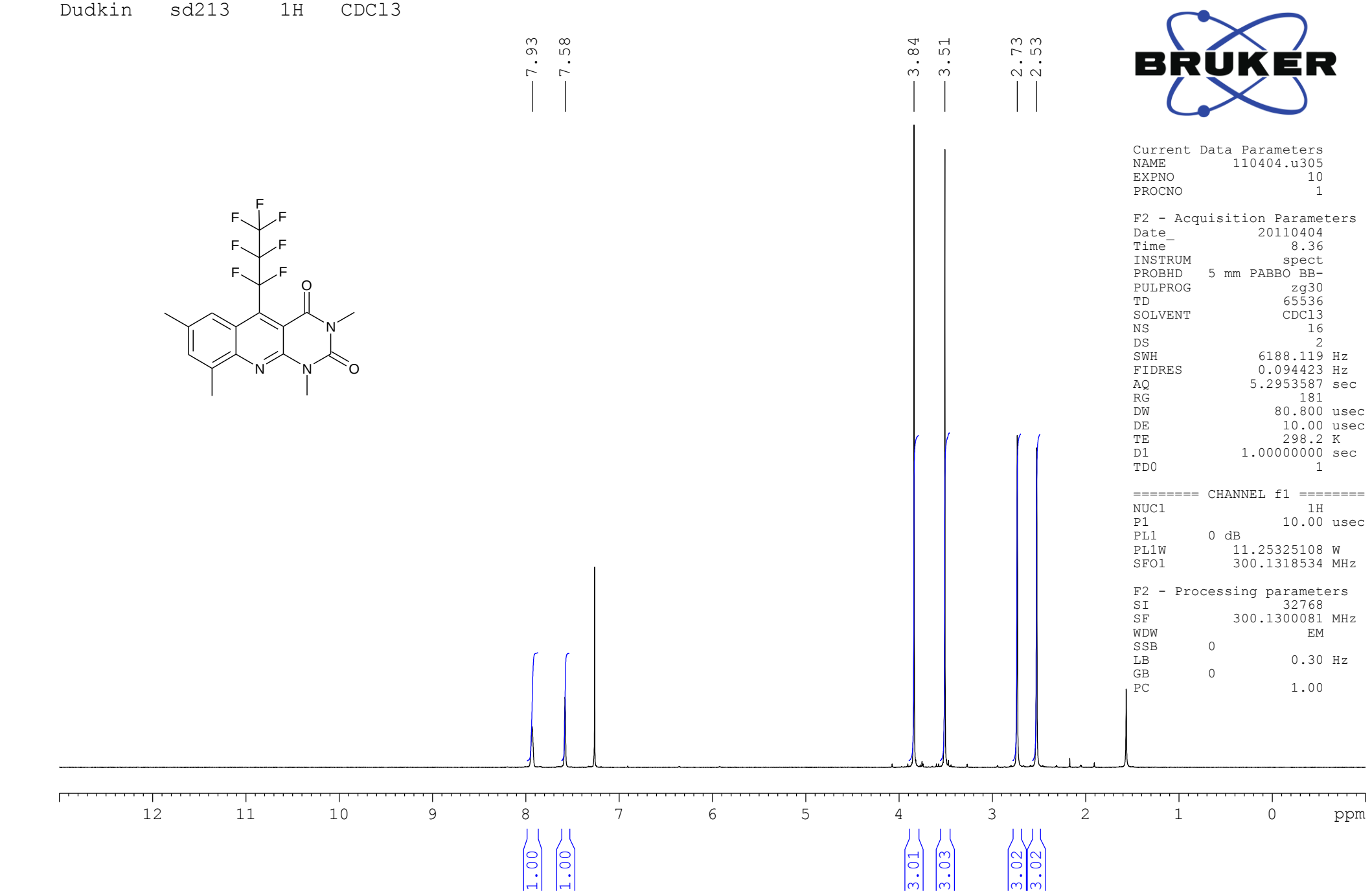
F2 - Acquisition Parameters
Date_ 20110510
Time 8.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1600
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.2 K
D1 5.00000000 sec
d11 0.03000000 sec
DELTA 4.90000010 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952171 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd213 1H CDCl3



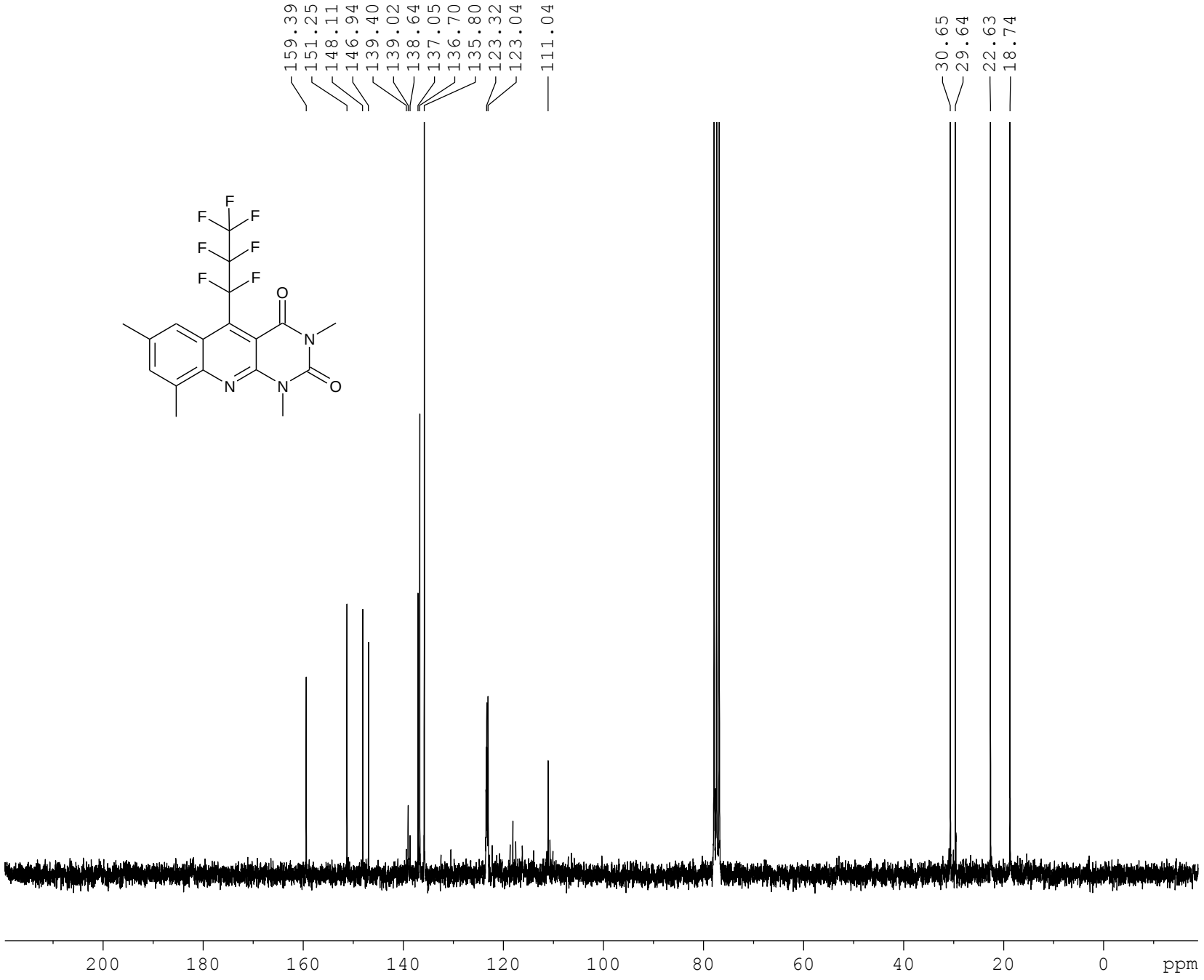

```
Current Data Parameters
NAME          110404.u305
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20110404
Time                8.36
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   181
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300081 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin, sd 213 , CDCl3, 13C



Current Data Parameters
NAME 110624.207
EXPNO 10
PROCNO 1

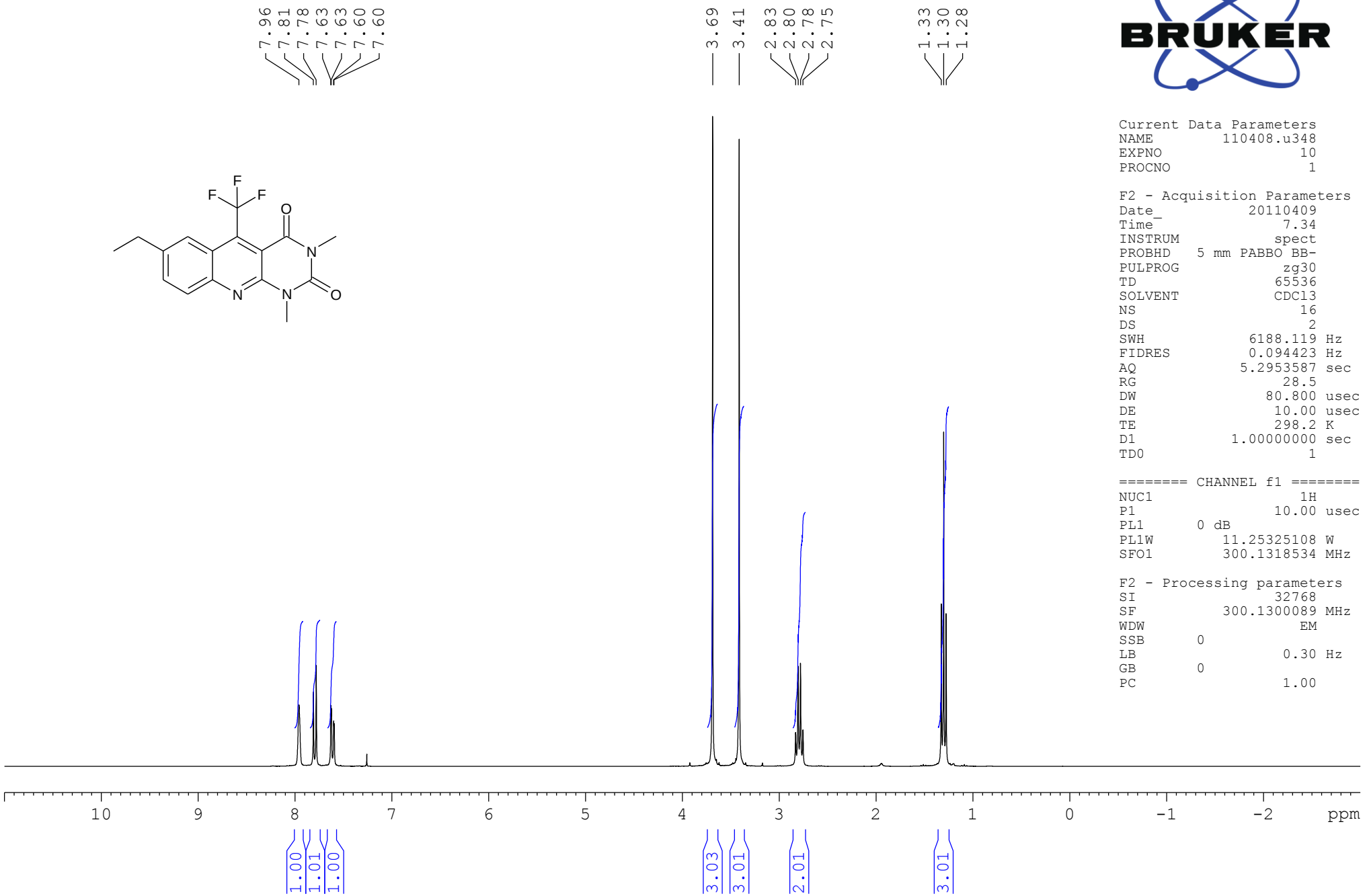
F2 - Acquisition Parameters
Date_ 20110626
Time 7.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 299.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952157 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd 195 1H CDCl3



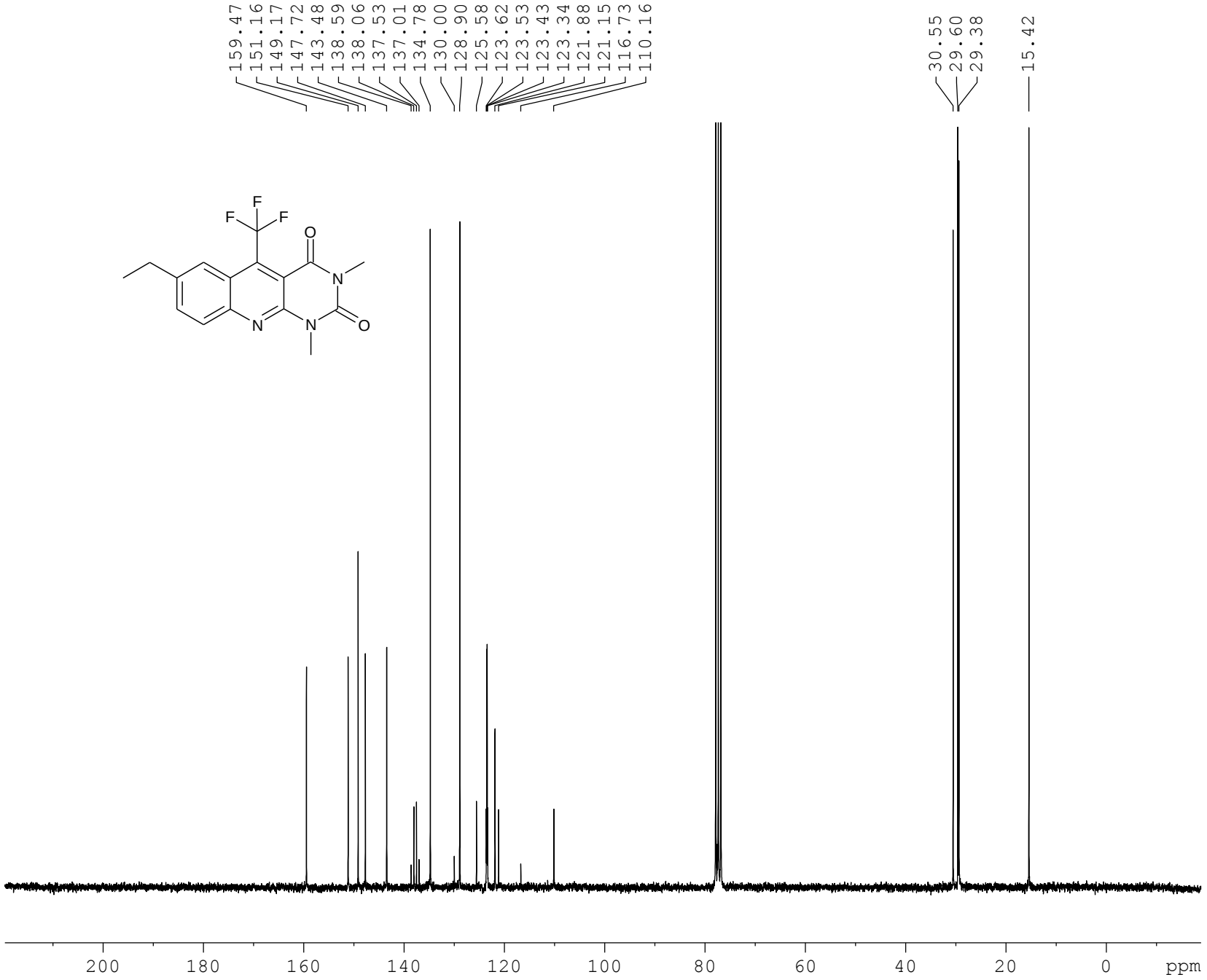

```
Current Data Parameters
NAME          110408.u348
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20110409
Time                7.34
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                  28.5
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300089 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin, sd 195, CDCl3, 13C



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Current Data Parameters
NAME 110708.212
EXPNO 10
PROCNO 1

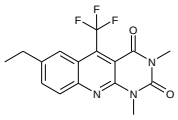
F2 - Acquisition Parameters
Date_ 20110711
Time 8.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 299.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952177 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd 195 COSY CDCl3



BRUKER

```
Current Data Parameters
NAME         110408.u348
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110409
Time                7.35
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG         cosygpqf
TD                  2048
SOLVENT             CDCl3
NS                     4
DS                     8
SWH              2631.579 Hz
FIDRES           1.284951 Hz
AQ               0.3891700 sec
RG                    16
DW                190.000 usec
DE                 10.00 usec
TE                 298.2 K
D0             0.00000300 sec
D1             1.35336196 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00038000 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                 10.00 usec
P1                 10.00 usec
PL1       0 dB
PL1W         11.25325108 W
SFO1        300.1313743 MHz

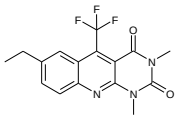
====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPZ1               10.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   128
SFO1            300.1314 MHz
FIDRES          20.559210 Hz
SW                8.768 ppm
FnMODE                QF

F2 - Processing parameters
SI                  1024
SF           300.1300115 MHz
WDW                 SINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           300.1300116 MHz
WDW               States
SSB       0
LB        0 Hz
GB        0
```

Dudkin sd 195 HSQC CDCl3




```
Current Data Parameters
NAME          110408.u348
EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
Date_            20110409
Time                7.52
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG     hsqcetgpsi2
TD                  1024
SOLVENT             CDCl3
NS                    12
DS                    16
SWH           2631.579 Hz
FIDRES        2.569901 Hz
AQ            0.1946100 sec
RG                  1820
DW             190.000 usec
DE              10.00 usec
TE              298.2 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.43343997 sec
D4            0.00172414 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00004000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
P2                 20.00 usec
P28              1000.00 usec
PL1        0 dB
PL1W         11.25325108 W
SFO1        300.1313743 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                  13C
P3                 10.00 usec
P4                 20.00 usec
PCPD2              72.00 usec
PL2                -0.50 dB
PL12               17.00 dB
PL2W         33.25691986 W
PL12W         0.59140092 W
SFO2          75.4734070 MHz

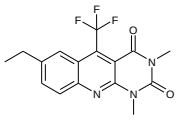
====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPNAM3          SINE.100
GPNAM4          SINE.100
GPZ1               80.00 %
GPZ2               20.10 %
GPZ3               11.00 %
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

F1 - Acquisition parameters
TD                    256
SFO1           75.47341 MHz
FIDRES        48.836605 Hz
SW              165.650 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           300.1300104 MHz
WDW                 QSINE
SSB                     2
LB         0 Hz
GB         0
PC                   1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           75.4677373 MHz
WDW
SSB                     2
LB         0 Hz
GB         0
```

Dudkin sd 195 HMBC CDCl3




```
Current Data Parameters
NAME         110408.u348
EXPNO                 13
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110409
Time                9.19
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG       hmbcgpndqf
TD                  4096
SOLVENT             CDCl3
NS                    48
DS                    16
SWH             2631.579 Hz
FIDRES          0.642475 Hz
AQ              0.7782900 sec
RG                  2050
DW               190.000 usec
DE                10.00 usec
TE                298.2 K
CNST13         8.0000000
D0            0.00000300 sec
D1            1.23376000 sec
D6            0.06250000 sec
D16           0.00020000 sec
IN0           0.00002985 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1       300.1313743 MHz

======== CHANNEL f2 ========
NUC2                 13C
P3                10.00 usec
PL2               -0.50 dB
PL2W         33.25691986 W
SFO2          75.4752833 MHz

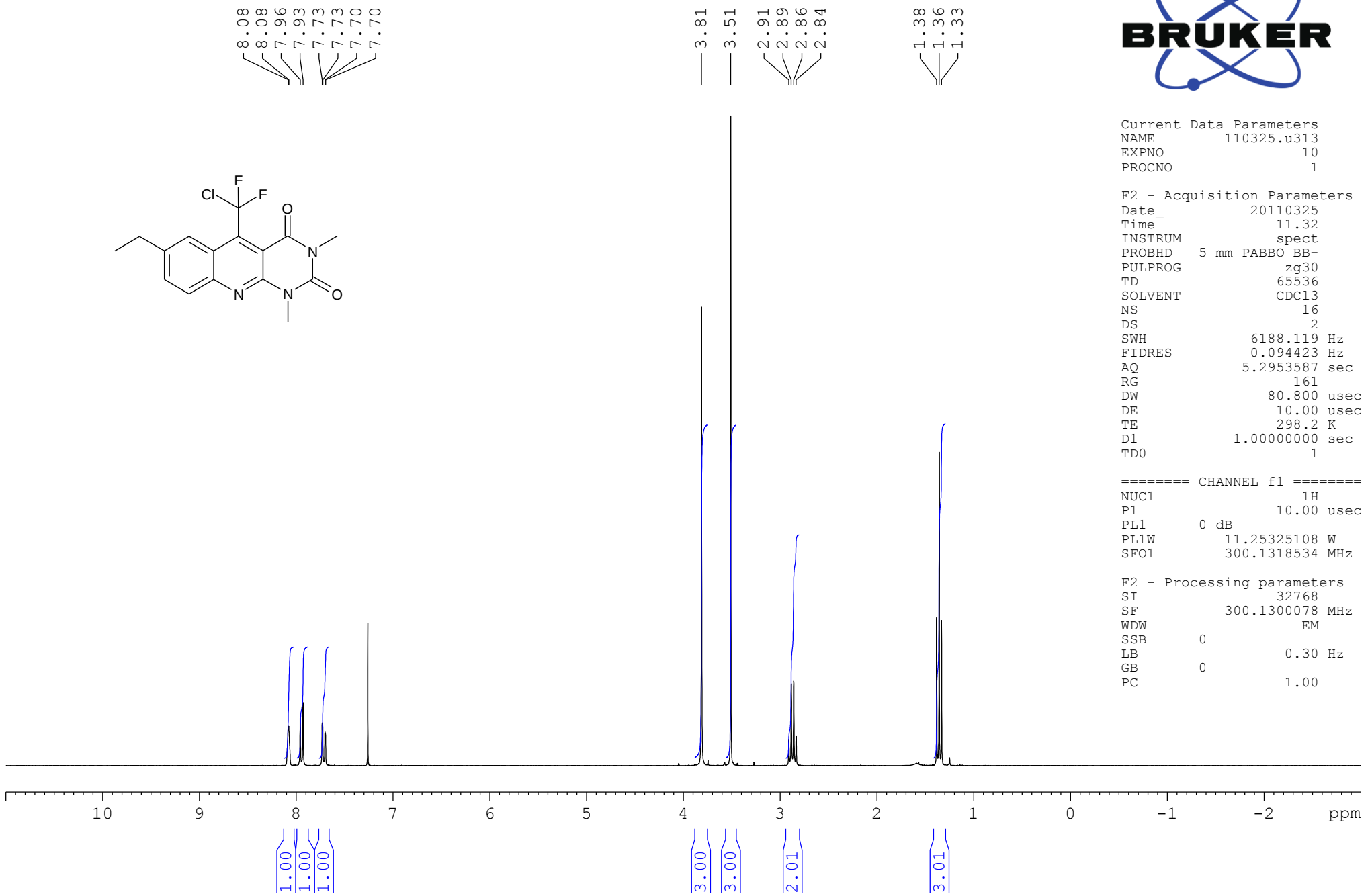
====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPNAM3          SINE.100
GPZ1               50.00 %
GPZ2               30.00 %
GPZ3               40.10 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   128
SFO1           75.47528 MHz
FIDRES        130.958496 Hz
SW              222.095 ppm
FnMODE                QF

F2 - Processing parameters
SI                  1024
SF           300.1300114 MHz
WDW                 SINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           75.4677099 MHz
WDW               States
SSB       0
LB        0 Hz
GB        0
```

Dudkin sd196 1H CDCl3



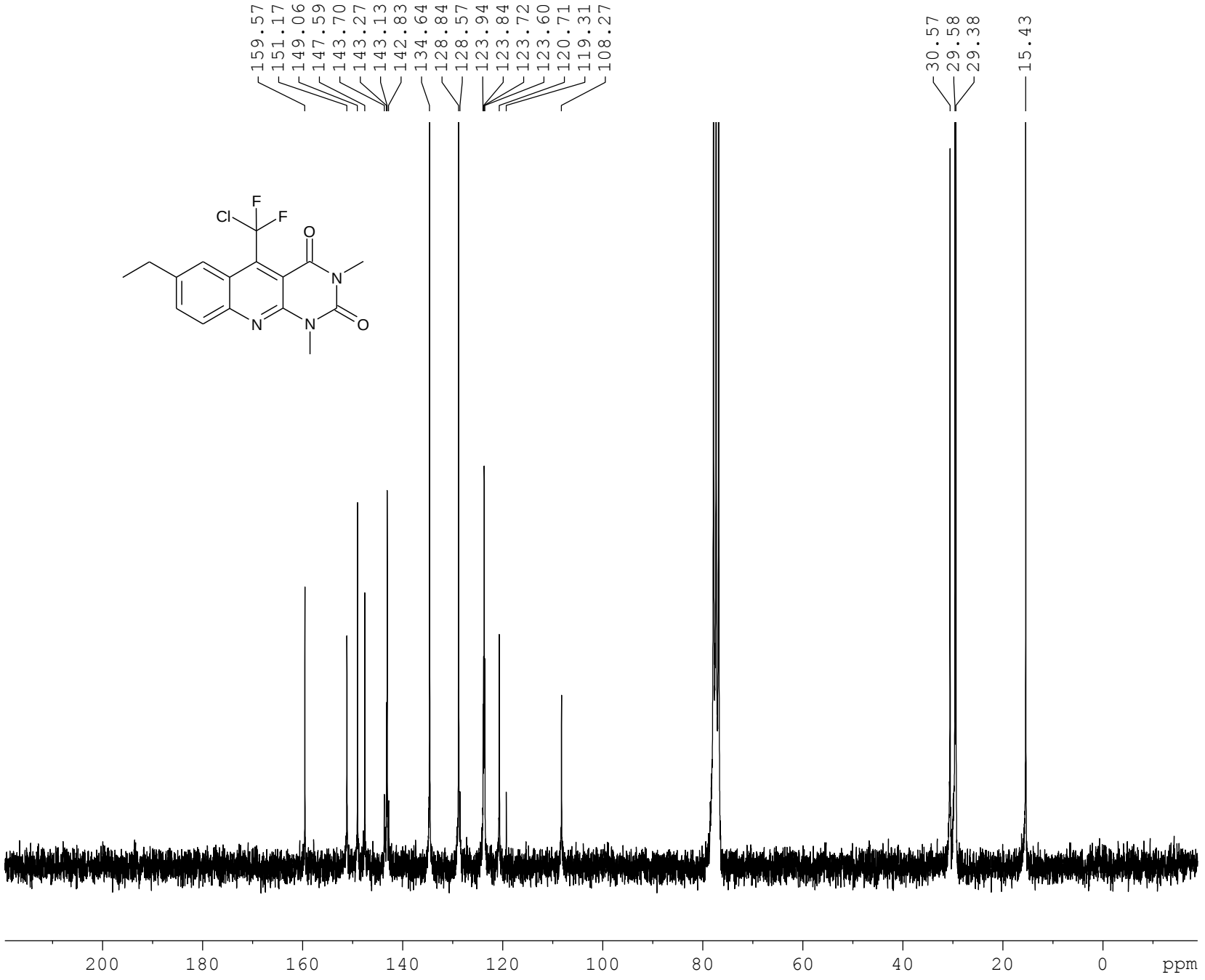

```
Current Data Parameters
NAME          110325.u313
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20110325
Time                11.32
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.094423 Hz
AQ               5.2953587 sec
RG                    161
DW                 80.800 usec
DE                 10.00 usec
TE                 298.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1        0 dB
PL1W          11.25325108 W
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF            300.1300078 MHz
WDW                    EM
SSB        0
LB                  0.30 Hz
GB         0
PC                  1.00
```

Dudkin sd196 13C CDCl3




```
Current Data Parameters
NAME          110401.237
EXPNO                 10
PROCNO                 1

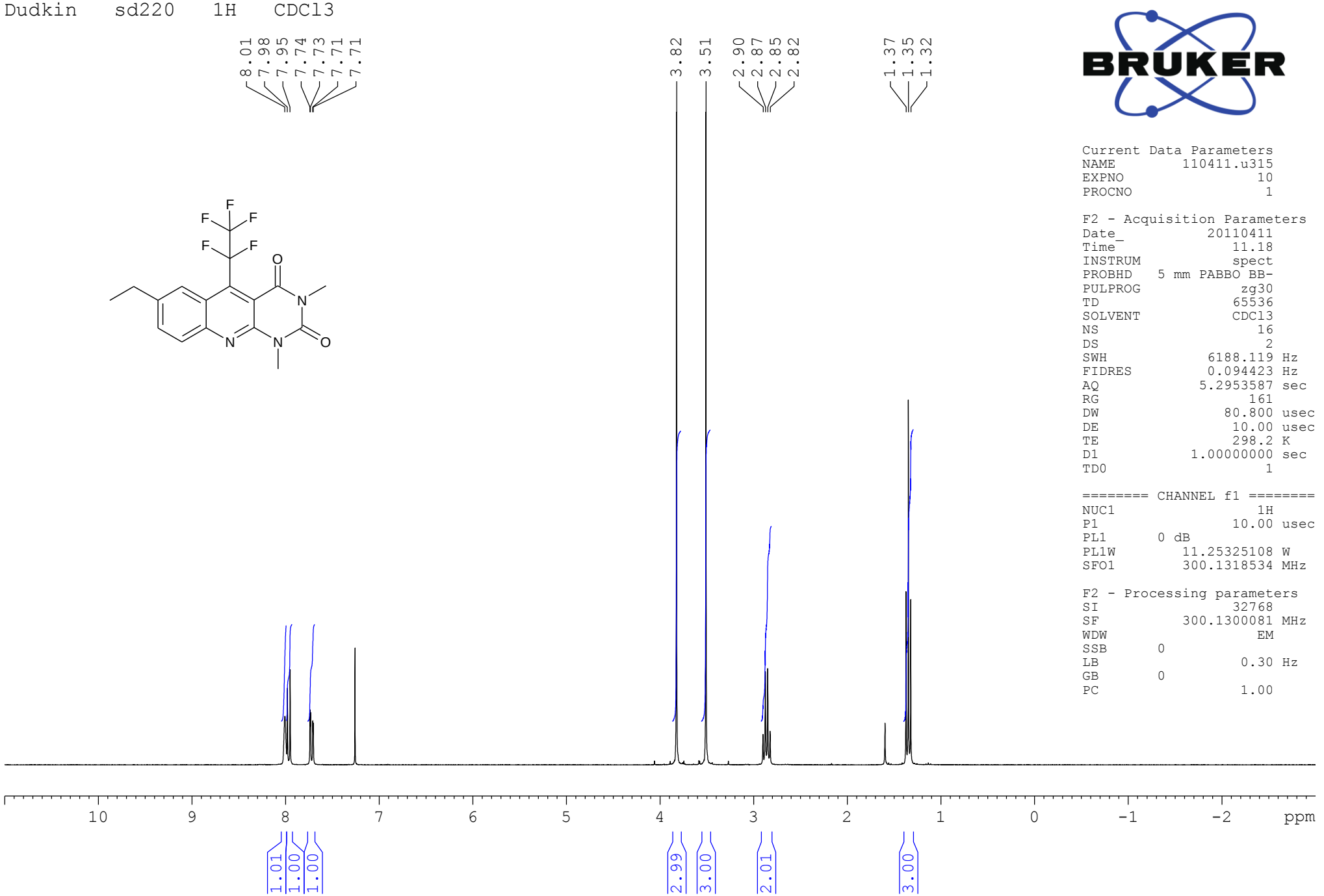
F2 - Acquisition Parameters
Date_           20110404
Time                3.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.2 K
D1           4.00000000 sec
d11          0.03000000 sec
DELTA        3.90000010 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF          62.8952197 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd220 1H CDCl3



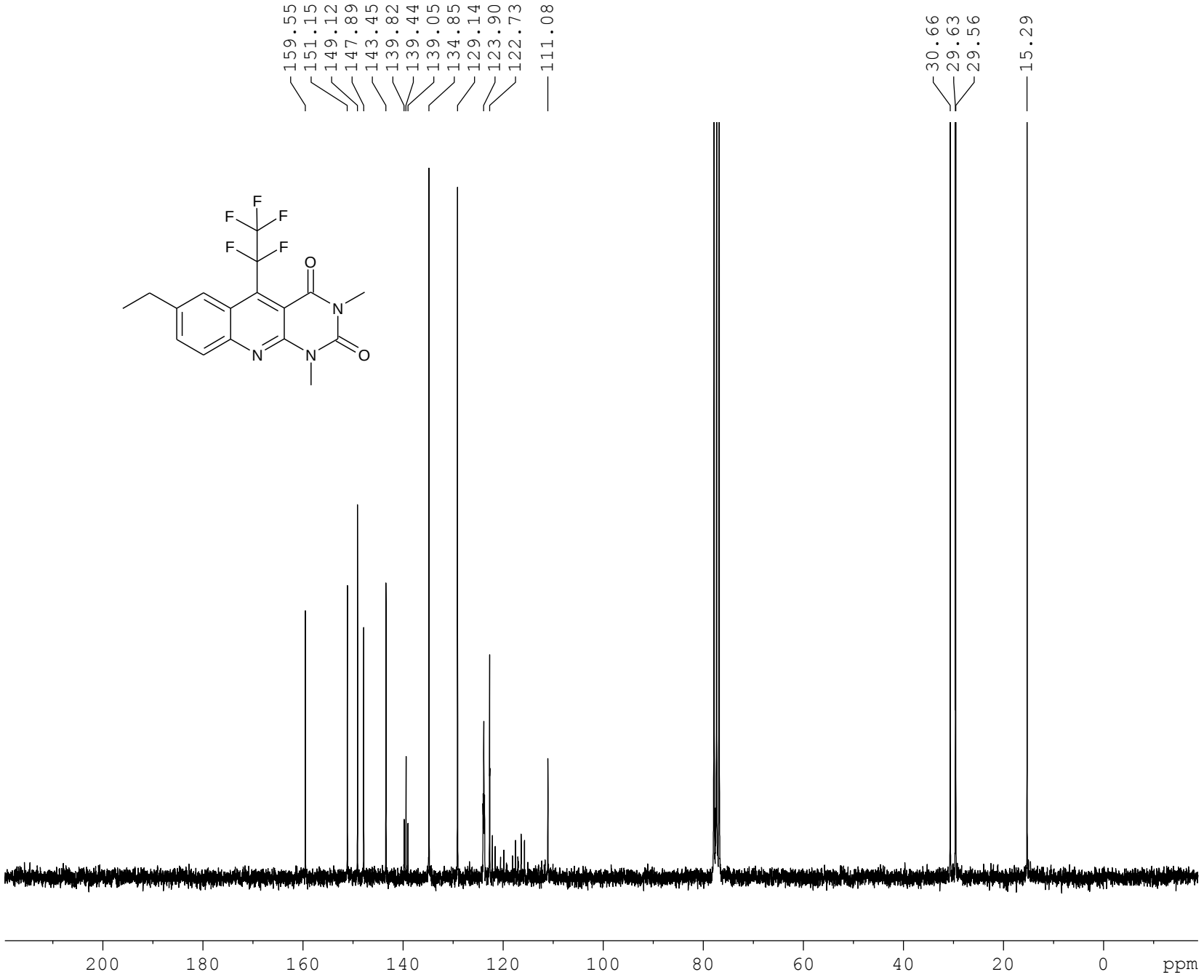
Current Data Parameters
NAME 110411.u315
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110411
Time 11.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 161
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd220 13C CDCl3



Current Data Parameters
NAME 110511.211
EXPNO 10
PROCNO 1

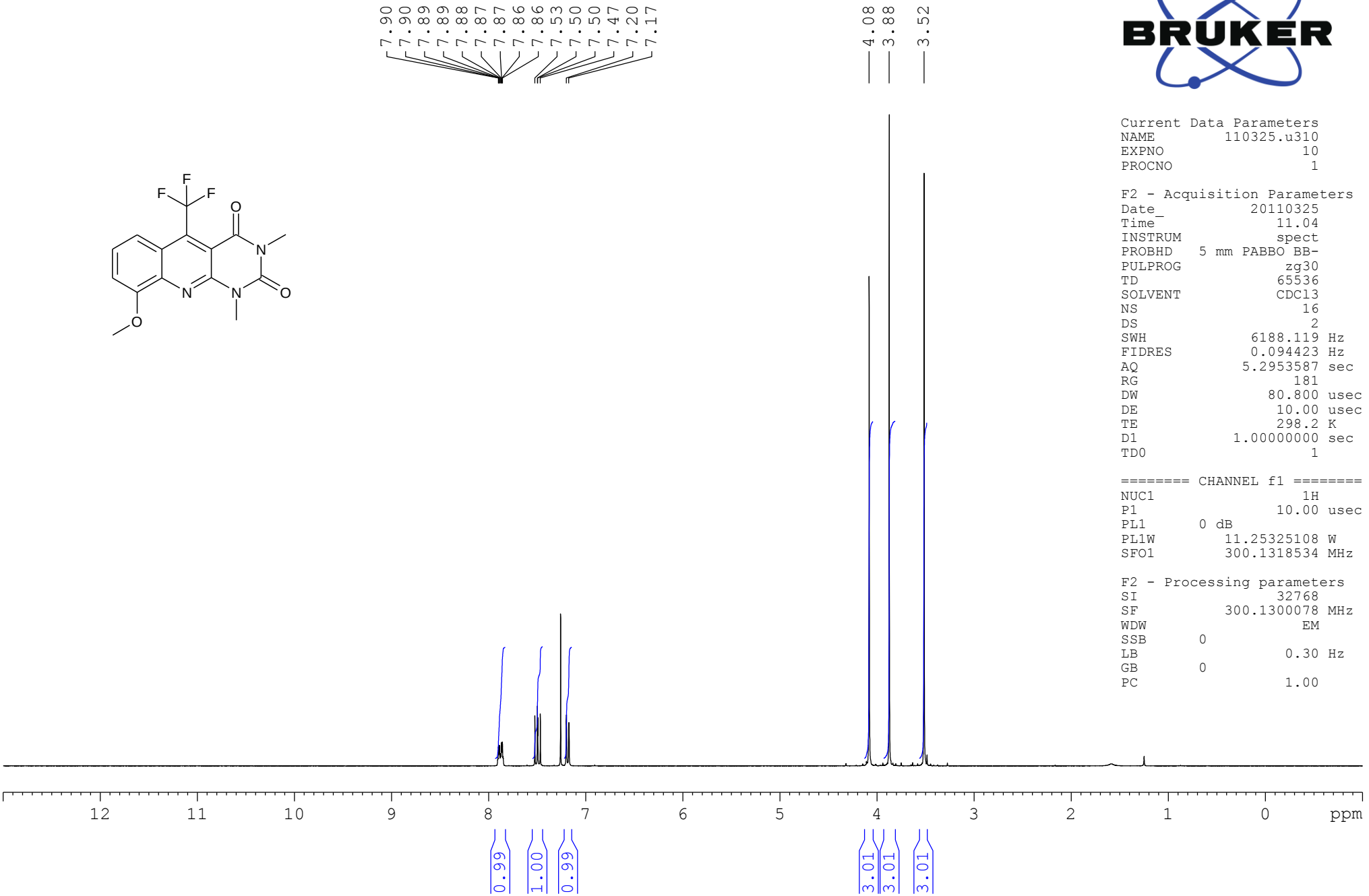
F2 - Acquisition Parameters
Date_ 20110512
Time 8.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1600
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 299.0 K
D1 5.00000000 sec
d11 0.03000000 sec
DELTA 4.90000010 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952166 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd193 1H CDCl3



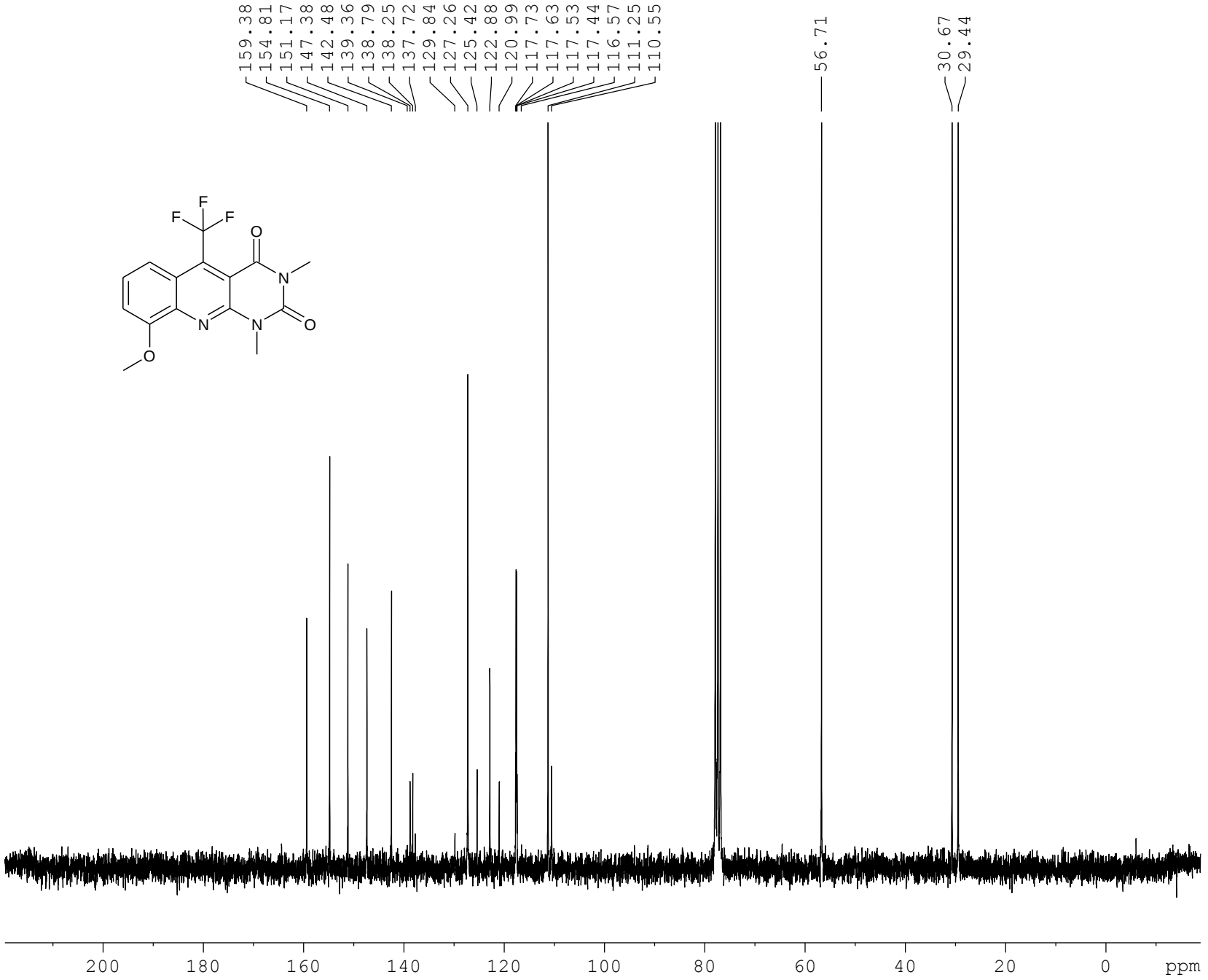

```
Current Data Parameters
NAME         110325.u310
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110325
Time               11.04
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   181
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300078 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd193 13C CDCl3



Current Data Parameters
NAME 110401.234
EXPNO 10
PROCNO 1

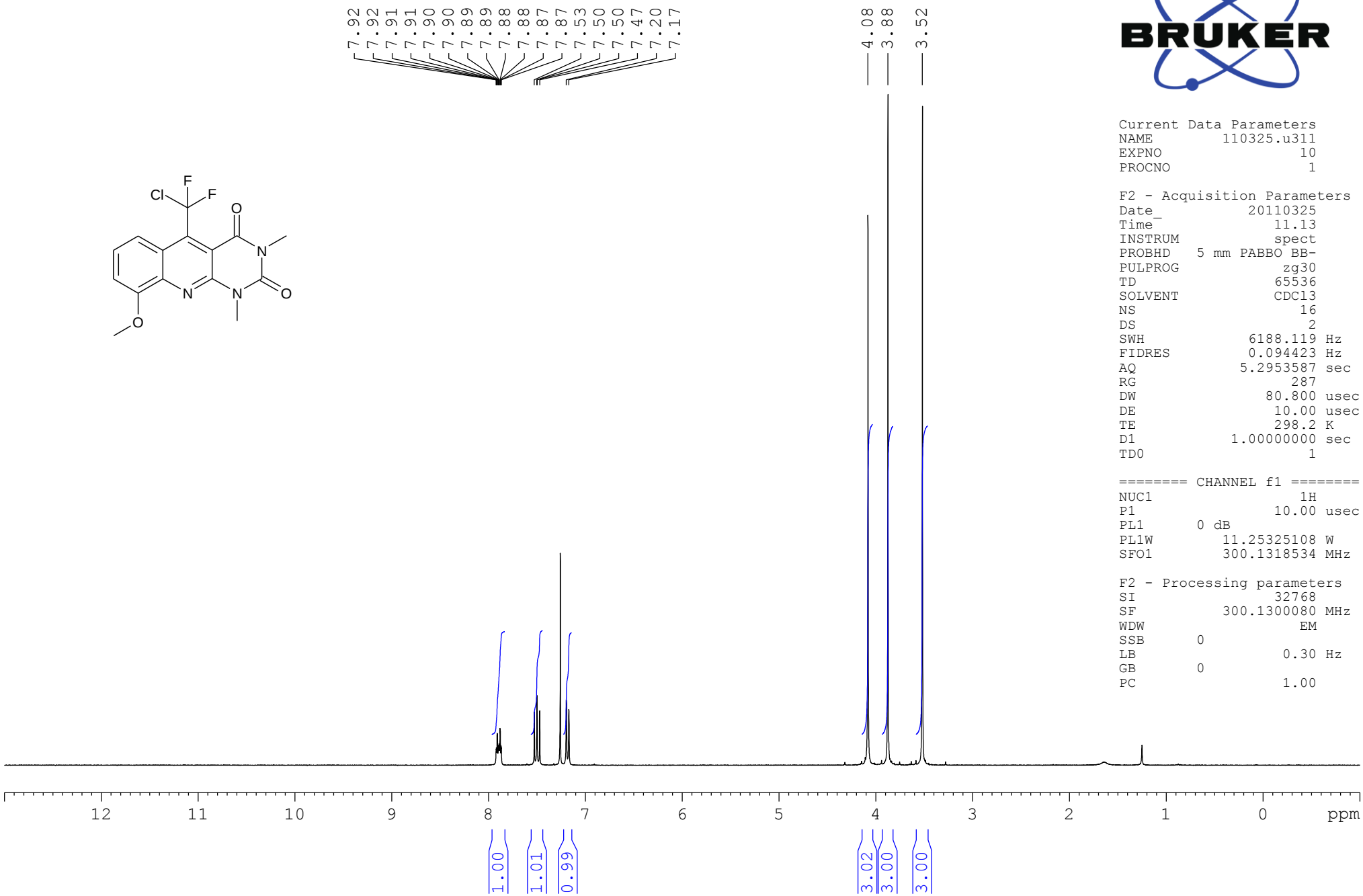
F2 - Acquisition Parameters
Date_ 20110403
Time 21.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.2 K
D1 4.00000000 sec
d11 0.03000000 sec
DELTA 3.90000010 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952178 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd194 1H CDCl3



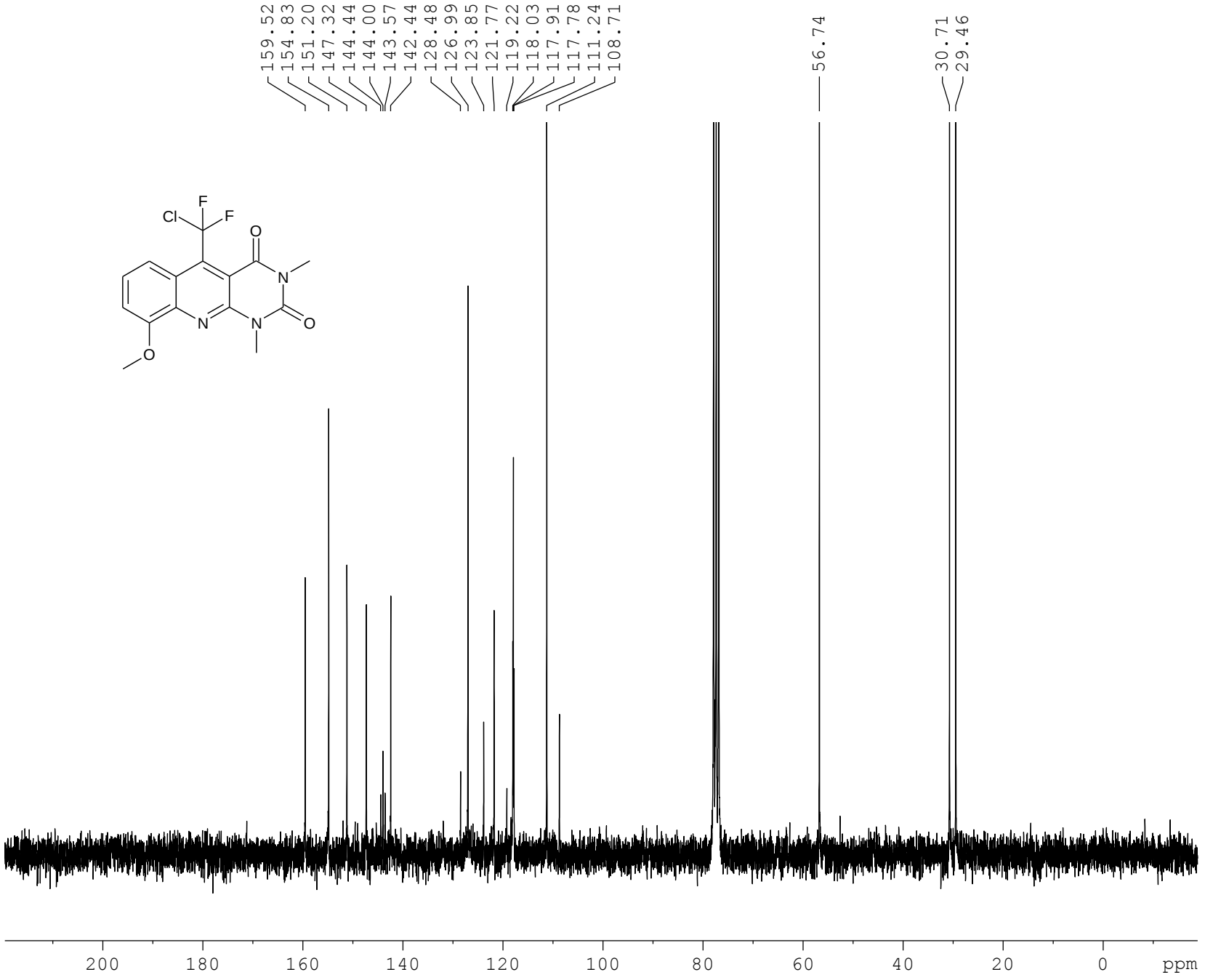

```
Current Data Parameters
NAME          110325.u311
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20110325
Time                11.13
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.094423 Hz
AQ               5.2953587 sec
RG                    287
DW                 80.800 usec
DE                 10.00 usec
TE                 298.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1       0 dB
PL1W         11.25325108 W
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF           300.1300080 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

Dudkin sd194 13C CDCl3



Current Data Parameters

NAME	110401.235
EXPNO	10
PROCNO	1

F2 - Acquisition Parameters

Date_	20110404
Time	0.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	1620
DW	33.333 usec
DE	10.00 usec
TE	298.1 K
D1	4.00000000 sec
d11	0.03000000 sec
DELTA	3.90000010 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz

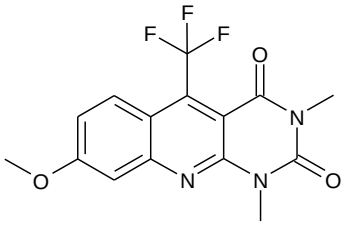
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz

F2 - Processing parameters

SI	32768
SF	62.8952180 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Dudkin sd216 1H CDCl3



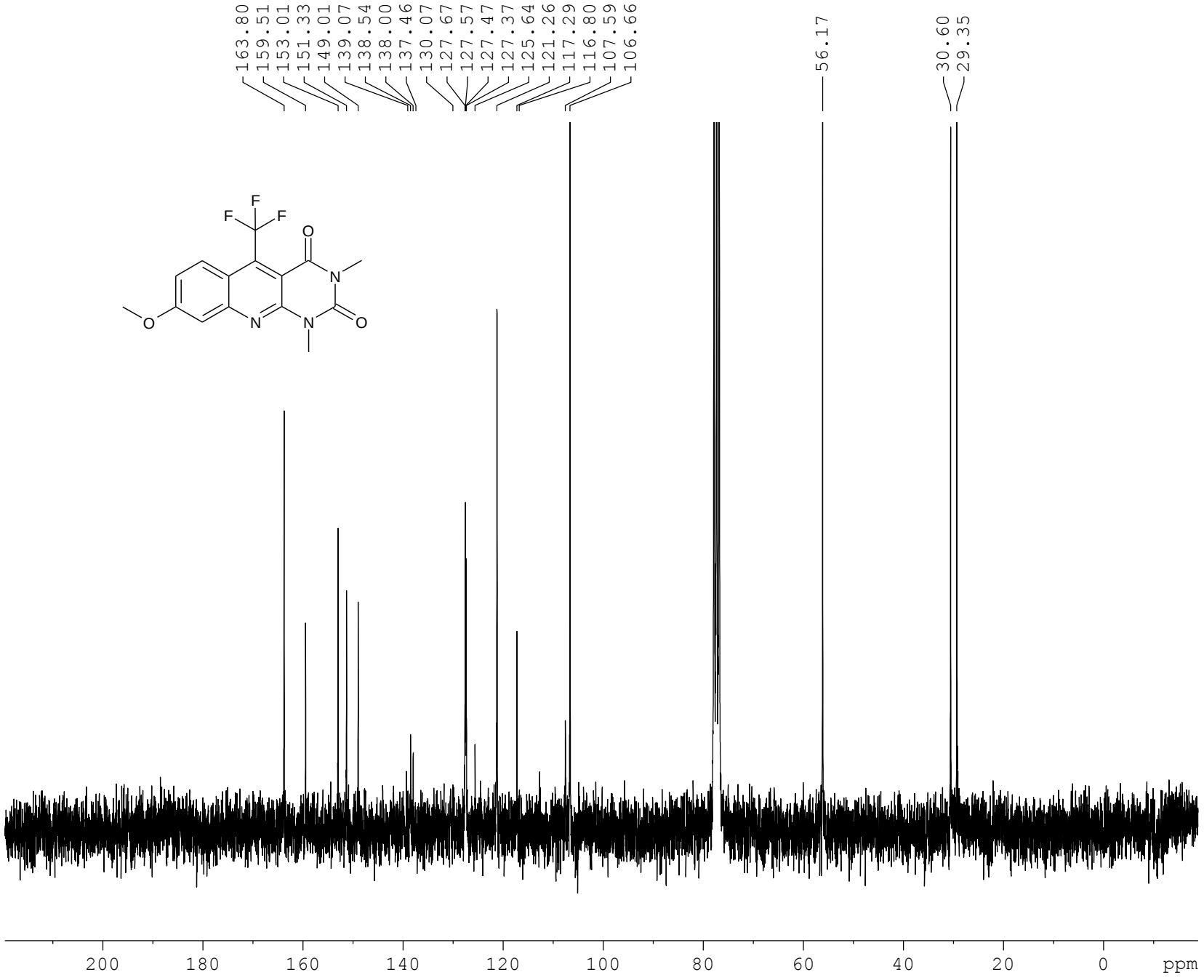

```
Current Data Parameters
NAME          110408.u302
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20110408
Time                9.02
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   181
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300081 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd216 13C CDCl3



Current Data Parameters

NAME	110411.207
EXPNO	10
PROCNO	1

F2 - Acquisition Parameters

Date_	20110412
Time	1.31
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2048
DS	4
SWH	15000.000 Hz
FIDRES	0.228882 Hz
AQ	2.1845834 sec
RG	1440
DW	33.333 usec
DE	10.00 usec
TE	298.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz

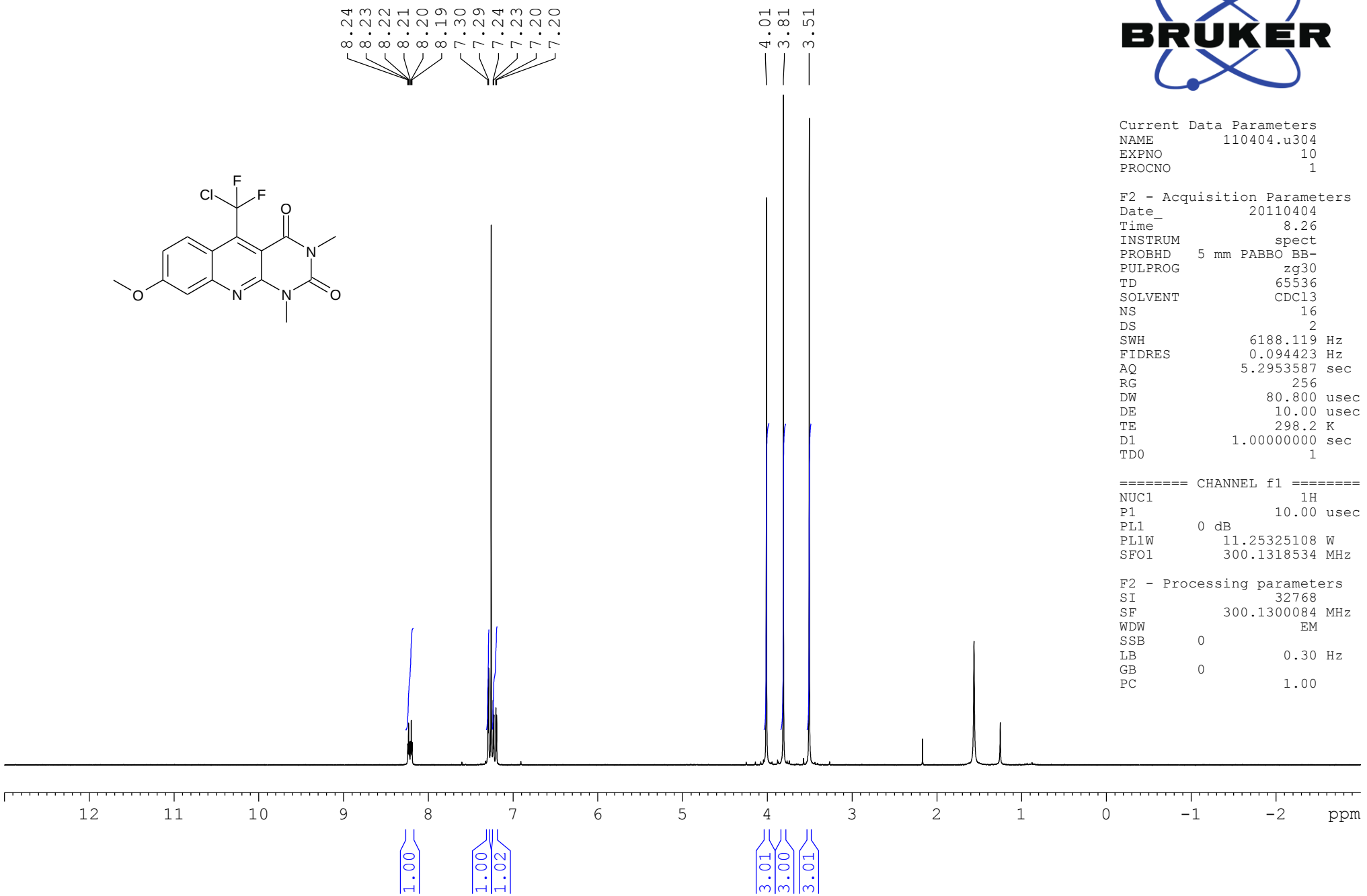
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz

F2 - Processing parameters

SI	32768
SF	62.8952162 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Dudkin sd212 1H CDCl3



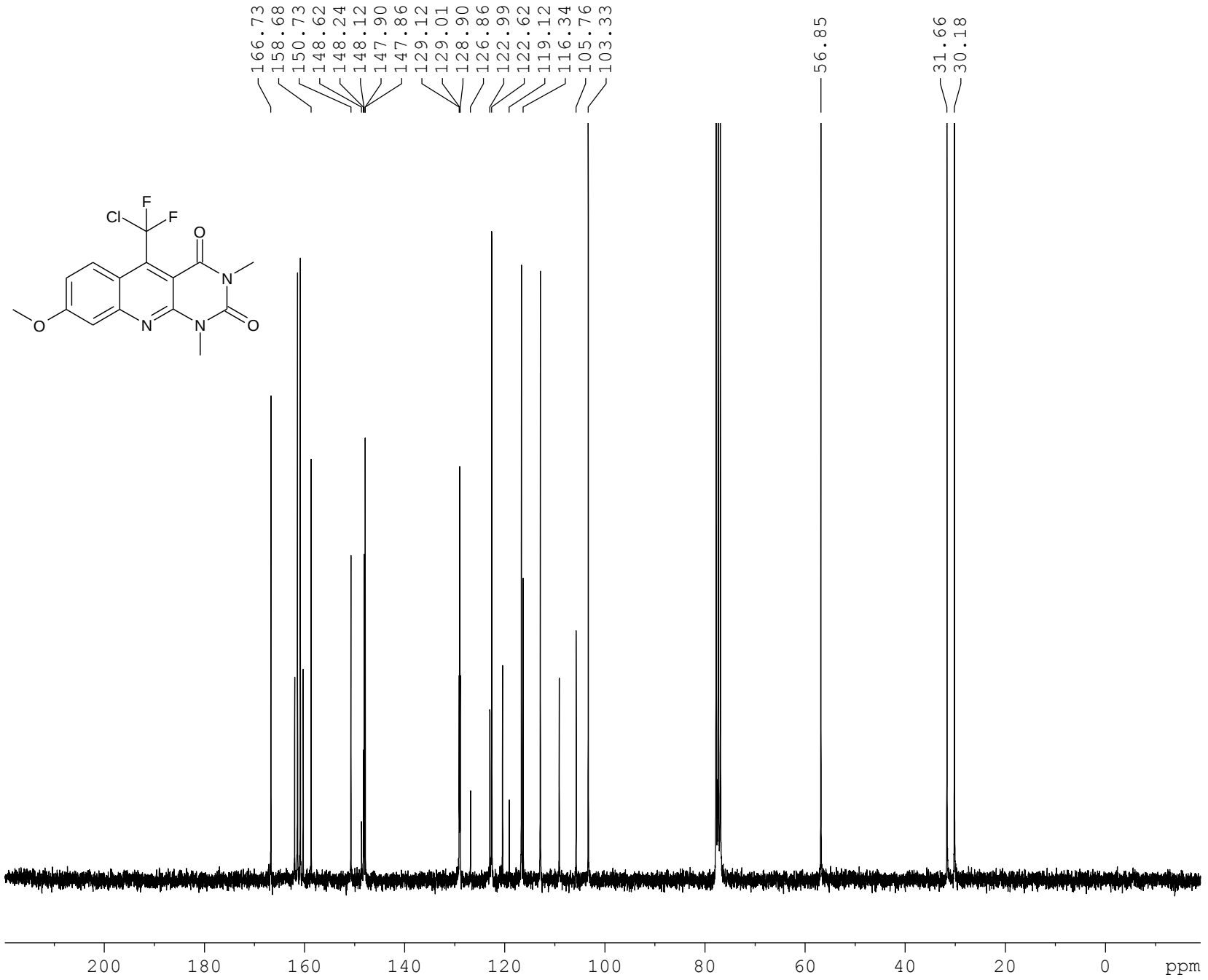
Current Data Parameters
NAME 110404.u304
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110404
Time 8.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 256
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd212 13C CDCl3/CF3COOD(12%)




```
Current Data Parameters
NAME         120425.u343
EXPNO                 10
PROCNO                 1

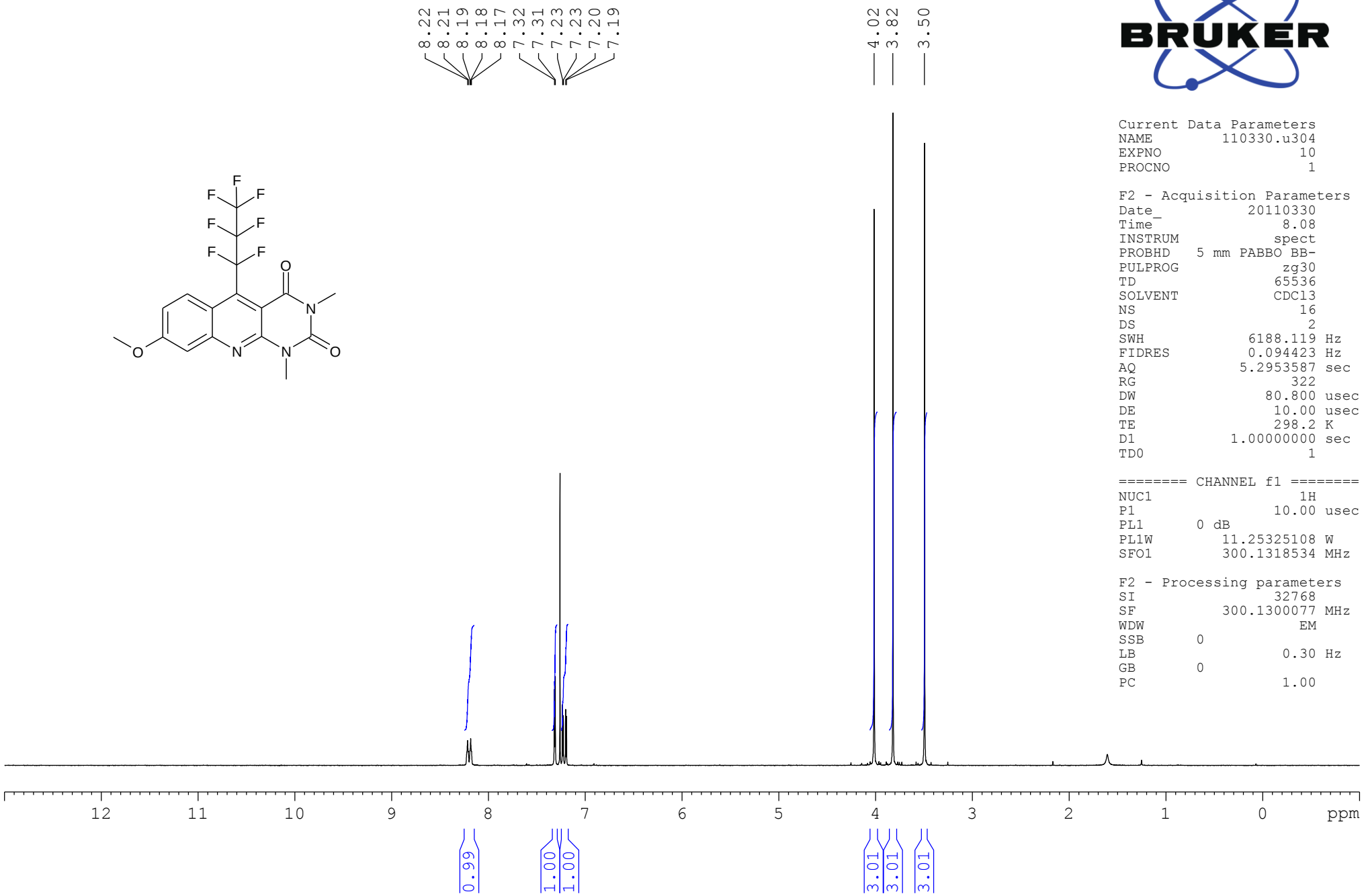
F2 - Acquisition Parameters
Date_           20120425
Time                19.32
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  3072
DS                     4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                  2050
DW                27.733 usec
DE                10.00 usec
TE                298.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              72.00 usec
PL2       0 dB
PL12               17.00 dB
PL13               17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677171 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Dudkin sd206 1H CDCl3



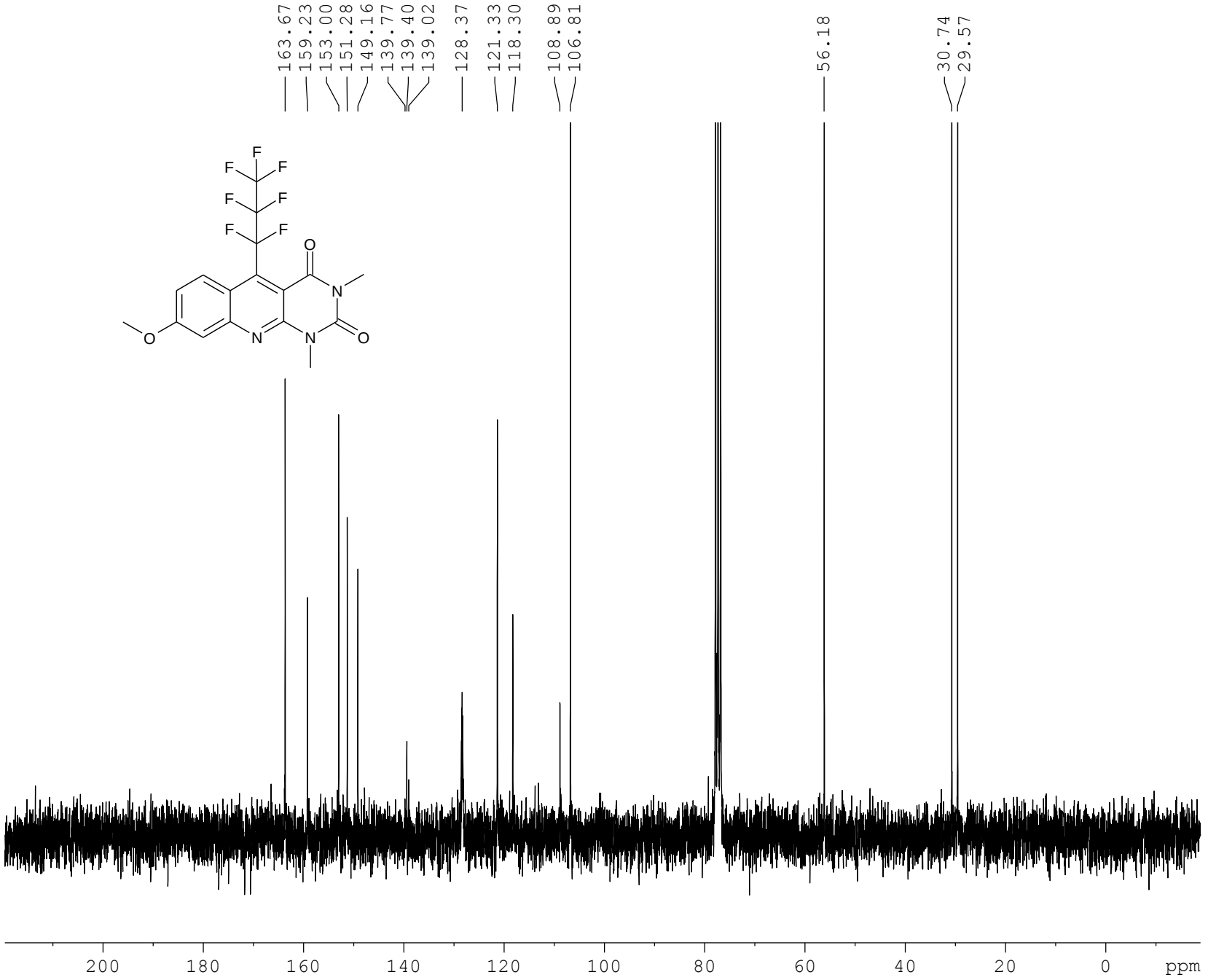

```
Current Data Parameters
NAME         110330.u304
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110330
Time               8.08
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6188.119 Hz
FIDRES         0.094423 Hz
AQ             5.2953587 sec
RG                  322
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300077 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd206 13C CDCl3




```
Current Data Parameters
NAME          110401.240
EXPNO                 10
PROCNO                 1

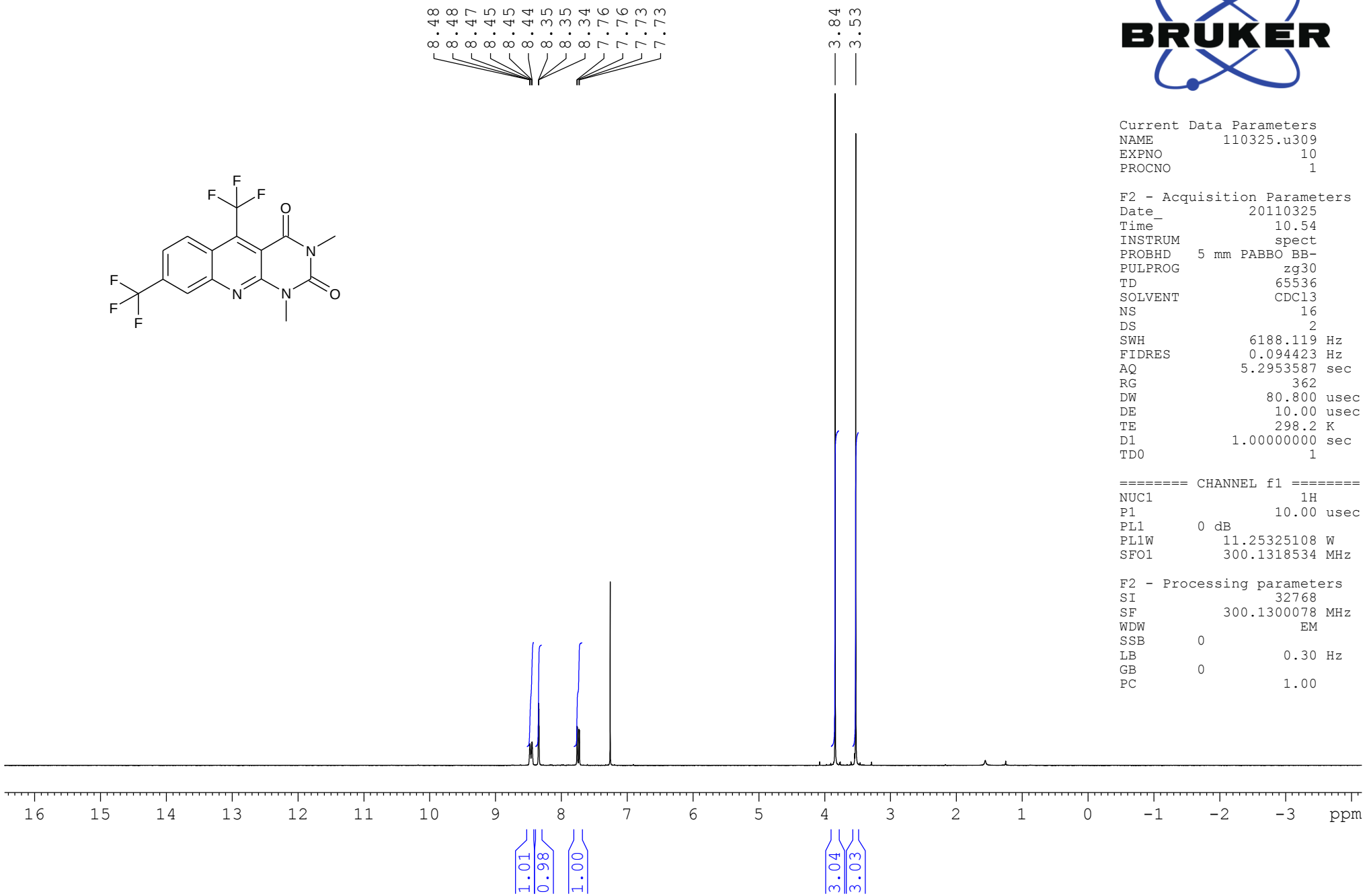
F2 - Acquisition Parameters
Date_           20110404
Time               9.45
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.2 K
D1           4.00000000 sec
d11          0.03000000 sec
DELTA        3.90000010 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF          62.8952157 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd192 1H CDCl3



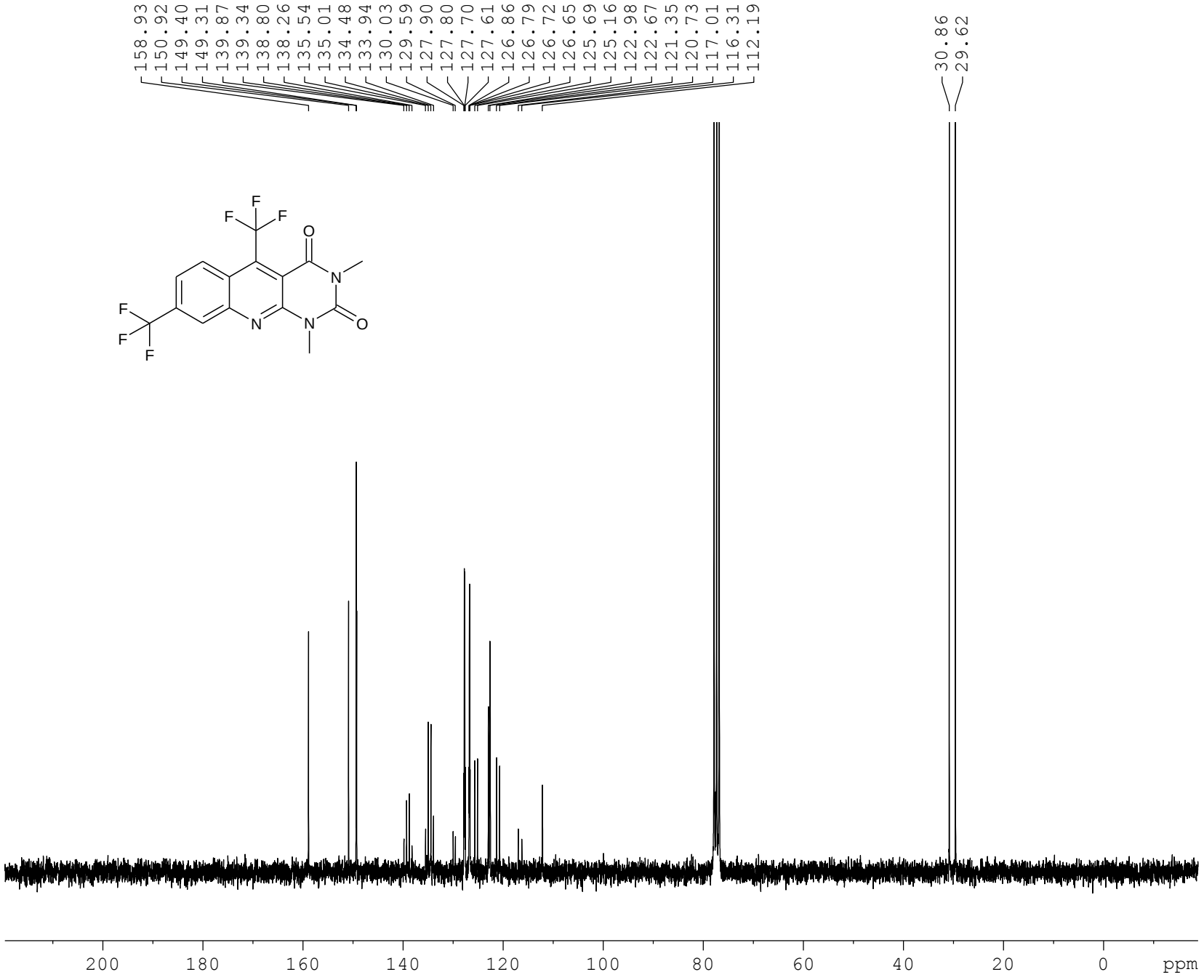
Current Data Parameters
NAME 110325.u309
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110325
Time 10.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 362
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd192 13C CDCl3



Current Data Parameters
NAME 110401.233
EXPNO 10
PROCNO 1

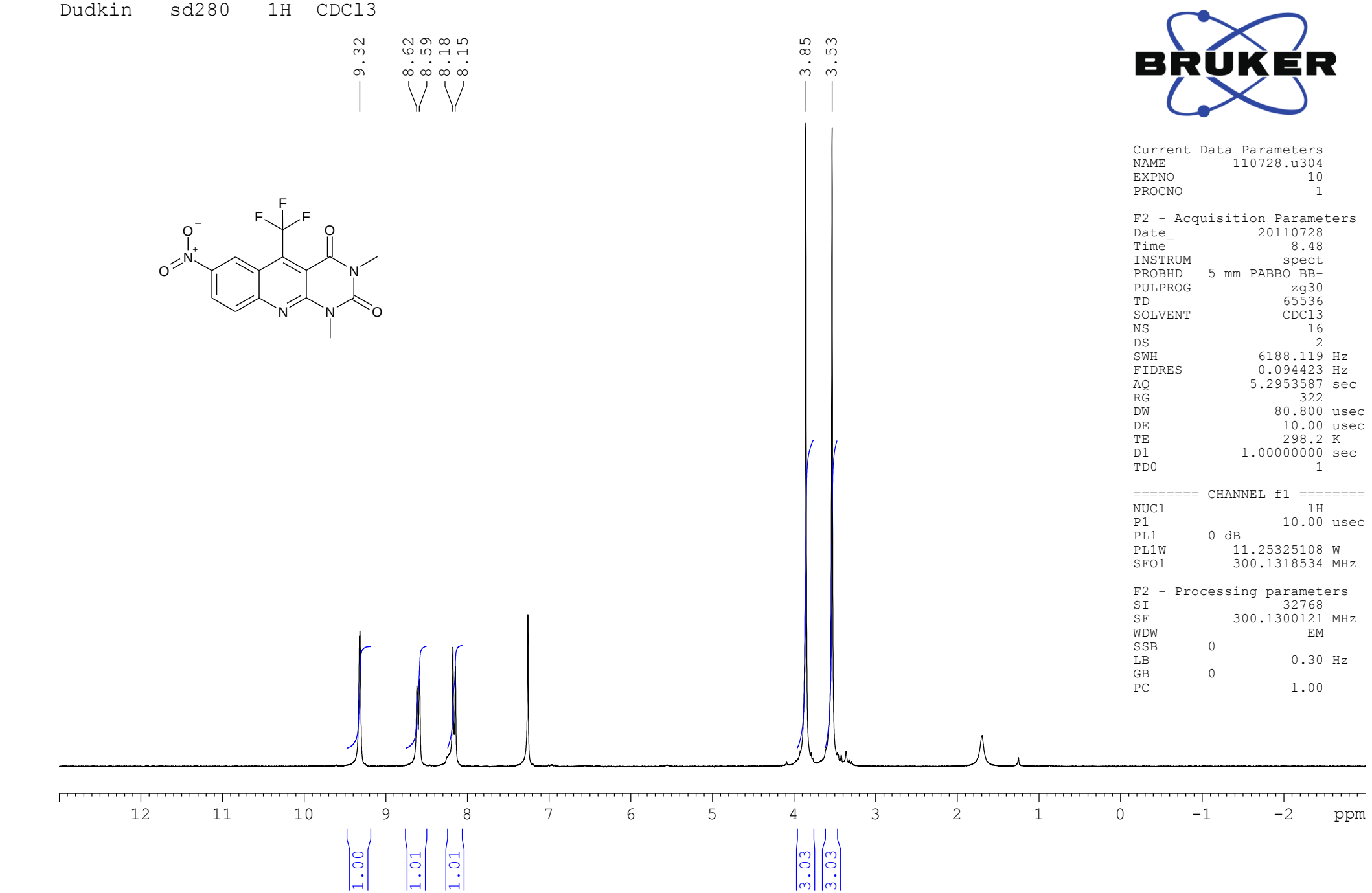
F2 - Acquisition Parameters
Date_ 20110403
Time 19.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.4 K
D1 4.00000000 sec
d11 0.03000000 sec
DELTA 3.90000010 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952160 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd280 1H CDCl3



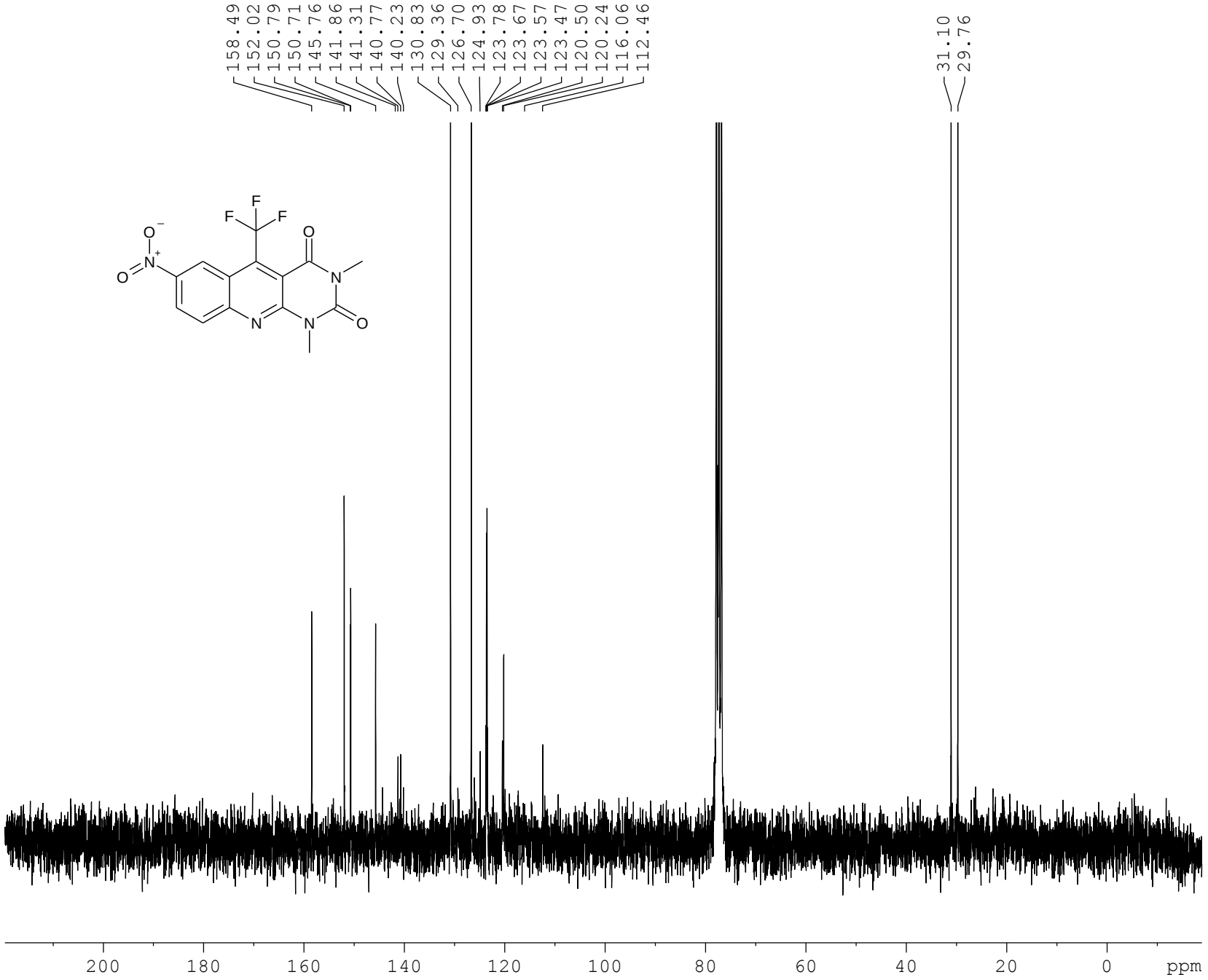
Current Data Parameters
NAME 110728.u304
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110728
Time 8.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 322
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd280 13C CDCl3




```
Current Data Parameters
NAME          110801.202
EXPNO                 10
PROCNO                 1

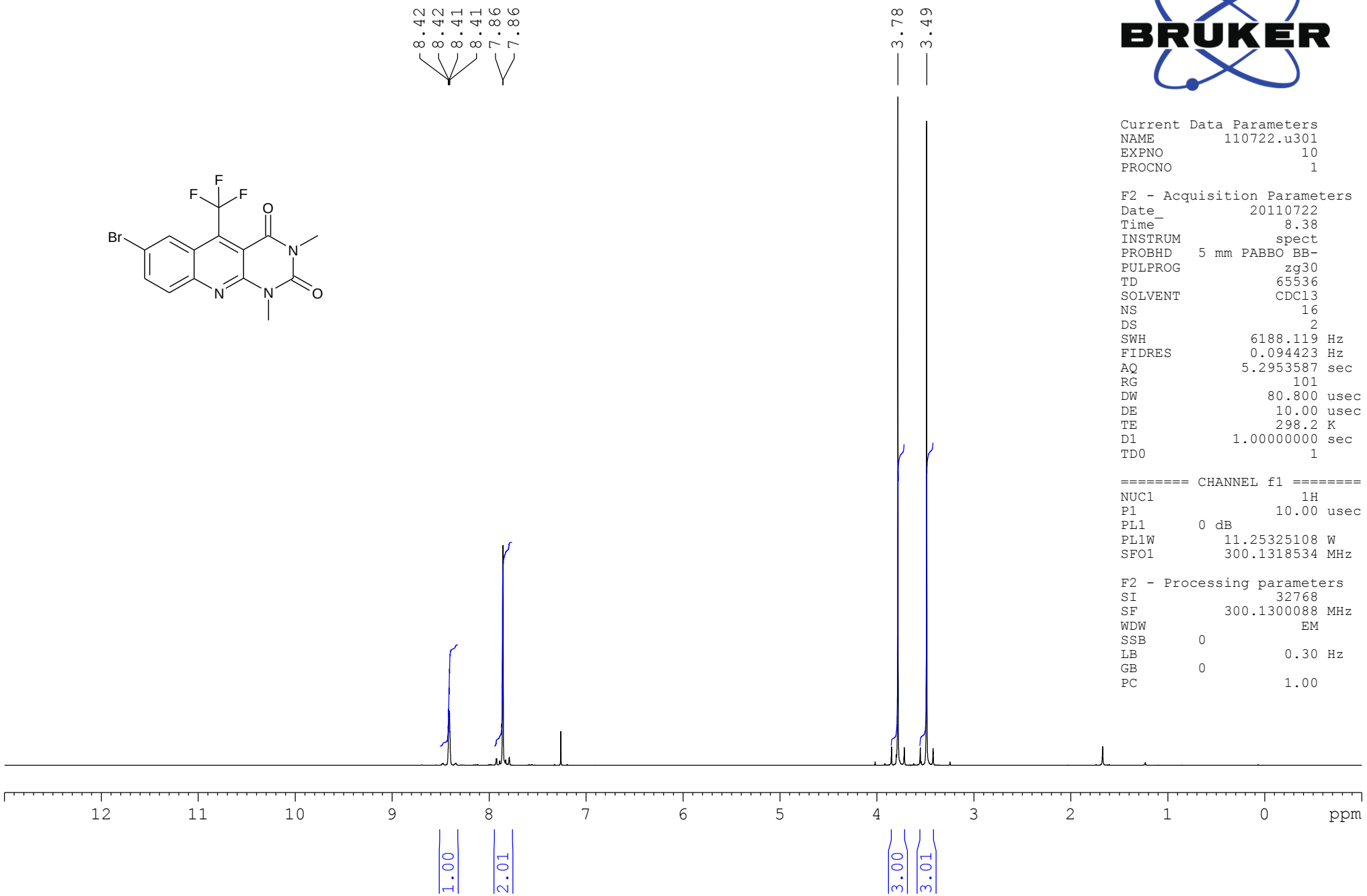
F2 - Acquisition Parameters
Date_          20110802
Time               0.26
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                 4096
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.1 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952159 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd276 1H CDCl3



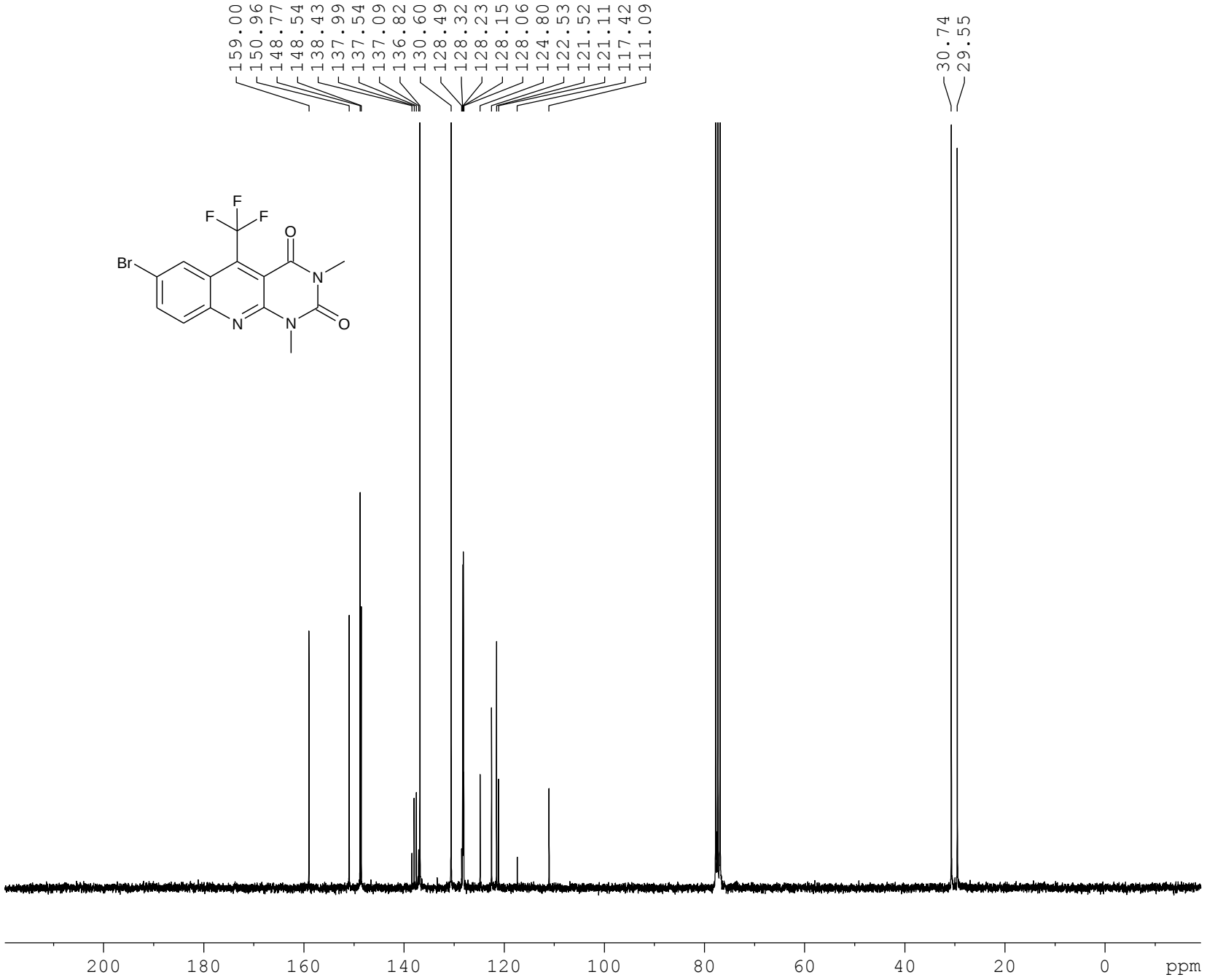
Current Data Parameters
NAME 110722.u301
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110722
Time 8.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 101
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd276 13C CDCl3




```
Current Data Parameters
NAME         110722.u301
EXPNO                 13
PROCNO                 1

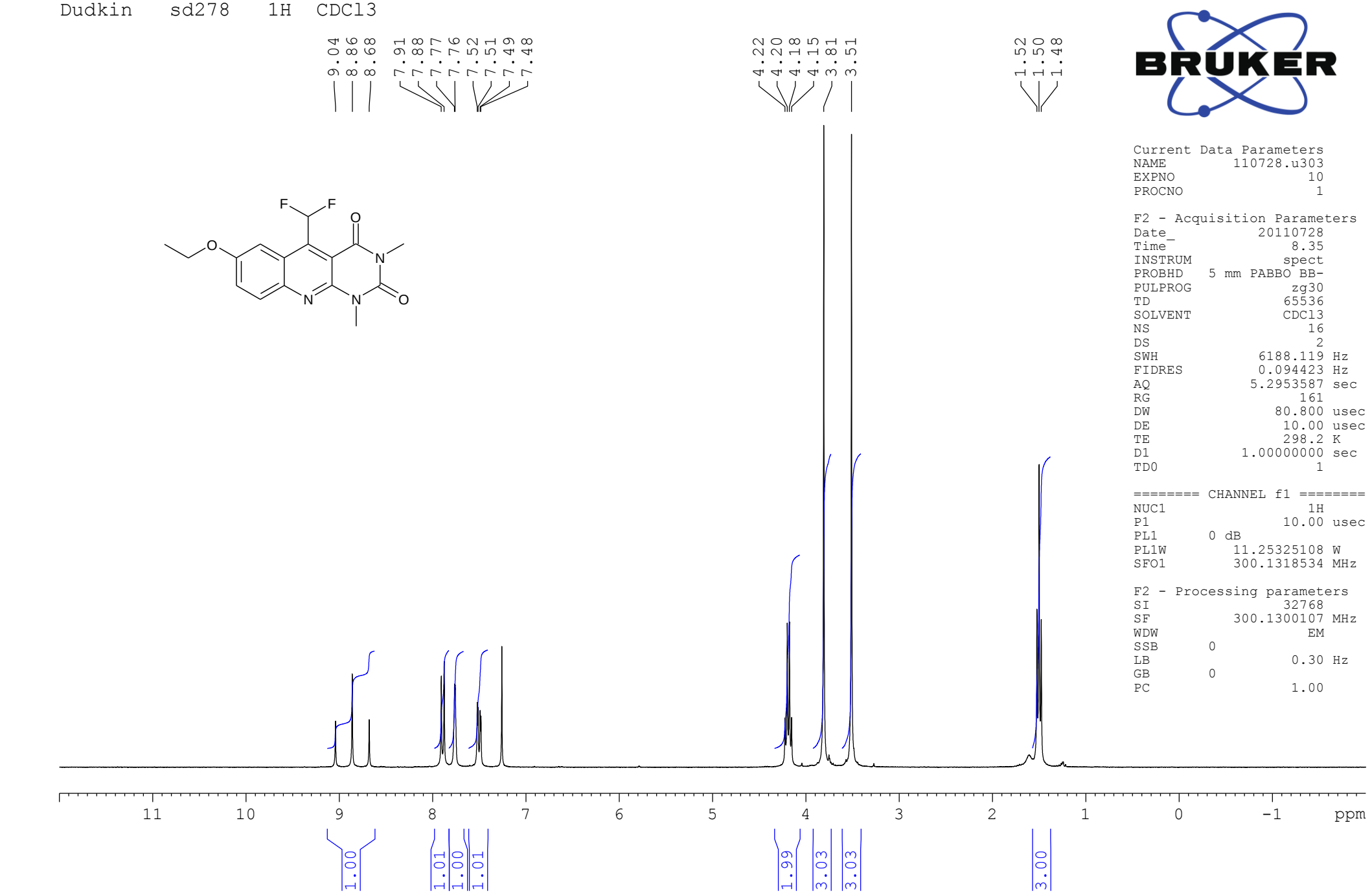
F2 - Acquisition Parameters
Date_           20110722
Time              18.30
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                 2050
DW               27.733 usec
DE               10.00 usec
TE               298.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             72.00 usec
PL2       0 dB
PL12              17.00 dB
PL13              17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677254 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd278 1H CDCl3



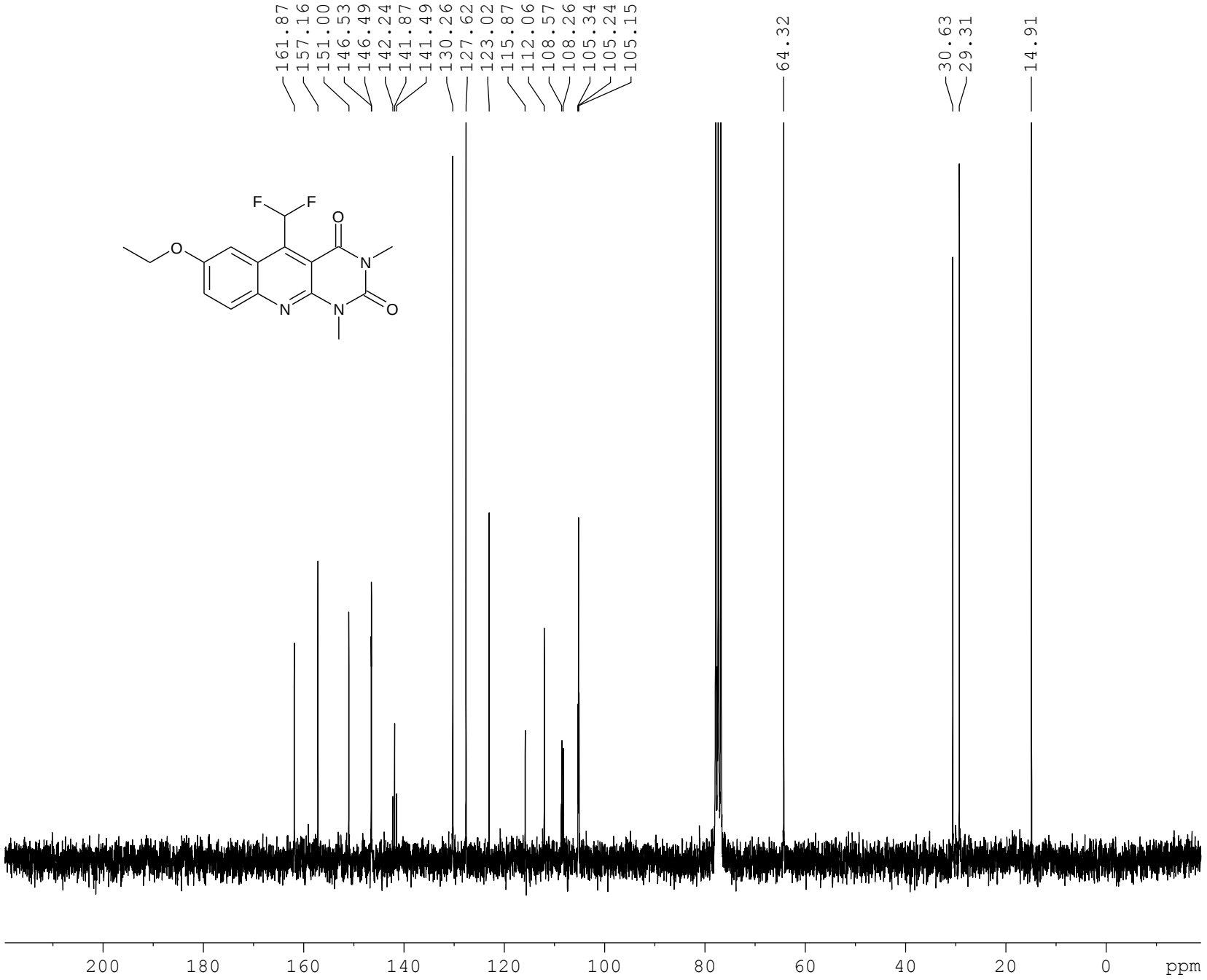
Current Data Parameters
NAME 110728.u303
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110728
Time 8.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 161
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300107 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd278 13C CDCl3




```
Current Data Parameters
NAME          110801.201
EXPNO                 10
PROCNO                 1

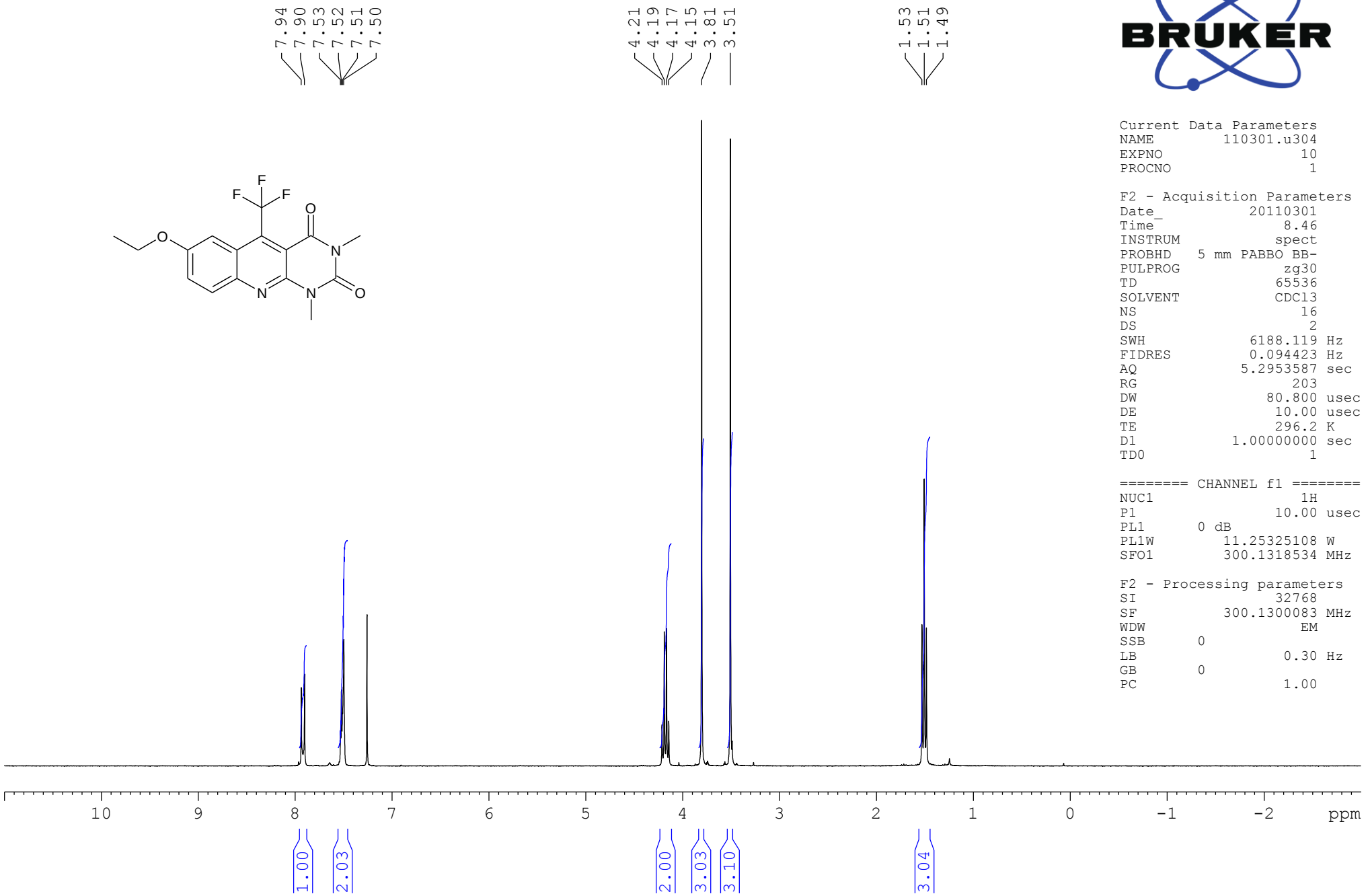
F2 - Acquisition Parameters
Date_           20110801
Time               12.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                299.5 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952157 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd184 1H CDCl3



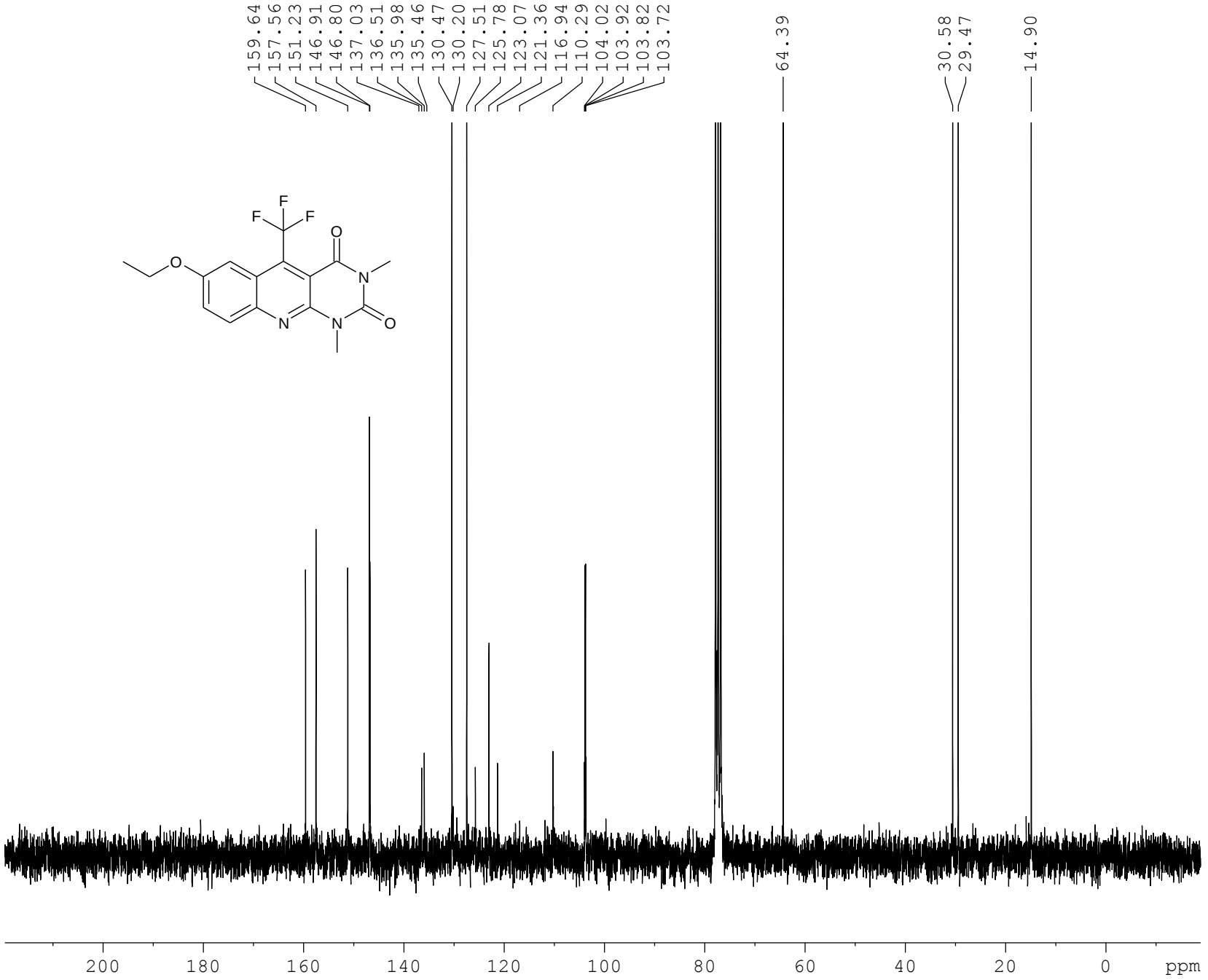
Current Data Parameters
NAME 110301.u304
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110301
Time 8.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 203
DW 80.800 usec
DE 10.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300083 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd184 13C CDCl3



Current Data Parameters
NAME 110318.215
EXPNO 10
PROCNO 1

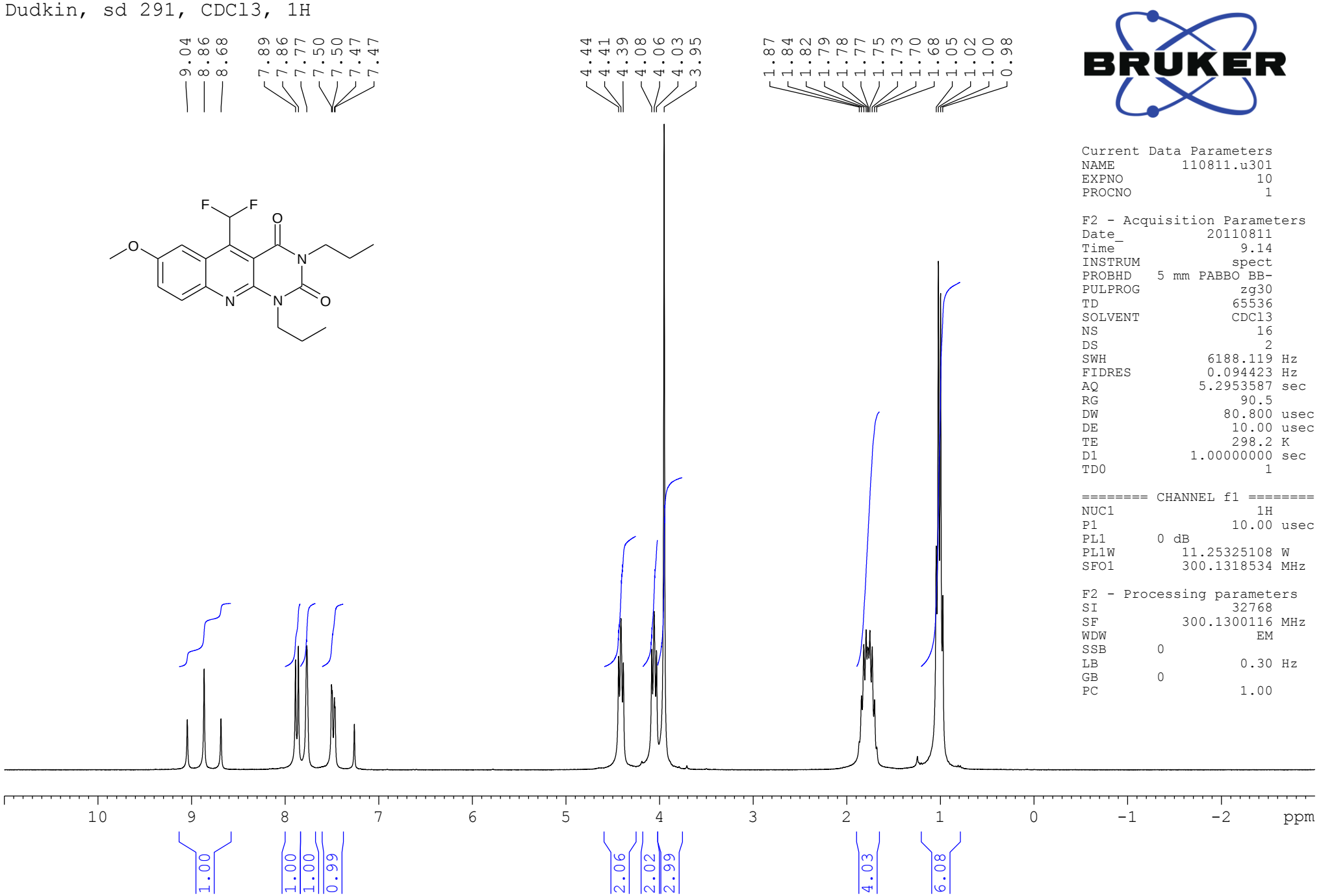
F2 - Acquisition Parameters
Date_ 20110319
Time 7.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.7 K
D1 5.00000000 sec
d11 0.03000000 sec
DELTA 4.90000010 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952162 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin, sd 291, CDCl3, 1H



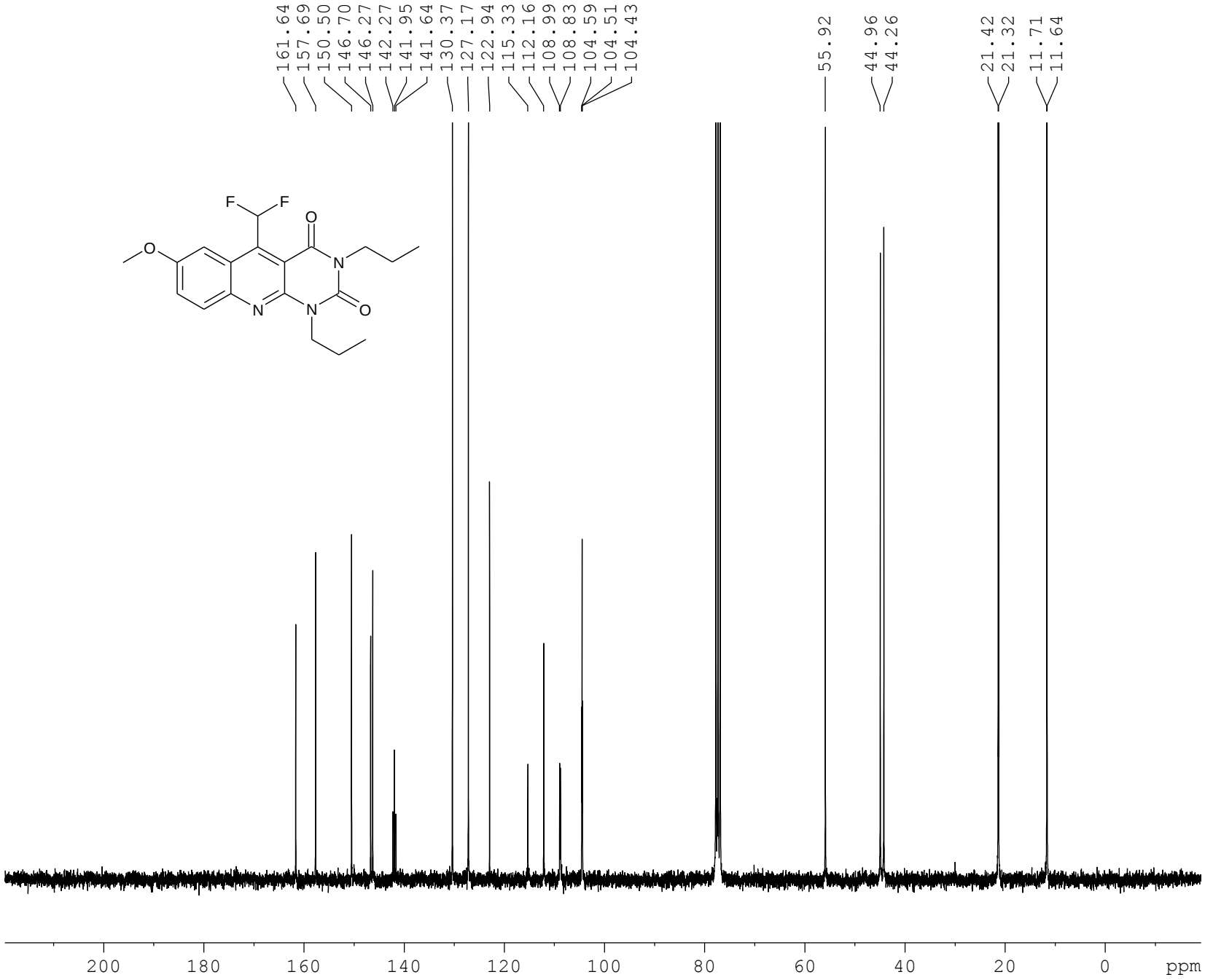
Current Data Parameters
NAME 110811.u301
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110811
Time 9.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 90.5
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin, sd 291, CDCl3, 13C




```
Current Data Parameters
NAME          110811.u301
EXPNO                  12
PROCNO                  1

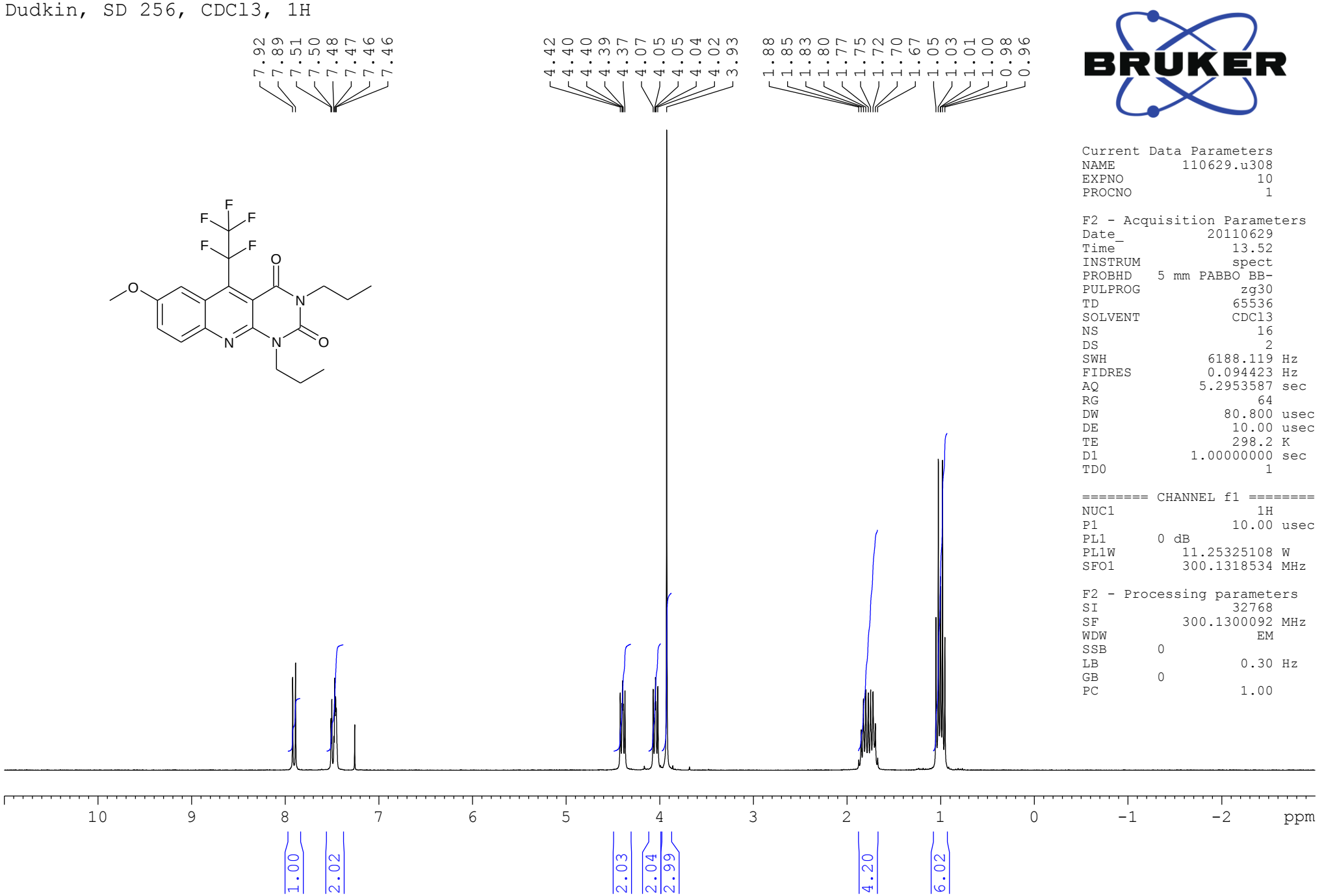
F2 - Acquisition Parameters
Date_            20110812
Time                 0.31
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   2500
DS                      4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                   2050
DW               27.733 usec
DE               10.00 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                10.00 usec
PL1               -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             72.00 usec
PL2       0 dB
PL12              17.00 dB
PL13              17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677245 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin, SD 256, CDCl3, 1H



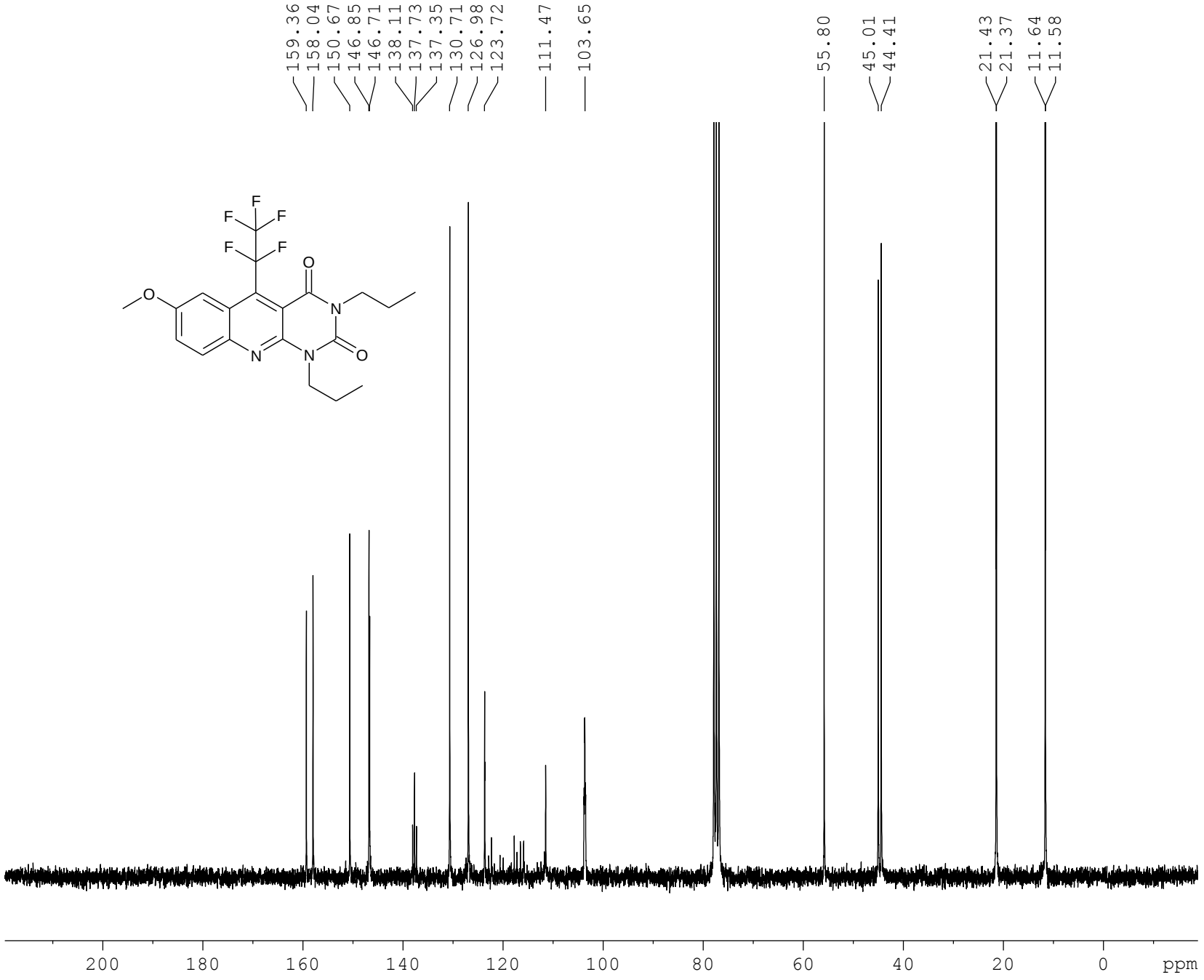

```
Current Data Parameters
NAME          110629.u308
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20110629
Time                13.52
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.094423 Hz
AQ               5.2953587 sec
RG                     64
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1        0 dB
PL1W         11.25325108 W
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF           300.1300092 MHz
WDW                    EM
SSB        0
LB                  0.30 Hz
GB         0
PC                  1.00
```

Dudkin, sd 256, CDCl3, 13C




```
Current Data Parameters
NAME          110630.206
EXPNO                 10
PROCNO                 1

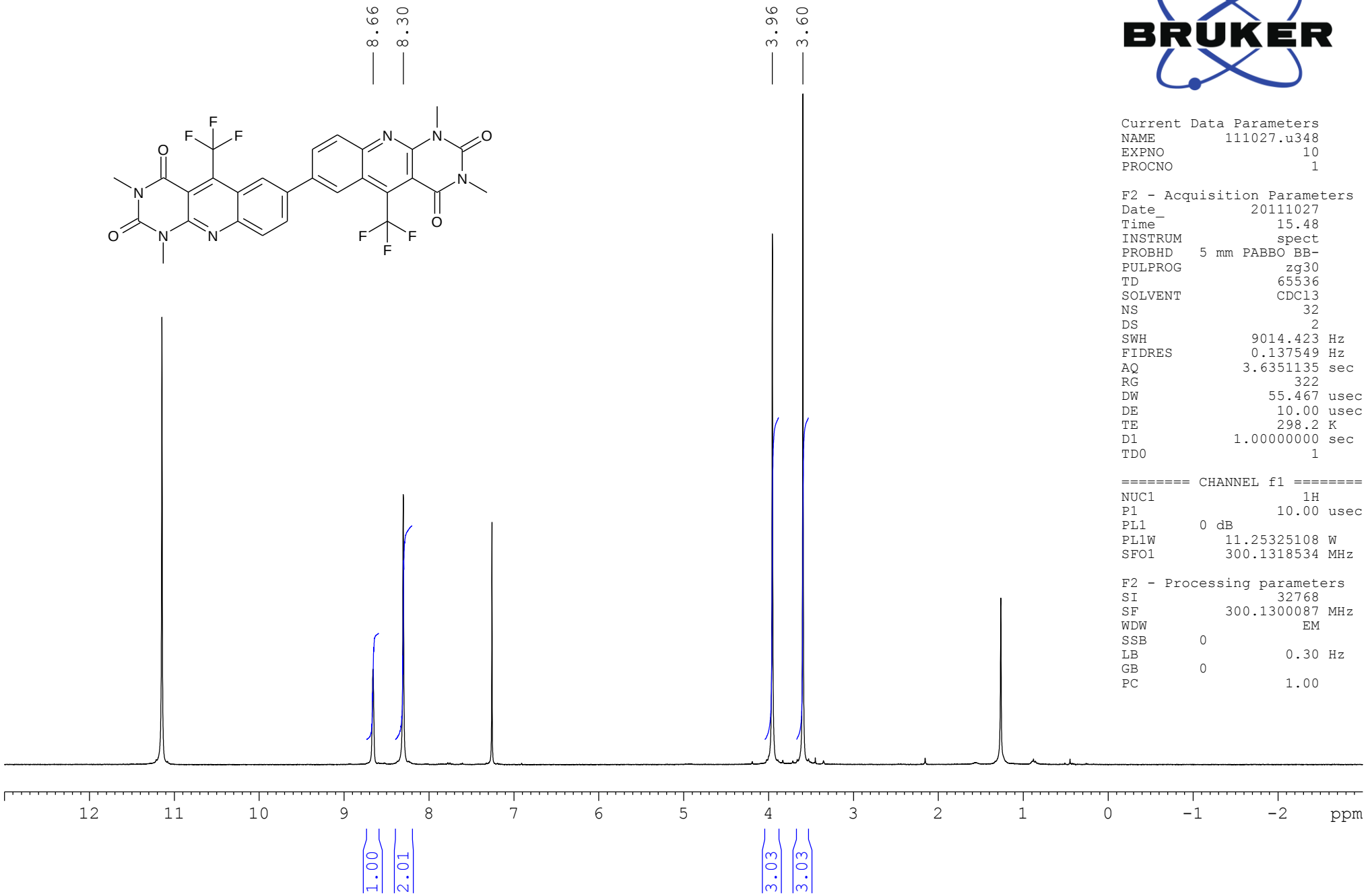
F2 - Acquisition Parameters
Date_           20110630
Time              21.38
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2500
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE               10.00 usec
TE               299.7 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952157 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd337 1H CDCl3/CF3COOD 12%



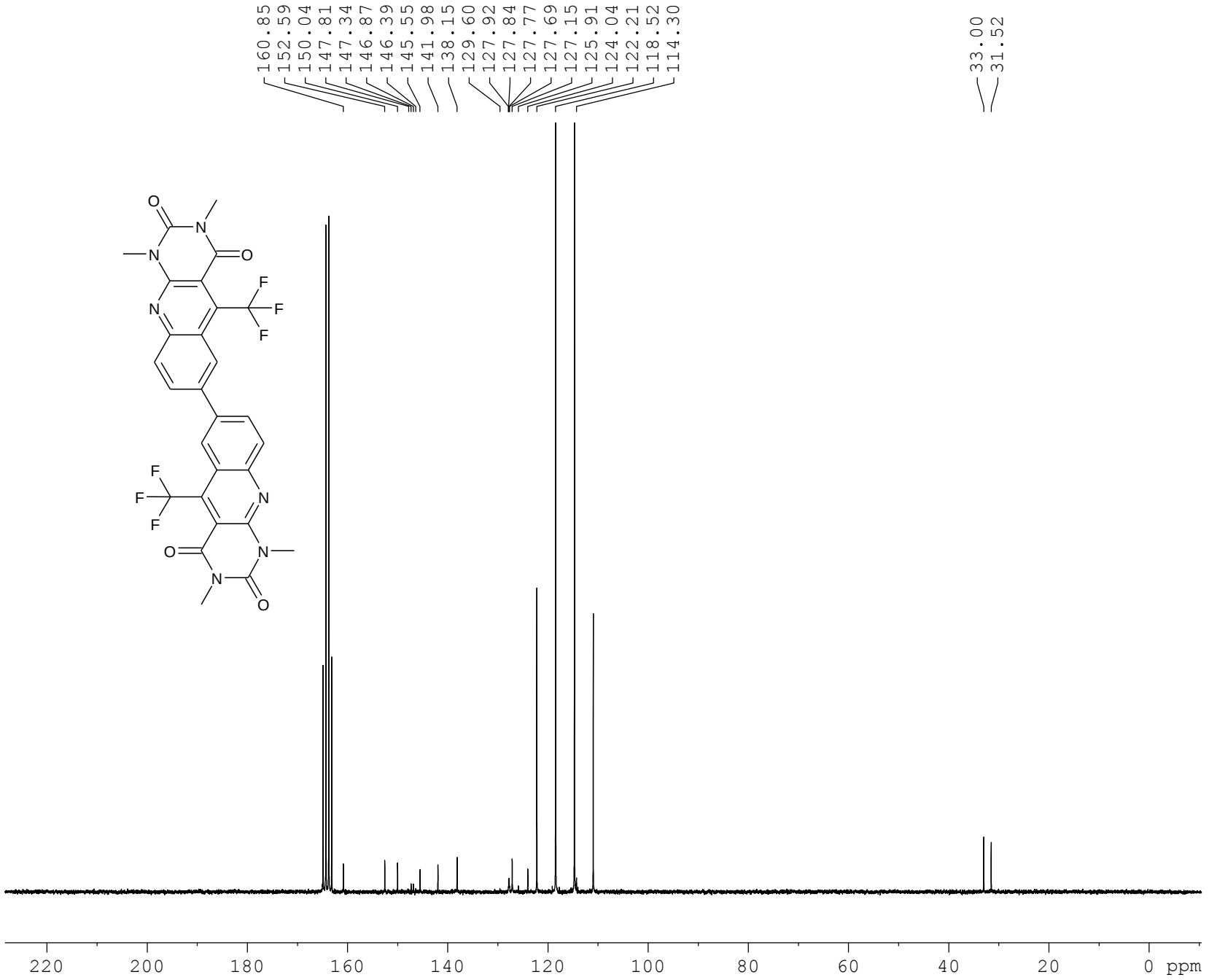

```
Current Data Parameters
NAME         111027.u348
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20111027
Time              15.48
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH            9014.423 Hz
FIDRES         0.137549 Hz
AQ            3.6351135 sec
RG                  322
DW               55.467 usec
DE               10.00 usec
TE               298.2 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1               10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300087 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Dudkin sd337 13C CF3COOD gem.auf D2O



Current Data Parameters
NAME 120615.u311
EXPNO 12
PROCNO 1

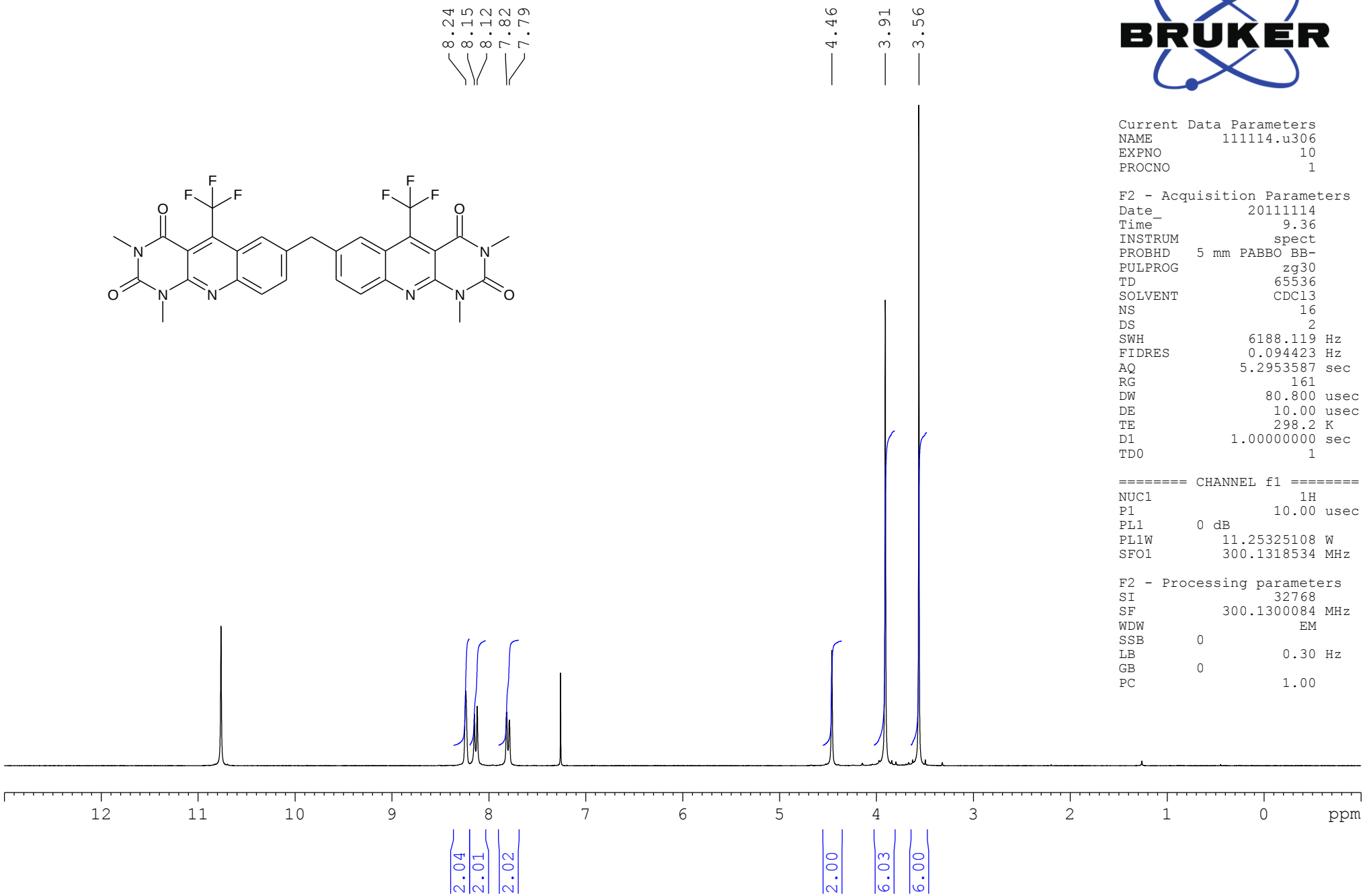
F2 - Acquisition Parameters
Date_ 20120616
Time 11.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4670728 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd219 1H CDCl3 + 12%CF3COOD



Current Data Parameters
NAME 111114.u306
EXPNO 10
PROCNO 1

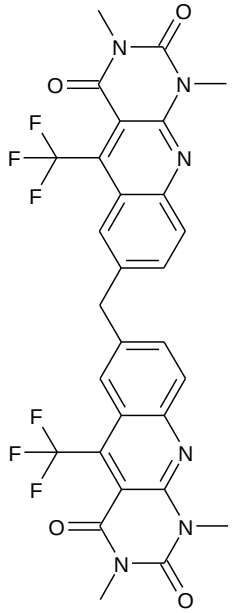
F2 - Acquisition Parameters
Date_ 20111114
Time 9.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 161
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd219 13C CDCl3+12%CF3COOD

160.16
152.17
149.15
147.67
140.30
139.81
139.78
139.28
138.74
136.02
129.68
129.44
125.78
125.68
125.59
125.49
125.24
122.37
120.82
116.39
110.21
42.82
31.28
30.06



Current Data Parameters
NAME 111118.208
EXPNO 10
PROCNO 1

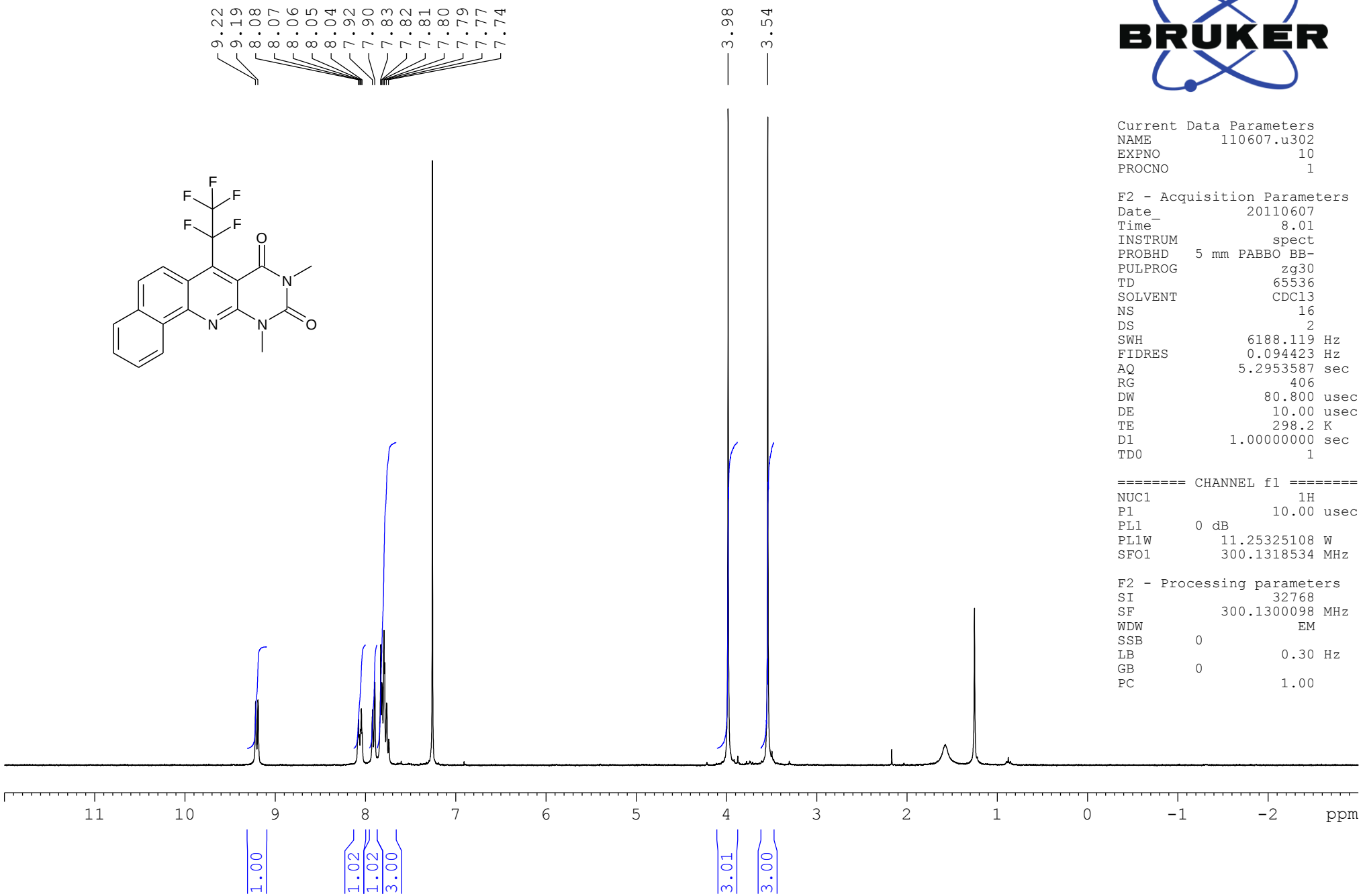
F2 - Acquisition Parameters
Date_ 20111119
Time 11.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952115 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd250 1H CDCl3



Current Data Parameters
NAME 110607.u302
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110607
Time 8.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 406
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

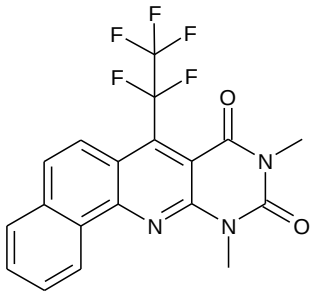
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd250 13C CDCl3/CF3COOD(12%)

160.29
152.50
150.65
147.64
139.82
139.44
139.05
134.66
131.67
130.13
129.69
128.49
128.23
126.47
122.19
122.00
109.45

31.24
30.13



BRUKER

```
Current Data Parameters
NAME          120427.218
EXPNO                 10
PROCNO                 1

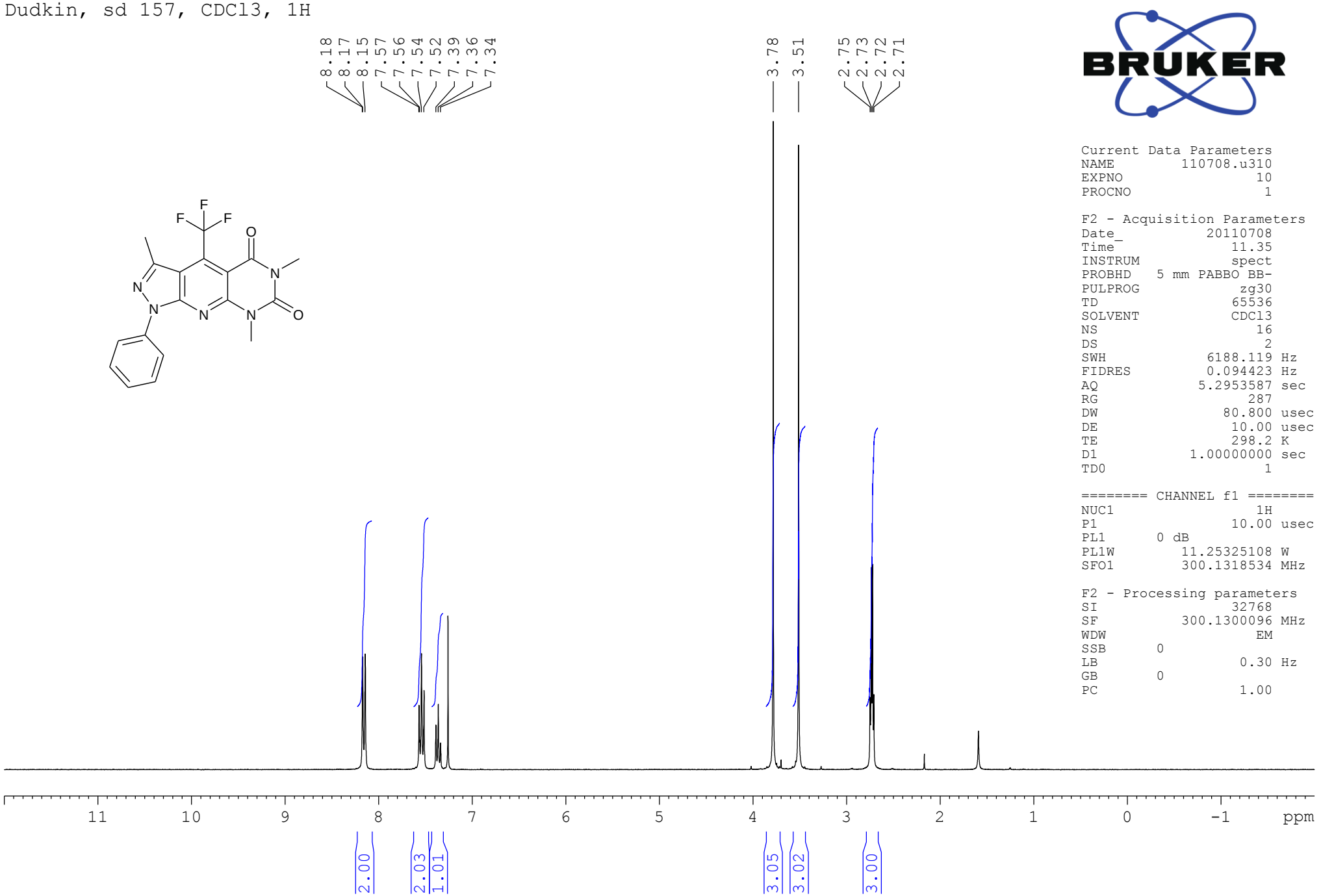
F2 - Acquisition Parameters
Date_           20120428
Time               19.56
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           15000.000 Hz
FIDRES            0.228882 Hz
AQ             2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                300.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952104 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin, sd 157, CDCl3, 1H



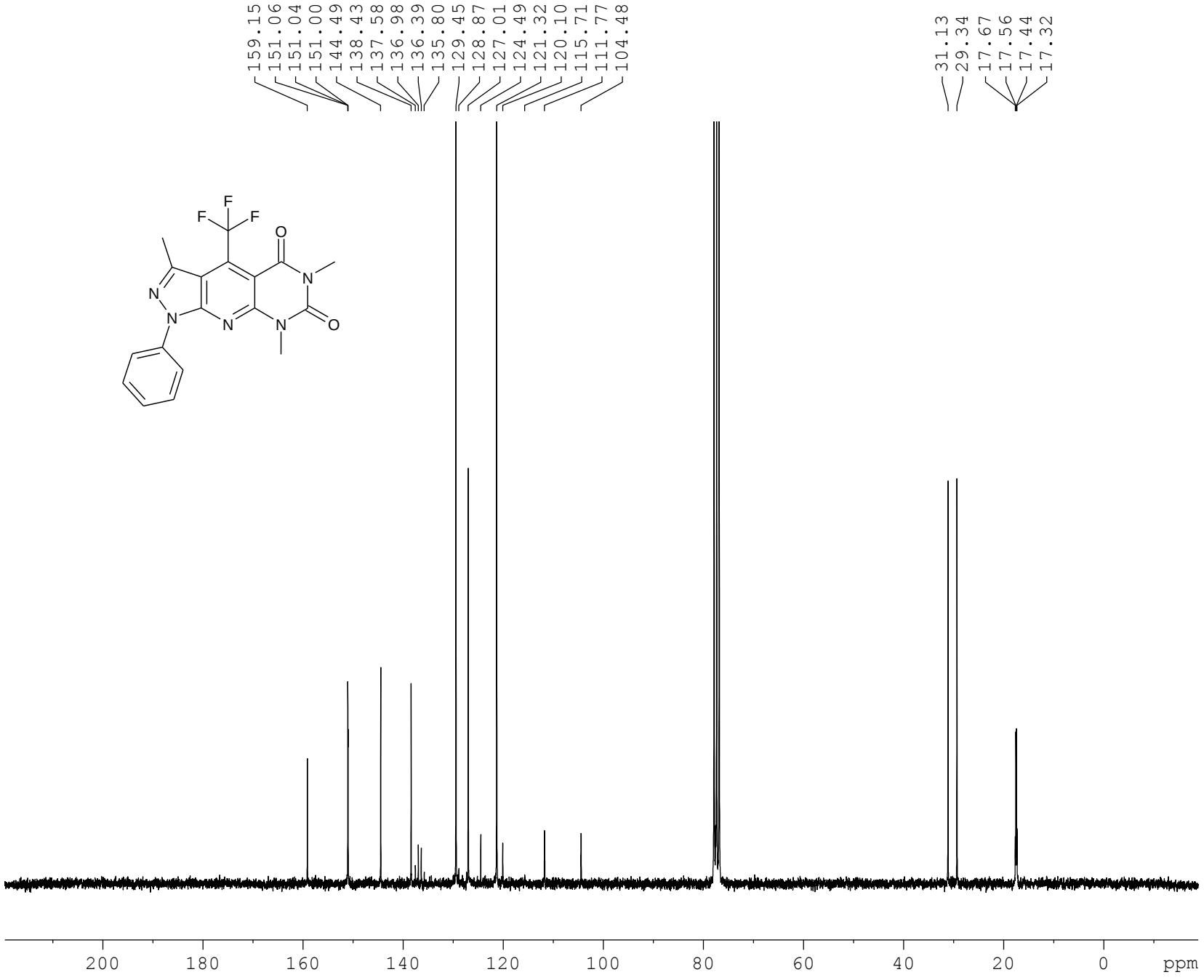
Current Data Parameters
NAME 110708.u310
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110708
Time 11.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 287
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd257 13C CDCl3



Current Data Parameters
NAME 110714.206
EXPNO 10
PROCNO 1

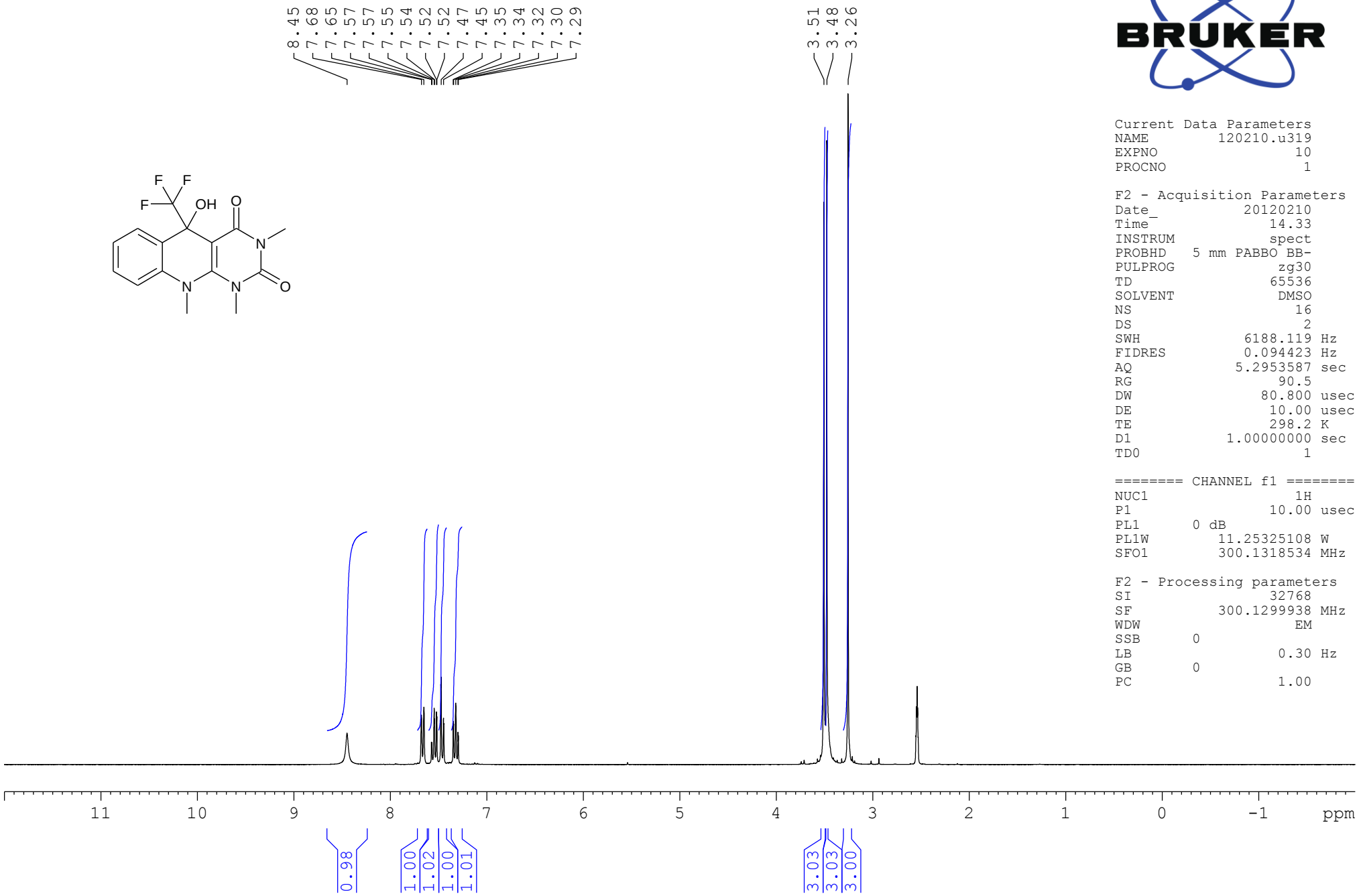
F2 - Acquisition Parameters
Date_ 20110715
Time 5.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5120
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 1290
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952175 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin, sd 367, DMSO, 1H



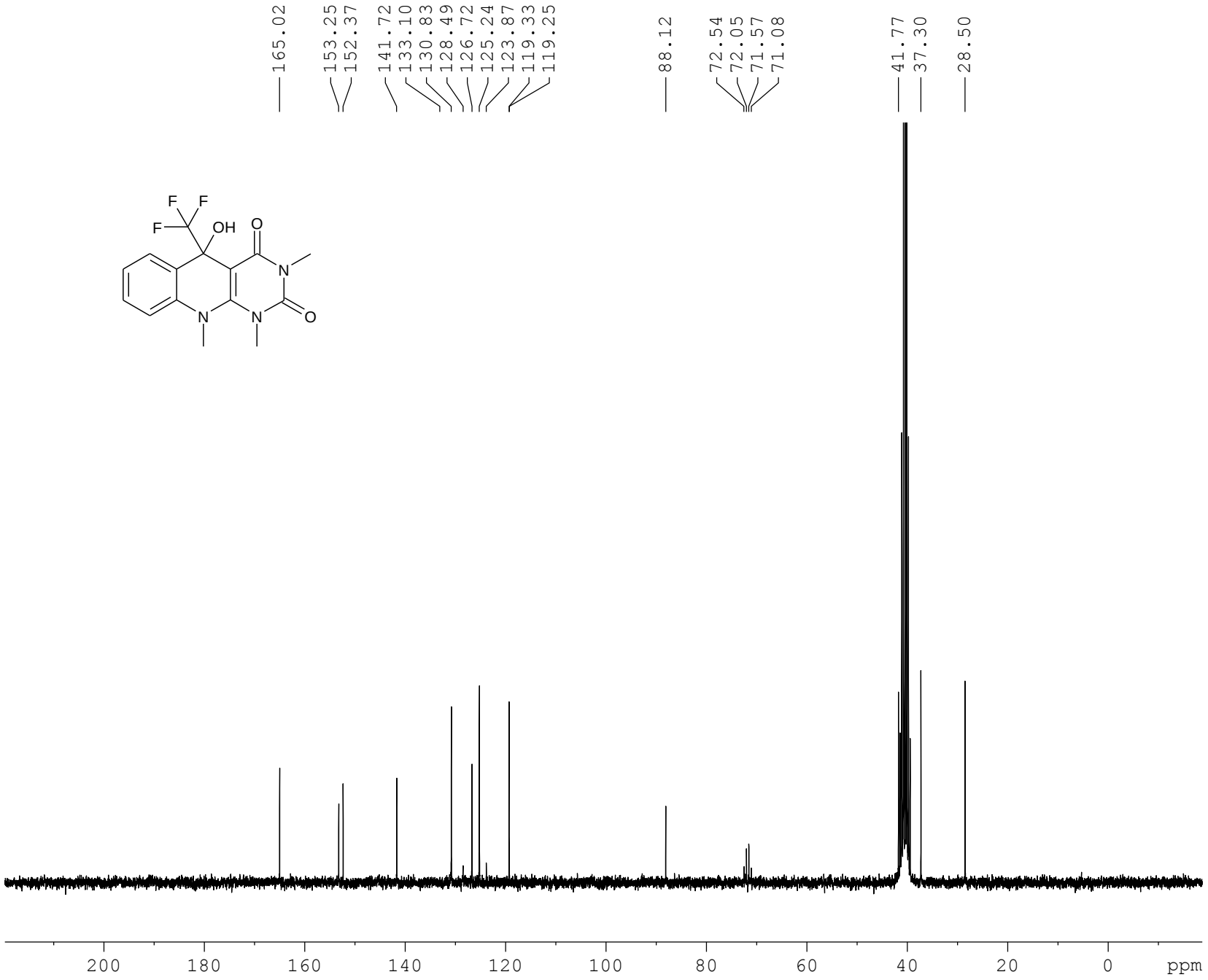

```
Current Data Parameters
NAME         120210.u319
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120210
Time               14.33
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                  90.5
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1299938 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Savych, IS-202.1, DMSO, 13C




```
Current Data Parameters
NAME          120215.203
EXPNO                 11
PROCNO                 1

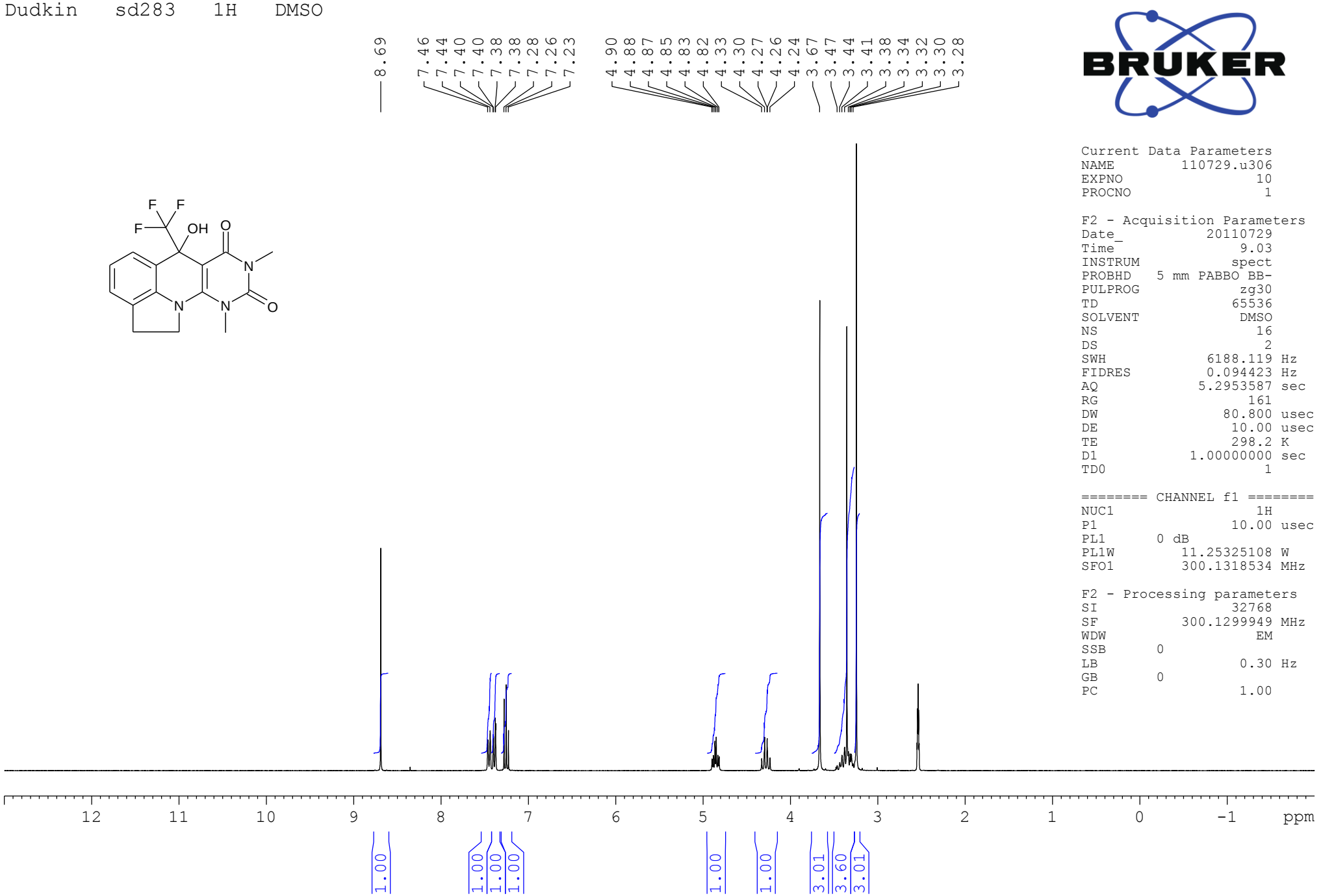
F2 - Acquisition Parameters
Date_           20120215
Time               15.28
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 1024
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1       0 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              14.00 dB
PL13              14.00 dB
PL2               -3.00 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952081 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd283 1H DMSO



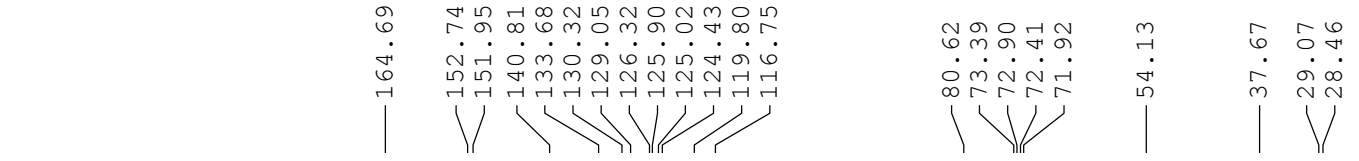

```
Current Data Parameters
NAME         110729.u306
EXPNO                 10
PROCNO                 1

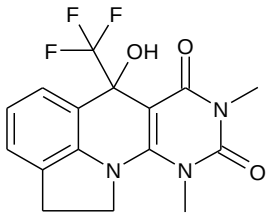
F2 - Acquisition Parameters
Date_           20110729
Time                9.03
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   161
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1299949 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd283 13C DMSO





Current Data Parameters
NAME 110801.203
EXPNO 10
PROCNO 1

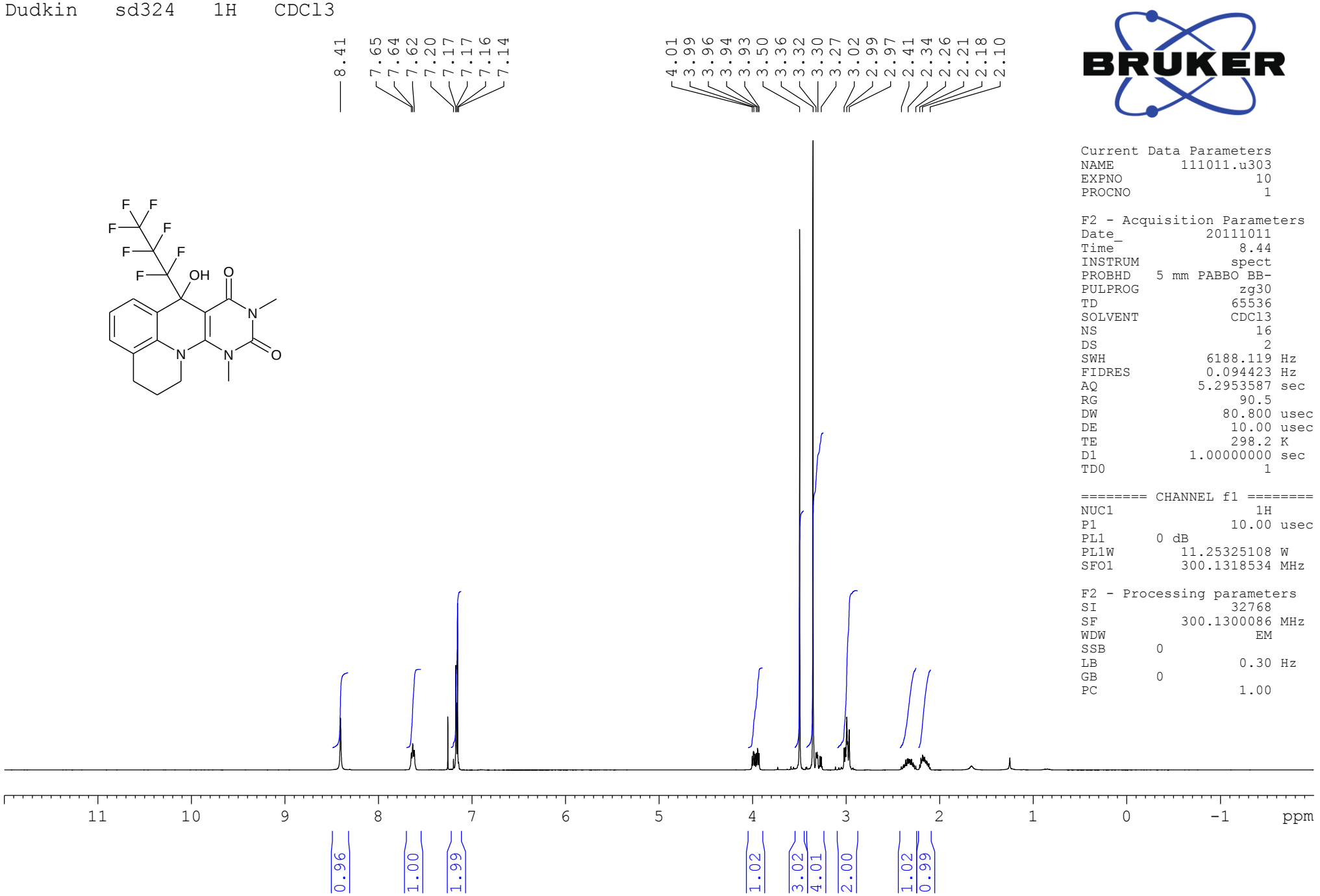
F2 - Acquisition Parameters
Date_ 20110801
Time 16.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952097 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd324 1H CDCl3



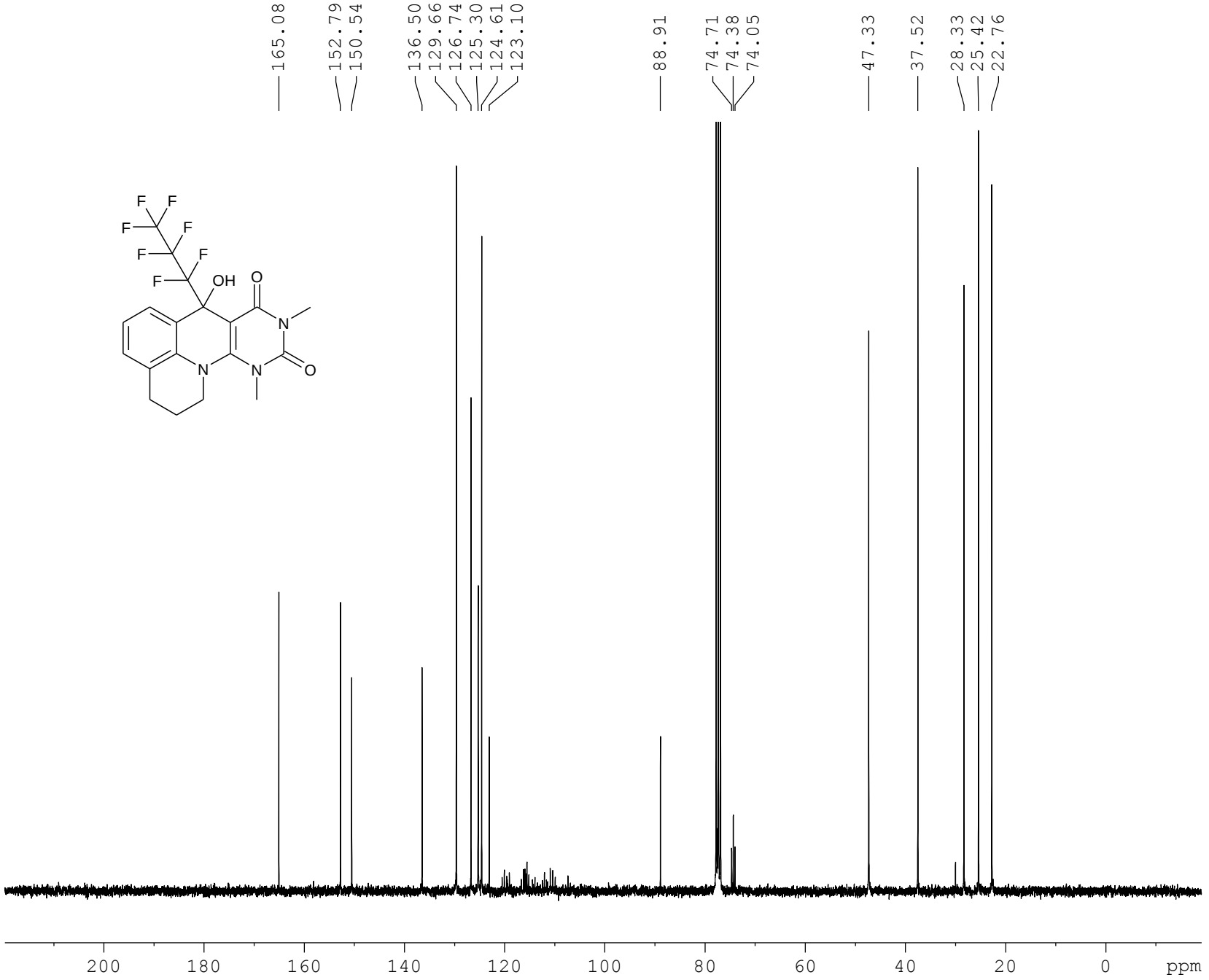

```
Current Data Parameters
NAME          111011.u303
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20111011
Time                8.44
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                  90.5
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300086 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd324 13C CDCl3




```
Current Data Parameters
NAME         111011.u303
EXPNO                 12
PROCNO                 1

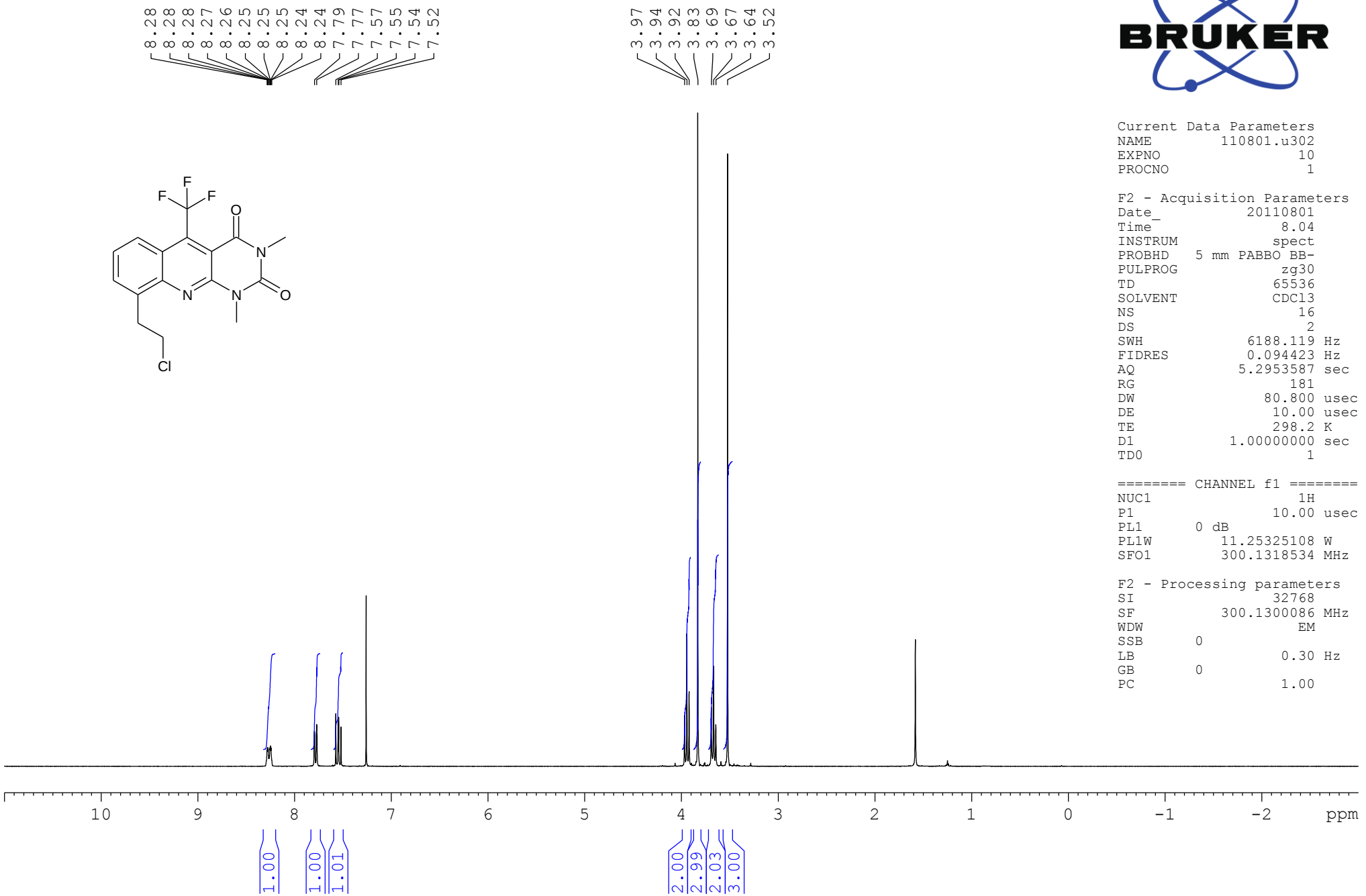
F2 - Acquisition Parameters
Date_           20111012
Time                4.16
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                 2050
DW               27.733 usec
DE               10.00 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                10.00 usec
PL1               -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             72.00 usec
PL2       0 dB
PL12              17.00 dB
PL13              17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677248 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd284 1H CDCl3



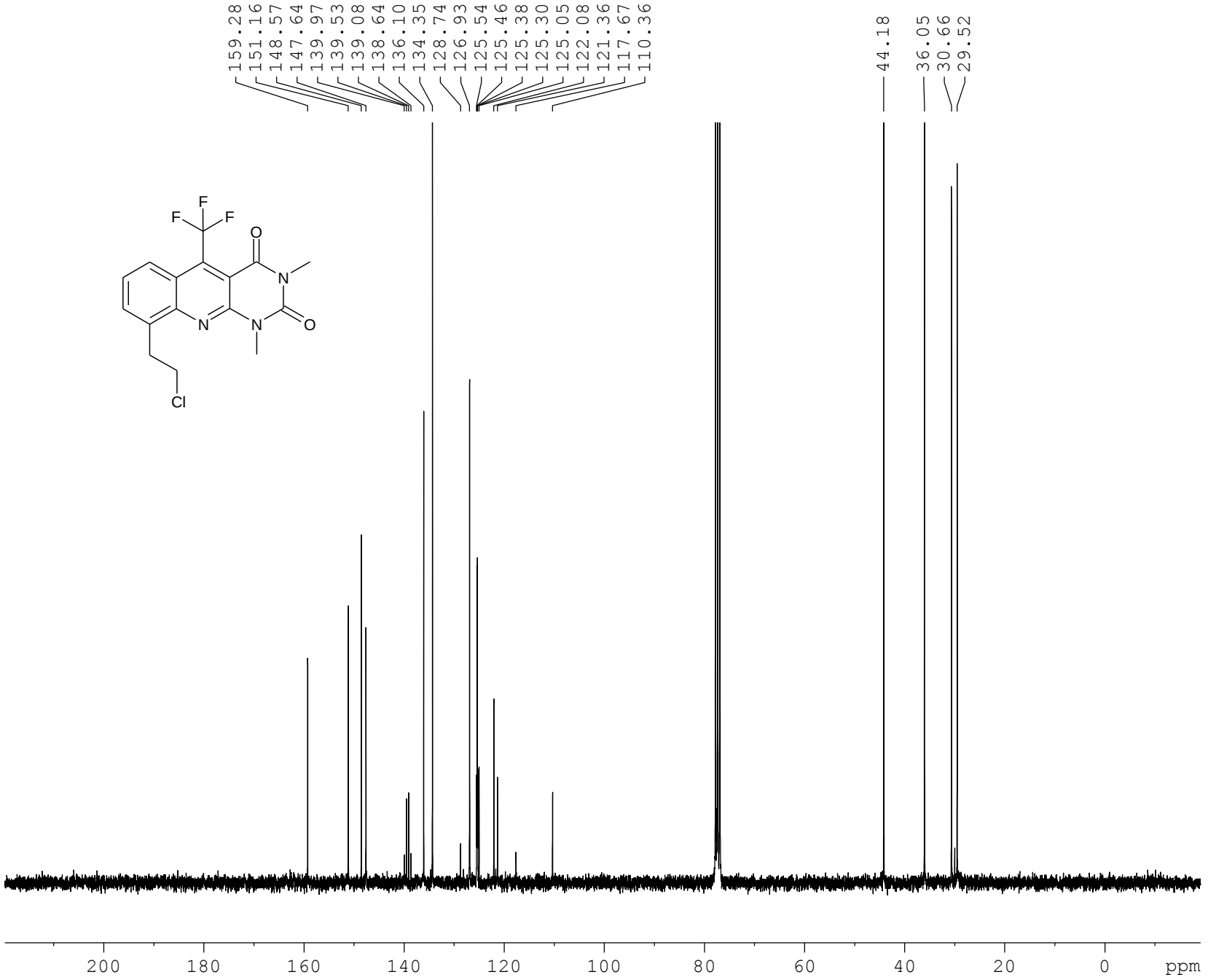
Current Data Parameters
NAME 110801.u302
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110801
Time 8.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 181
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin, sd 284, CDCl3, 13C




```
Current Data Parameters
NAME          110810.u331
EXPNO                  10
PROCNO                  1

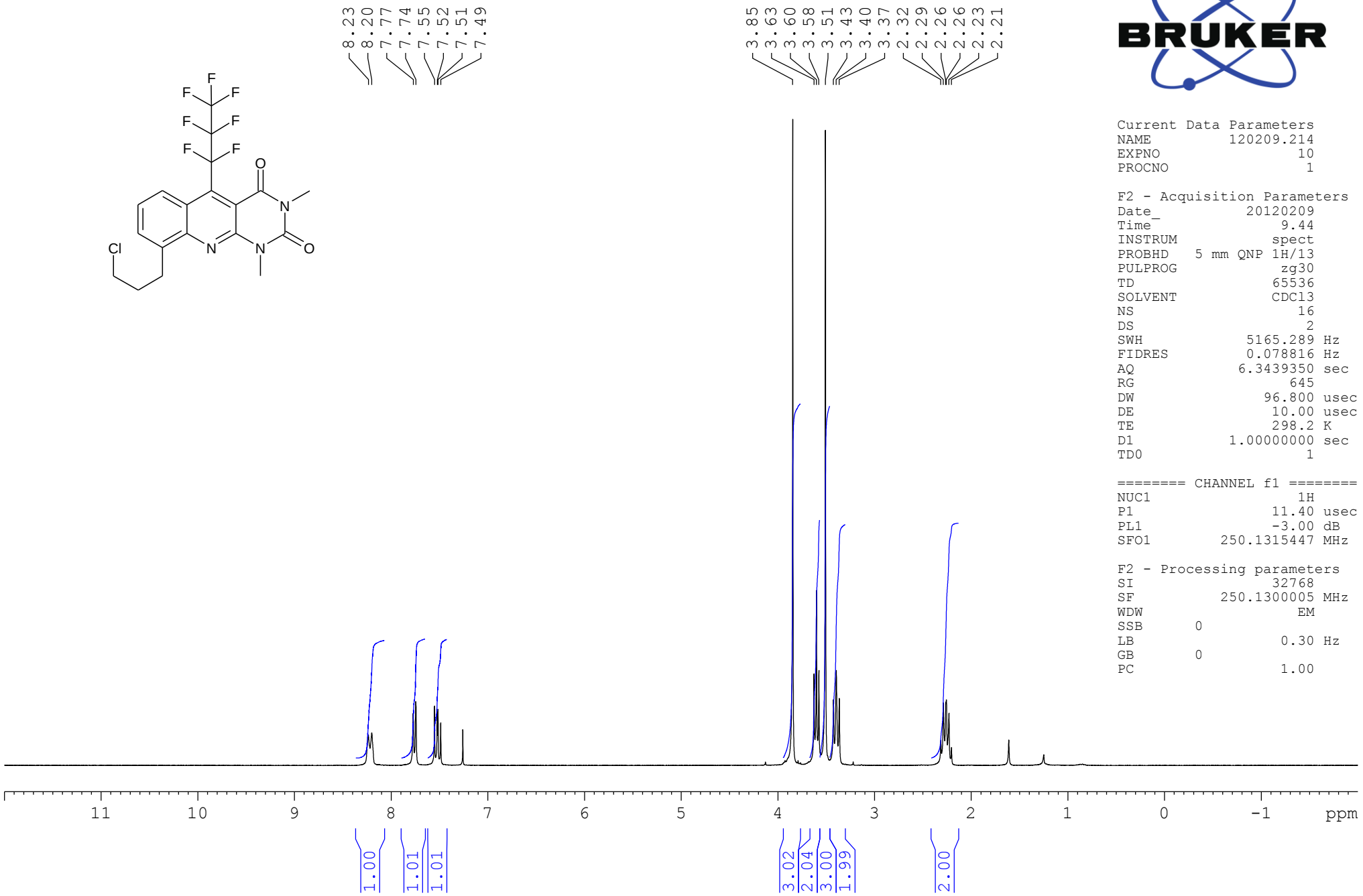
F2 - Acquisition Parameters
Date_            20110811
Time                5.30
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2500
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ             1.8175818 sec
RG                  2050
DW                27.733 usec
DE                10.00 usec
TE                298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                -0.50 dB
PL1W         33.25691986 W
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              72.00 usec
PL2       0 dB
PL12               17.00 dB
PL13               17.00 dB
PL2W         11.25325108 W
PL12W         0.22453187 W
PL13W         0.22453187 W
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677252 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Dudkin, sd 368, CDCl3, 1H



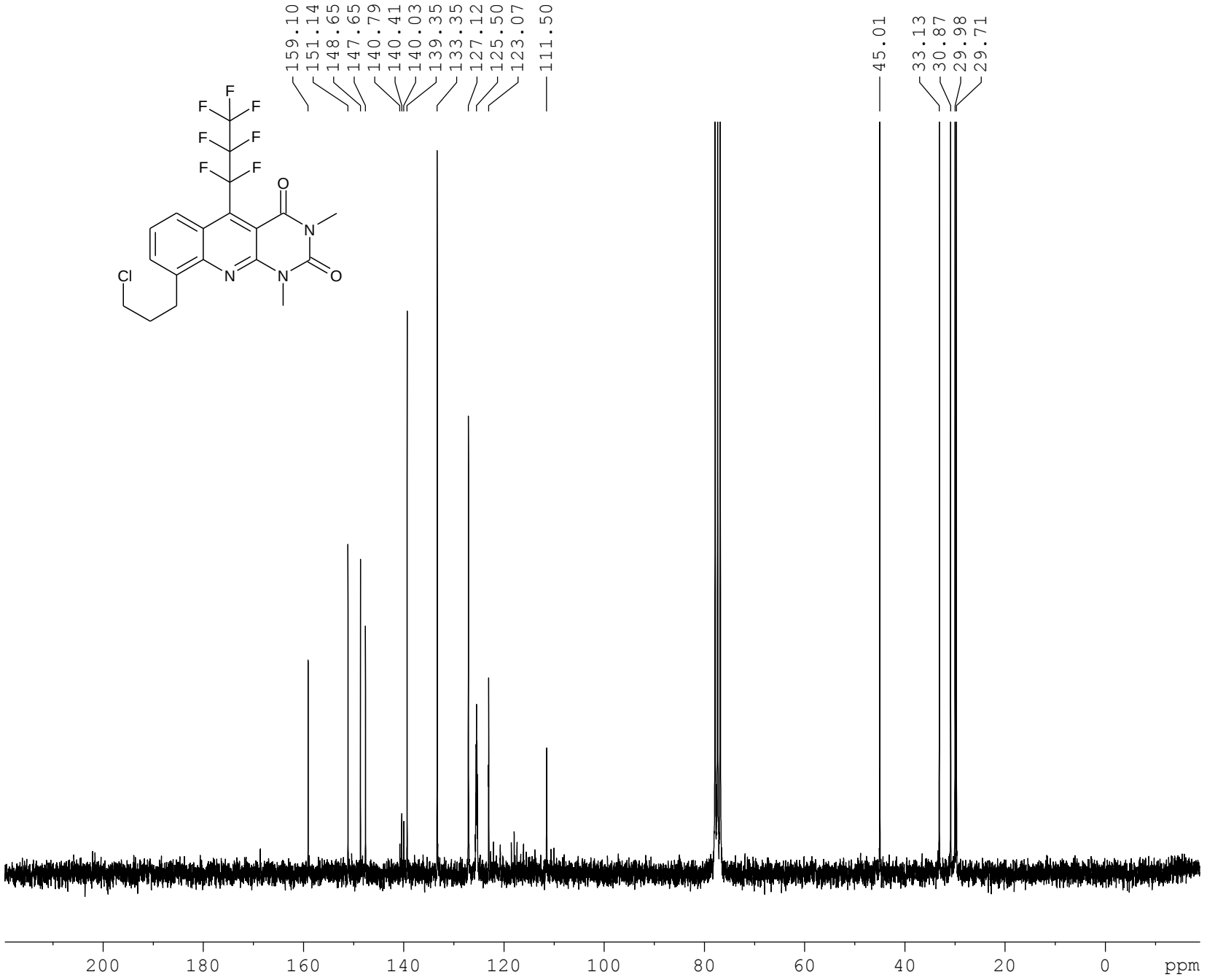

```
Current Data Parameters
NAME          120209.214
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120209
Time               9.44
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            5165.289 Hz
FIDRES         0.078816 Hz
AQ             6.3439350 sec
RG                  645
DW                96.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.40 usec
PL1               -3.00 dB
SFO1        250.1315447 MHz

F2 - Processing parameters
SI                32768
SF          250.1300005 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Dudkin, sd 368, CDCl3, 13C




```
Current Data Parameters
NAME          120210.204
EXPNO                 10
PROCNO                 1

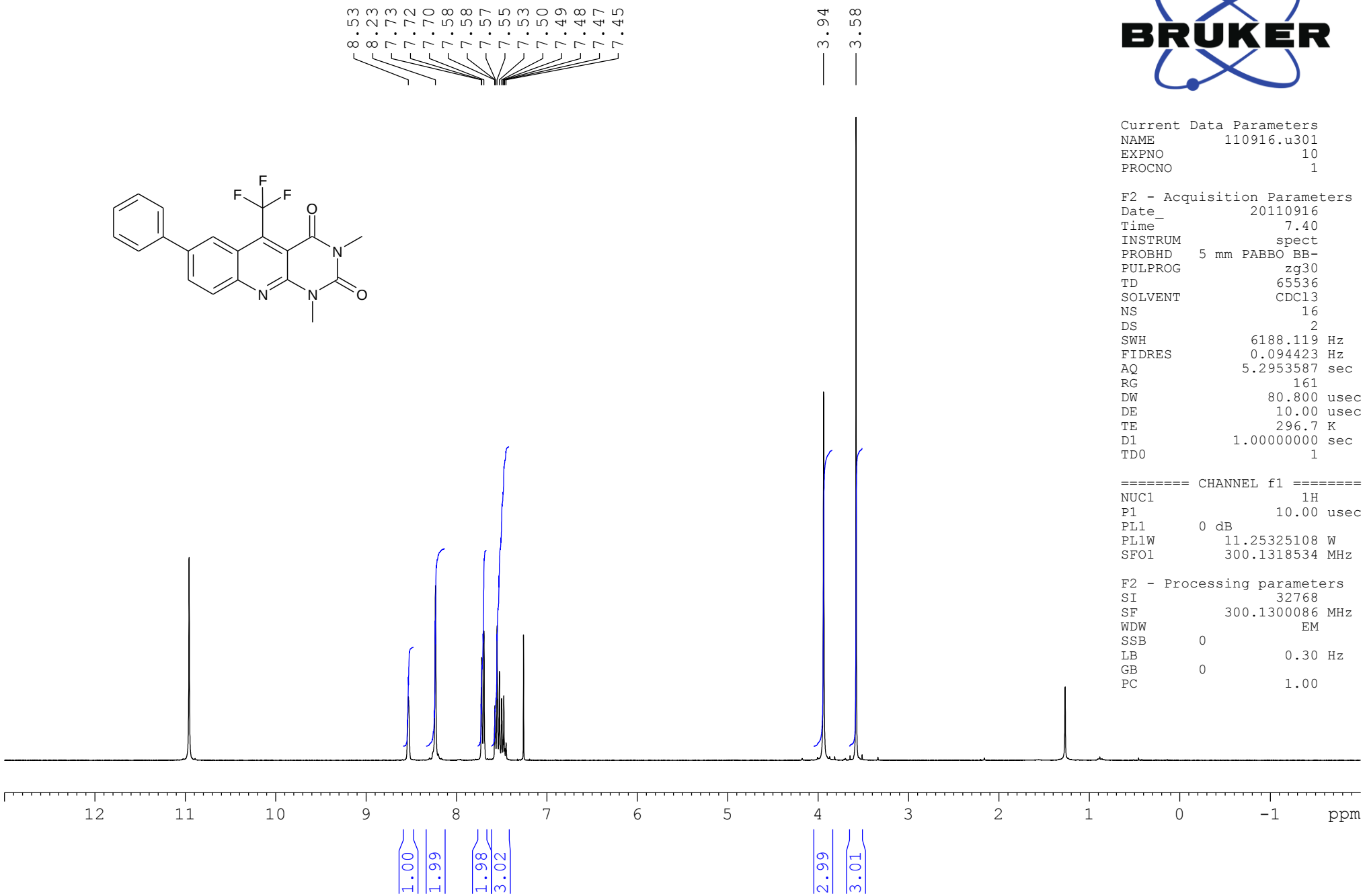
F2 - Acquisition Parameters
Date_           20120210
Time               22.07
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2500
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1       0 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              14.00 dB
PL13              14.00 dB
PL2               -3.00 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952162 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd292 1H CDCl3/CF3COOD



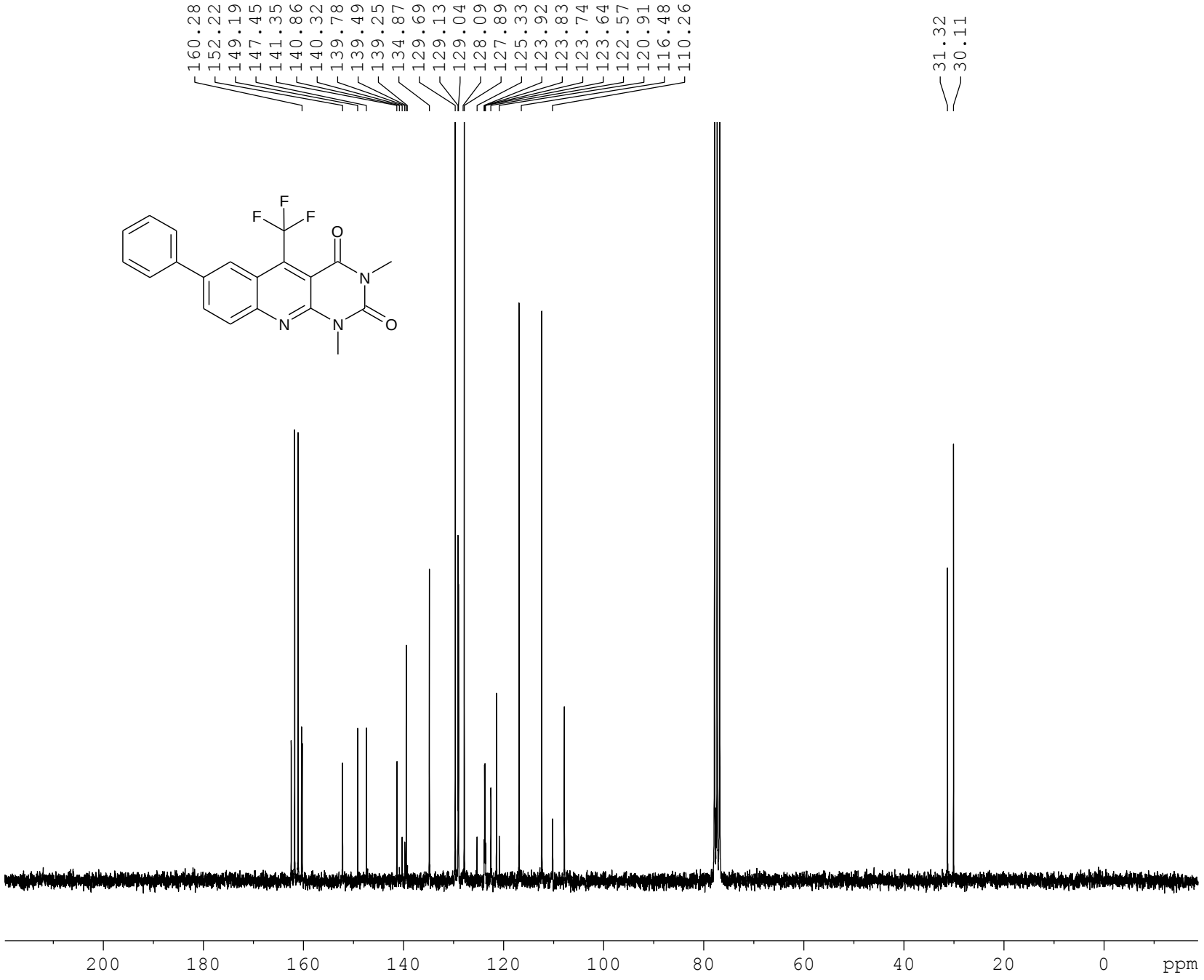

```
Current Data Parameters
NAME         110916.u301
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110916
Time                7.40
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   161
DW                80.800 usec
DE                10.00 usec
TE                296.7 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300086 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd292 13C CDCl3/CF3COOD



Current Data Parameters
NAME 110921.202
EXPNO 10
PROCNO 1

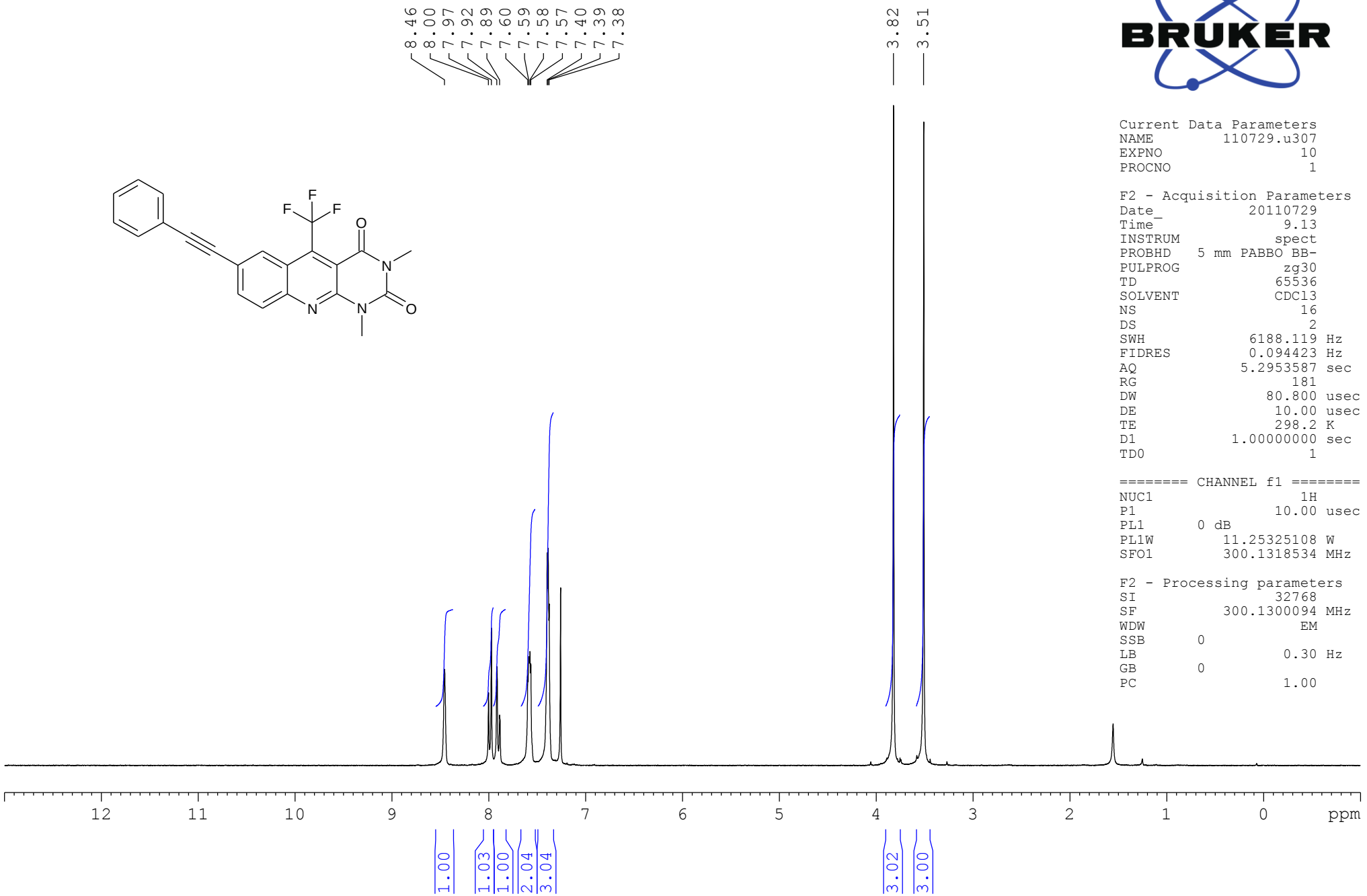
F2 - Acquisition Parameters
Date_ 20110921
Time 14.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952103 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd281 1H CDCl3



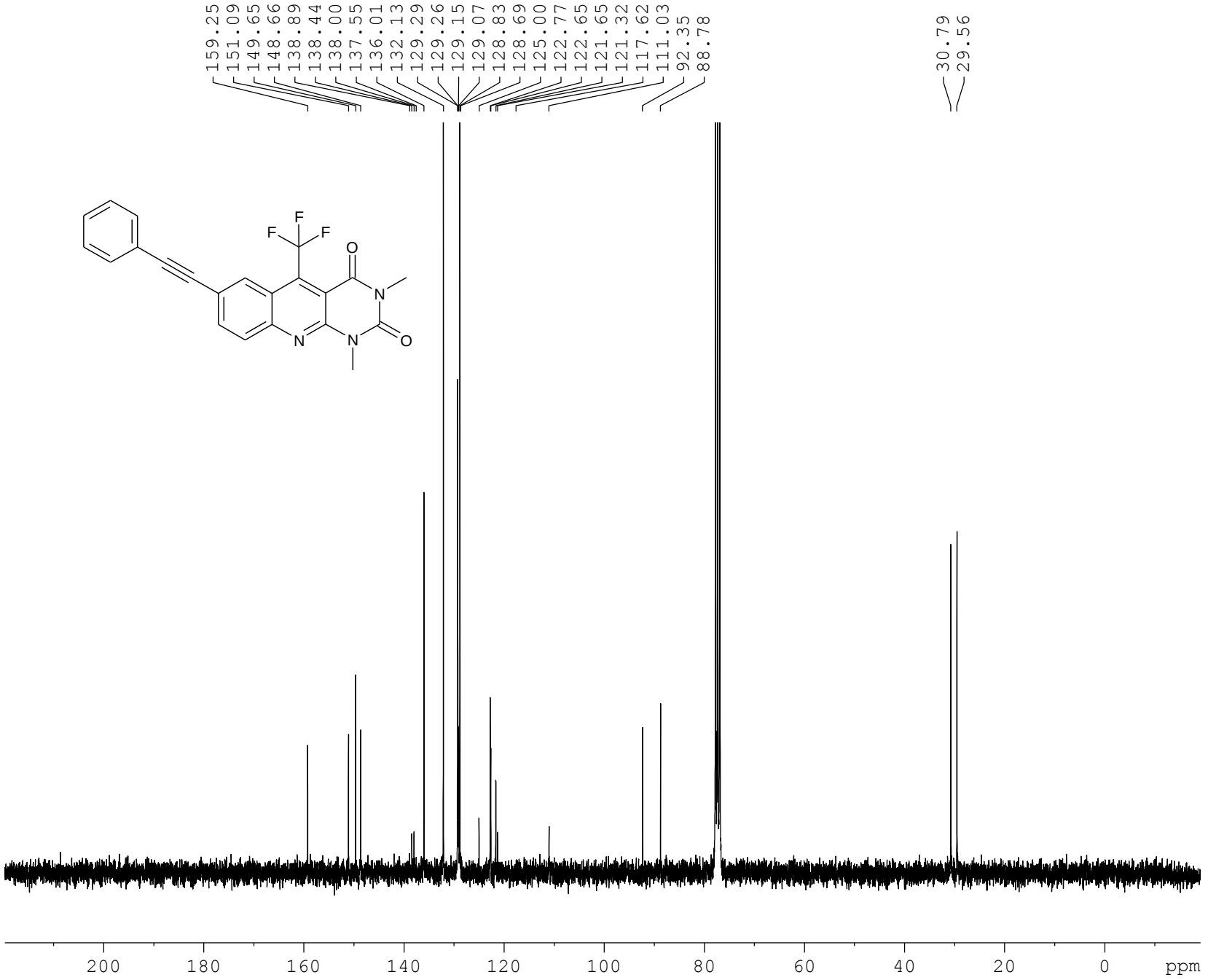
Current Data Parameters
NAME 110729.u307
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110729
Time 9.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 181
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd281 13C CDCl3



BRUKER

```
Current Data Parameters
NAME         110729.u307
EXPNO                 12
PROCNO                 1

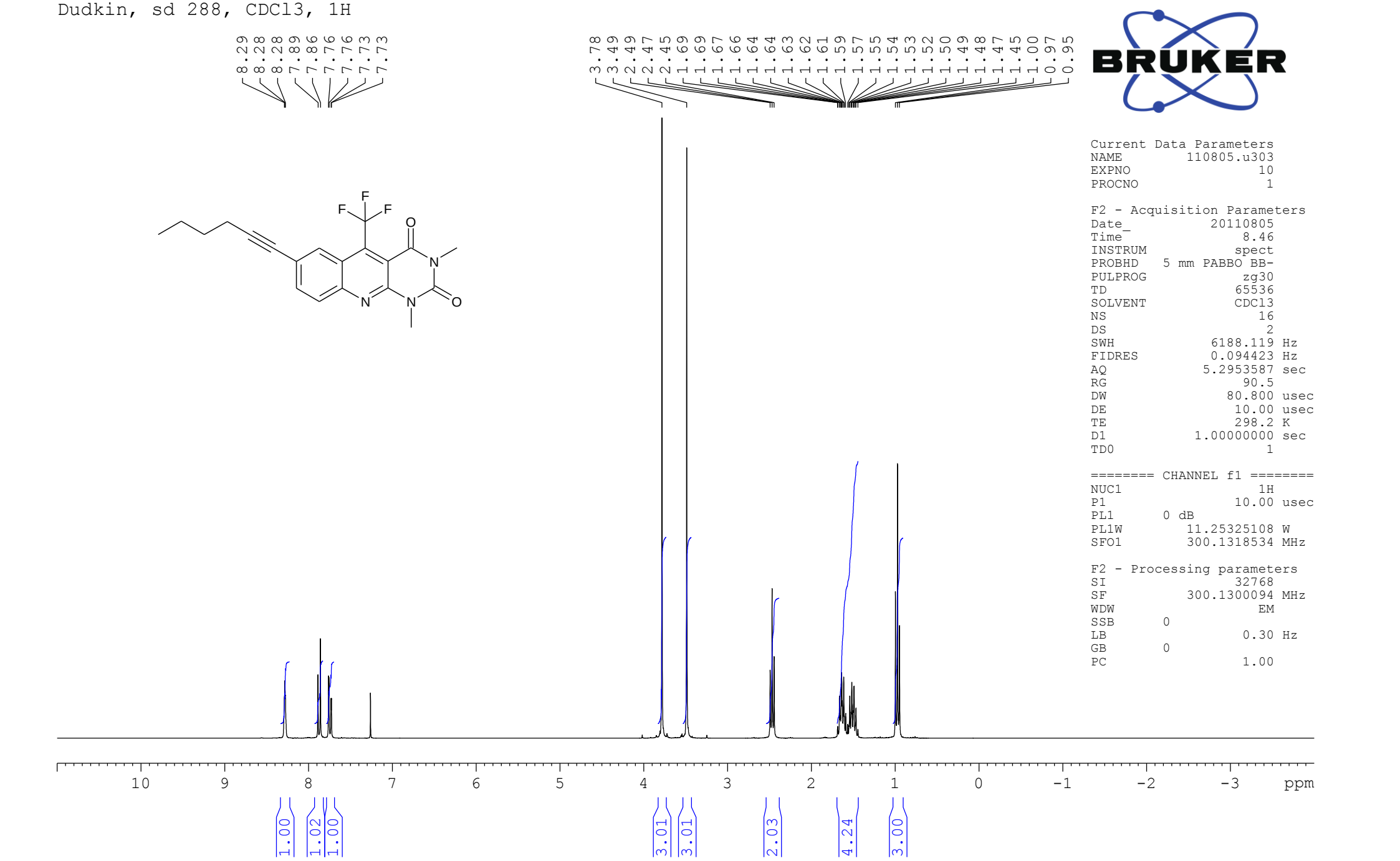
F2 - Acquisition Parameters
Date_           20110730
Time                4.19
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                 2050
DW               27.733 usec
DE               10.00 usec
TE               298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             72.00 usec
PL2       0 dB
PL12              17.00 dB
PL13              17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677239 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin, sd 288, CDCl3, 1H



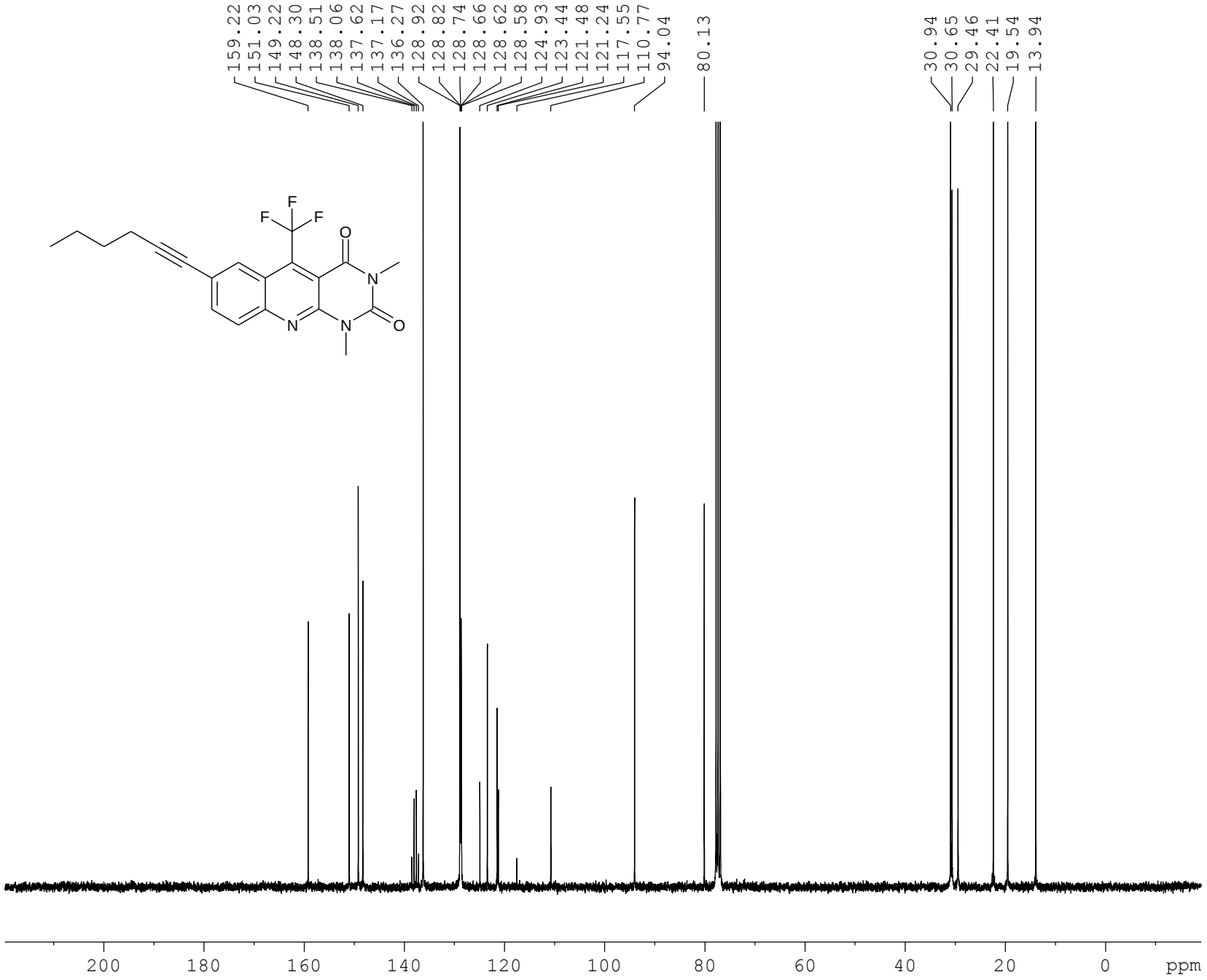
Current Data Parameters
NAME 110805.u303
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110805
Time 8.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 90.5
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin, sd 288, CDCl3, 13C



Current Data Parameters
NAME 110810.u332
EXPNO 10
PROCNO 1

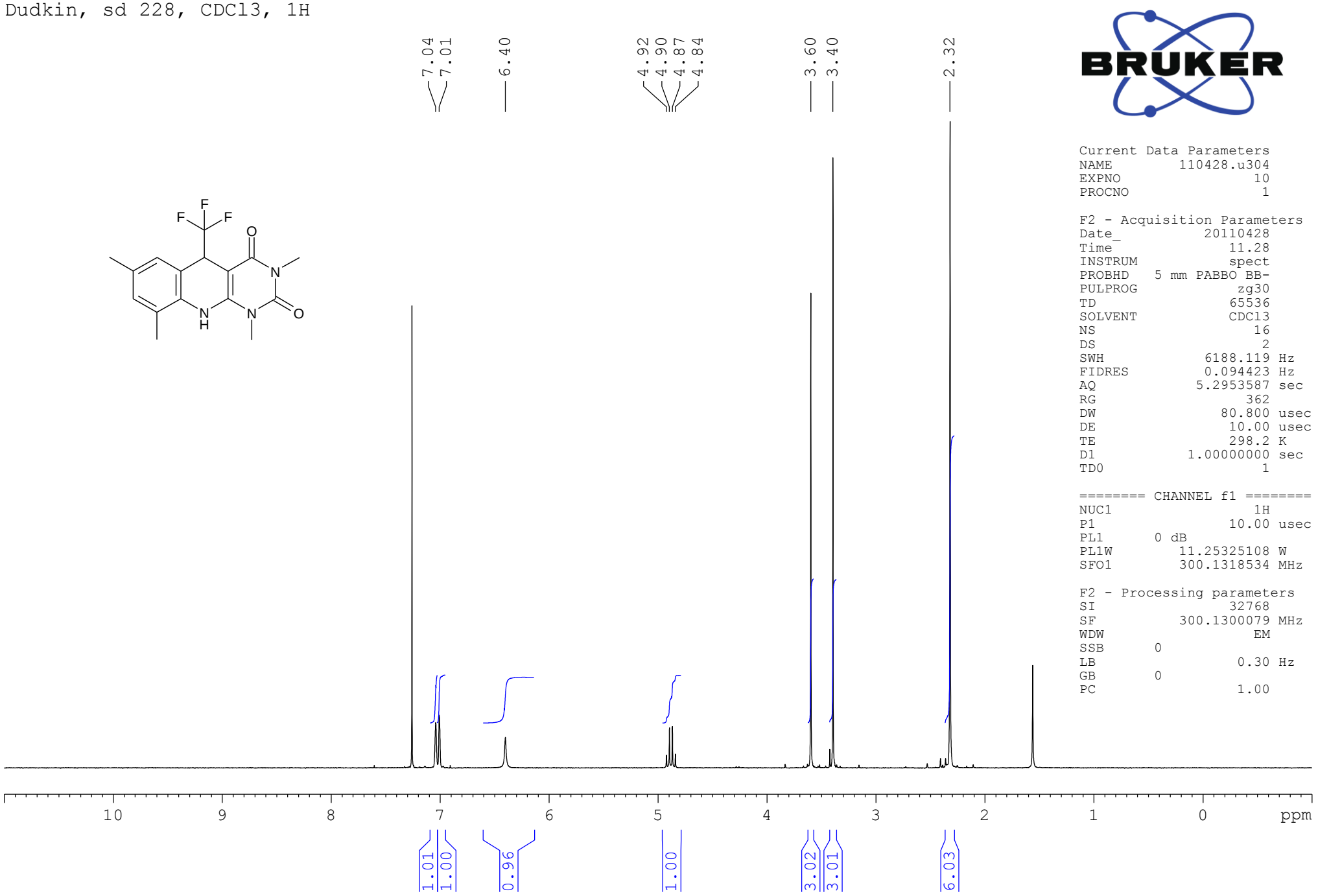
F2 - Acquisition Parameters
Date_ 20110811
Time 8.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2500
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677254 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin, sd 228, CDCl3, 1H



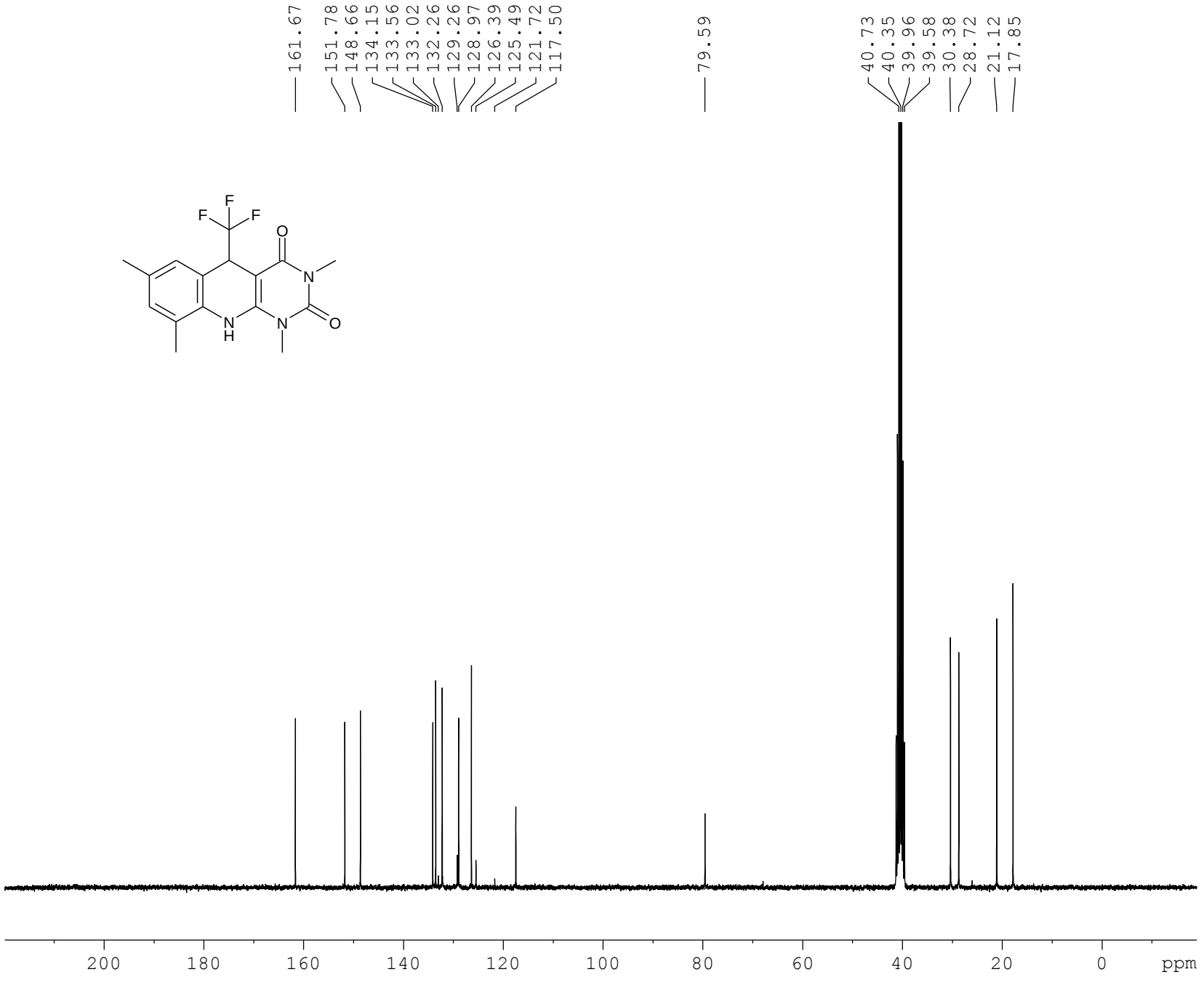

```
Current Data Parameters
NAME          110428.u304
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20110428
Time                11.28
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.094423 Hz
AQ               5.2953587 sec
RG                    362
DW                 80.800 usec
DE                 10.00 usec
TE                 298.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1        0 dB
PL1W          11.25325108 W
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF            300.1300079 MHz
WDW                    EM
SSB        0
LB                  0.30 Hz
GB         0
PC                  1.00
```

Dudkin sd228 13C DMSO



Current Data Parameters
NAME 120615.u310
EXPNO 12
PROCNO 1

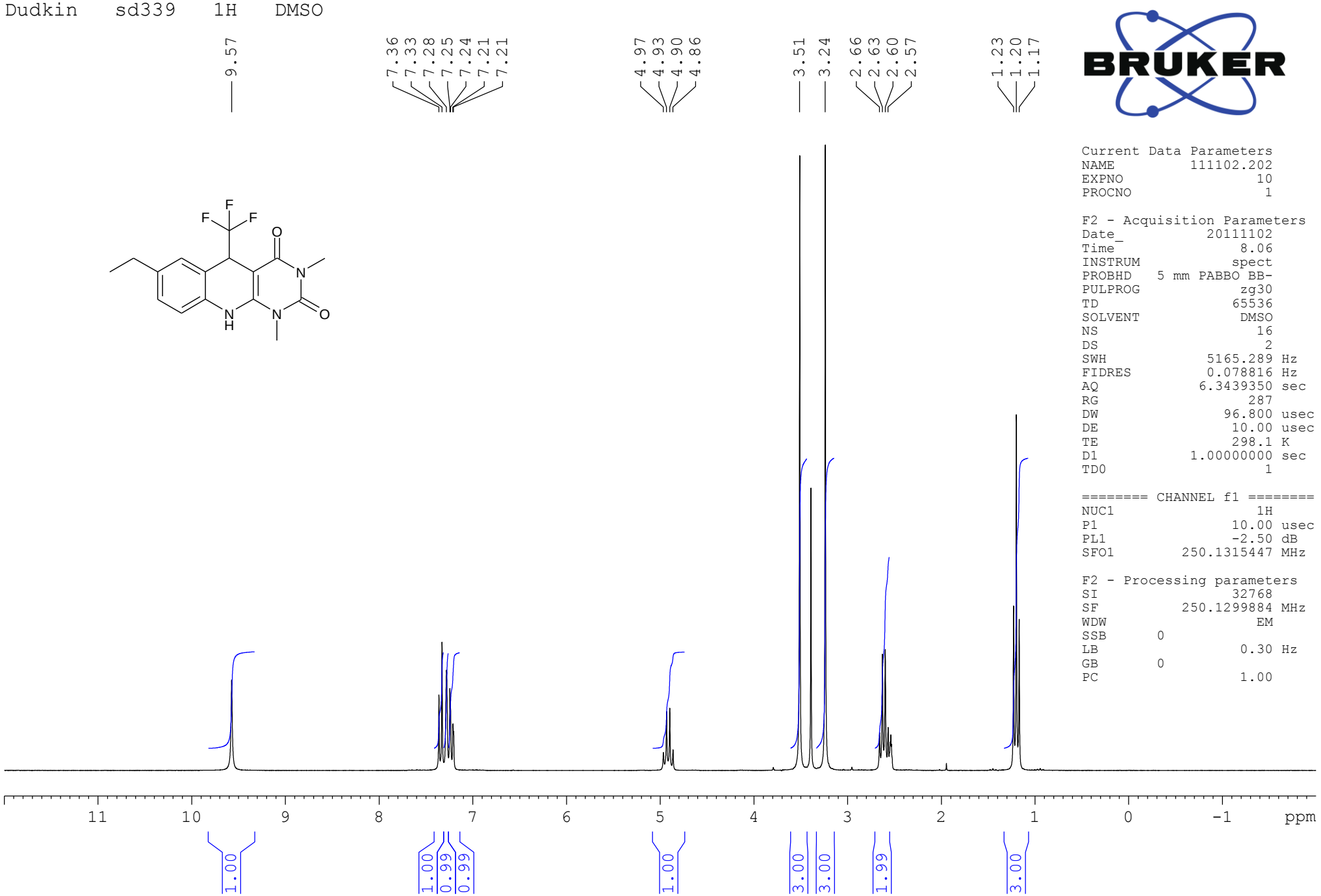
F2 - Acquisition Parameters
Date_ 20120616
Time 9.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677152 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd339 1H DMSO



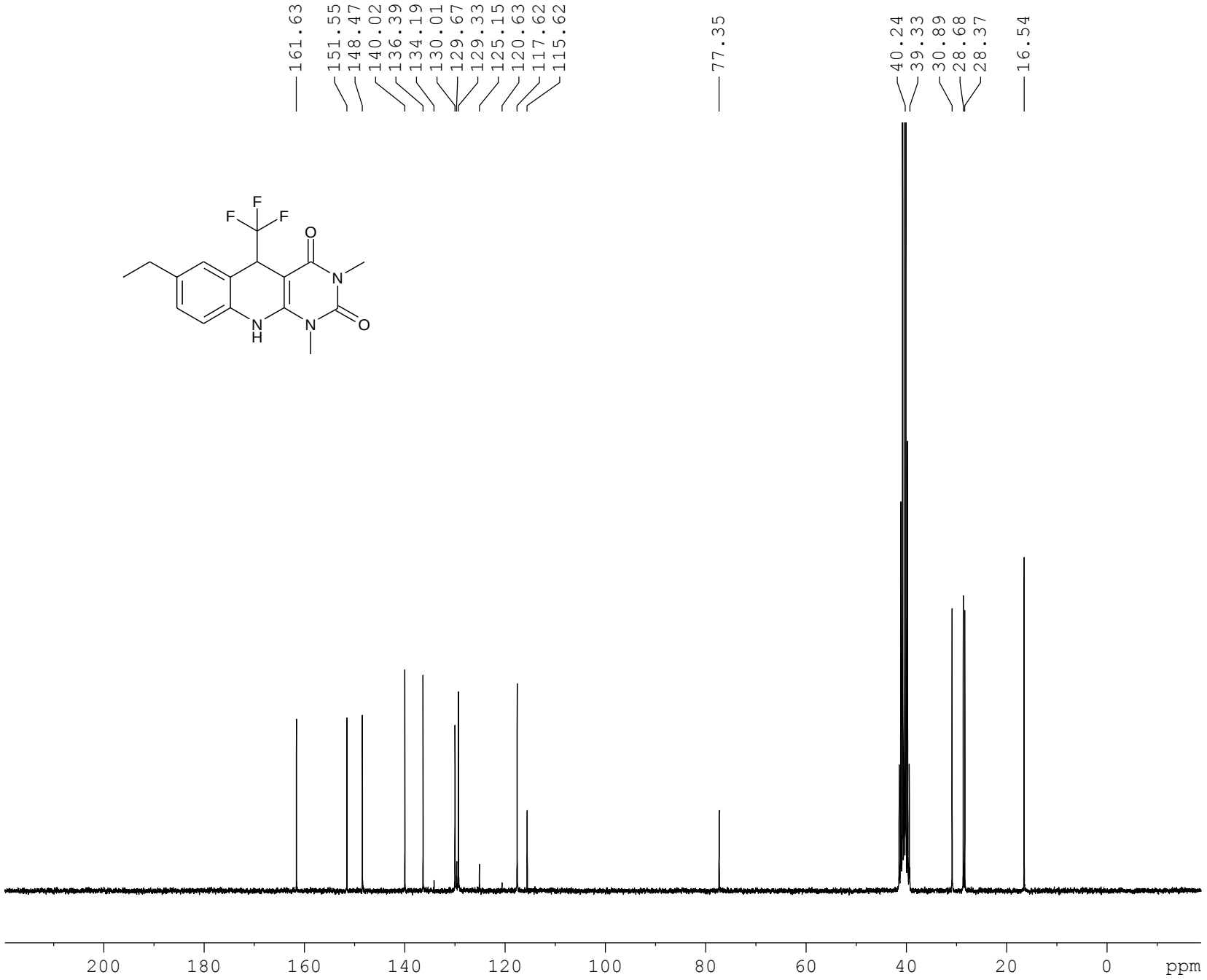

```
Current Data Parameters
NAME          111102.202
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20111102
Time                8.06
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             5165.289 Hz
FIDRES          0.078816 Hz
AQ              6.3439350 sec
RG                   287
DW                96.800 usec
DE                10.00 usec
TE                298.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1               -2.50 dB
SFO1        250.1315447 MHz

F2 - Processing parameters
SI                 32768
SF          250.1299884 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Dudkin sd339 13C DMSO




```
Current Data Parameters
NAME          111104.211
EXPNO                 10
PROCNO                 1

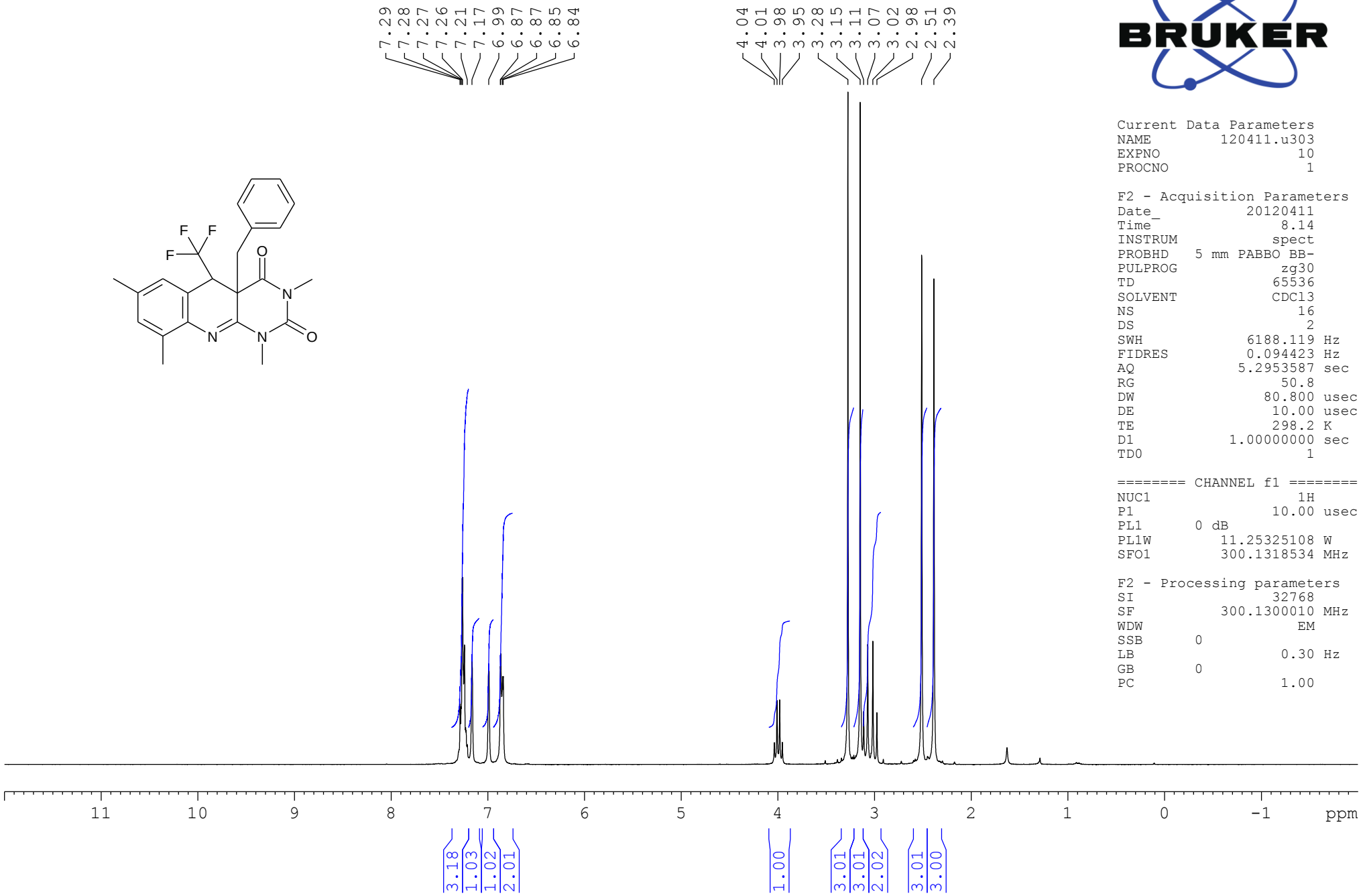
F2 - Acquisition Parameters
Date_           20111105
Time               14.34
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.4 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952079 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd402 1H CDCl3



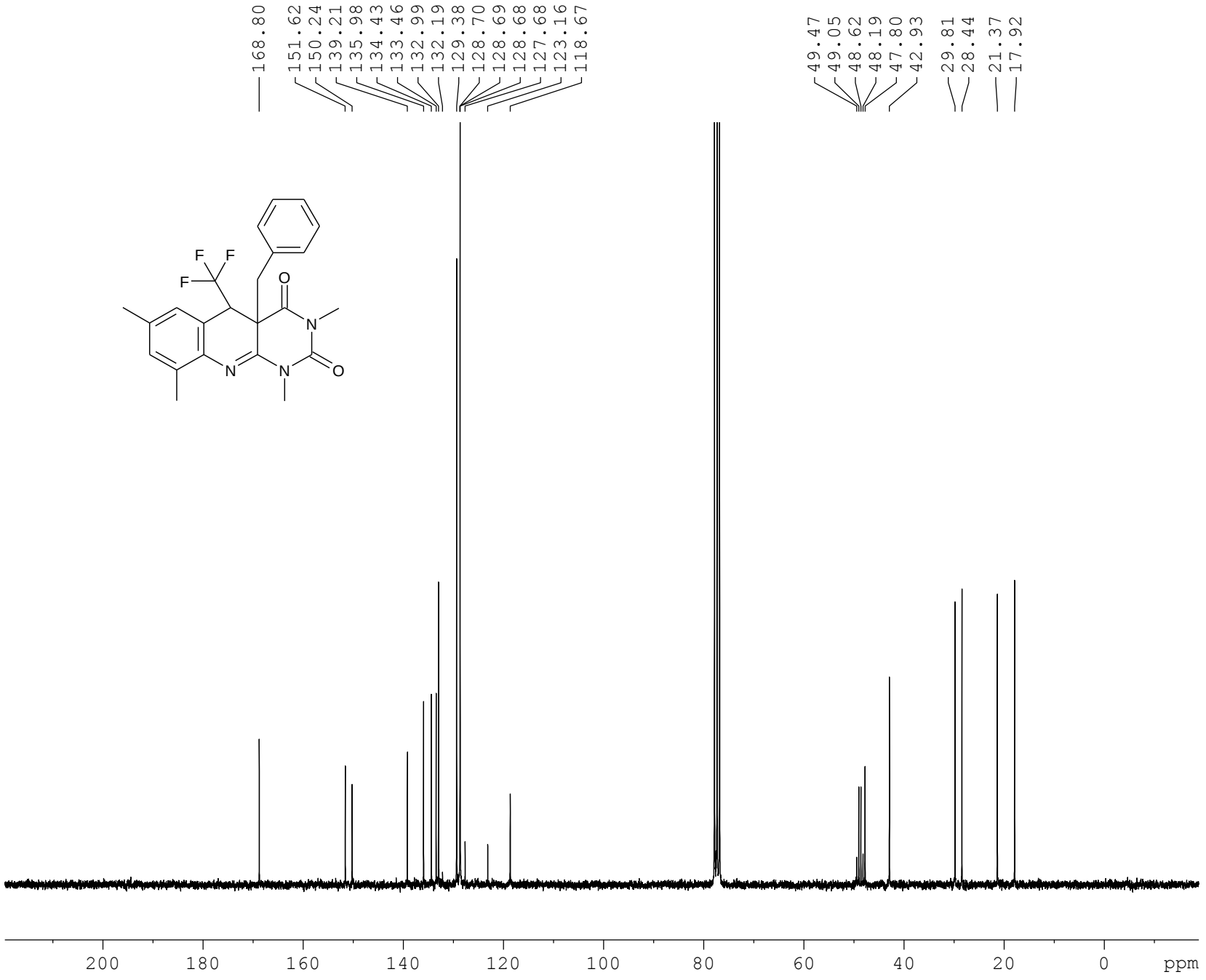

```
Current Data Parameters
NAME          120411.u303
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120411
Time                8.14
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                  50.8
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300010 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Dudkin sd402 13C CDCl3



Current Data Parameters
NAME 120412.202
EXPNO 10
PROCNO 1

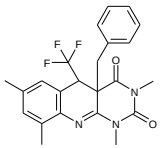
F2 - Acquisition Parameters
Date_ 20120412
Time 14.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952168 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd402 NOESY CDCl3



Current Data Parameters
NAME 121210.u339
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121210
Time 16.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG noesyph
TD 2048
SOLVENT CDCl3
NS 16
DS 4
SWH 2183.406 Hz
FIDRES 1.066116 Hz
AQ 0.4690420 sec
RG 64
DW 229.000 usec
DE 10.00 usec
TE 298.2 K
D0 0.00021627 sec
D1 1.86524105 sec
D8 1.50000000 sec
IN0 0.00045800 sec

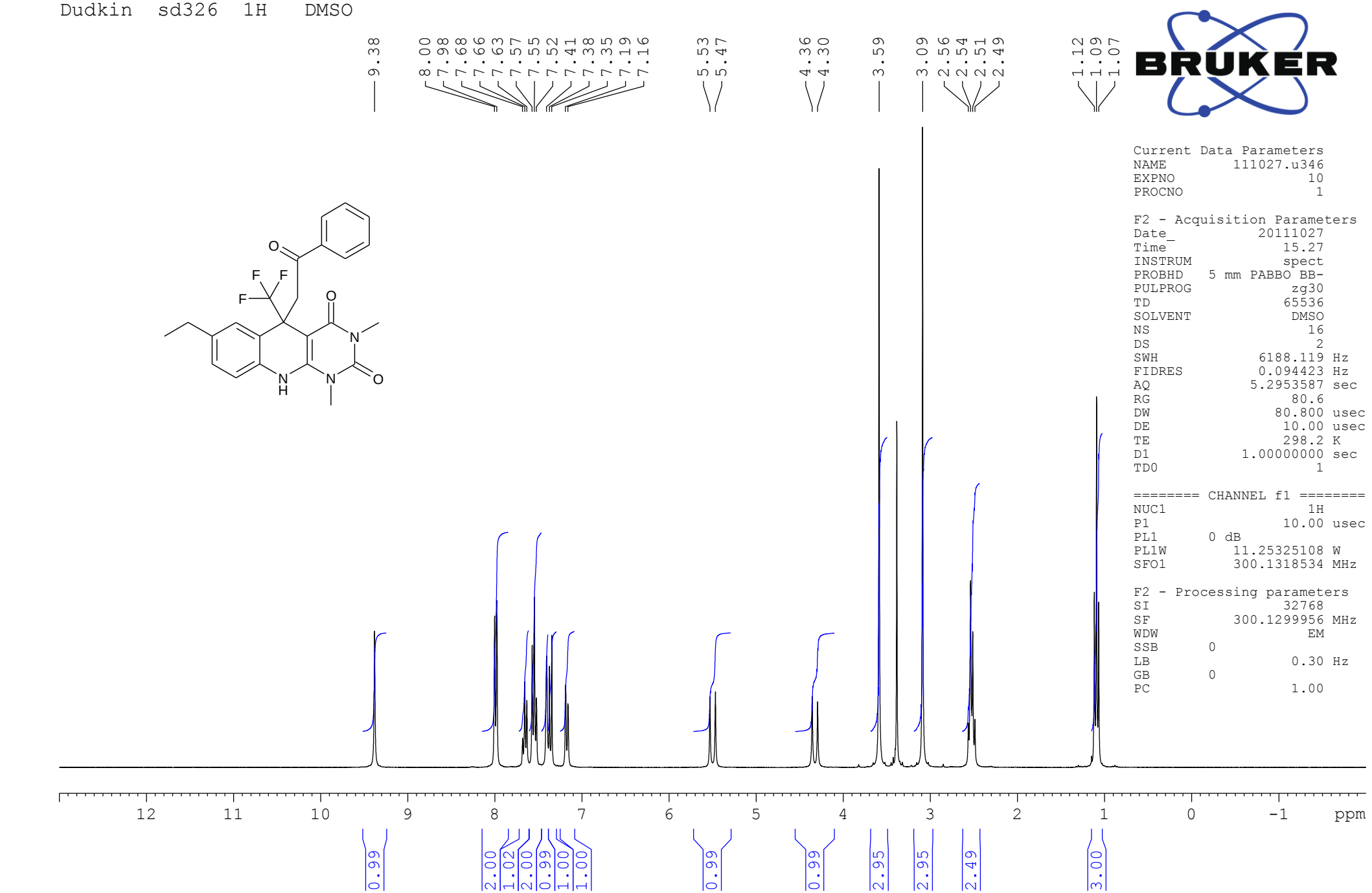
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1313142 MHz

F1 - Acquisition parameters
TD 256
SFO1 300.1313 MHz
FIDRES 8.528930 Hz
SW 7.275 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 300.1300009 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

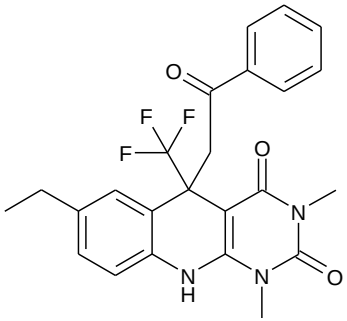
F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 300.1300009 MHz
WDW
SSB 2
LB 0 Hz
GB 0

Dudkin sd326 1H DMSO



Dudkin sd326 13C DMSO

195.82 161.61 151.10 148.13 139.60 137.63 134.99 134.27 133.90 130.47 129.52 128.87 128.67 126.95 126.66 122.85 119.94 117.58 79.95 48.03 47.69 47.35 47.00 38.55 31.22 28.61 28.51 16.60




```
Current Data Parameters
NAME         111028.u319
EXPNO                 10
PROCNO                 1

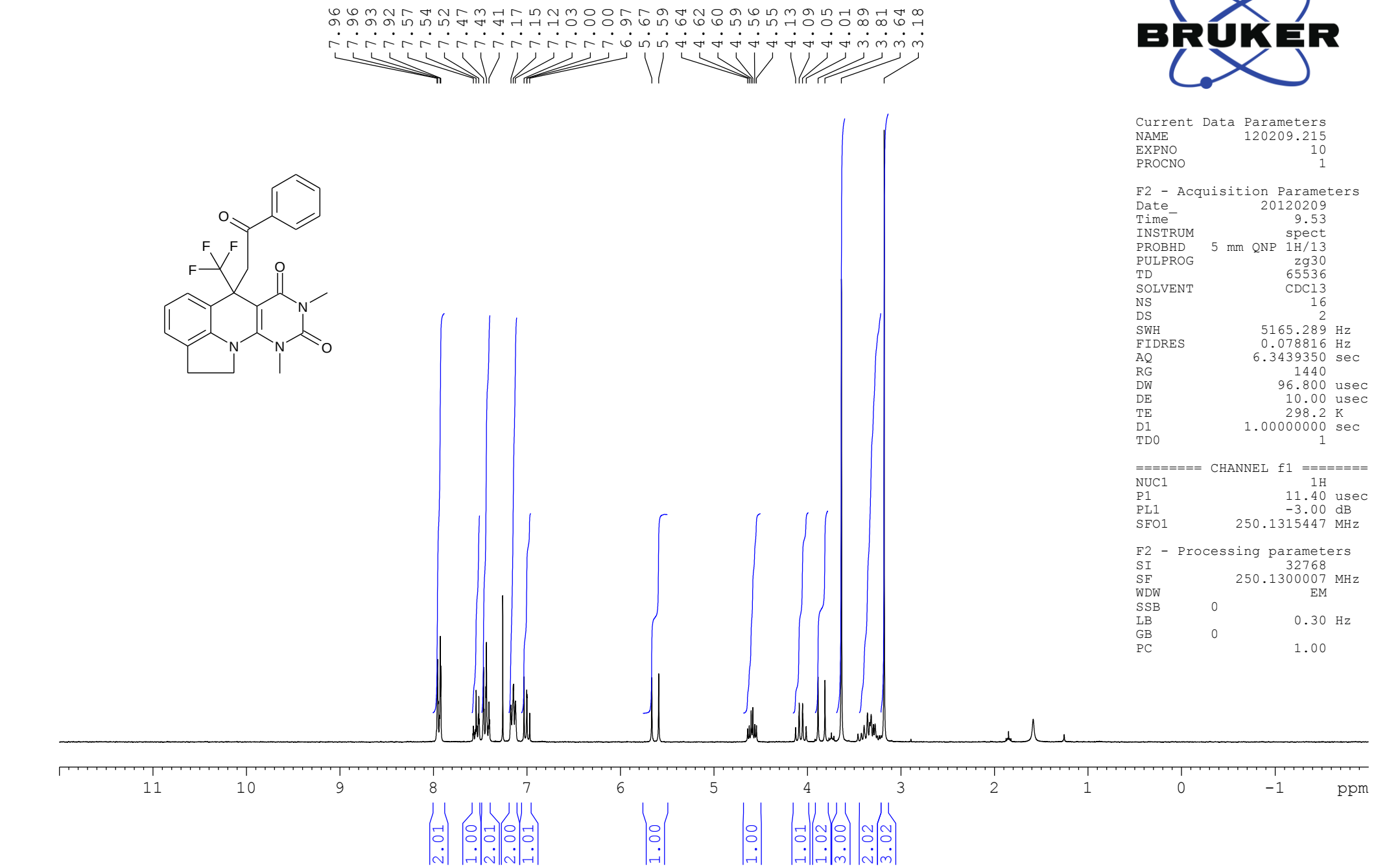
F2 - Acquisition Parameters
Date_           20111029
Time               15.56
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                 2050
DW               27.733 usec
DE               10.00 usec
TE               298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1               10.00 usec
PL1              -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            72.00 usec
PL2       0 dB
PL12             17.00 dB
PL13             17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677153 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

Dudkin, sd 370, CDCl3, 1H



BRUKER

```
Current Data Parameters
NAME          120209.215
EXPNO                 10
PROCNO                 1

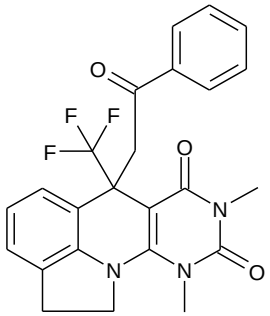
F2 - Acquisition Parameters
Date_           20120209
Time               9.53
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            5165.289 Hz
FIDRES         0.078816 Hz
AQ             6.3439350 sec
RG                 1440
DW                96.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.40 usec
PL1               -3.00 dB
SFO1         250.1315447 MHz

F2 - Processing parameters
SI                32768
SF           250.1300007 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Dudkin, sd 370, CDCl3, 13C

195.75
161.99
152.90
152.88
141.77
137.18
134.38
133.34
129.83
128.87
128.82
128.21
125.27
125.04
124.83
124.45
120.71
117.65
84.74
53.41
48.47
48.04
47.62
47.19
38.55
38.40
28.93
28.52



Current Data Parameters
NAME 120210.206
EXPNO 10
PROCNO 1

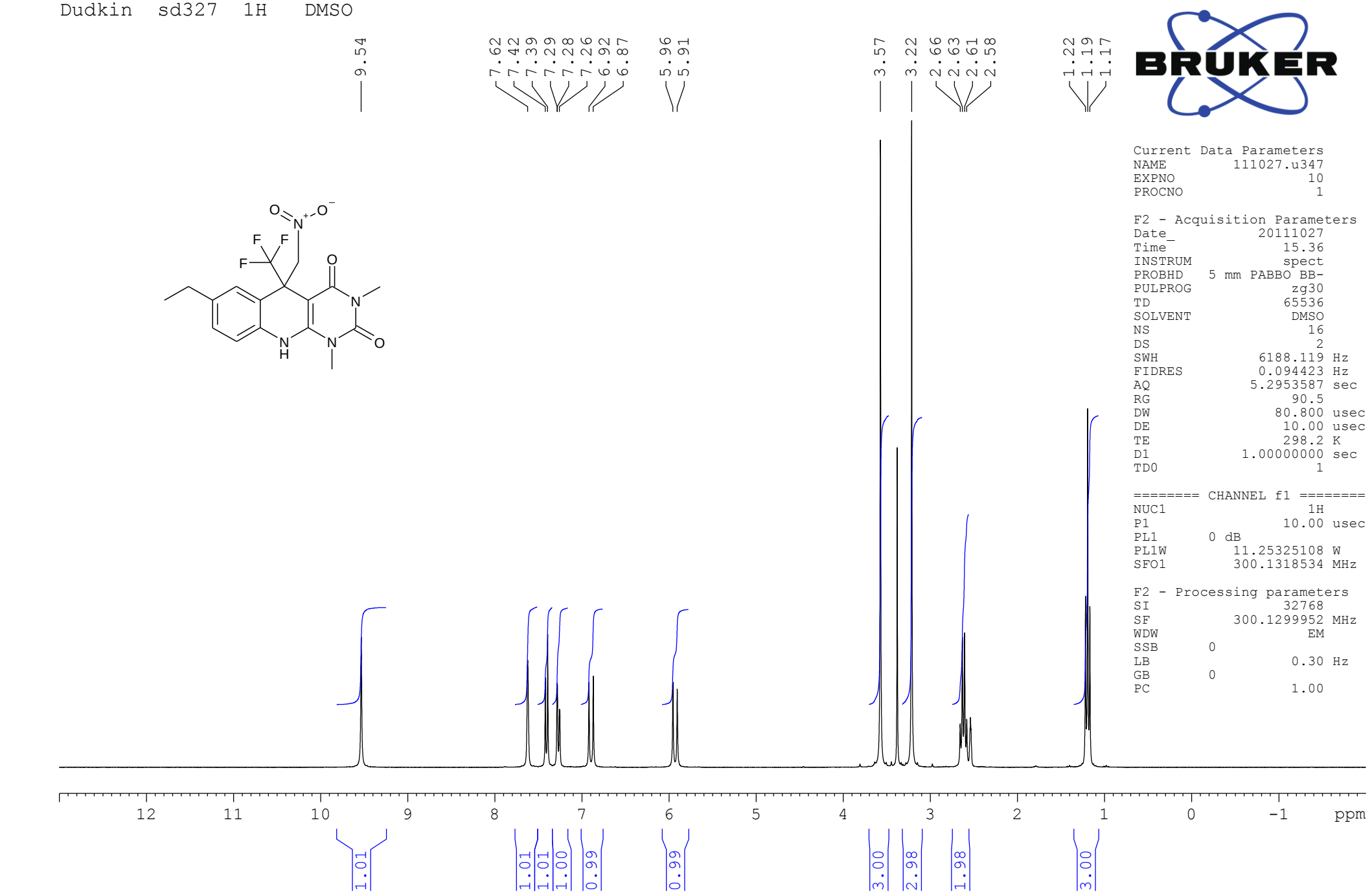
F2 - Acquisition Parameters
Date_ 20120211
Time 3.19
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2500
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.20 usec
PL1 0 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 14.00 dB
PL13 14.00 dB
PL2 -3.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952176 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd327 1H DMSO



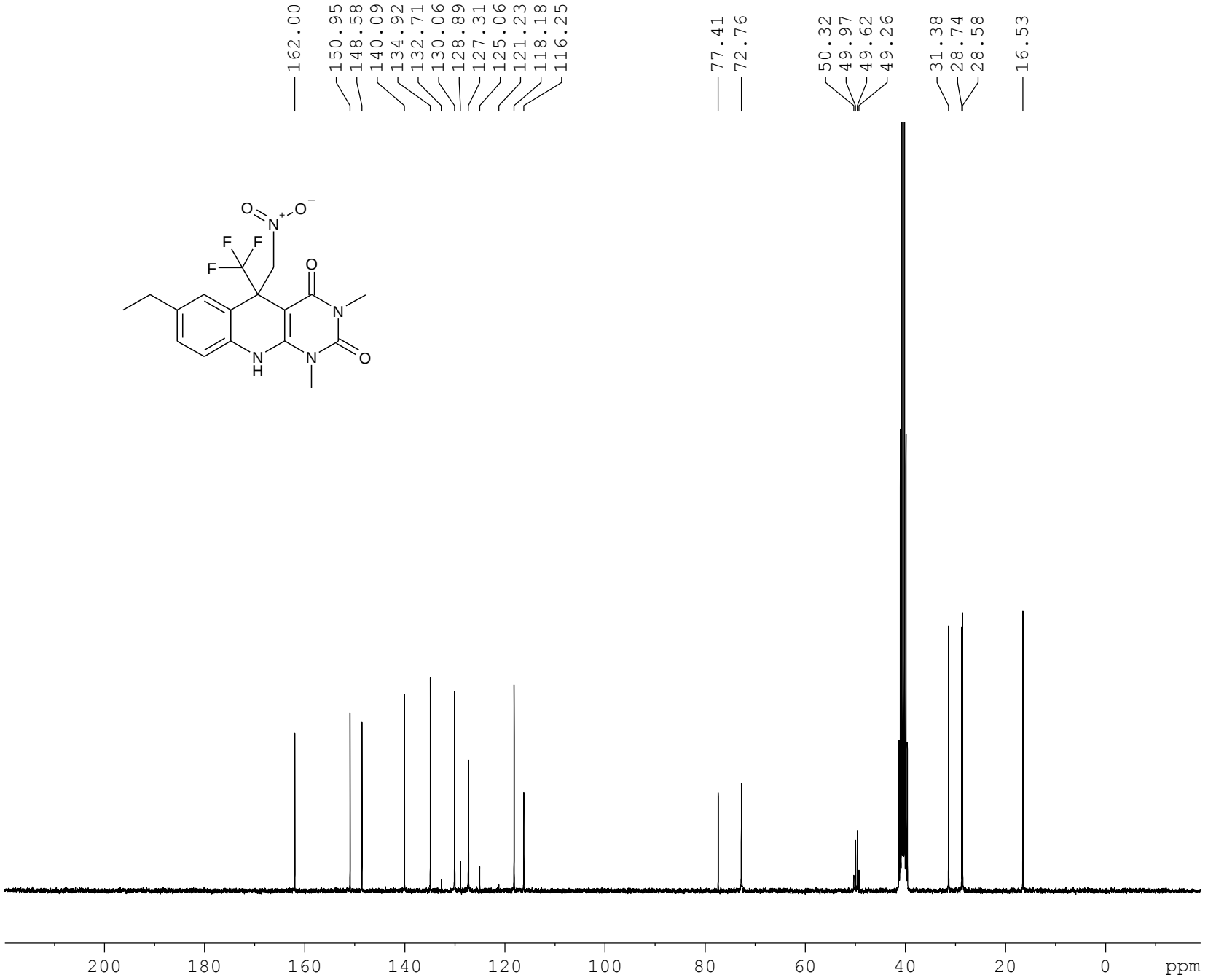
Current Data Parameters
NAME 111027.u347
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111027
Time 15.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 90.5
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299952 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd327 13C DMSO



Current Data Parameters
NAME 111028.u320
EXPNO 10
PROCNO 1

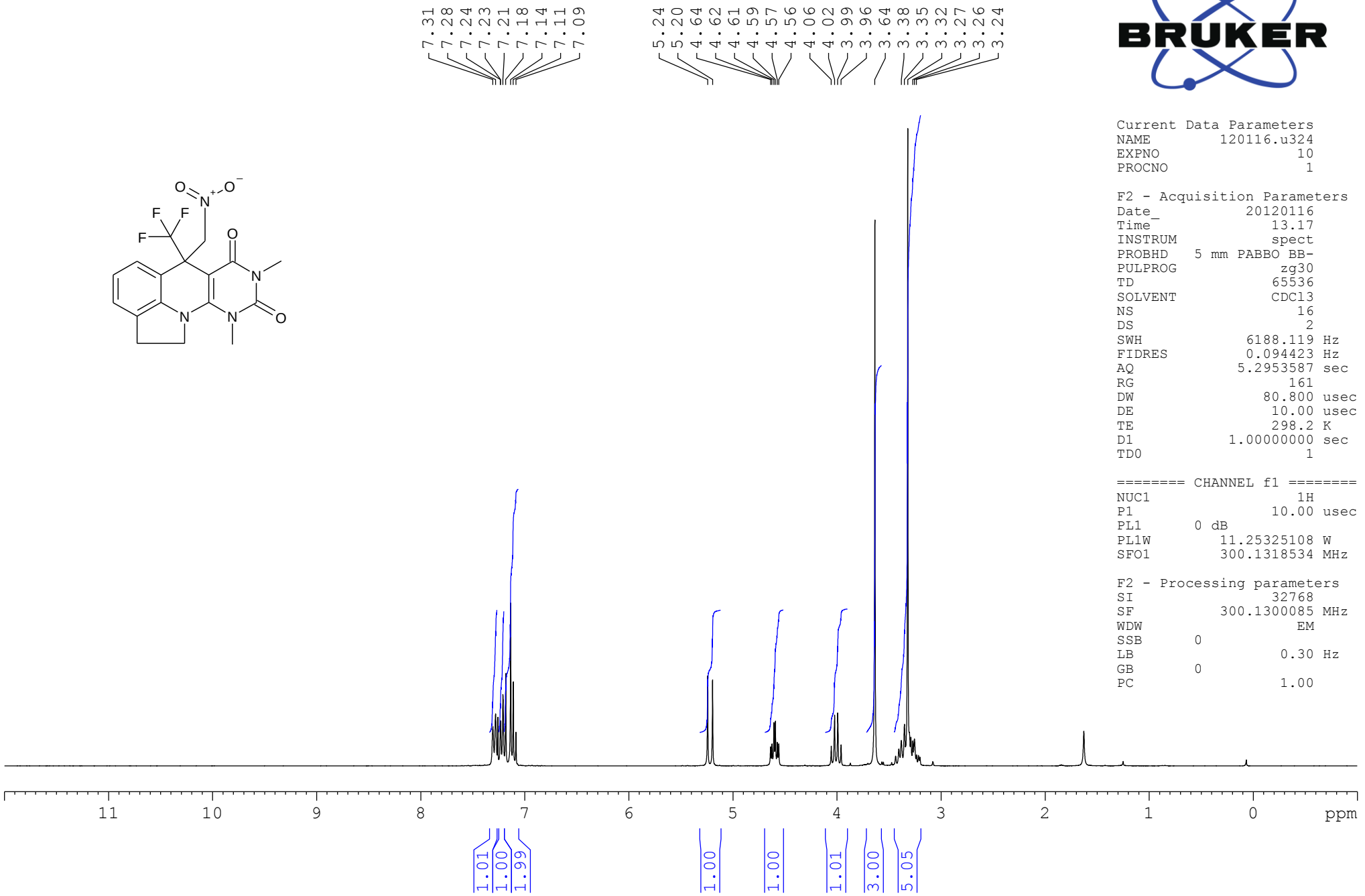
F2 - Acquisition Parameters
Date_ 20111029
Time 20.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

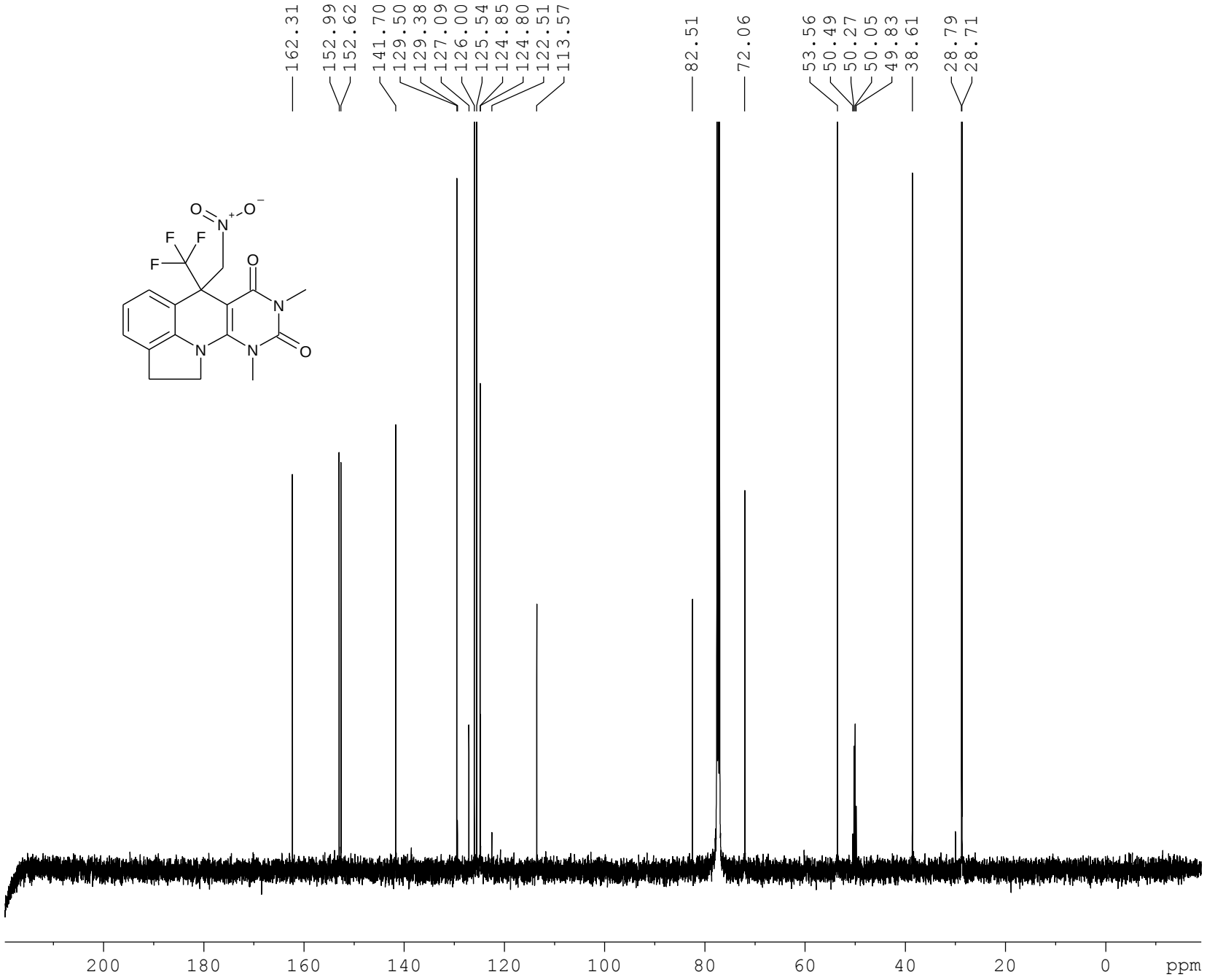
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677143 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin, sd 348, CDCl3, 1H



Sergii Dudkin, sd 348, 13C in CDCl3




```
Current Data Parameters
NAME          120124.501
EXPNO                 12
PROCNO                 1

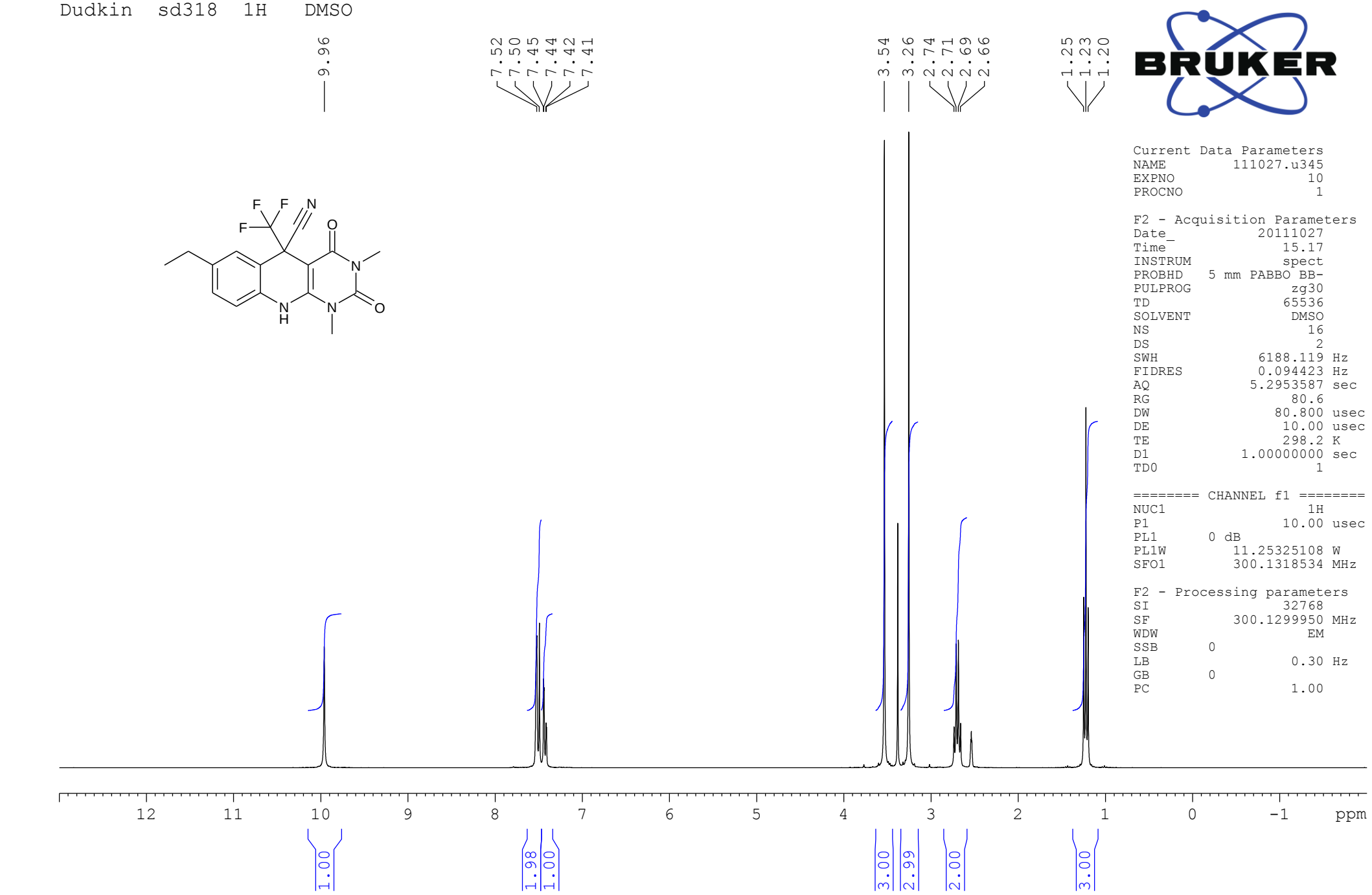
F2 - Acquisition Parameters
Date_           20120124
Time               14.49
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3762
DS                    4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912244 sec
RG               4597.6
DW              16.650 usec
DE               6.50 usec
TE              300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                9.00 usec
PL1               4.50 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            70.00 usec
PL2              -3.00 dB
PL12             14.08 dB
PL13            120.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577466 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd318 1H DMSO



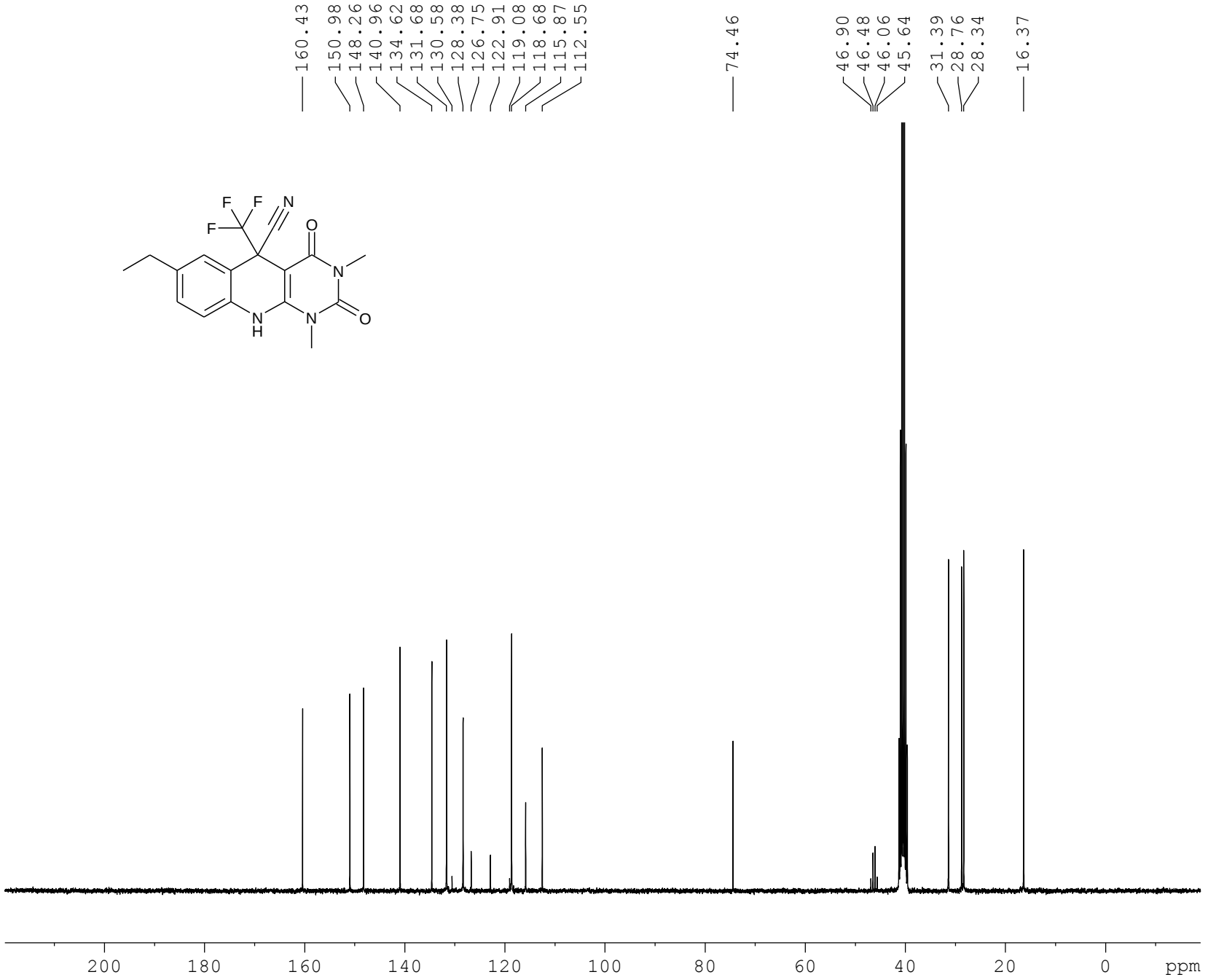

```
Current Data Parameters
NAME          111027.u345
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20111027
Time                15.17
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ              5.2953587 sec
RG                   80.6
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1        0 dB
PL1W         11.25325108 W
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF           300.1299950 MHz
WDW                    EM
SSB        0
LB                  0.30 Hz
GB         0
PC                  1.00
```

Dudkin sd318 13C DMSO




```
Current Data Parameters
NAME         111028.u318
EXPNO                 10
PROCNO                 1

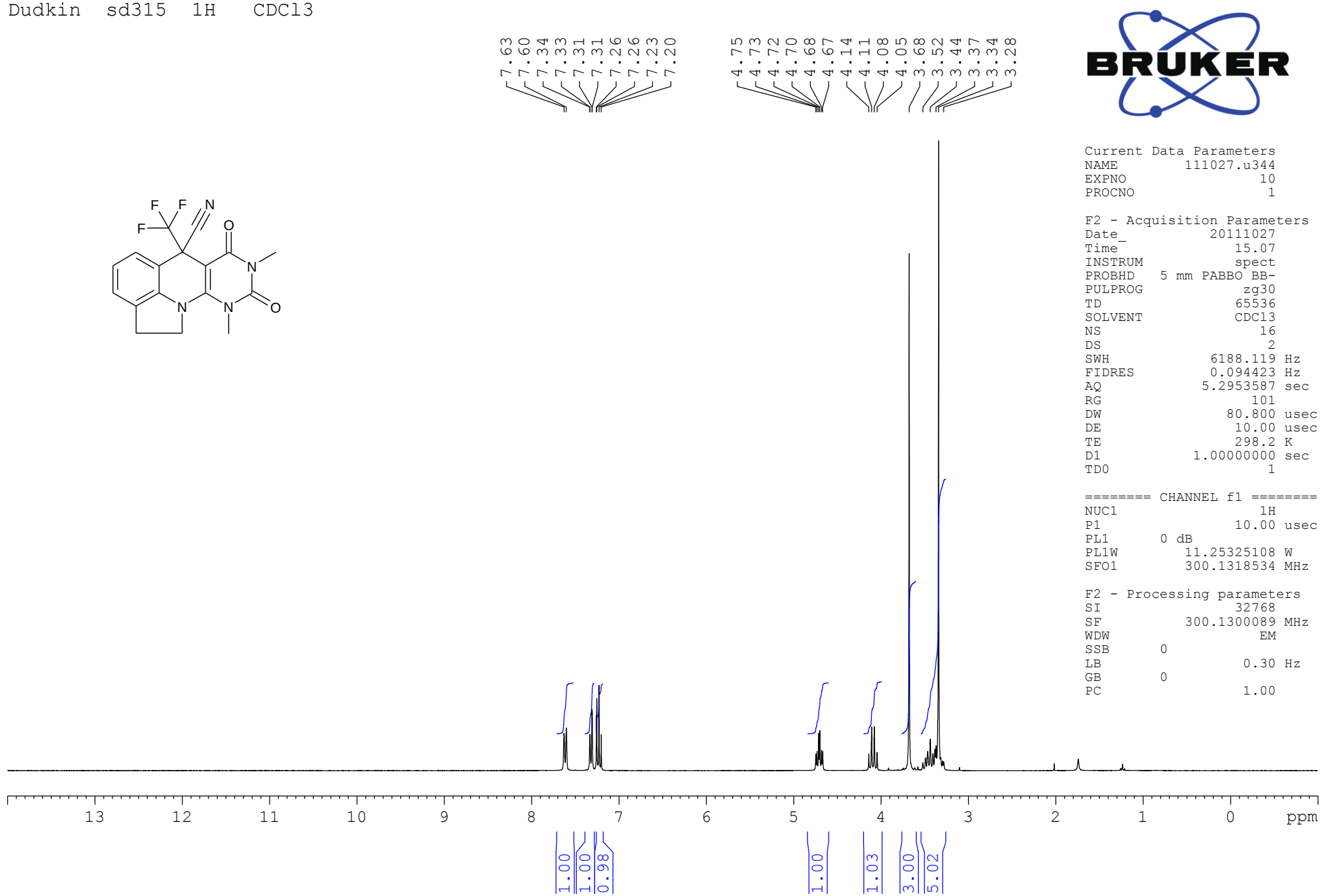
F2 - Acquisition Parameters
Date_           20111029
Time               11.42
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                 2050
DW               27.733 usec
DE               10.00 usec
TE               298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -0.50 dB
PL1W        33.25691986 W
SFO1         75.4752953 MHz

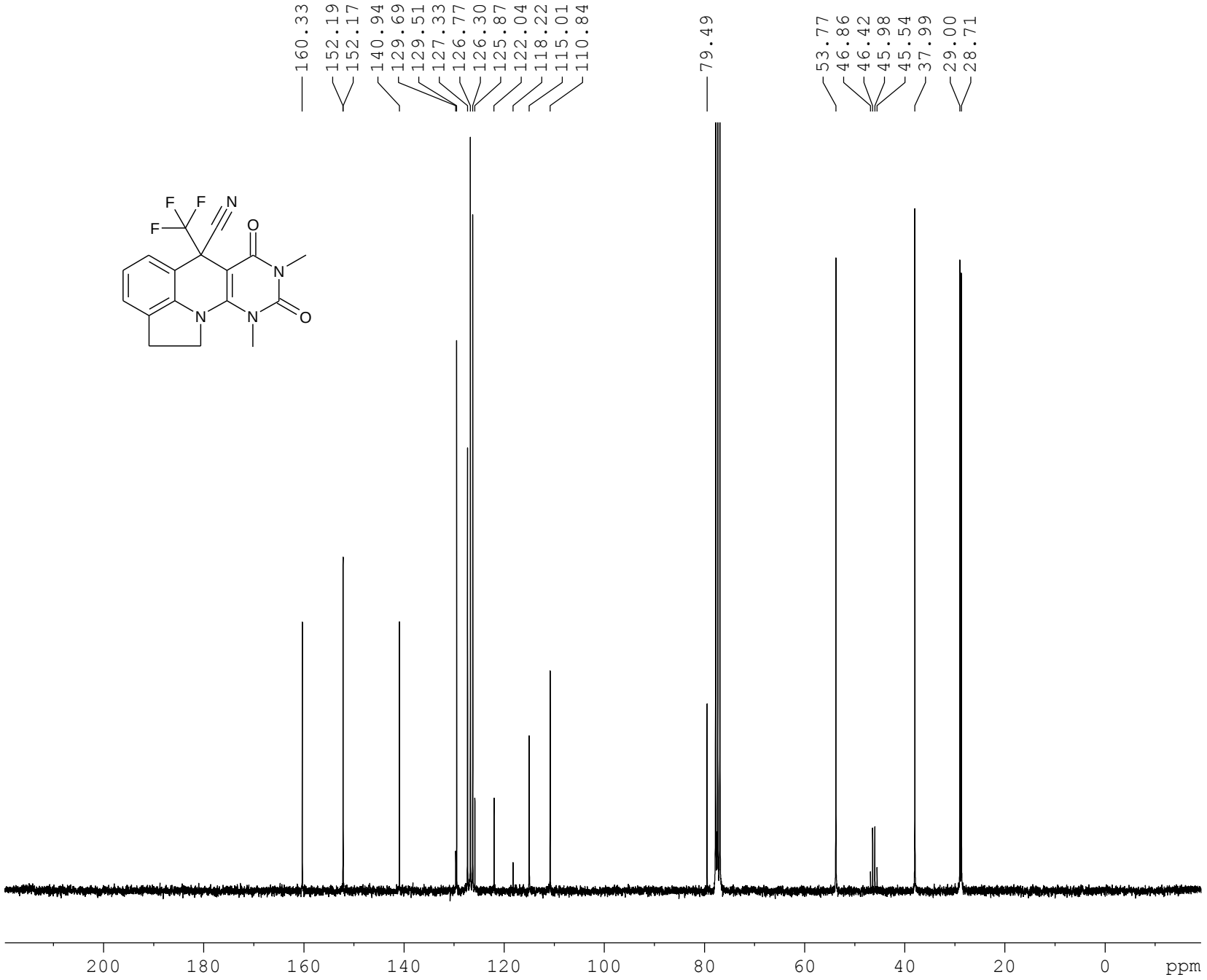
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             72.00 usec
PL2       0 dB
PL12              17.00 dB
PL13              17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677147 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin sd315 1H CDCl3



Dudkin sd315 13C CDCl3



Current Data Parameters
NAME 111028.u317
EXPNO 10
PROCNO 1

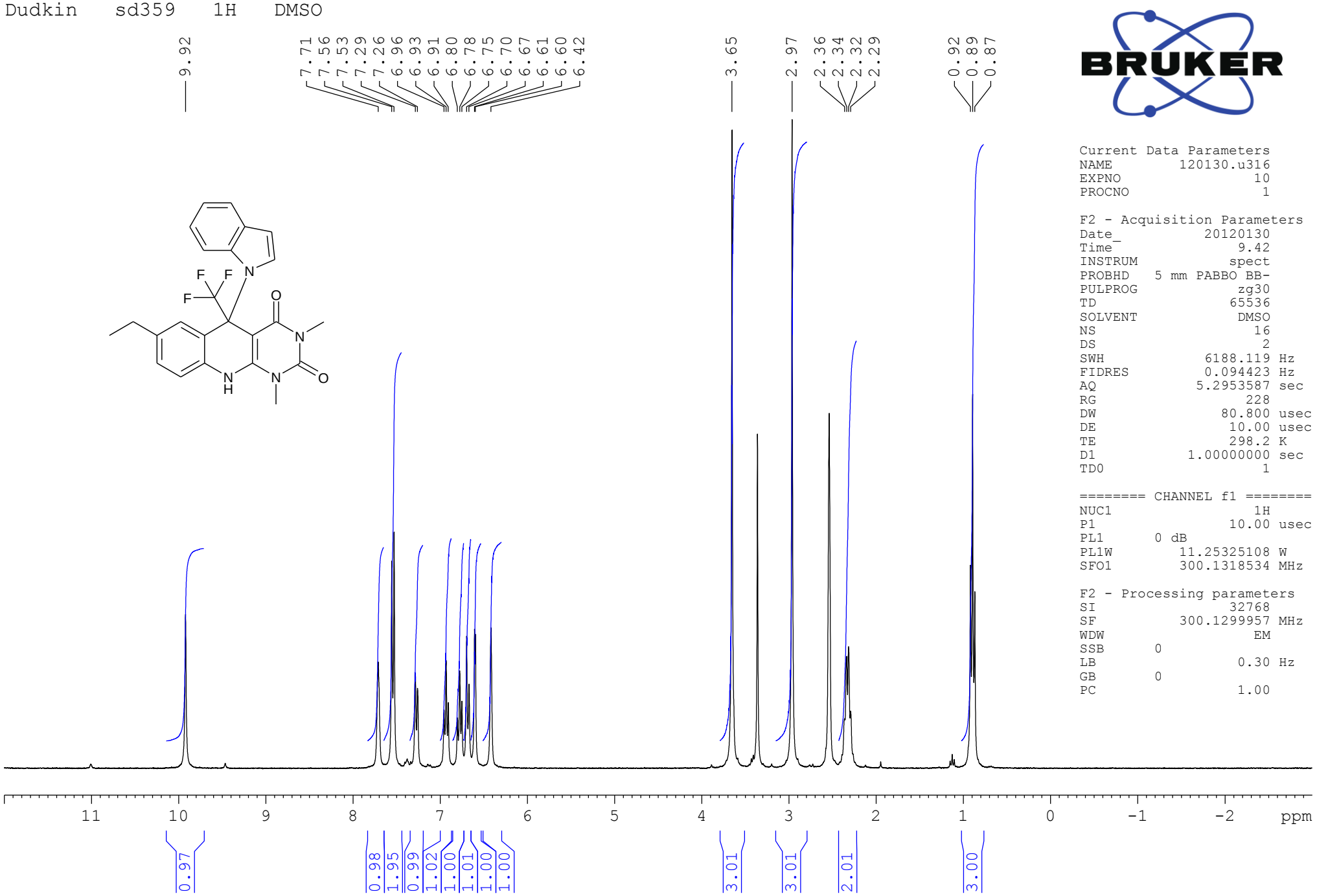
F2 - Acquisition Parameters
Date_ 20111029
Time 7.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677287 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd359 1H DMSO



Current Data Parameters
NAME 120130.u316
EXPNO 10
PROCNO 1

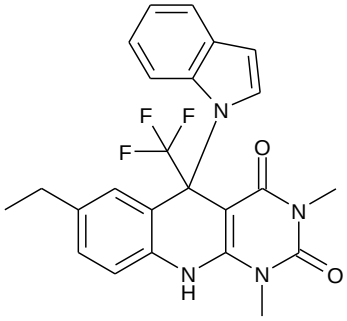
F2 - Acquisition Parameters
Date_ 20120130
Time 9.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 228
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299957 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd359 13C DMSO

159.42 151.16 147.89 139.79 135.66 134.12 133.41 130.70 130.24 129.63 128.69 127.22 124.10 121.69 121.41 120.09 119.55 117.83 117.69 112.89 101.93 78.65 65.99 65.52 65.05 64.57 31.47 28.26 28.24 16.24



Current Data Parameters
NAME 120203.207
EXPNO 11
PROCNO 1

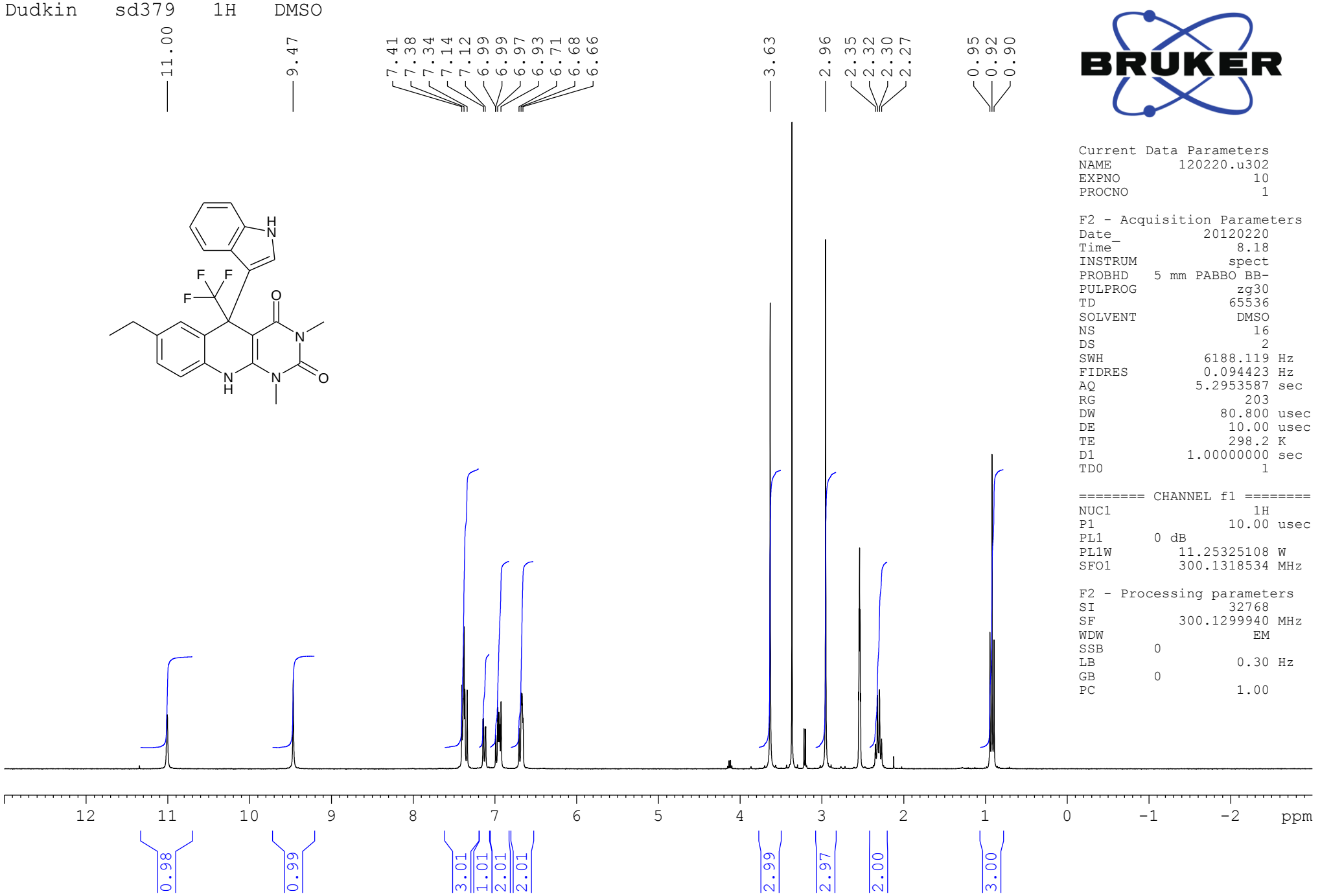
F2 - Acquisition Parameters
Date_ 20120204
Time 2.16
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.20 usec
PL1 0 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 14.00 dB
PL13 14.00 dB
PL2 -3.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin sd379 1H DMSO



Current Data Parameters
NAME 120220.u302
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120220
Time 8.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 203
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

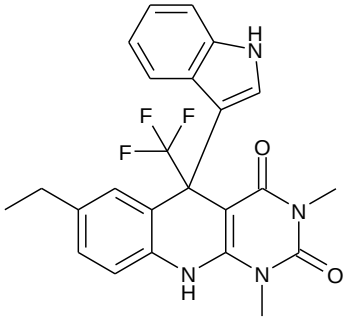
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299940 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd379 13C DMSO

159.73 151.43 148.02 138.70 137.00 135.44 134.72 130.85 130.15 129.08 126.77 126.26 123.91 121.67 121.40 120.36 120.09 118.91 117.16 114.38 112.30 81.11

50.36 49.93 49.50 49.07 31.24 28.33 28.32 16.35



Current Data Parameters
NAME 120301.205
EXPNO 10
PROCNO 1

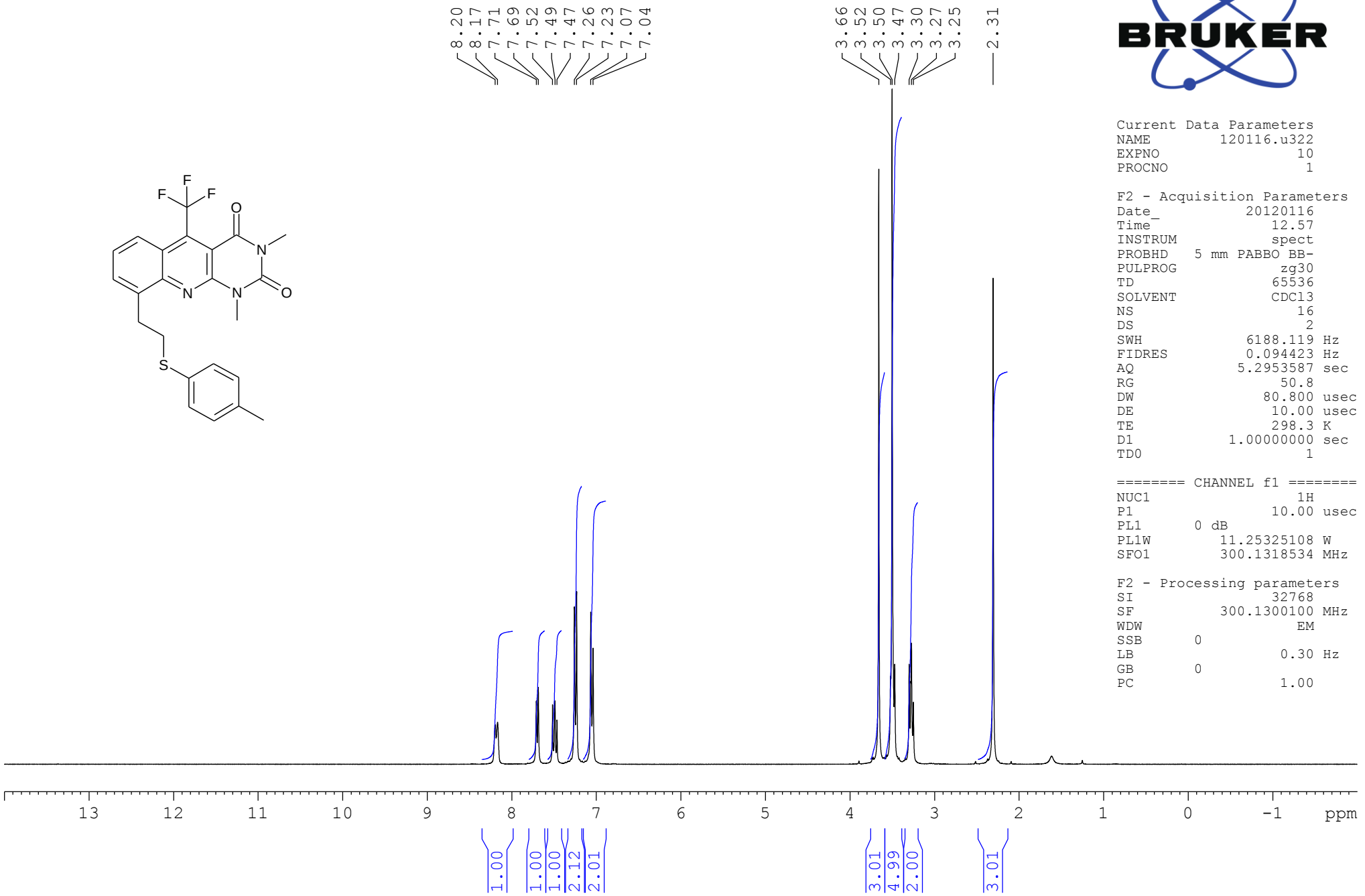
F2 - Acquisition Parameters
Date_ 20120301
Time 22.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952090 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Dudkin, sd 346, CDCl3, 1H



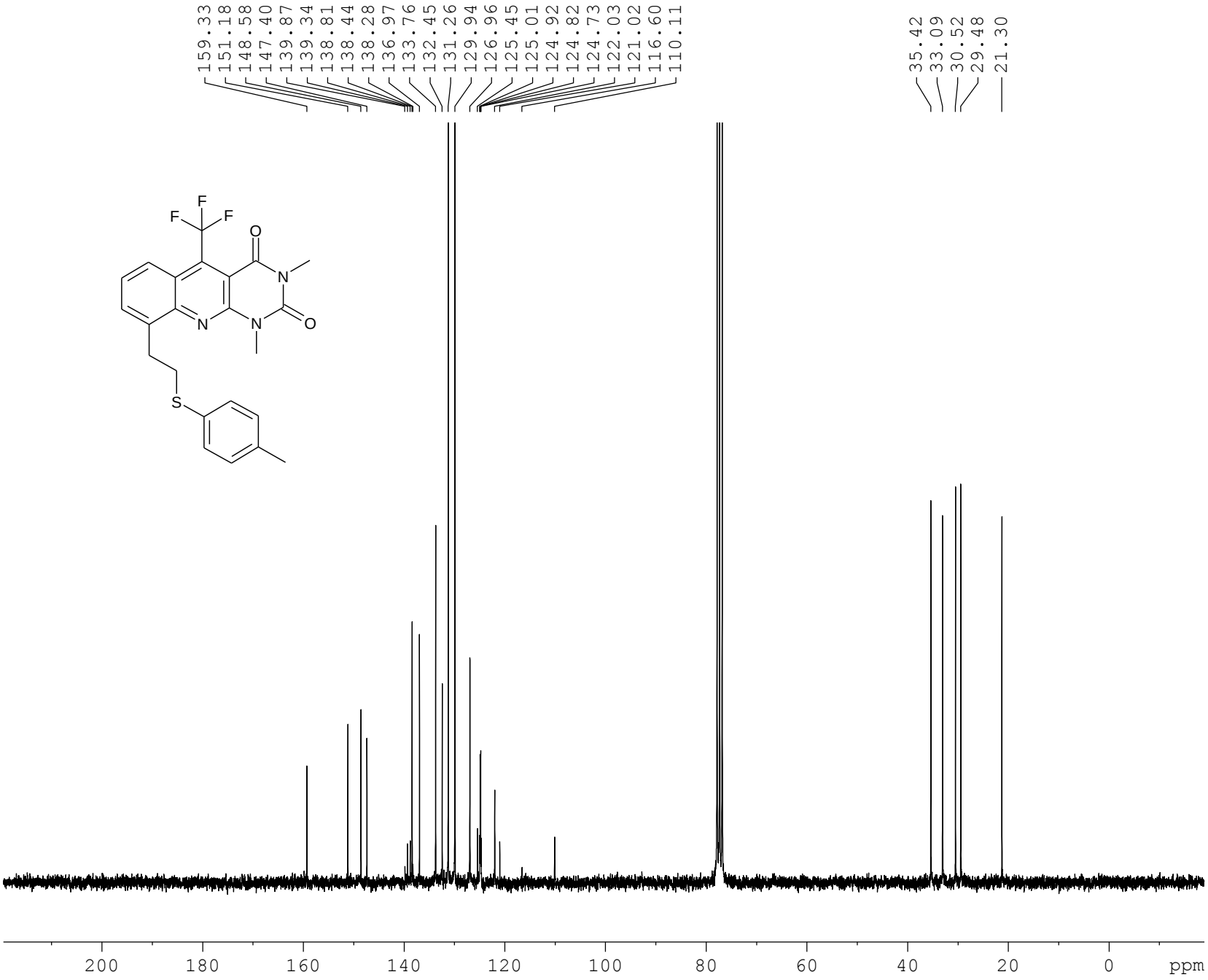
Current Data Parameters
NAME 120116.u322
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120116
Time 12.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 50.8
DW 80.800 usec
DE 10.00 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd346 13C CDCl3




```
Current Data Parameters
NAME          120118.201
EXPNO                 10
PROCNO                 1

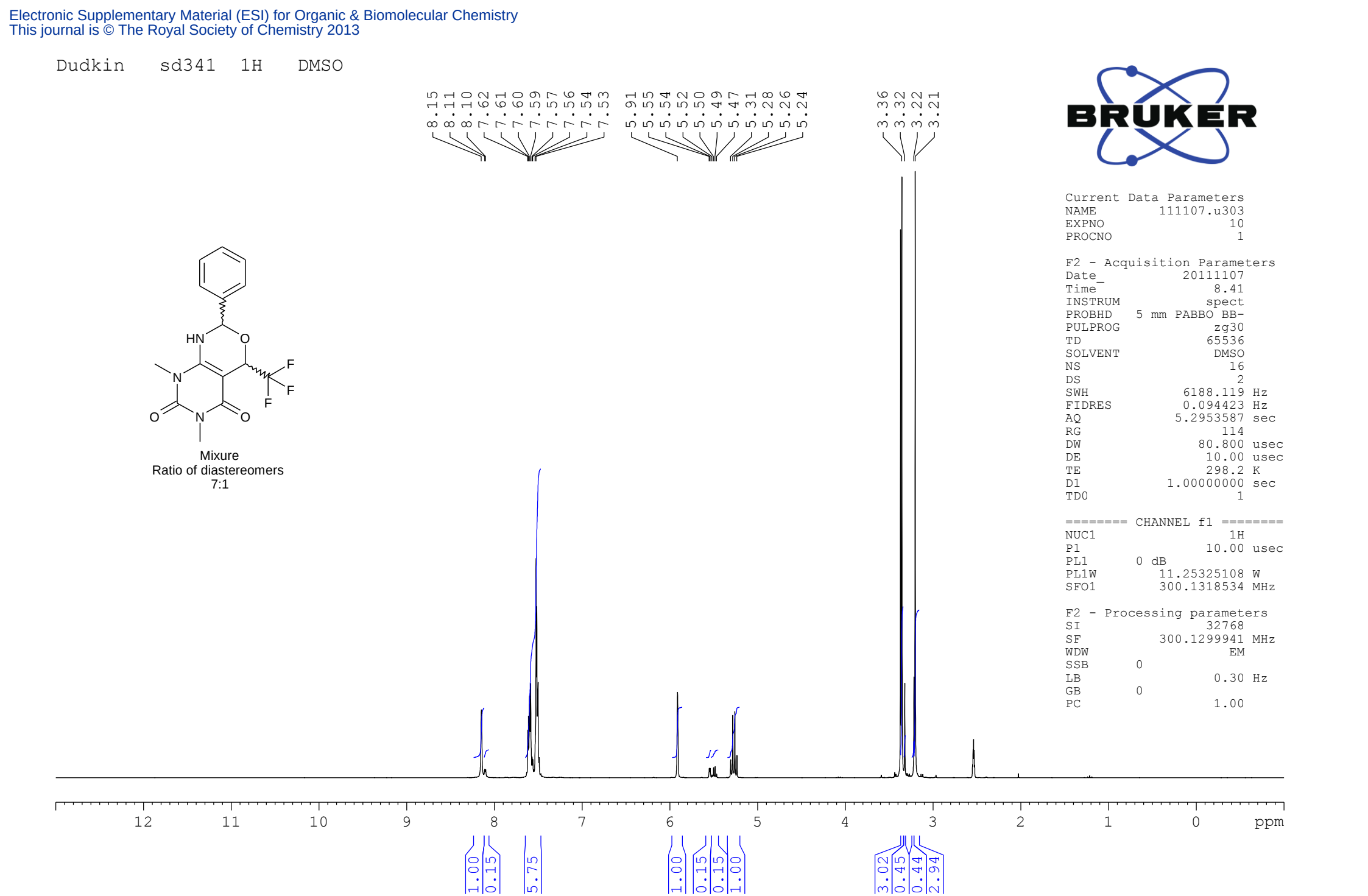
F2 - Acquisition Parameters
Date_           20120118
Time               12.53
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2869
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1       0 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              14.00 dB
PL13              14.00 dB
PL2               -3.00 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952180 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Dudkin sd341 1H DMSO



Current Data Parameters
NAME 111107.u303
EXPNO 10
PROCNO 1

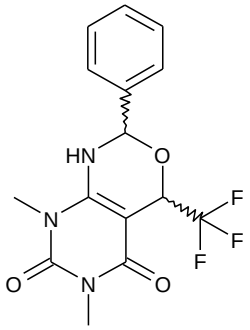
F2 - Acquisition Parameters
Date_ 20111107
Time 8.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 114
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299941 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dudkin sd378 13C DMSO

160.36 160.23 154.03 151.60 151.54 150.49 137.57 136.97 132.58 130.77 130.43 129.44 129.31 128.57 128.47 128.00 123.43 118.86 82.97 82.22 81.90 81.86 77.21 77.18 71.60 71.10 70.59 70.40 70.08 69.90 69.40 68.90 30.40 30.13 28.24



Mixure
Ratio of diastereomers
7:1


```
Current Data Parameters
NAME          120224.202
EXPNO                 10
PROCNO                 1

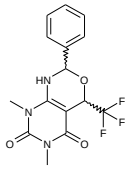
F2 - Acquisition Parameters
Date_           20120224
Time               19.14
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ             2.1845834 sec
RG                 2050
DW               33.333 usec
DE                10.00 usec
TE                298.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1       0 dB
SFO1          62.9015280 MHz

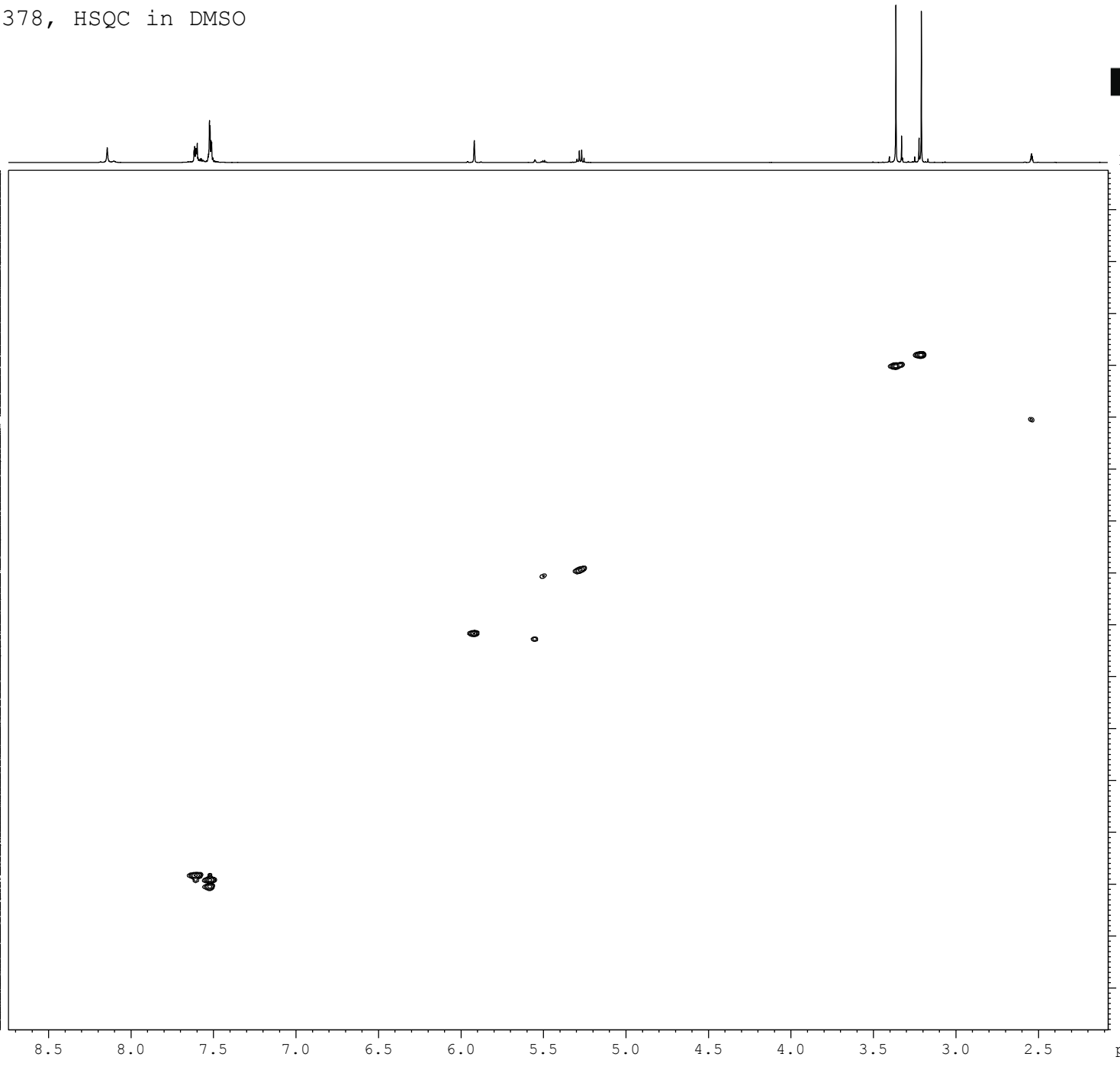
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              14.00 dB
PL13              14.00 dB
PL2               -3.00 dB
SFO2         250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952076 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Dudkin, sd 378, HSQC in DMSO



Mixure
Ratio of diastereomers
7:1




```
Current Data Parameters
NAME            120302.502
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120302
Time                 14.24
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG     hsqcetgpsi2
TD                   1024
SOLVENT               DMSO
NS                       2
DS                      16
SWH             3333.333 Hz
FIDRES          3.255208 Hz
AQ            0.1536500 sec
RG                   13004
DW               150.000 usec
DE                 6.50 usec
TE                 300.1 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.42320001 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00002400 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                   9.80 usec
P2                  19.60 usec
P28       0 usec
PL1                 -3.00 dB
SFO1         500.1326829 MHz

======== CHANNEL f2 ========
CPDPRG2               garp
NUC2                   13C
P3                   9.00 usec
P4                  18.00 usec
PCPD2               72.00 usec
PL2                  4.50 dB
PL12                22.00 dB
SFO2         125.7672177 MHz

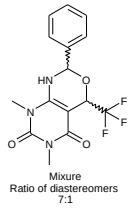
====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPNAM3           SINE.100
GPNAM4           SINE.100
GPZ1                80.00 %
GPZ2                20.10 %
GPZ3                11.00 %
GPZ4                -5.00 %
P16               1000.00 usec
P19                600.00 usec

F1 - Acquisition parameters
TD                     256
SFO1           125.7672 MHz
FIDRES         81.380234 Hz
SW               165.650 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                    1024
SF           500.1299769 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                    1024
MC2        echo-antiecho
SF           125.7577541 MHz
WDW                 SINE
SSB                     2
LB        0 Hz
GB        0
```

Dudkin, sd 378, HMBC in DMSO



Mixure
Ratio of diastereomers
7:1


```
Current Data Parameters
NAME          120302.502
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120302
Time               14.41
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG       hmbcgpndqf
TD                  4096
SOLVENT              DMSO
NS                     16
DS                     16
SWH            3333.333 Hz
FIDRES          0.813802 Hz
AQ             0.6144500 sec
RG                 16384
DW               150.000 usec
DE                 6.50 usec
TE                300.1 K
CNST13         8.0000000
D0             0.00000300 sec
D1             1.19280005 sec
D6             0.06250000 sec
D16            0.00020000 sec
IN0            0.00001790 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   9.80 usec
P2                  19.60 usec
PL1                 -3.00 dB
SFO1         500.1326829 MHz

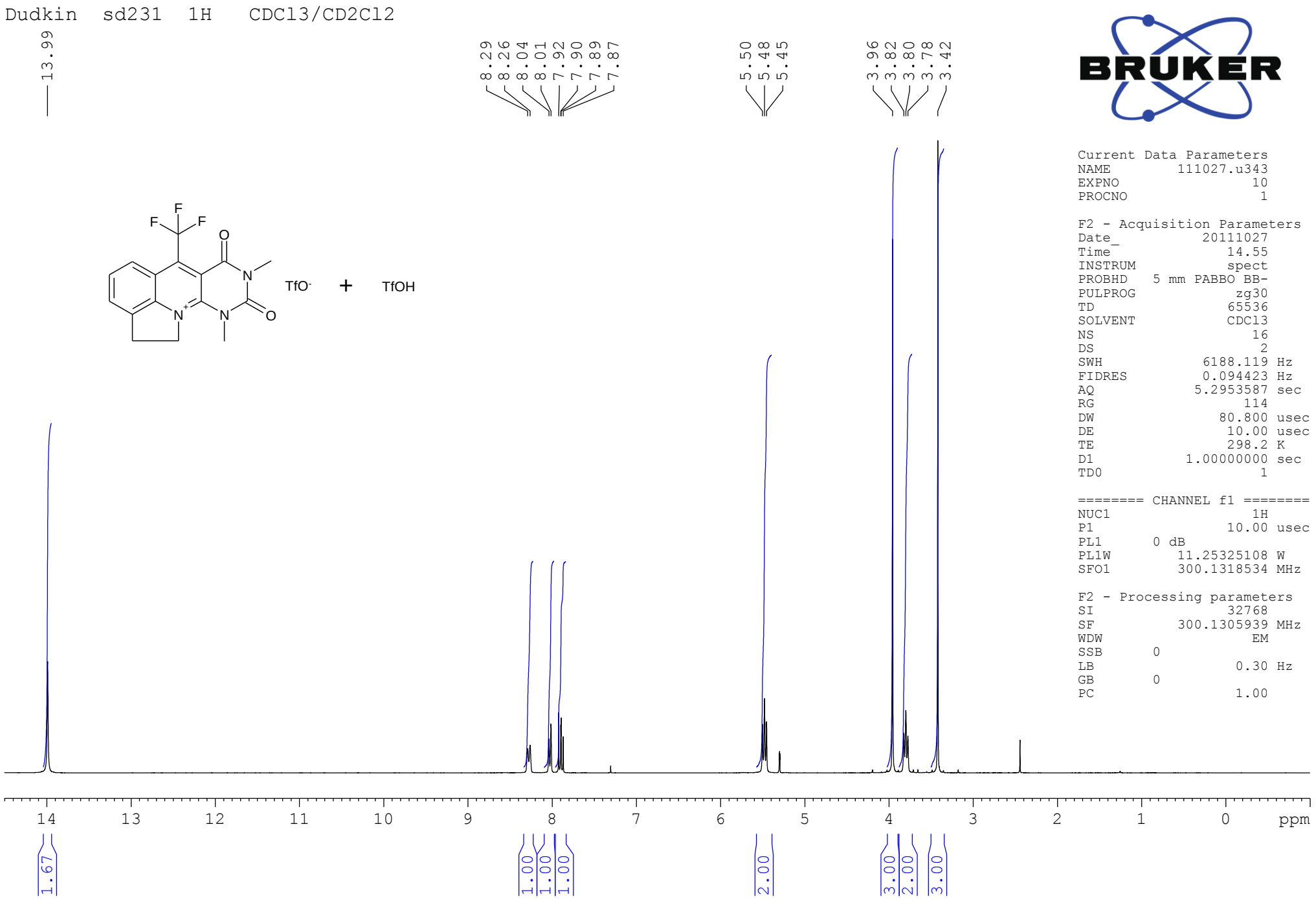
======== CHANNEL f2 ========
NUC2                  13C
P3                   9.00 usec
PL2                  4.50 dB
SFO2         125.7703443 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPNAM3           SINE.100
GPZ1                50.00 %
GPZ2                30.00 %
GPZ3                40.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    128
SFO1           125.7703 MHz
FIDRES         218.226349 Hz
SW               222.095 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF           500.1299724 MHz
WDW                  SINE
SSB       0
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF           125.7577246 MHz
WDW                States
SSB       0
LB        0 Hz
GB        0
```

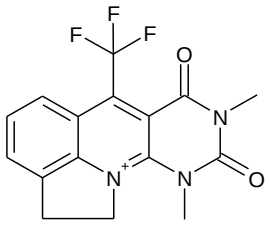


Dudkin sd231 13C CDCl3/CD2Cl2

155.85
149.33
149.22
145.86
145.39
144.91
144.44
143.35
134.47
133.13
131.89
127.12
125.14
124.68
124.60
124.52
124.45
123.41
120.93
120.46
119.71
116.72
116.01
115.61
112.52

60.02

36.60
30.02
27.84



TfO⁻ + TfOH

Current Data Parameters
NAME 111028.u316
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111029
Time 3.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4678811 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40