3-Methoxalylchromone – A Novel Versatile Reagent for the Regioselective Purine Isostere Synthesis

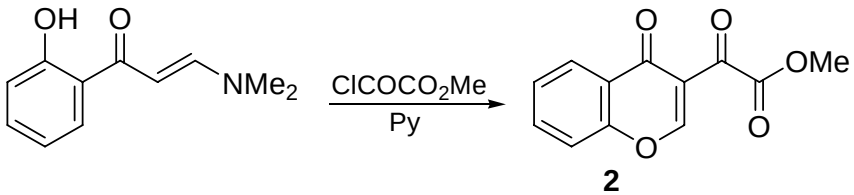
Satenik Mkrtchyan,[a] Viktor O. Iaroshenko,[a,b]* Sergii Dudkin,[a] Ashot Gevorgyan,[a] Marcelo Vilches-Herrera,[a] Gagik Ghazaryan,[a] Dmitriy M. Volochnyuk,[b,c] Dmytro Ostrovskyi,[a] Zeeshan Ahmed,[a] Alexander Villinger,[a] Vyacheslav Ya. Sosnovskikh,[d] Peter Langer[a,e]*

[a] *Institut für Chemie, Universität Rostock,, Albert-Einstein-Str. 3a, 18059 Rostock, Germany. Fax: 00 49 381 49864112; Tel: 0049 381 4986410; E-mail: viktor.iaroshenko@uni-rostock.de, iva108@googlemail.com, peter.langer@uni-rostock.de*
[b] *National Taras Shevchenko University, 62 Volodymyrska st., Kyiv-33, 01033, Ukraine.E-mail: iva108@googlemail.com.*
[c] *"Enamine Ltd." 23 A. Matrosova st., 01103 Kyiv, Ukraine.*
[d] *Department of Chemistry, Ural State University, 620083 Ekaterinburg, Russian Federation*
[e] *Leibniz-Institut für Katalyse e. V. an der Universität Rostock,, Albert-Einstein-Str. 29a, 18059 Rostock, Germany.*

General: Reactions were monitored by thin layer chromatography using UV light to visualize the course of reaction. Purification of reaction products were carried out by flash chromatography on silica gel. Column chromatography was performed on silica gel (63 – 200 mesh, Merck). Silica gel Merck 60F254 plates were used for TLC. Satisfactory microanalysis obtained C ± 0.33; H ± 0.45; N ± 0.25.

Chemical yields refer to pure isolated substances. ^{1}H and ^{13}C NMR spectra were obtained using a Bruker DPX-300 spectrometer. Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, h = heptet, m = multiplet, br = broad.

General procedures for the synthesis of 3-methoxalylchromone **(2)**

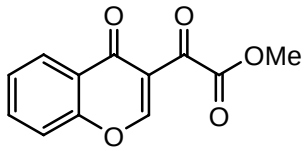


2

To a round-bottom 250 ml flask, fitted with a septum, containing 20 g (0.105 mol) of 3-(dimethylamino)-1-(2-hydroxyphenyl)prop-2-en-1-one, dissolved in 100 ml of dry dichloromethane, 28 ml of dry pyridine (3,3 eq.) was added. The solution was set on stirring

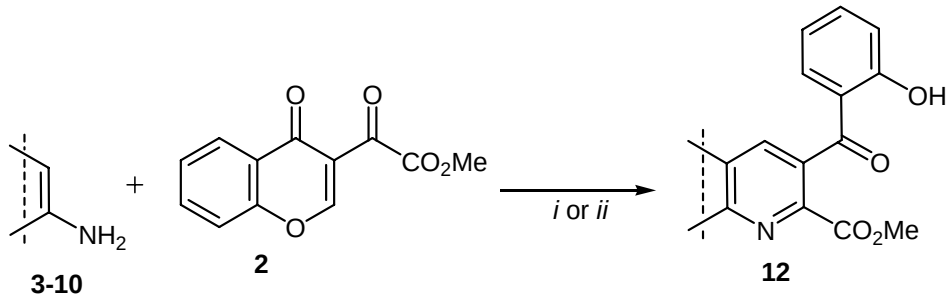
on ice bath, and 10,60 ml (1,1 eq.) of methyloxalylchloride was added dropwise. The reaction mixture stirred at the room temperature for 8 hours, and after was stripped of solvents and liquid residues. The obtained solid was washed well with water to give 19,1 g (79%) of 3-methoxalylchromone, as light pink crystals.

(2)



Yellow solid (0.8 mol, 18.6g, 80 %) mp 133-135 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 3.88 (s, 3H, OMe), 7.61 (t, 1H, ^{3}J = 7.3 Hz, CH_{Ar}), 7.78-7.81 (m, 1H, CH_{Ar}), 7.90-7.95 (m, 1H, CH_{Ar}), 8.11 (dd, 1H, ^{3}J = 7.9 Hz, ^{4}J = 1.5 Hz, CH_{Ar}), 9.12 (s, 1H, Pyranone).
^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 52.7, 118.5, 118.9, 123.9, 125.2, 127.0, 135.6, 155.6, 164.0, 164.6, 174.1, 184.6.
MS (GC, 70 eV): *m/z* (%) = 232 (M^+, 3), 204 (21), 189 (16), 173 (100), 121 (40).
HRMS (ESI): calcd for $C_{12}H_8O_5$ (M+H) 233.0459, found 233.0461.

General procedures for the synthesis of pyridines **(12)**



Reagents and conditions: (i): AcOH, reflux, 2–5 h (for **3**, **4**, **6**, **7**, **8**); (ii): DMF/TMSCl, 80–100 ^{o}C (for **5**).

A: In acetic acid

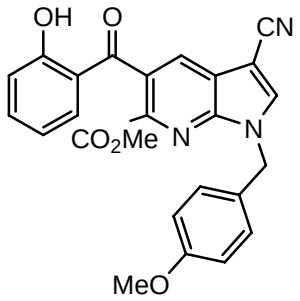
1.56 mmol of the corresponding amine and 1.2 mmol of 3-methoxalylchromone (**2**) were dissolved in 20 ml of acetic acid and heated under reflux in the inert atmosphere during 2–5 h (controlled by TLC). Then the solution was evaporated under reduced pressure, treated with water, filtrated, dried on the air and recrystallized from an appropriate solvent, or was subjected to a column chromatography over silica gel.

B: In DMF/TMSCl

In the pressure tube, 1.56 mmol of the corresponding amine and 1.2 mmol of 3-methoxalylchromone (**2**) in inert atmosphere were dissolved in 8 ml of dry DMF and 1 ml of TMSCl was added. The reaction mixture was heated at 80–100 ^{o}C for 5 h (controlled by TLC). Then the solution was evaporated under reduced pressure, treated with water, filtrated, dried on the air and recrystallized from an appropriate solvent, or was subjected to a column chromatography over silica gel.

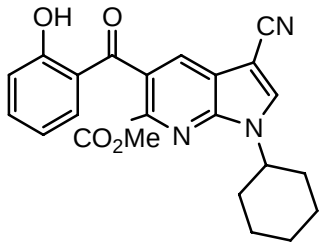
Compounds:

(12a)



Brown solid (1.01 mmol, 447 mg, 78%), mp 186-187 ^{0}C. ^{1}H NMR (250 MHz, DMSO-d_6): δ = 3.72 (s, 6 H, 2 MeO), 5.54 (s, 2 H, CH_2), 6.91–7.02 (m, 4 H, Ar), 7.34–7.55 (m, 4 H, Ar), 8.39 (s, 1 H, Py), 8.88 (s, 1 H, =CHN), 11.06 (s, 1 H, OH);
^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 47.9, 52.7, 55.1, 84.3, 114.1, 114.2, 117.4, 119.3, 120.4, 121.8, 128.2, 128.5, 129.4, 131.2, 132.1, 135.8, 141.6, 142.1, 145.1, 159.1, 159.8, 165.4, 197.7;
MS (EI, 70 eV): *m/z* (%) = 441 (M^+, 27), 121 (100), 91 (13), 77 (20);
HRMS (ESI): calcd for $C_{25}H_{19}O_4N_4$ (M+H) 442.1244, found 442.1242;
IR (ATR): ν = 3056 (w), 2946 (w), 2236 (w), 1645 (m), 1627 (m), 1600 (m), 1515 (m), 1481 (w), 1458 (m), 1446 (m), 1409 (m), 1360 (s), 1332 (w), 1309 (m), 1291 (s), 1256 (m), 1244 (m), 1217 (m), 1209 (m), 1155 (w), 1142 (m), 1114 (w), 1084 (w), 1038 (w), 993 (w), 932 (w), 918 (m), 905 (m), 887 (w), 857 (w), 827 (w), 781 (m), 763 (s), 751 (s),741 (s), 726 (s), 675 (w), 653 (m), 616 (m), 575 (w), 560 (m), 531 (w) cm^{-1}.

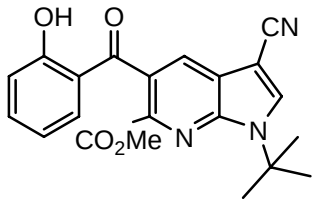
(12b)



Brown solid (0.98 mmol, 393 mg, 75%), mp 185–187 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 1.25-2.05 (m, 10 H, 5 CH_2), 3.71 (s, 3 H, MeO), 4.79–4.81 (m, 1 H, NCH), 6.90 (td, 1 H, ^{3}J

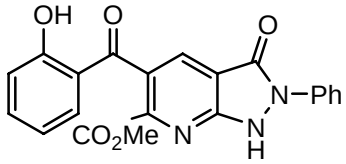
= 8.0 Hz, ^4J = 0.9 Hz, H-5′), 6.99 (d, 1 H, ^3J = 8.3 Hz, H-3′), 7.37 (dd, 1 H, ^3J = 7.7 Hz, ^4J = 1.7 Hz, H-6′), 7.50–7.53 (m, 1 H, H-4′), 8.36 (s, 1 H, Py), 8.99 (s, 1 H, =CHN), 11.05 (s, 1 H, OH);
^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 24.7, 25.1, 32.4, 52.8, 54.3, 84.1, 114.5, 117.4, 119.3, 120.4, 121.9, 128.5, 131.0, 132.0, 135.8, 139.5, 141.9, 144.7, 160.0, 165.5, 197.6;
MS (GC, 70 eV): *m/z* (%) = 403 (M^+, 6), 371 (5), 344 (M^+ – CO_2Me, 100), 289 (23), 262 (38);
HRMS (ESI): calcd for $C_{23}H_{21}O_4N_3$ (M^+ + 1) 404.1605, found 404.1607;
IR (ATR): ν = 3113 (w), 2933 (w), 2855 (w), 2226 (m), 1719 (m), 1636 (m), 1607 (m), 1524 (w), 1483 (w), 1448 (m), 1425 (m), 1399 (m), 1374 (m), 1341 (w), 1300 (m), 1263 (s), 1247 (s), 1202 (s), 1164 (m), 1147 (s), 1119 (m), 1083 (m), 1034 (w), 1008 (w), 958 (w), 919 (w), 903 (w), 874 (w), 858 (w), 818 (w), 785 (w), 748 (s), 706 (m), 671 (m), 644 (m), 630 (m), 614 (m), 529 (m) cm^{-1}.

(12c)



Yellow solid (1.16 mmol, 436 mg, 89%), mp 145-147 ^{0}C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.88 (s, 9 H, 3 CH_3), 3.78 (s, 3 H, MeO), 6.79 (td, 1 H, ^3J = 8.0 Hz, ^4J = 0.9 Hz, H-5′), 7.06 (d, 1 H, ^3J = 8.0 Hz, H-3′), 7.16 (dd, 1 H, ^3J = 7.8 Hz, ^4J = 1.5 Hz, H-6′), 7.45–7.51 (m, 1 H, H-4′), 8.10 (s, 1 H, Py), 8.12 (s, 1 H, =CHN), 11.82 (s, 1 H, OH);
^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 28.6, 52.7, 59.4, 83.0, 114.6, 117.4, 119.3, 121.7, 121.8, 127.9, 130.7, 132.1, 135.8, 140.2, 140.5, 145.3, 159.8, 165.4, 197.8;
MS (GC, 70 eV): *m/z* (%) = 377 (M^+, 4), 318 (49), 289 (35), 262 (100);
HRMS (ESI): calcd for $C_{21}H_{19}O_4N_3$ (M^+ + 1) 378.1448, found 378.1448;
IR (ATR): ν = 3140 (w), 2224 (m), 1709 (m), 1628 (m), 1606 (m), 1519 (w), 1484 (w), 1452 (m), 1436 (m), 1417 (m), 1377 (m), 1326 (w), 1301 (m), 1264 (s), 1244 (s), 1198 (s), 1163 (m), 1147 (m), 1119 (m), 1102 (m), 1073 (w), 1031 (w), 947 (m), 877 (m), 821 (m), 764 (m), 729 (s), 973 (m), 622 (m) cm^{-1}.

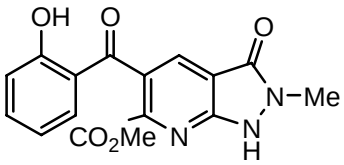
(12d)



Green solid (0.74 mmol, 288 mg, 57%), mp 222-224 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 3.76 (s, 3 H, MeO), 6.93–7.02 (m, 2 H, H-5′, H-3′), 7.33 (t, 1 H, ^3J = 7.6 Hz, Ph), 7.46–7.58 (m, 4 H, H-6′, H-4′, Ph), 7.88 (d, 2 H, ^3J = 8.1 Hz, Ph), 8.34 (s, 1 H, Py), 10.77 (s, 1 H, OH);
^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 52.8, 110.0, 117.2, 119.4, 120.1, 122.6, 126.0, 128.0, 129.2, 131.5, 135.2, 135.8, 136.4, 152.0, 155.2, 157.0, 158.5, 165.6, 195.2;
MS (EI, 70 eV): *m/z* (%) = 389 (M^+, 14), 357 (28), 344 (11), 330 (M^+ – CO_2Me, 100);
HRMS (ESI): calcd for $C_{21}H_{15}O_5N_3$ (M^+ + 1) 390.1084, found 390.1083;

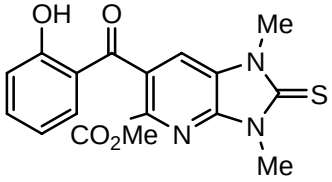
IR (ATR): ν = 3033 (w), 2957 (w), 2916 (w), 2849 (w), 1720 (w), 1643 (s), 1626 (m), 1609 (m), 1596 (m), 1573 (w), 1496 (w), 1482 (w), 1463 (w), 1438 (w), 1414 (w), 1356 (m), 1296 (m), 1253 (m), 1237 (s), 1201 (m), 1182 (m), 1147 (m), 1120 (m), 1088 (m), 1053 (w), 1033 (w), 962 (w), 949 (w), 928 (w), 870 (w), 828 (w), 807 (w), 799 (w), 784 (w), 752 (s), 684 (s), 662 (m), 644 (m), 602 (m), 569 (m), 540 (m) cm^{-1}.

(12e)



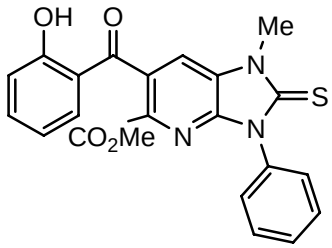
White solid (1.04 mmol, 340 mg, 80%), mp 245-247 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 3.49 (s, 3 H, NMe), 3.73 (s, 3 H, MeO), 6.91–7.01 (m, 2 H, H-5′, H-3′), 7.41 (t, 1 H, ^3J = 7.8 Hz, H-6′), 7.50 (d, 2 H, ^3J = 7.5 Hz, H-4′), 8.22 (s, 1 H, Py), 10.71 (s, 1 H, OH), 12.37 (s, 1 H, NH);
^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 30.7, 52.7, 108.4, 117.2, 119.3, 122.8, 126.5, 131.4, 135.0, 135.3, 151.7, 153.4, 156.6, 158.3, 165.9, 195.3;
MS (EI, 70 eV): *m/z* (%) = 327 (M^+, 9), 295 (10), 268 (100), 239 (12), 196 (10), 121 (18),
HRMS (ESI): calcd for $C_{16}H_{13}O_5N_3$ (M+1) 328.0928, found 328.0927;
IR (ATR): ν = 3106 (w), 1715 (m), 1682 (s), 1614 (s), 1598 (m), 1567 (w), 1480 (w), 1439 (m), 1404 (w), 1360 (w), 1310 (m), 1241 (s), 1196 (m), 1174 (m), 1148 (s), 1115 (w), 1080 (w), 1031 (w), 973 (w), 936 (m), 918 (m), 850 (w), 825 (w), 803 (w), 786 (m), 767 (s), 731 (s), 723 (s), 651 (s), 632 (m), 614 (s) cm^{-1}.

(12f)



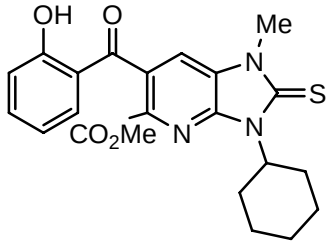
White solid (0.92 mmol, 330 mg, 71%), mp 273-275 ^{0}C. ^{1}H NMR (250 MHz, DMSO-d_6): δ = 3.33 (br s, 3 H, MeN), 3.73 (br s, 6 H, MeN, MeO), 6.88–7.01 (m, 2 H, H-5′, H-3′), 7.32–7.54 (m, 2 H, H-6′, H-4′), 8.07 (s, 1 H, Py), 11.20 (s, 1 H, OH);
^{13}C NMR (75.5 MHz, DMSO-*d*): δ = 26.2, 32.5, 52.6, 115.4, 117.6, 119.4, 121.3, 131.7, 136.3, 137.9, 138.1, 140.2, 145.6, 160.0, 163.9, 175.4, 195.7;
MS (GC, 70 eV): *m/z* (%) = 357 (M^+, 1), 325 (100), 297 (M^+ – 1 – CO_2Me, 22), 281 (14), 264 (23), 207 (18);
HRMS (ESI): calcd for $C_{17}H_{15}N_3O_4S$ (M+H) 358.0856, found 358.0849;
IR (ATR): ν = 3072 (w), 2950 (w), 1716 (m), 1631 (m), 1614 (w), 1582 (w), 1485 (m), 1444 (m), 1417 (s), 1397 (m), 1350 (m), 1328 (m), 1302 (s), 1272 (s), 1246 (s), 1215 (s), 1163 (m), 1149 (m), 1123 (s), 1056 (w), 1033 (w), 987 (w), 961 (w), 912 (w), 872 (m), 822 (m), 797 (m), 749 (s), 711 (m), 675 (m), 664 (w), 631 (m), 586 (w), 567 (m) cm^{-1}.

(12g)



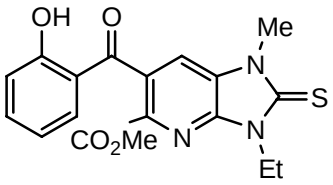
White solid (0.95 mmol, 398 mg, 73%), mp 291-292 ^{0}C. ^{1}H NMR (250 MHz, DMSO-d_6, 80^{0}C): δ = 3.57 (s, 3 H, MeN), 3.81 (s, 3 H, MeO), 6.88 (t, 1 H, ^3J = 7.2 Hz, H-5′), 7.02 (d, 1 H, ^3J = 8.0 Hz, H-3′), 7.35 (d, 1 H, ^3J = 7.1 Hz, H-6′), 7.54–7.63 (m, 6 H, H-4′, Ph), 8.04 (s, 1 H, Py), 11.10 (s, 1 H, OH);
^{13}C NMR (125.7 MHz, DMSO-d_6, 303 K): δ = 31.3, 52.4, 115.7, 117.4, 119.1, 121.1, 128.0, 128.5, 129.0, 129.1, 132.0, 133.3, 134.2, 136.0, 138.3, 145.1, 160.1, 164.7, 173.5, 197.6;
MS (EI, 70 eV): *m/z* (%) = 419 (M^+, 10), 387 (55), 360 (M^+ – CO_2Me, 100), 342 (15), 121 (14), 93 (10), 77 (33), 65 (18), 51 (11);
HRMS (EI): calcd for $C_{22}H_{17}N_3O_4S$ (M^+) 419.09343, found 419.09360;
IR (ATR): ν = 3053 (w), 2958 (w), 1710 (m), 1668 (w), 1621 (m), 1607 (s), 1580 (w), 1498 (m), 1489 (m), 1469 (m), 1447 (s), 1419 (s), 1387 (s), 1340 (s), 1328 (s), 1296 (m), 1267 (s),1237 (s), 1224 (s), 1192 (m), 1165 (m), 1148 (m), 1125 (s), 1109 (m), 1073 (w), 1055 (m), 1030 (m), 970 (w), 954 (m), 924 (w), 904 (w), 879 (m), 864 (m), 824 (w), 816 (w), 798 (m), 786 (w), 760 (s), 704 (s), 689 (s), 672 (m), 631 (m), 570 (m), 545 (m) cm^{-1}.

(12h)



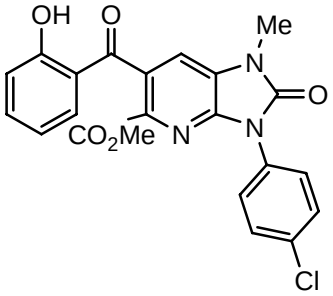
Pink solid (0.83 mmol, 354 mg, 64%), mp 220-222 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 1.16–1.95 (m, 10 H), 3.37 (m, 1 H, CHN), 3.70 (s, 3 H, MeN), 3.75 (s, 3 H, MeO), 6.89–6.94 (m, 1 H, H-5′), 7.03 (d, 1 H, ^3J = 7.7 Hz, H-3′), 7.46–7.56 (m, 2 H, H-4′, H-6′), 8.08 (s, 1 H, Py), 11.01 (s, 1 H, OH);
^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 24.2, 24.7, 31.8, 48.6, 53.0, 112.4, 117.6, 119.3, 120.2, 121.3, 128.6, 131.7, 134.2, 136.2, 137.9, 138.1, 145.8, 160.0, 163.9, 195.7;
MS (GC, 70 eV): *m/z* (%) = 425 (M^+, 33), 382 (100), 366 (M^+ – CO_2Me, 62), 310 (9), 284 (17);
HRMS (EI): calcd for $C_{22}H_{23}N_3O_4S$ (M^+) 425.14038, found 425.14045;
IR (ATR): ν = 3062 (w), 2929 (w), 2853 (w), 2677 (w), 2509 (w), 2414 (w), 2139 (w), 1947 (w), 1737 (m), 1627 (s), 1614 (s), 1574 (s), 1495 (w), 1452 (m), 1438 (m), 1408 (w), 1377 (w), 1340 (m), 1297 (m), 1275 (w), 1241 (s), 1178 (m), 1150 (m), 1129 (m), 1069 (w), 1031 (w), 1002 (w), 976 (w), 912 (w), 887 (m), 834 (w), 822 (m), 793 (m), 758 (s), 7.24 (m), 712 (s), 679 (m), 663 (m), 603 (m), 559 (m) cm^{-1}.

(12i)



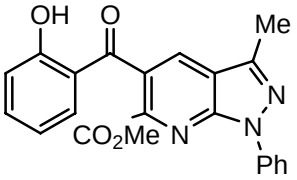
Yellow solid (0.91 mmol, 338 mg, 70%), mp 212-213 ^{0}C ^{1}H NMR (500 MHz, DMSO-d_6, 70 ^{0}C): δ = 1.34 (t, 3 H, ^3J = 7.2 Hz, Me), 3.48 (q, 2 H, ^3J = 7.2 Hz, CH_2), 3.69 (s, 6 H, MeO, MeN), 6.90 (t, 1 H, ^3J = 8.0 Hz, H-5′), 7.04 (d, 1 H, ^3J = 8.0 Hz, H-3′), 7.10–7.42 (m, 1 H, H-4′), 7.52-7.55 (m, 1 H, H-6′), 7.94 (s, 1 H, Py), 11.0 (s, 1 H, OH);
^{13}C NMR (125.8 MHz, DMSO-d_6, 70 ^{0}C): δ = 13.8, 31.9, 46.0, 52.1, 116.3, 117.4, 118.9, 120.9, 131.5, 135.9, 137.0, 137.7, 138.2, 141.6, 145.8, 160.0, 163.6, 196.1;
MS (GC, 70 eV): *m/z* (%) = 371 (M^+, 11), 356 (23), 324 (18), 312 (100);
HRMS (ESI): calcd for $C_{18}H_{17}N_3O_4S$ (M^+ + 1) 372.1013, found 372.1015;
IR (ATR): ν = 3078 (w), 2983 (w), 2952 (w), 2561 (w), 1719 (m), 1625 (s), 1609 (s), 1575 (s), 1555 (m), 1485 (m), 1438 (m), 1404 (w), 1369 (m), 1348 (m), 1328 (m), 1299 (s), 1261 (s), 1243 (s), 1216 (s), 1184 (s), 1148 (m), 1126 (s), 1107 (m), 1088 (m), 1032 (w), 998 (w), 953 (w), 922 (w), 910 (m), 887 (m), 821 (m), 800 (m), 759 (s), 731 (s), 710 (m), 985 (s), 666 (m), 603 (w), 656 (w), 549 (w) cm^{-1}.

(12j)



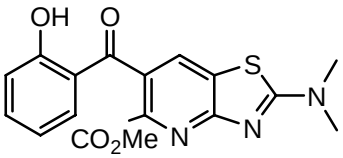
White solid (0.90 mmol, 392 mg, 69%), mp 275-277 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 3.46 (s, 3 H, MeN), 3.60 (s, 3 H, MeO), 6.87 (td, 1 H, ^3J = 8.0 Hz, ^4J = 0.9 Hz, H-5′), 7.03 (dd, 1 H, ^3J = 8.0 Hz, ^4J = 0.9 Hz, H-3′), 7.30 (dd, 1 H, ^3J = 8.0 Hz, ^4J = 1.6 Hz, H-6′), 7.55 (td, 1 H, ^3J = 8.0 Hz, ^4J = 1.6 Hz, H-4′), 7.66–7.76 (m, 4 H, C_6H_4), 7.88 (s, 1 H, Py), 11.30 (s, 1 H, OH);
^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 27.5, 52.3, 113.5, 117.6, 119.3, 121.1, 127.1, 128.2, 129.1, 131.8, 132.1, 132.3, 133.0, 135.7, 136.2, 142.6, 152.8, 160.4, 164.9, 198.6;
MS (EI, 70 eV): *m/z* (%) = 437 (M^+, 3), 405 (24), 378 (M^+ – CO_2Me, 100), 348 (11);
HRMS (EI): calcd for $C_{22}H_{16}ClN_3O_5$ (M^+) 437.07730, found 437.07733;
IR (ATR): ν = 3063 (w), 2953 (w), 1735 (s), 1713 (s), 1628 (s), 1612 (m), 1583 (w), 1499 (m), 1482 (s), 1450 (m), 1420 (m), 1399 (m), 1318 (w), 1301 (m), 1260 (s), 1245 (s), 1217 (s), 1190 (m), 1165 (m), 11550 (m), 1133 (w), 1118 (m), 1106 (m), 1095 (m), 1086 (m), 1058 (w), 1032 (w), 1015 (m), 961 (w), 929 (s), 910 (m), 874 (w), 846 (m), 835 (w), 826 (m), 799 (w), 758 (s), 742 (s), 733 (s), 708 (m), 674 (m), 624 (w), 587 (s), 566 (m) cm^{-1}.

(12k)



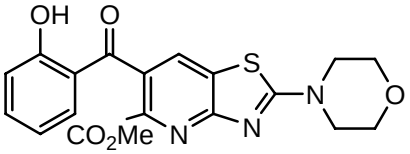
Yellow solid (0.95 mmol, 368 mg, 73%), mp 179-180 ^{0}C. ^{1}H NMR (500 MHz, DMSO-d_6): δ = 2.65 (s, 3 H, Me), 3.72 (s, 3 H, MeO), 6.93 (t, 1 H, ^3J = 7.8 Hz, H-5′), 7.01 (d, 1 H, ^3J = 8.0 Hz, H-3′), 7.37 (t, 1 H, ^3J = 7.4 Hz, H-4′), 7.48 (dd, 1 H, ^3J = 8.2 Hz, ^4J = 1.6 Hz, H-6′), 7.52–7.60 (m, 3 H, Ph), 8.23 (d, 2 H, ^3J = 7.7 Hz, Ph), 8.65 (s, 1 H, Py), 10.94 (s, 1 H, OH);
^{13}C NMR (125.7 MHz, DMSO-d_6): δ = 12.2, 52.8, 116.9, 117.4, 119.3, 120.4, 122.1, 126.2, 129.3, 129.6, 131.9, 132.2, 135.7, 138.5, 144.3, 147.0, 148.8, 159.4, 165.5, 196.8;
MS (GC, 70 eV): *m/z* (%) = 387 (M^+, 5), 328 (M^+ – CO_2Me, 100);
HRMS (ESI): calcd for $C_{22}H_{17}N_3O_6$ (M^+ + 1) 388.1292, found 388.1297;
IR (ATR): ν = 3049 (w), 2925 (w), 1710 (m), 1625 (w), 1610 (w), 1595 (m), 1556 (w), 1504 (w), 1486 (m), 1441 ‘(m), 1415 (w), 1377 (w), 1330 (w), 1292 (m), 1266 (s), 1240 (s), 1223 (s), 1166 (s), 1151 (m), 1119 (m), 1102 (m), 1050 (w), 1034 (w), 1011 (w), 943 (m), 874 (w), 837 (w), 819 (w), 800 (w), 780 (m), 752 (s), 709 (m), 691 (s), 667 (s), 637 (s), 618 (m), 588 (m), 569 (m), 530 (m) cm^{-1}.

(12l)



Yellow solid (0.88 mmol, 316 mg, 68%), mp 190-192 ^{0}C. ^{1}H NMR (250 MHz, DMSO-d_6): δ = 3.23 (s, 6 H, 2 MeN), 3.67 (s, 3 H, MeO), 6.90 (td, 1 H, ^3J = 8.0 Hz, ^4J = 1.0 Hz, H-5′), 7.00 (dd, 1 H, ^3J = 8.0 Hz, ^4J = 1.0 Hz, H-3′), 7.36 (dd, 1 H, ^3J = 7.8 Hz, ^4J = 1.7 Hz, H-6′), 7.48–7.54 (m, 1 H, H-4′), 8.40 (s, 1 H, Py), 11.00 (s, 1 H, OH);
^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 40.0, 52.3, 117.4, 119.3, 122.1, 127.5, 127.6, 130.1, 131.7, 135.5, 144.8, 159.4, 164.5, 165.9, 171.9, 197.3;
MS (GC, 70 eV): *m/z* (%) = 357 (M^+, 1), 298 (M^+ – CO_2Me, 100);
HRMS (ESI): calcd for $C_{17}H_{15}N_3O_4S$ (M^+ + 1) 358.0856, found 358.0856;
IR (ATR): ν = 3031 (w), 2947 (w), 1712 (m), 1625 (w), 1601 (s), 1562 (m), 1504 (w), 1483 (w), 1436 (m), 1417 (m), 1386 (w), 1352 (m), 1335 (s), 1286 (s), 1254 (s), 1228 (s), 1151 (m), 1122 (s), 1104 (s), 1062 (w), 1030 (w), 960 (w), 943 (m), 927 (w), 915 (w), 877 (w), 832 (w), 811 (m), 771 (s), 760 (s), 725 (m), 705 (w), 678 (m), 632 (w), 619 (m), 566 (w), 535 (w) cm^{-1}.

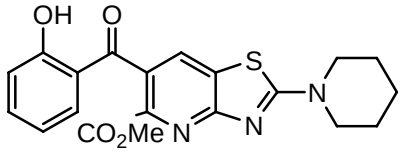
(12m)



Brown solid (0.92 mmol, 368 mg, 71%), mp. 244-246 ^{0}C. ^{1}H NMR (500 MHz, DMSO-d_6): δ = 3.67 (s, 3 H, MeO), 3.70–3.77 (m, 8 H, morph.), 6.90 (td, 1 H, ^3J = 8.1 Hz, ^4J = 1.0 Hz, H-5′), 7.00 (dd, 1 H, ^3J = 8.0 Hz, ^4J = 1.0 Hz, H-3′), 7.36 (dd, 1 H, ^3J = 8.0 Hz, ^4J = 1.6 Hz, H-6′), 7.50–7.53 (m, 1 H, H-4′), 8.44 (s, 1 H, Py), 10.97 (s, 1 H, OH);

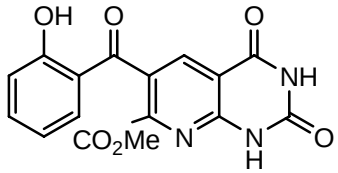
^{13}C NMR (125.8 MHz, DMSO-d_6): δ = 48.0, 52.3, 65.4, 117.4, 119.3, 122.0, 127.2, 128.2, 130.4, 131.7, 135.5, 144.7, 159.4, 164.1, 165.8, 172.1, 197.2;
MS (EI, 70 eV): *m/z* (%) = 399 (M^+, 3), 367 (10), 340 (M^+ – CO_2Me, 100), 282 (13), 69 (12);
HRMS (ESI): calcd for $C_{19}H_{17}N_3O_5S$ (M^+ + 1) 400.0962, found 400.0964;
IR (ATR): ν = 3065 (w), 2970 (w), 2922 (w), 2854 (w), 1716 (m), 1623 (w), 1598 (m), 1558 (s), 1507 (w), 1484 (w), 1437 (m), 1423 (m), 1389 (m), 1350 (m), 1331 (s), 1299 (m), 1280 (s), 1257 (s), 1240)s), 1205 (s), 1146 (m), 1124 (m), 1105 (s), 1063 (s), 1024 (m), 957 (w), 939 (m), 885 (m), 862 (w), 829 (w), 808 (w), 795 (w), 757 (s), 743 (s), 717 (m), 677 (m), 624 (m), 603 (m), 567 (w) cm^{-1}.

(12n)



Orange solid (1.00 mmol, 397 mg, 77%), mp 166-168 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 1.66 (s, 6 H, 3 CH_2), 3.66 (s, 7 H, 2 CH_2N, MeO), 6.88–6.93 (m, 1 H, H-5′), 7.00 (dd, 1 H, ^3J = 8.2 Hz, ^4J = 0.8 Hz, H-3′), 7.35 (dd, 1 H, ^3J = 7.8 Hz, ^4J = 1.6 Hz, H-6′), 7.48–7.54 (m, 1 H, H-4′), 8.38 (s, 1 H, Py), 11.00 (s, 1 H, OH);
^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 23.4, 24.9, 49.2, 52.3, 117.4, 119.2, 122.0, 127.3, 127.7, 130.0, 131.7, 135.5, 144.7, 159.5, 164.6, 165.9, 171.3, 197.3;
MS (EI, 70 eV): *m/z* (%) = 397 (M^+, 14), 365 (48), 338 (M^+ – CO_2Me, 100), 308 (24), 282 (38), 269 (18), 121 (11), 69 (10), 41 (15);
HRMS (ESI): calcd for $C_{20}H_{19}O_4N_3S$ (M^+ + 1) 398.1169, found 398.1177;
IR (ATR): ν = 3057 (w), 2938 (w), 2852 (w), 1711 (m), 1672 (m), 1586 (m), 1547 (s), 1505 (m), 1487 (m), 1461 (w), 1439 (m), 1428 (m), 1392 (m), 1346 (s), 1324 (s), 1296 (m), 1283 (s), 1274 (s), 1238 (s), 1215 (s), 1155 (m), 1124 (s), 1106 (s), 1033 (w), 1008 (w), 960 (w), 941 (m), 890 (m), 883 (m), 855 (m), 830 (w), 813 (w), 799 (w), 756 (s), 730 (s), 719 (s), 699 (m), 677 (m), 655 (w), 632 (s), 579 (w), 566 (w), 534 (w)cm^{-1}.

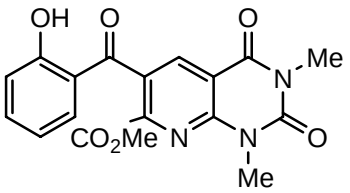
(12o)



White solid (0.83 mmol, 284 mg, 64%), mp 262-264 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 3.73 (s, 3 H, MeO), 6.92–7.00 (m, 2 H, H-5′, H-3′), 7.43 (dd, 1 H, ^3J = 7.9 Hz, ^4J = 1.6 Hz, H-6′), 7.48–7.54 (m, 1 H, H-4′), 8.32 (s, 1 H, Py), 10.68 (s, 1 H, OH), 11.73 (s, 1 H, NH), 12.22 (s, 1 H, NH);
^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 52.9, 111.0, 117.2, 119.5, 122.7, 129.1, 131.3, 135.3, 138.4, 150.3, 152.3, 153.1, 158.3, 161.5, 165.2, 194.3;
MS (EI, 70 eV): *m/z* (%) = 341 (M^+, 7), 282 (M^+ – CO_2Me, 100), 238 (41), 210 (22), 121 (19), 65 (10);
HRMS (ESI): calcd for $C_{16}H_{11}N_3O_6$ (M^+ + 1) 342.0721, found 342.0726;
IR (ATR): ν = 3197 (w), 3095 (w), 2811 (w), 1748 (w), 1731 (m), 1692 (m), 1636 (m), 1604 (m), 1574 (m), 1505 (w), 1484 (w), 1447 (w), 1399 (w), 1360 (w), 1328 (m), 1309 (w), 1270

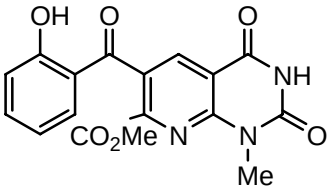
(s), 1243 (m), 1218 (m), 1170 (w), 1147 (m), 1116 (w), 1053 (w), 1015 (w), 962 (w), 920 (w), 829 (m), 818 (m), 805 (m), 793 (w), 759 (s), 722 (m), 688 (m), 657 (m), 627 (w), 584 (w), 555 (m), 532 (s) cm^{-1}.

(12p)



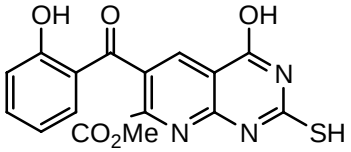
White solid (0.72 mmol, 264 mg, 55%), mp 203-204 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 3.31 (s, 3 H, NMe), 3.59 (s, 3 H, NMe), 3.74 (s, 3 H, MeO), 6.93-7.00 (m, 2 H, H-5′, H-3′), 7.45 (dd, 1H, ^3J = 7.4 Hz, ^4J = 1.6 Hz, H-6′), 7.49-7.55 (m, 1 H, H-4′), 8.44 (s, 1 H, Py), 10.66 (s, 1 H, OH);
^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 28.3, 29.5, 52.9 , 111.3, 117.2, 119.4, 122.7, 129.3, 131.2, 135.3, 138.7, 150.8, 151.1, 151.5, 158.2, 160.0, 165.1, 193.9;
MS (EI, 70 eV): *m/z* (%) = 369 (M^+, 1), 337 (71), 309 (51), 280 (21), 225 (10), 197 (100), 140 (9), 81 (10);
HRMS (ESI): calcd for $C_{18}H_{15}O_6N_3$ (M+1) 370.1034, found 370.1034;
IR (ATR): ν = 3060 (w), 1714 (m), 1660 (s), 1633 (s), 1603 (s), 1574 (m), 1464 (m), 1409 (w), 1352 (m), 1290 (s), 1264 (s), 1239 (s), 1214 (s), 1163 (m), 1151 (m), 1128 (w), 1081 (w), 1052 (w), 959 (w), 906 (m), 868 (m), 812 (w), 788 (s), 751 (s), 713 (m), 689 (m), 663 (m) cm^{-1}.

(12q)



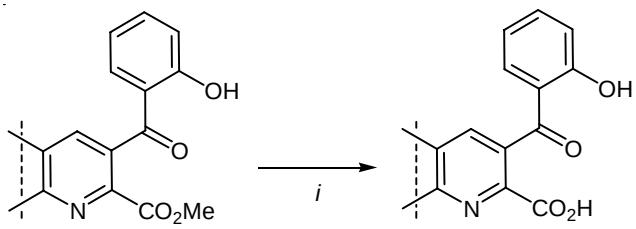
Yellow solid (0.78 mmol, 277 mg, 60%), mp 243-245 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 3.51 (s, 3 H, MeN), 3.74 (s, 3 H, MeO), 6.93-7.00 (m, 2 H, H-5′, H-3′), 7.43-7.54 (m, 2 H, H-6′, H-4′), 8.38 (s, 1 H, Py), 10.66 (s, 1 H, OH), 12.00 (s, 1 H, NH);
^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 28.6, 52.9, 112.1, 117.2, 119.4, 122.7, 128.9, 131.2, 135.3, 138.4, 150.5, 151.6, 152.6, 158.2, 160.4, 165.2, 194.0;
MS (EI, 70 eV): *m/z* (%) = 355 (M^+, 2), 296 (100), 253 (29), 197 (33), 121 (12);
HRMS (ESI): calcd for $C_{17}H_{12}N_3O_6$ (M^+ -1) 354.0732, found 354.0737;
IR (ATR): ν = 3051 (w), 1724 (m), 1690 (s), 1630 (s), 1598 (s), 1577 (m), 1470 (m), 1449 (m), 1371 (w), 1338 (m), 1297 (m), 1241 (s), 1207 (s), 1144 (m), 1122 (m), 1101 (m), 1024 (s), 965 (w), 940 (w), 896 (m), 854 (m), 828 (m), 785 (s), 751 (s), 711 (s), 672 (s), 640 (m) cm^{-1}.

(12r)



Yellow solid (0.57 mmol, 204 mg, 44%), mp 260-262 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 3.73 (s, 3 H, MeO), 6.93–7.00 (m, 2 H, H-5′, H-3′), 7.44–7.55 (m, 2 H, 6′, H-4′), 8.33 (s, 1 H, Py), 10.69 (s, 1 H, OH), 12.83 (s, 1 H, OH), 13.54 (s, 1 H, SH);
^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 52.9, 113.0, 117.2, 119.4, 122.5, 130.4, 131.3, 135.4, 138.1, 151.9, 152.3, 158.3, 158.9, 164.9, 176.6, 193.9;
MS (EI, 70 eV): *m/z* (%) = 357 (M^+, 15), 325 (13), 298 (M^+ – CO_2Me, 100), 281 (15), 239 (58), 210 (9), 121 (16), 78 (12), 63 (13);
HRMS (ESI): calcd for $C_{16}H_{11}O_5N_3S$ (M^+ + 1) 358.0492, found 358.0493;
IR (ATR): ν = 3090 (w), 3023 (w), 2916 (w), 1728 (m), 1682 (m), 1615 (s), 1594 (s), 1573 (m), 1551 (s), 1488 (w), 1450 (m), 1403 (w), 1368 (m), 1340 (m), 1317 (m), 1275 (s), 1245 (m), 1227 (s), 1135 (s), 1052 (m), 1027 (w), 968 (w), 954 (w), 921 (m), 861 (w), 835 (m), 813 (m), 799 (m), 783 (m), 760 (s), 733 (m), 705 (m), 694 (m), 652 (m), 640 (m), 613 (w), 566 (m), 554 (s), 528 (m) cm^{-1}

General procedures for the synthesis of acids **(13)**

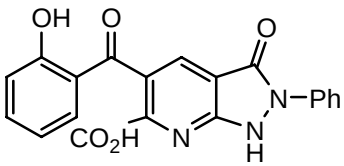


12d,k,l,p **13d,k,l,p**

Reagents and conditions: (i): a) MeOH, KOH, reflux, 2 h; b) conc. HCl.

Compound **12** (1 mmol) was dissolved in 15 ml of methanol and 0.224 g (4 mmol) of KOH was added, then the reaction mixture was kept under reflux for 2-3 hours. Afterwards reaction mixture was chilled to the room temperature and conc. HCl was added dropwise till the pH turned to be slightly acidic (pH = 4-5). The precipitate formed was filtrate, washed once with methanol and three times with distilled water, and dried on the air.

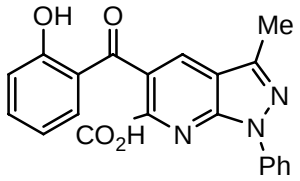
(13d)



White solid (0.80 mmol, 300 mg, 80%), mp 165-166 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 6.93-7.04 (m, 2 H, H-5′, H-3′), 7.34 (t, 1 H, ^3J = 7.4 Hz, Ph), 7.46-7.60 (m, 4 H, H-6′, H-4′,

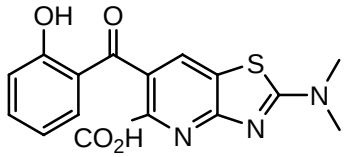
Ph), 7.91 (d, 2 H, ^3J = 7.6 Hz, Ph), 8.33 (s, 1 H, Py), 10.99 (s, 1 H, OH), 12.57 (s, 1 H, NH), 13.85 (s, 1 H, OH);
^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 110.0, 117.4, 119.3, 120.0, 122.2, 125.9, 128.1, 129.2, 131.9, 135.1, 135.5, 136.5, 153.3, 157.3, 166.5, 196.4;
MS (EI, 70 eV): *m/z* (%) = 375 (M^+, 14), 330 (100), 253 (37);
HRMS (ESI): calcd for $C_{20}H_{13}O_5N_3$ (M+1) 376.0928, found 376.0924;
IR (ATR): ν = 3401 (w), 3046 (w), 2910 (w), 1722 (m), 1682 (w), 1653 (s), 1625 (m), 1596 (s), 1575 (m), 1490 (s), 1461 (w), 1446 (m), 1348 (m), 1325 (w), 1304 (m), 1245 (s), 1199 (m), 1186 (m), 1156 (s), 1080 (w), 951 (w), 925 (m), 847 (w), 824 (m), 812 (m),762 (s), 706 (m), 691 (s), 655 (s), 635 (s) cm^{-1}.

(13k)



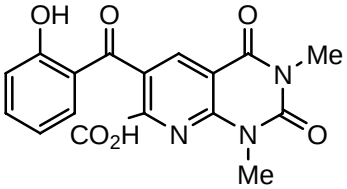
White solid (0.81 mmol, 302 mg, 82%), mp 128-130 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 2.65 (s, 3 H, Me), 6.89-7.02 (m, 2 H, H-5′, H-3′), 7.35-7.63 (m, 5 H, H-6′, Ph), 8.36 (d, 2 H, ^3J = 7.7 Hz, Ph), 8.61 (s, 1 H, Py), 11.19 (s, 1 H, OH), 13.71 (s, 1 H, OH);
^{13}C NMR (75.5 MHz, DMSO-d_6): δ = 12.2, 116.8, 117.5, 119.3, 120.3, 121.7, 126.1, 129.3, 129.7, 131.5, 132.3, 135.9, 138.6, 144.1, 137.9, 148.8, 160.1, 166.5, 198.0;
MS (EI, 70 eV): *m/z* (%) = 373 (M^+, 11), 328 (100), 251 (23), 236 (19);
HRMS (ESI): calcd for $C_{21}H_{15}O_4N_3$ (M+1) 374.1136, found 374.1135;
IR (ATR): ν = 3371 (w), 2920 (w), 1742 (m), 1721 (w), 1629 (s), 1598 (m), 1563 (w), 1484 (m), 1460 (m), 1444 (m), 1425 (m), 1397 (m), 1330 (m), 1294 (s), 1242 (s), 1142 (m), 1117 (m), 1103 (m), 1029 (m), 945 (s), 909 (m), 787 (m), 760 (s), 746 (s), 687 (s), 668 (s), 640 (s).

(13l)



White solid (0.79 mmol, 271 mg, 79%), mp 132-134 ^{0}C. ^{1}H NMR (250 MHz, DMSO-d_6): δ = 3.25 (s, 6 H, NMe_2), 6.89 (t, 1 H, ^3J = 7.7 Hz, H-5′), 6.99 (d, 1 H, ^3J = 8.1 Hz, H-3′), 7.31 (t, 1 H, ^3J = 7.8 Hz, ^4J = 1.3 Hz, H-6′), 7.48-7.55 (m, 1 H, H-4′), 8.36 (s, 1H, Py), 11.28 (s, 1 H, OH);
^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 39.7, 117.5, 119.3, 121.5, 127.7, 127.9, 129.6, 132.1, 135.8, 145.0, 160.3, 164.2, 166.7, 171.7, 198.7;
MS (EI, 70 eV): *m/z* (%) = 343 (M^+, 9), 298 (100), 254 (23);
HRMS (ESI): calcd for $C_{16}H_{13}O_4N_3S$ (M+1) 344.0689, found 344.0690;
IR (ATR): ν = 2924 (w), 2535 (w), 1706 (m), 1620 (m), 1597 (s), 1565 (s), 1519 (w), 1486 (w), 1449 (w), 1403 (s), 1339 (s), 1286 (s), 1239 (s), 1215 (s), 1151 (m), 1127 (m), 1106 (m), 1036 (w), 945 (m), 914 (w), 896 (m), 829 (w), 798 (w), 781 (w), 758 (s), 720 (s), 681 (m), 627 (m).

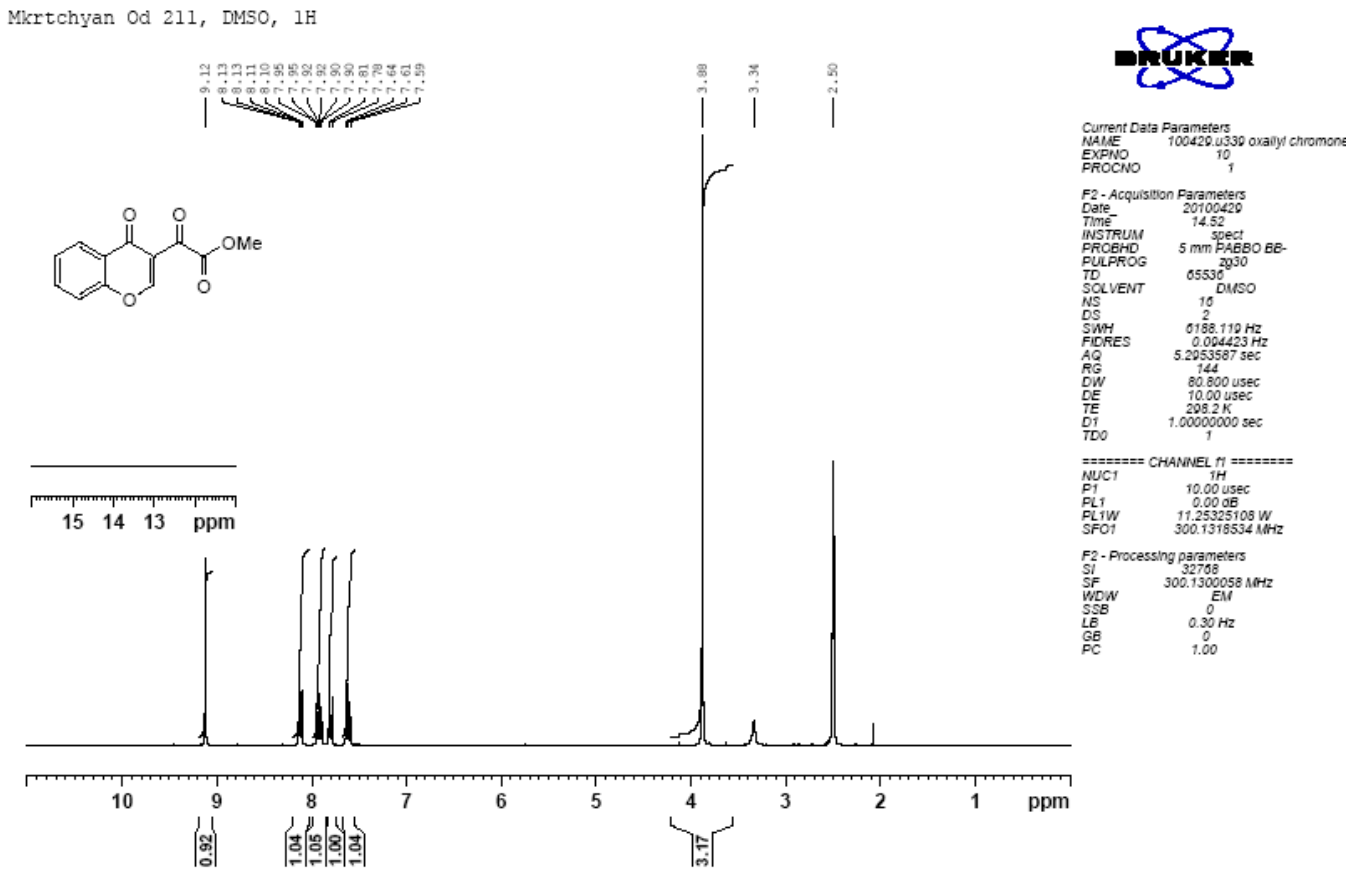
(13p)



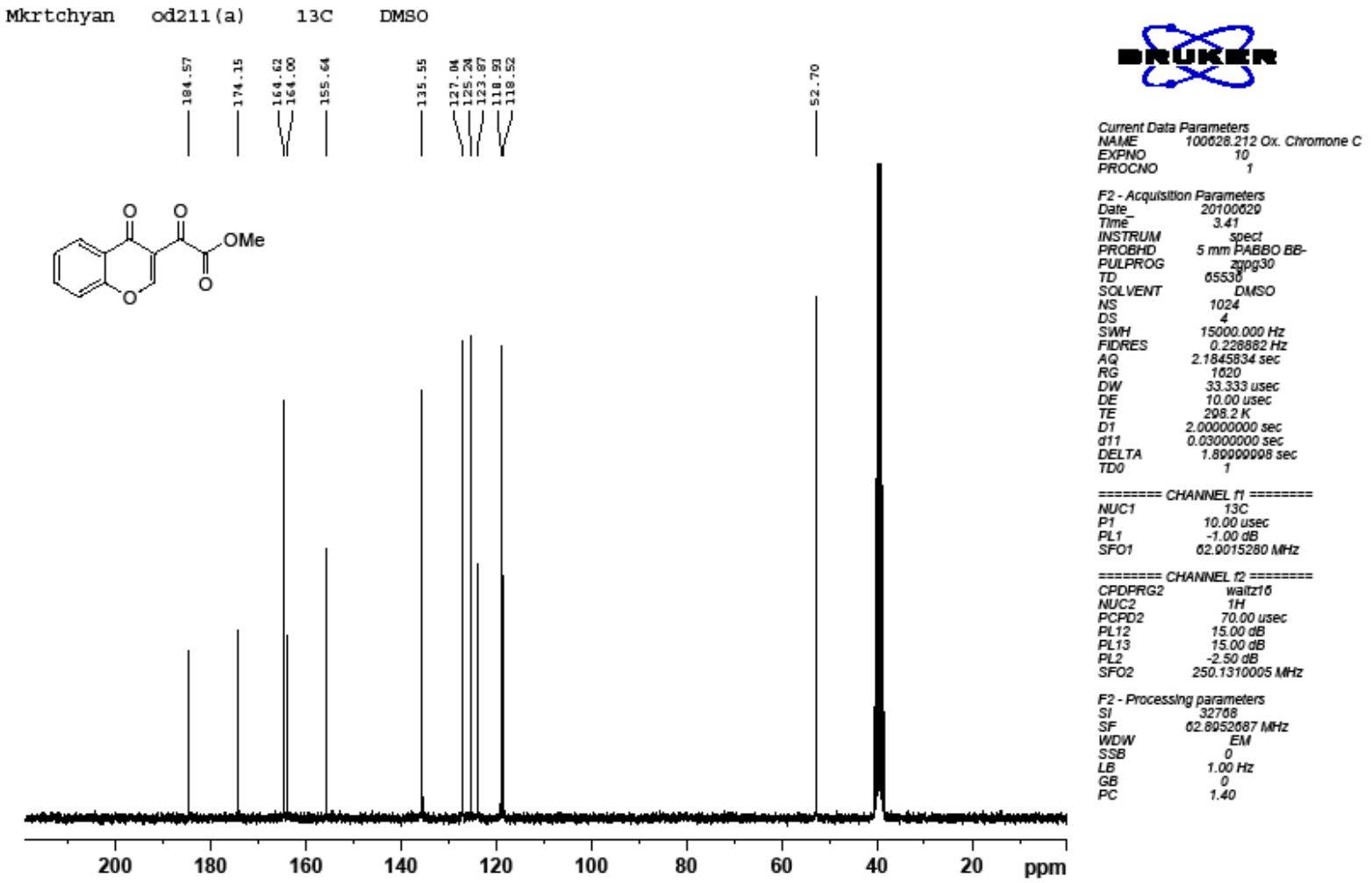
White solid (0.82 mmol, 291 mg, 81%), mp 254-256 ^{0}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ = 3.31 (s, 1 H, NMe), 3.62 (s, 1 H, NMe), 6.91-7.00 (m, 2 H, H-5´, H-3´), 7.41-7.55 (m, 2 H, H-6´, H-4´), 8.41 (s, 1 H, Py), 10.84 (s, 1 H, OH), 13.94 (s, 1 H, OH);
^{13}C NMR (62.9 MHz, DMSO-d_6): δ = 28.3, 29.5, 111.0, 117.3, 119.3, 122.2, 129.6, 131.5, 135.6, 138.1, 150.8, 150.9, 152.3, 160.0, 161.1, 166.0, 195.1;
MS (EI, 70 eV): *m/z* (%) = 355 (M^+, 7), 310 (100), 280 (15);
HRMS (ESI): calcd for $C_{17}H_{13}O_6N_3$ (M+1) 356.0877, found 356.087;
IR (ATR): ν = 3052 (w), 1706 (m), 1650 (s), 1625 (s), 1598 (s), 1471 (m), 1449 (m), 1409 (w), 1358 (m), 1288 (m), 1262 (w), 1213 (s), 1152 (s), 1085 ‘(w), 1052 (m), 954 (w), 908 (m), 870 (w), 812 (w), 790 (m), 763 (m), 751 (s), 704 (m), 663 (s).

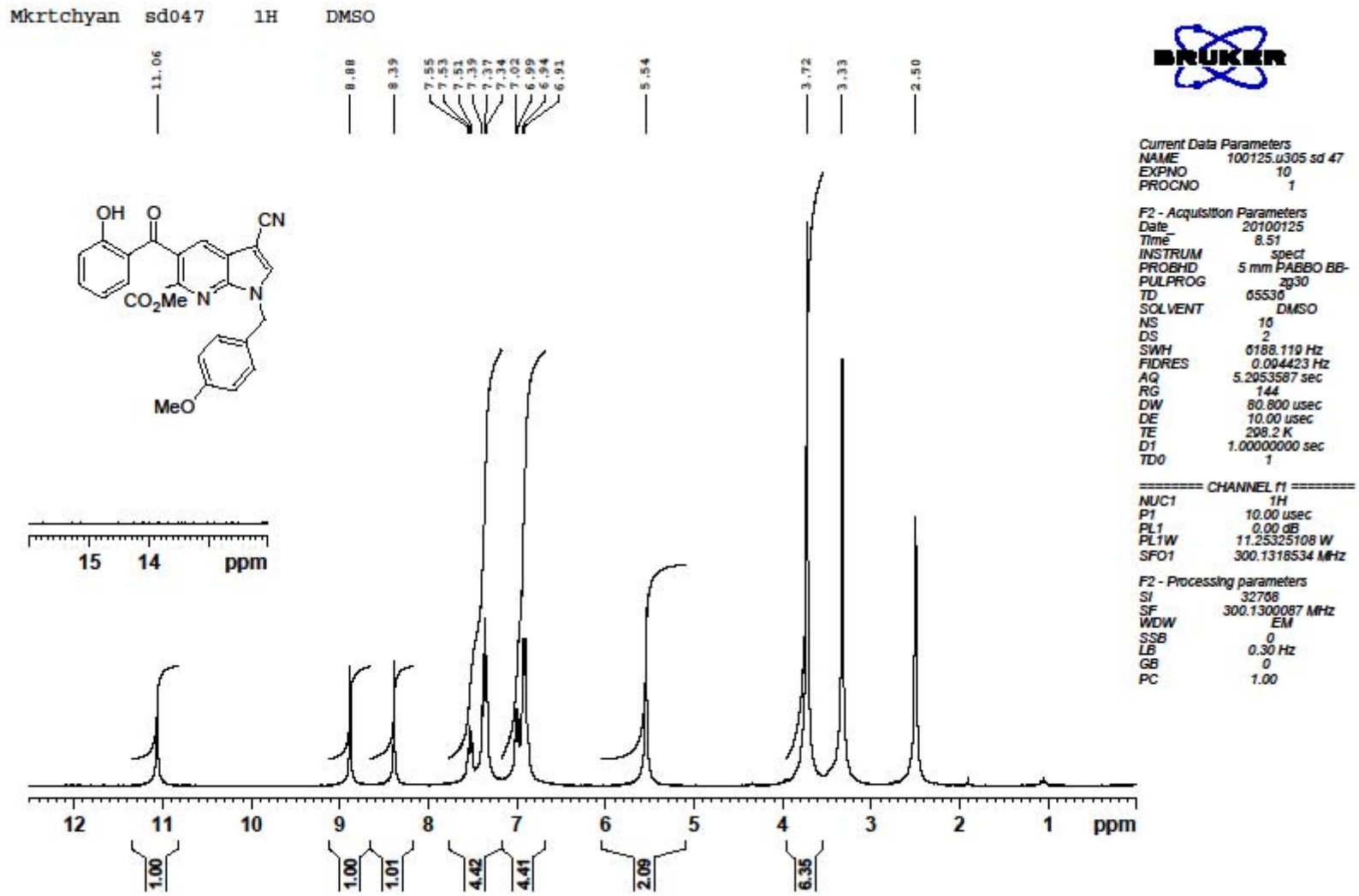
Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information
^{1}H and ^{13}C NMR Spectra

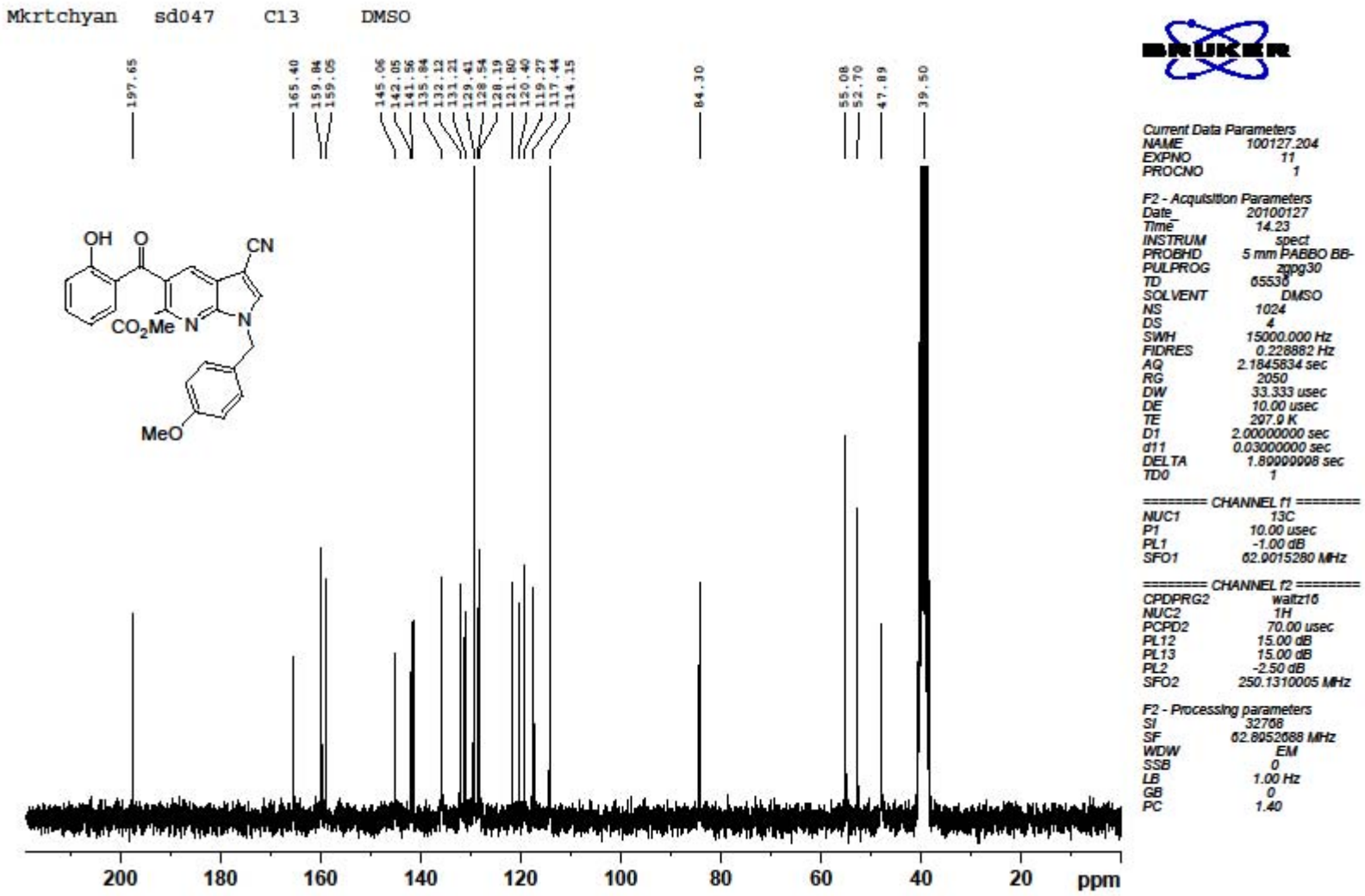

Mkrtchyan Od 211, DMSO, 1H
9.12
8.13
8.13
8.11
8.10
7.95
7.92
7.92
7.90
7.90
7.81
7.78
7.64
7.61
7.59
3.88
3.34
2.50
OMe
15 14 13 ppm
10 9 8 7 6 5 4 3 2 1 ppm
0.92
1.04
1.05
1.00
1.04
3.17
Current Data Parameters
NAME 100429.u339 oxallyl chromone
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100429
Time 14.52
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 144
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 0.00 dB
PL1W 11.25325108 W
SFO1 300.1316534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300058 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

2


Mkrtchyan od211(a) 13C DMSO
184.57
174.15
164.62
164.00
155.64
135.55
127.04
125.24
123.87
118.93
118.52
52.70
OMe
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 100628.212 Ox. Chromone C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100629
Time 3.41
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 1620
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 62.8952687 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Mkrtchyan sd047 1H DMSO
11.06
8.88
8.39
7.55
7.53
7.51
7.39
7.37
7.34
7.02
6.99
6.94
6.91
5.54
3.72
3.33
2.50
OH
O
CN
CO2Me
N
N
MeO
15 14 ppm
12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.00
1.01
4.42
4.41
2.09
6.35
Current Data Parameters
NAME 100125.u305 sd 47
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100125
Time 8.51
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 144
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 0.00 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

12 a



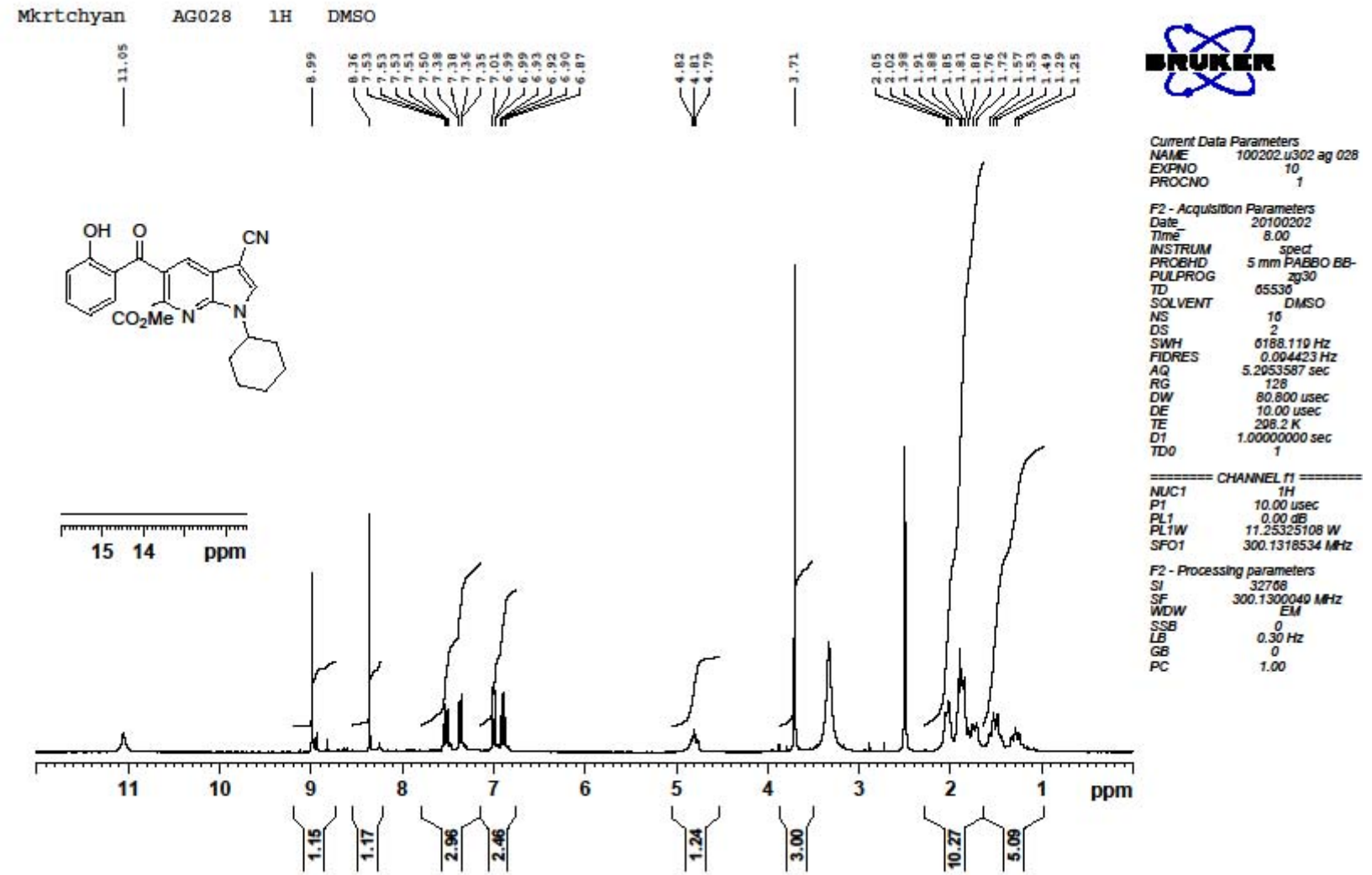
Current Data Parameters
NAME 100127.204
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date 20100127
Time 14.23
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 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

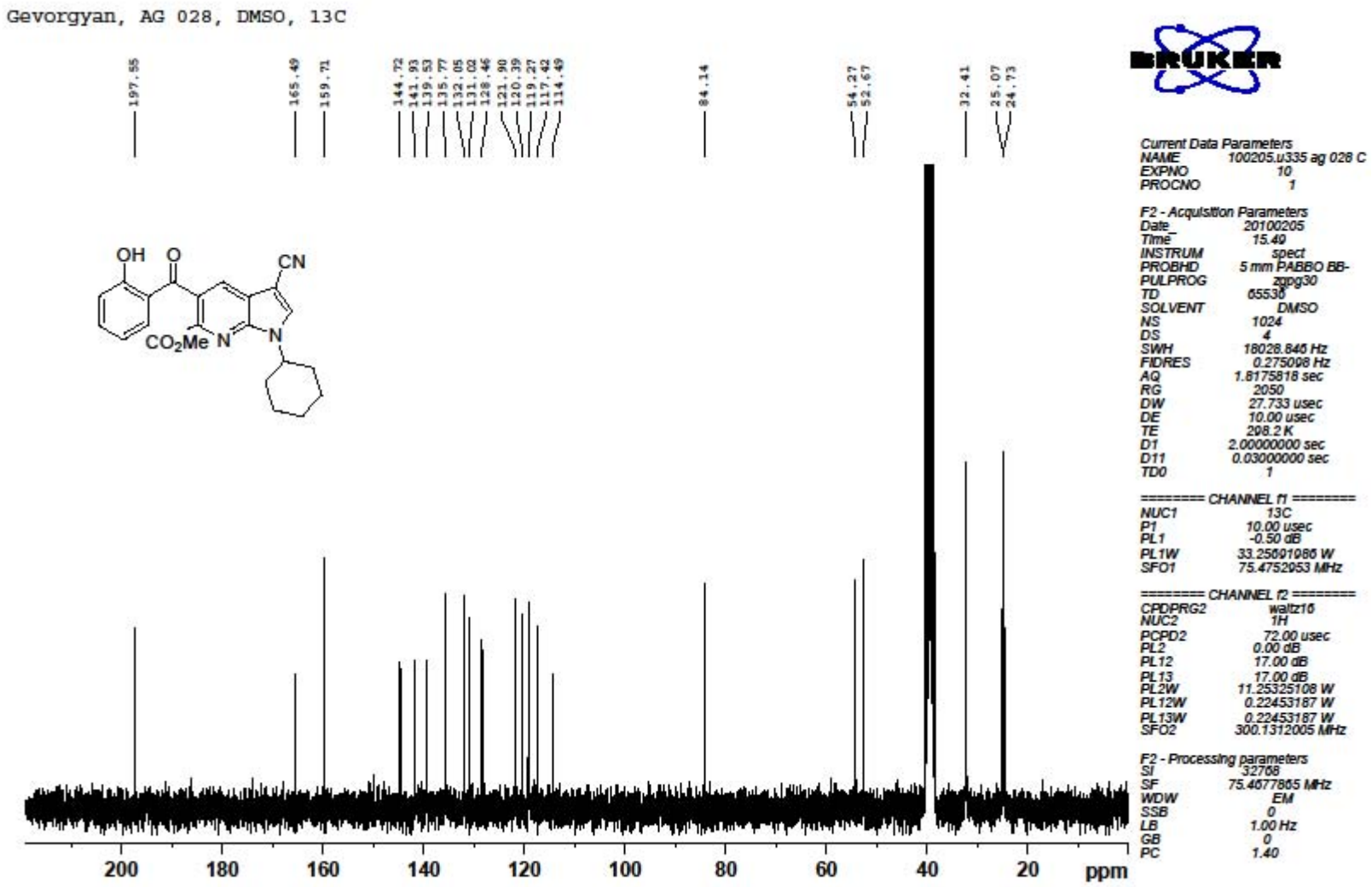
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

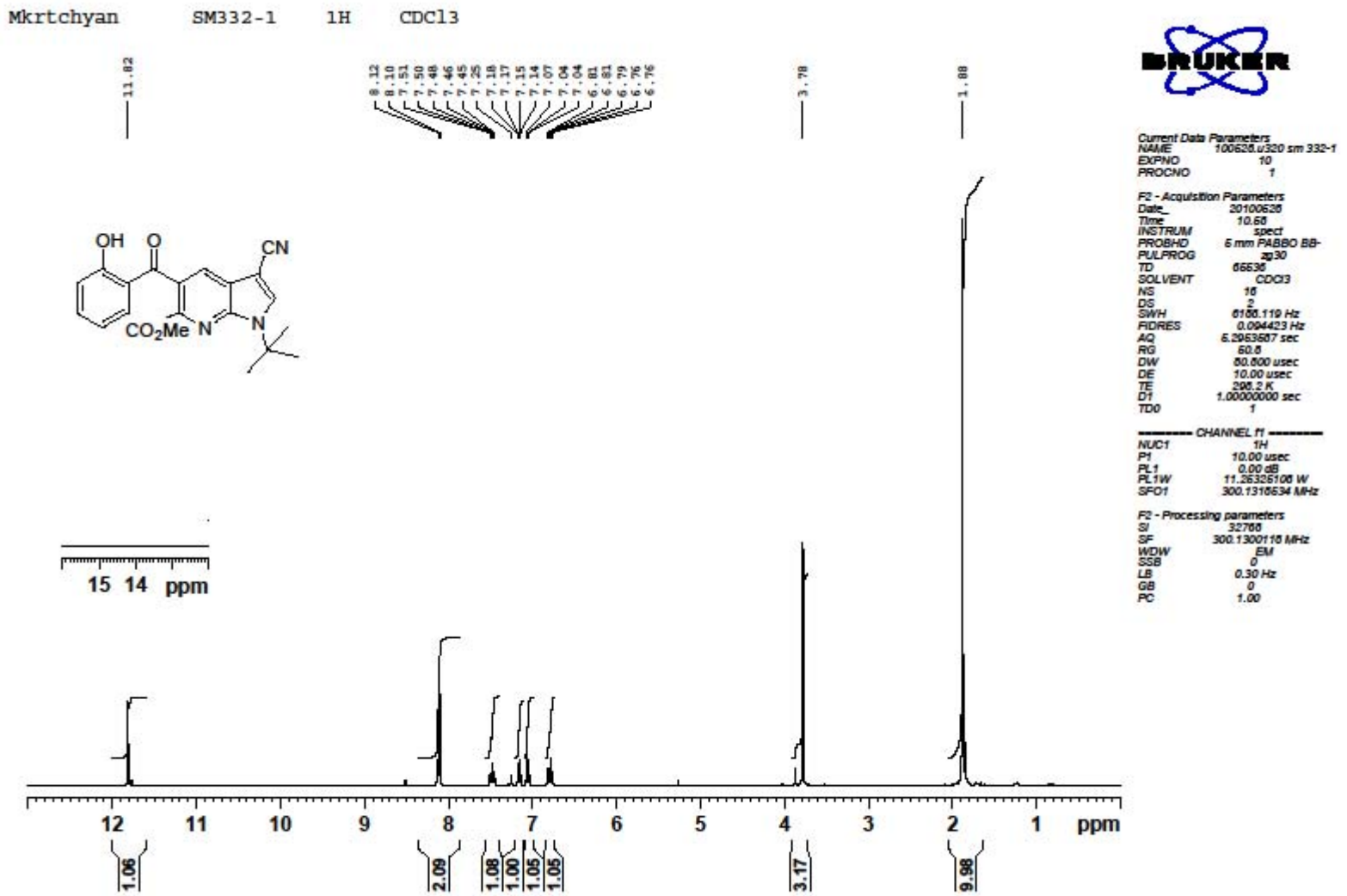
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952688 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

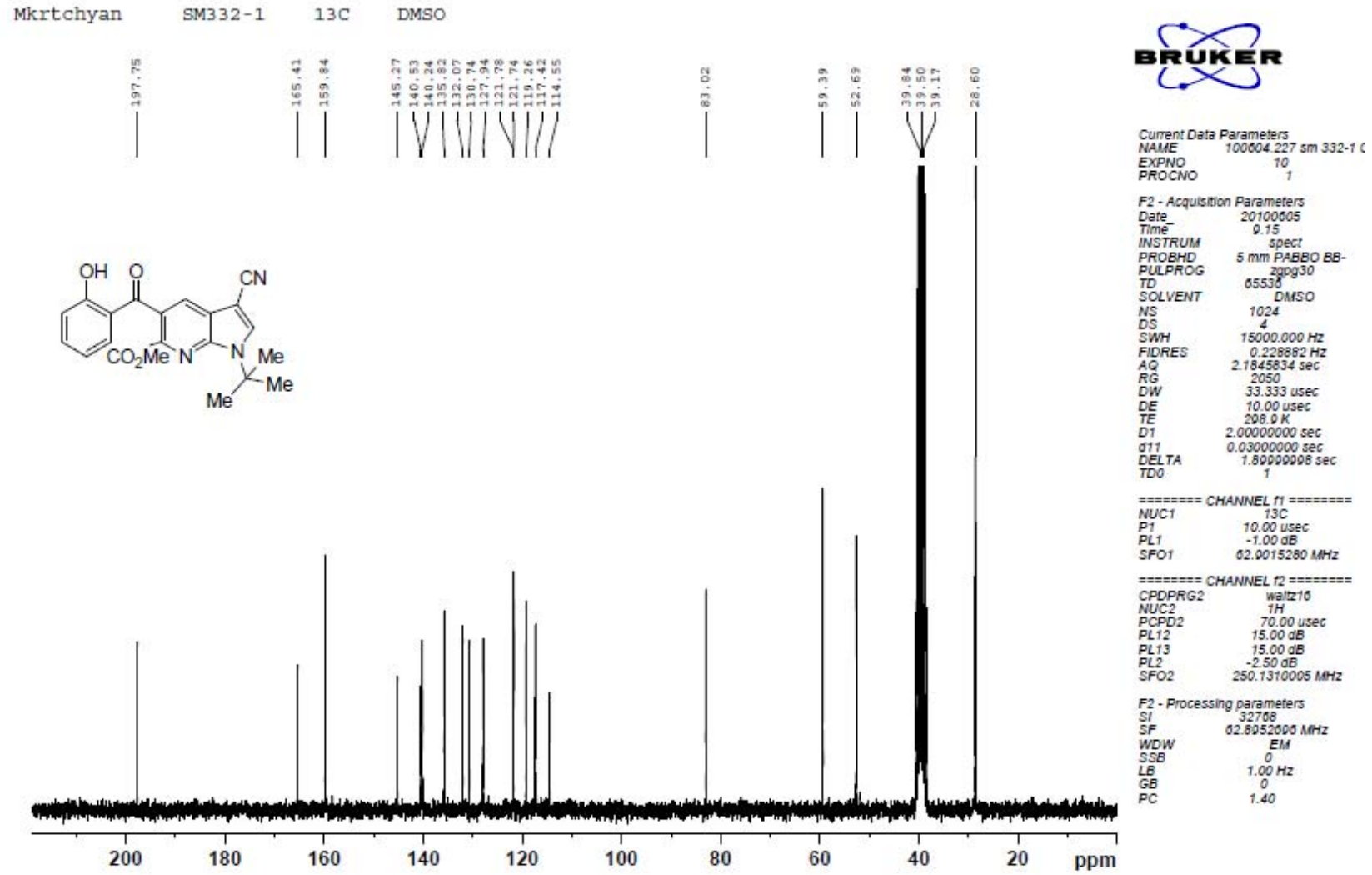

Mkrtchyan AG028 1H DMSO
11.05
8.99
8.36
7.53
7.53
7.51
7.50
7.38
7.36
7.35
7.01
6.99
6.99
6.93
6.92
6.90
6.87
4.82
4.81
4.79
3.71
2.05
2.02
1.98
1.91
1.88
1.85
1.81
1.80
1.76
1.72
1.57
1.53
1.49
1.29
1.25
OH
O
CN
CO2Me
N
N
15 14 ppm
11 10 9 8 7 6 5 4 3 2 1 ppm
1.15
1.17
2.96
2.46
1.24
3.00
10.27
5.09
BRUKER
Current Data Parameters
NAME 100202.u302 ag 028
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100202
Time 8.00
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 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300040 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

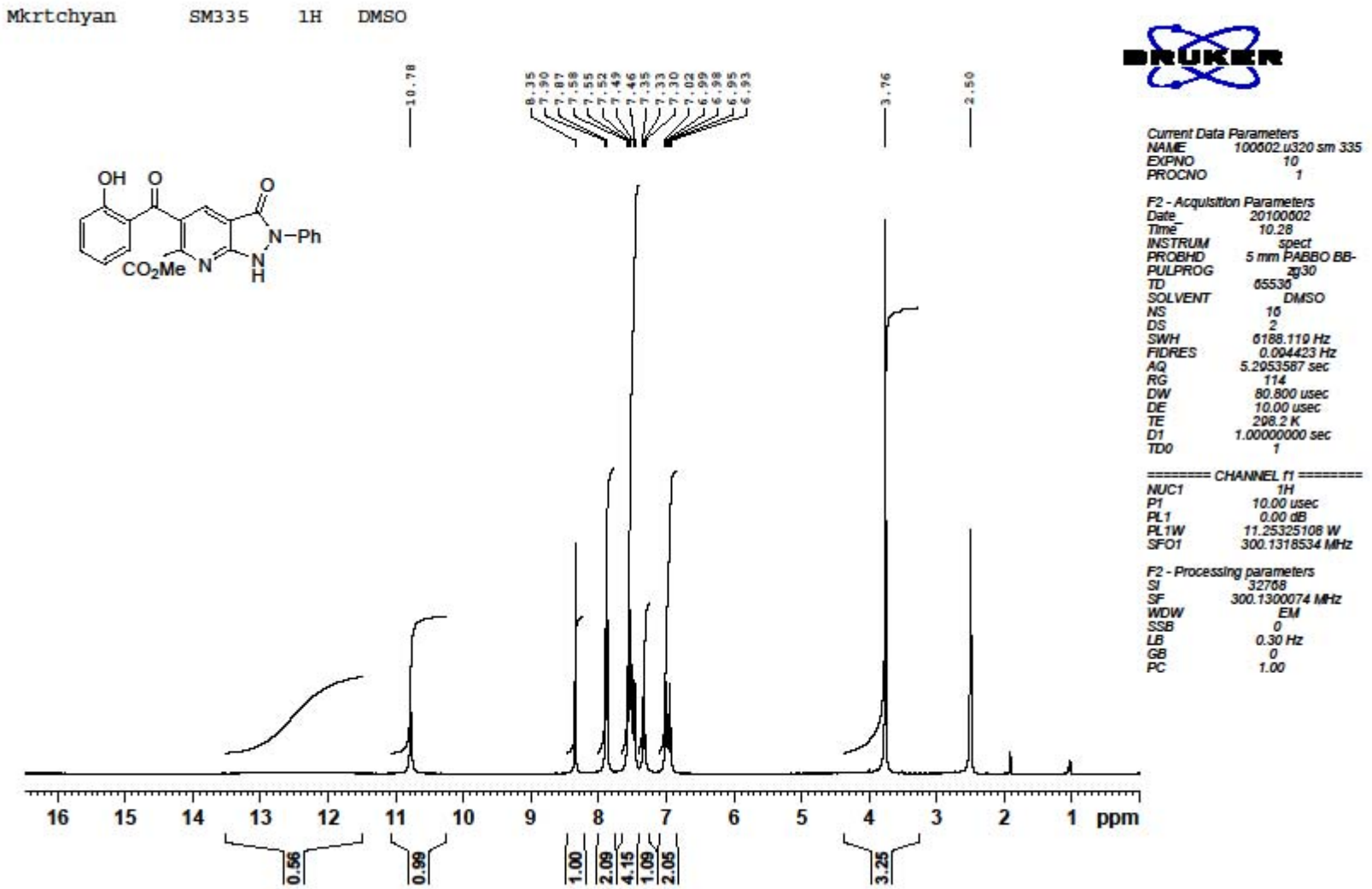
12 b


Gevorgyan, AG 028, DMSO, 13C
197.55
165.49
159.71
144.72
141.93
139.53
135.77
132.05
131.02
128.46
121.90
120.39
119.27
117.42
114.49
84.14
54.27
52.67
32.41
25.07
24.73
OH
O
CN
CO2Me
N
N
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME 100205.u335 ag 028 C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100205
Time 15.49
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 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25091086 W
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 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 75.4677865 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

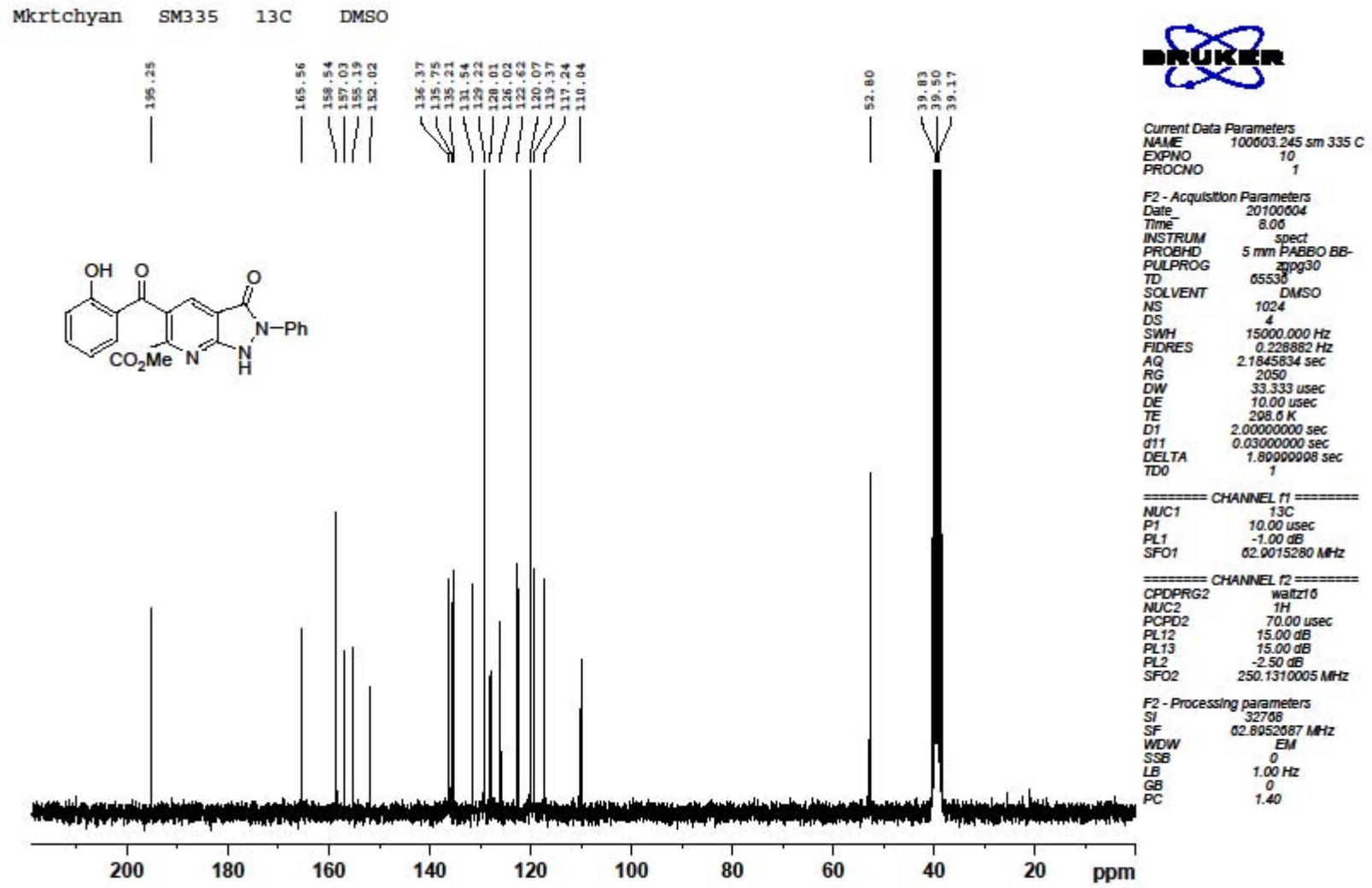

Mkrtchyan SM332-1 1H CDCl3
11.82
8.12
8.10
7.51
7.50
7.48
7.46
7.45
7.25
7.18
7.17
7.15
7.14
7.07
7.04
7.04
6.81
6.79
6.76
6.76
3.78
1.88
OH
O
CN
CO2Me
N
N
15 14 ppm
12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.06
2.09
1.08
1.00
1.05
1.05
3.17
9.98
Current Data Parameters
NAME 100626.u320 sm 332-1
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100626
Time 10.56
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 50.6
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 0.00 dB
PL1W 11.26326106 W
SFO1 300.1316634 MHz
F2 - Processing parameters
SI 32768
SF 300.1300116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12 c


Mkrtchyan SM332-1 13C DMSO
197.75
165.41
159.84
145.27
140.53
140.24
135.82
132.07
130.74
127.94
121.78
121.74
119.26
117.42
114.55
83.02
59.39
52.69
39.84
39.50
39.17
28.60
OH
O
CN
CO2Me
N
N
Me
Me
Me
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME 100604.227 sm 332-1 C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100605
Time 9.15
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 2050
DW 33.333 usec
DE 10.00 usec
TE 298.9 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 62.8952696 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Mkrtchyan SM335 1H DMSO
10.78
8.35
7.90
7.87
7.58
7.55
7.52
7.49
7.46
7.35
7.33
7.30
7.02
6.99
6.98
6.95
6.93
3.76
2.50
OH
O
O
N–Ph
CO2Me
N
N
H
Current Data Parameters
NAME 100602.u320 sm 335
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100602
Time 10.28
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 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.56
0.99
1.00
2.09
4.15
1.09
2.05
3.25

12 d



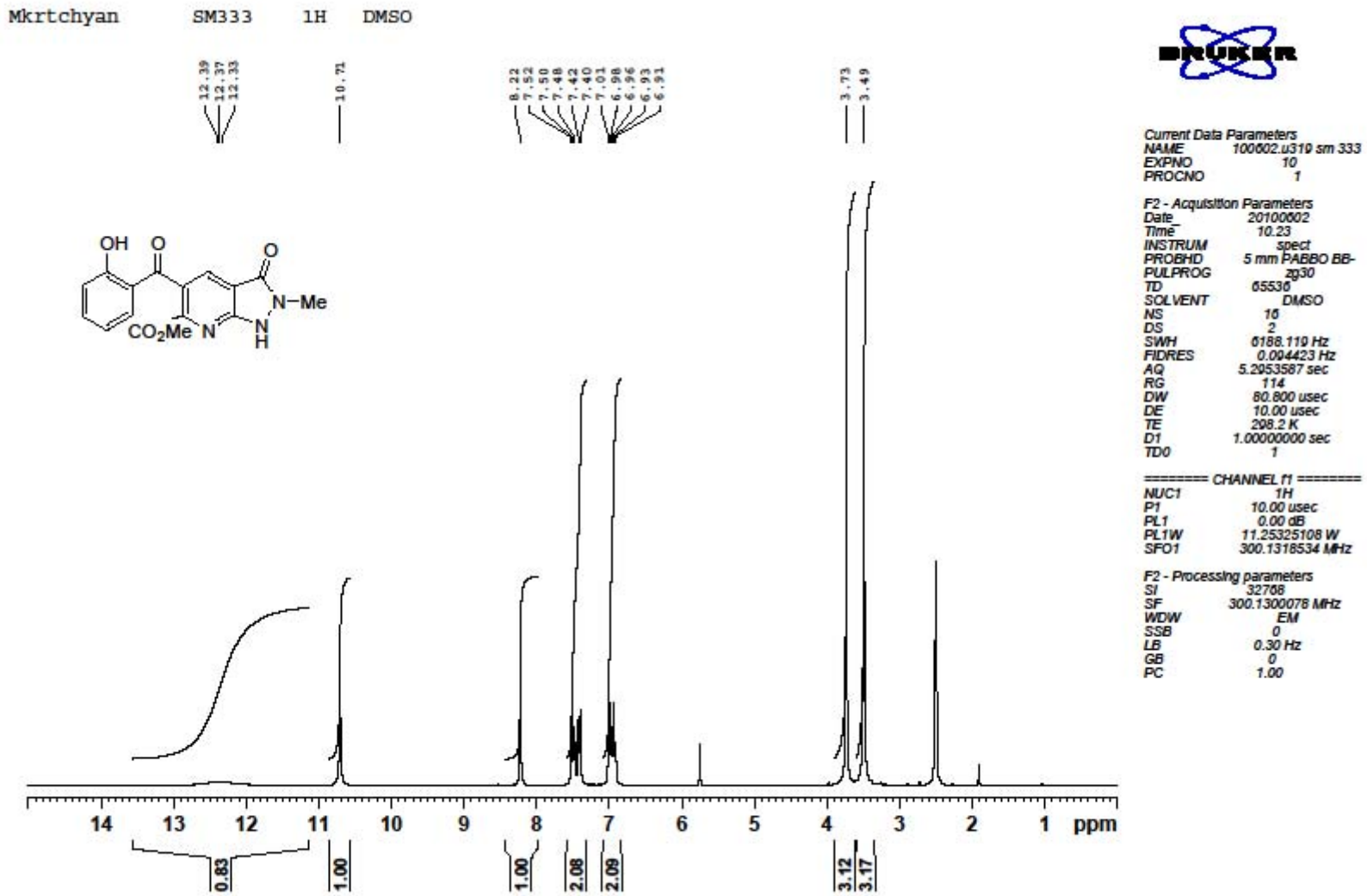
Current Data Parameters
NAME 100603.245 sm 335 C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20100604
Time 8.06
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 2050
DW 33.333 usec
DE 10.00 usec
TE 298.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.80000008 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 62.8952687 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



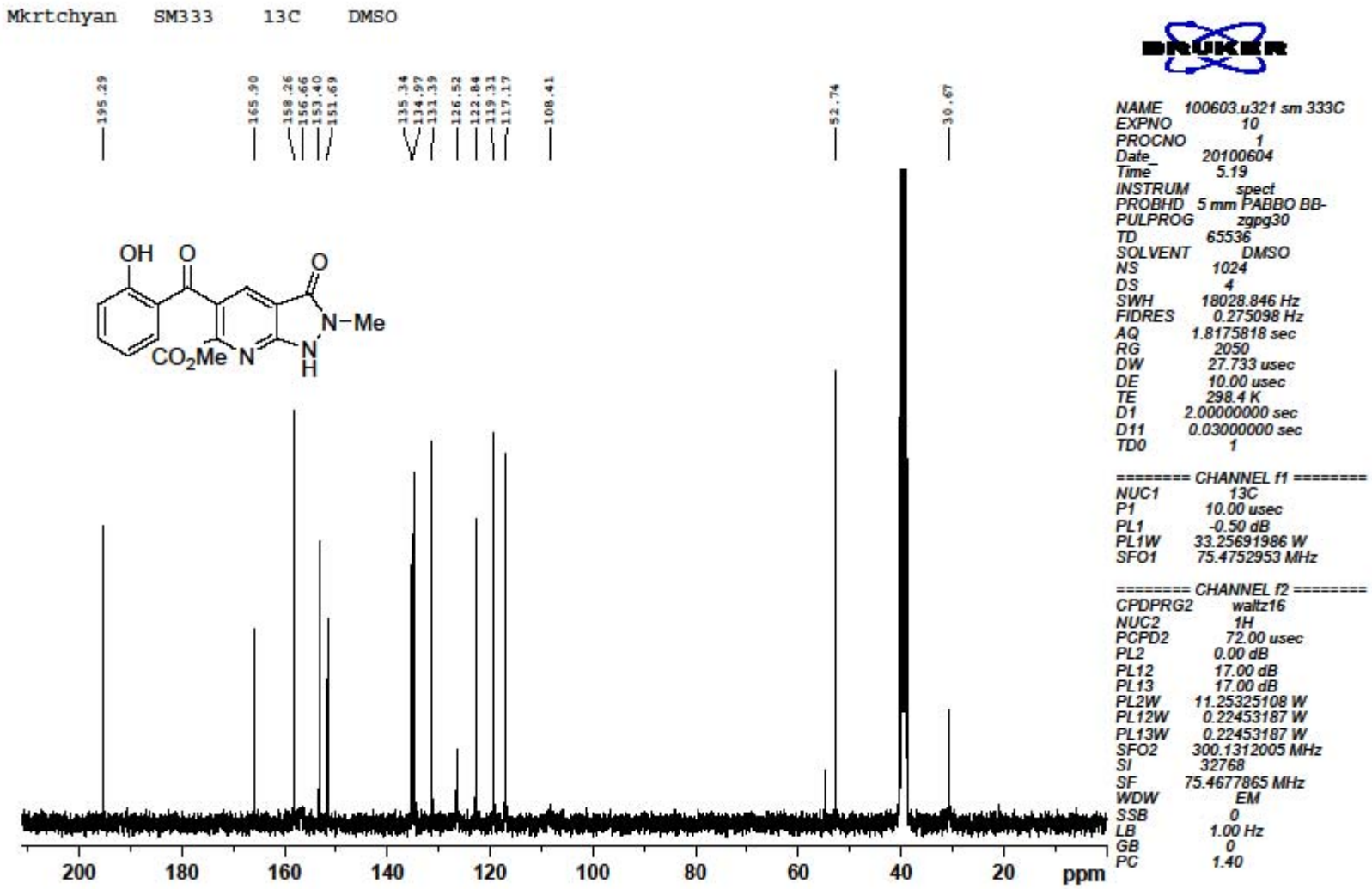
Current Data Parameters
NAME 100602.u319 sm 333
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100602
Time 10.23
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 0.00 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

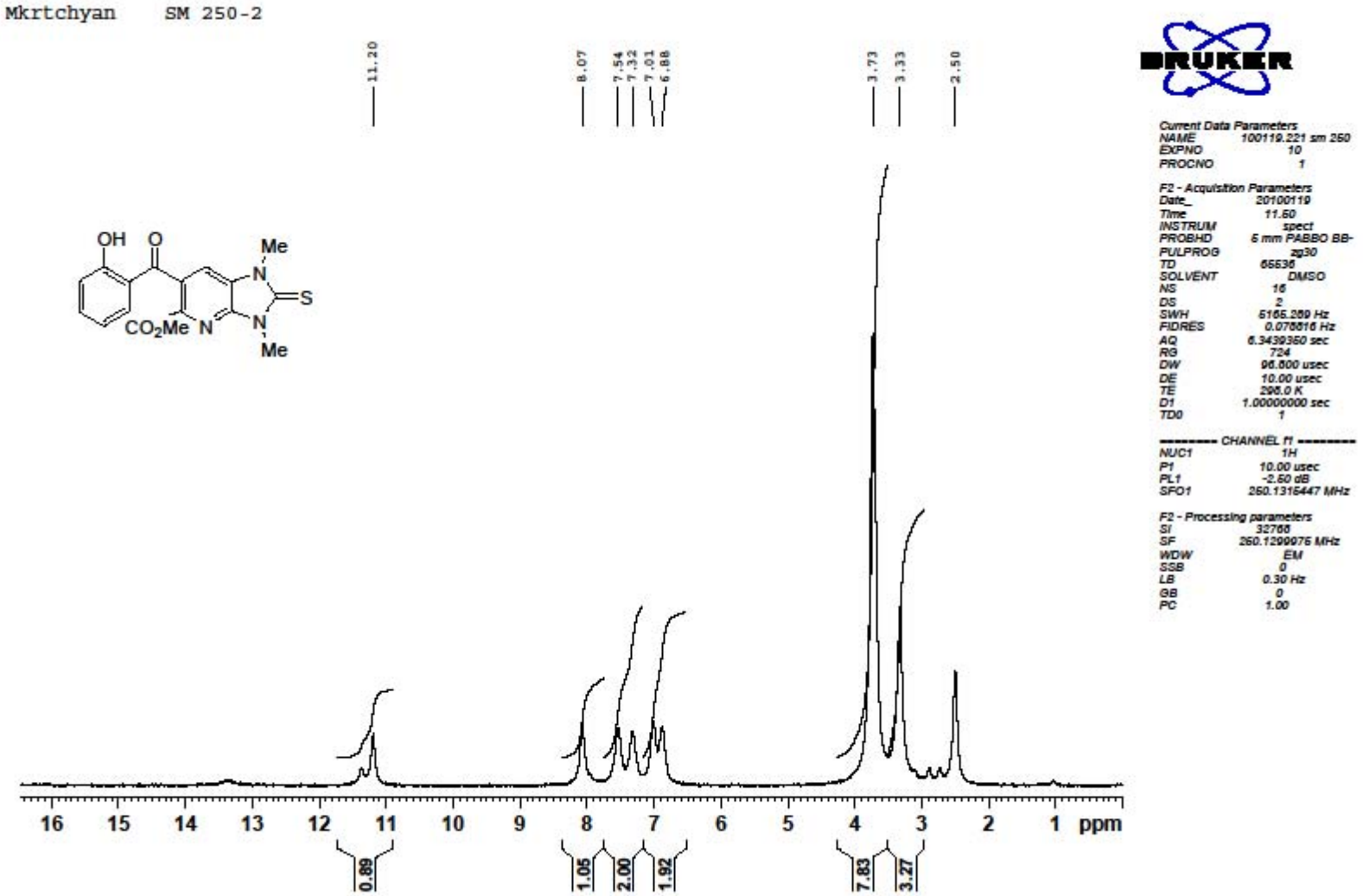
12 e



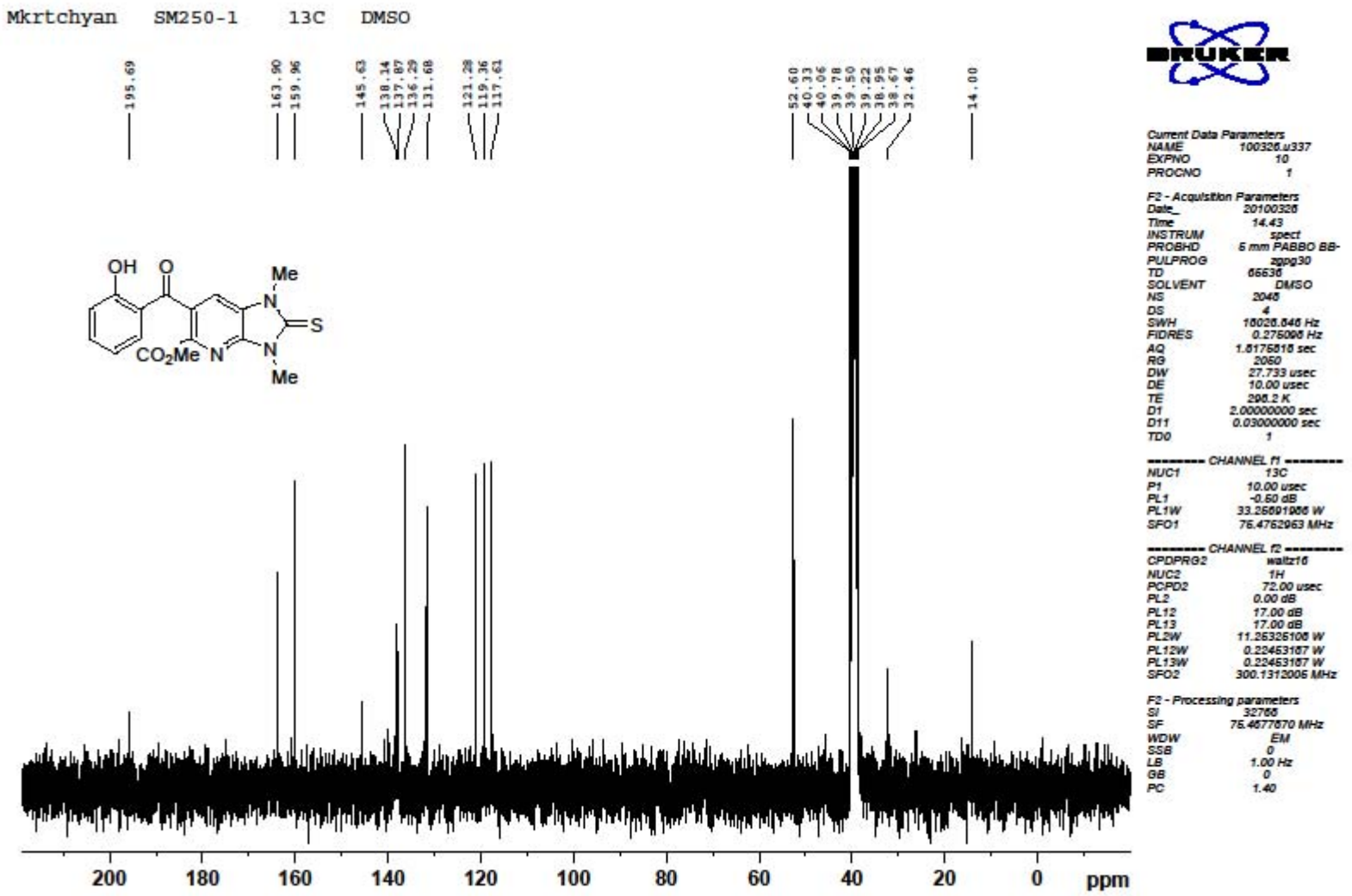
NAME 100603.u321 sm 333C
EXPNO 10
PROCNO 1
Date_ 20100604
Time 5.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== 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 0.00 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
SI 32768
SF 75.4677865 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Mkrtchyan SM 250-2
11.20
8.07
7.54
7.32
7.01
6.88
3.73
3.33
2.50
OH
O
Me
N
S
CO2Me
N
N
Me
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.89
1.05
2.00
1.92
7.83
3.27
BRUKER
Current Data Parameters
NAME 100119.221 sm 250
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100119
Time 11.50
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 724
DW 96.800 usec
DE 10.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.60 dB
SFO1 250.1315447 MHz
F2 - Processing parameters
SI 32768
SF 250.1299976 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12 f



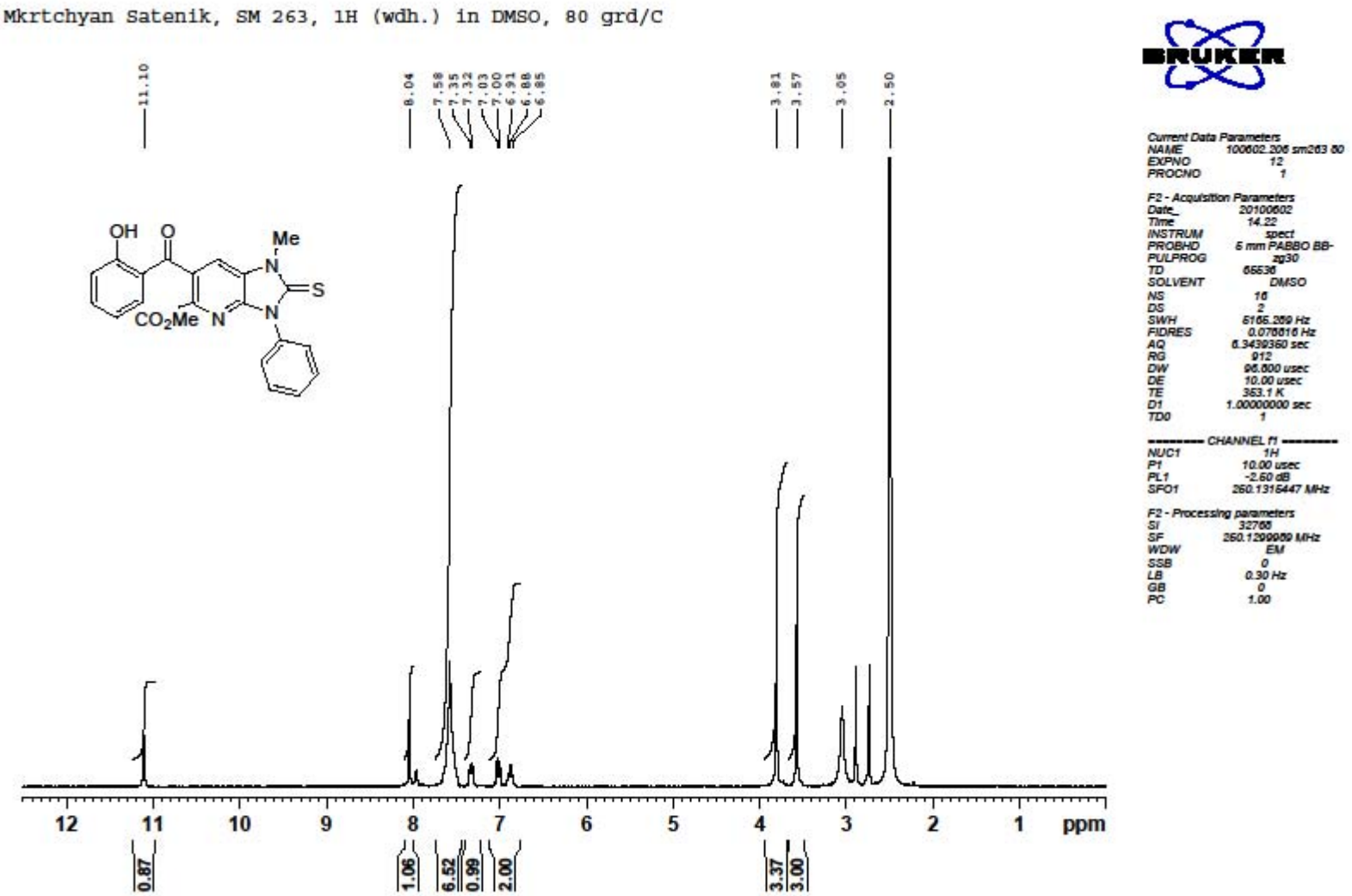
Current Data Parameters
NAME 100326.u337
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100326
Time 14.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 19026.846 Hz
FIDRES 0.276096 Hz
AQ 1.5175516 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

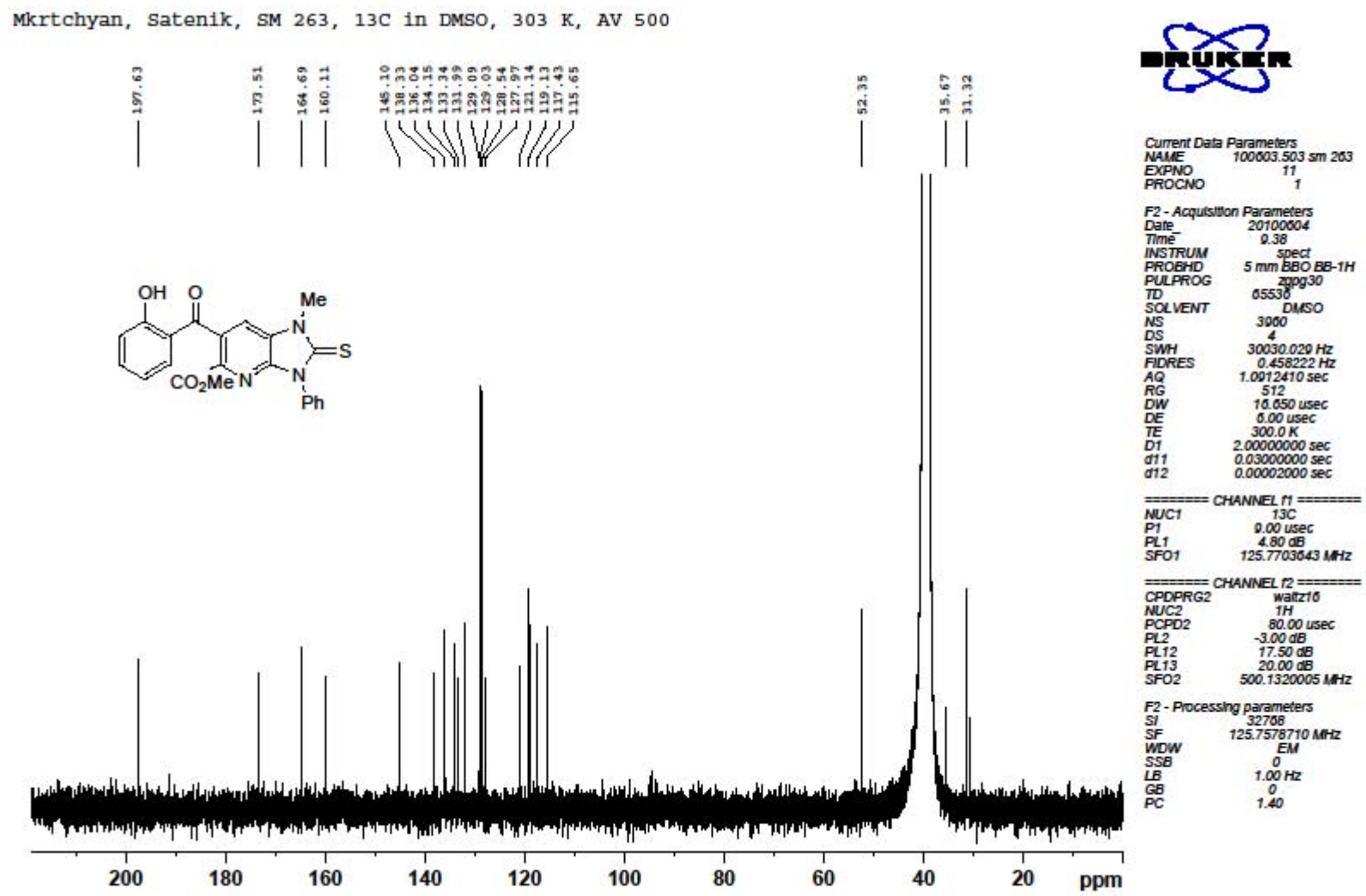
--------- CHANNEL f1 ---------
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 76.4762963 MHz

--------- CHANNEL f2 ---------
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25326106 W
PL12W 0.22463167 W
PL13W 0.22463167 W
SFO2 300.1312006 MHz

F2 - Processing parameters
SI 32768
SF 75.4677670 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Mkrtchyan Satenik, SM 263, 1H (wdh.) in DMSO, 80 grd/C
11.10
8.04
7.58
7.35
7.32
7.03
7.00
6.91
6.88
6.85
3.81
3.57
3.05
2.50
OH
O
Me
N
S
CO2Me
N
N
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.87
1.06
6.52
0.99
2.00
3.37
3.00
Current Data Parameters
NAME 100602.206 sm263 80
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100602
Time 14.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6166.359 Hz
FIDRES 0.076616 Hz
AQ 5.3439360 sec
RG 912
DW 96.800 usec
DE 10.00 usec
TE 363.1 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.60 dB
SFO1 250.1315447 MHz
F2 - Processing parameters
SI 32768
SF 250.1299959 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12 g



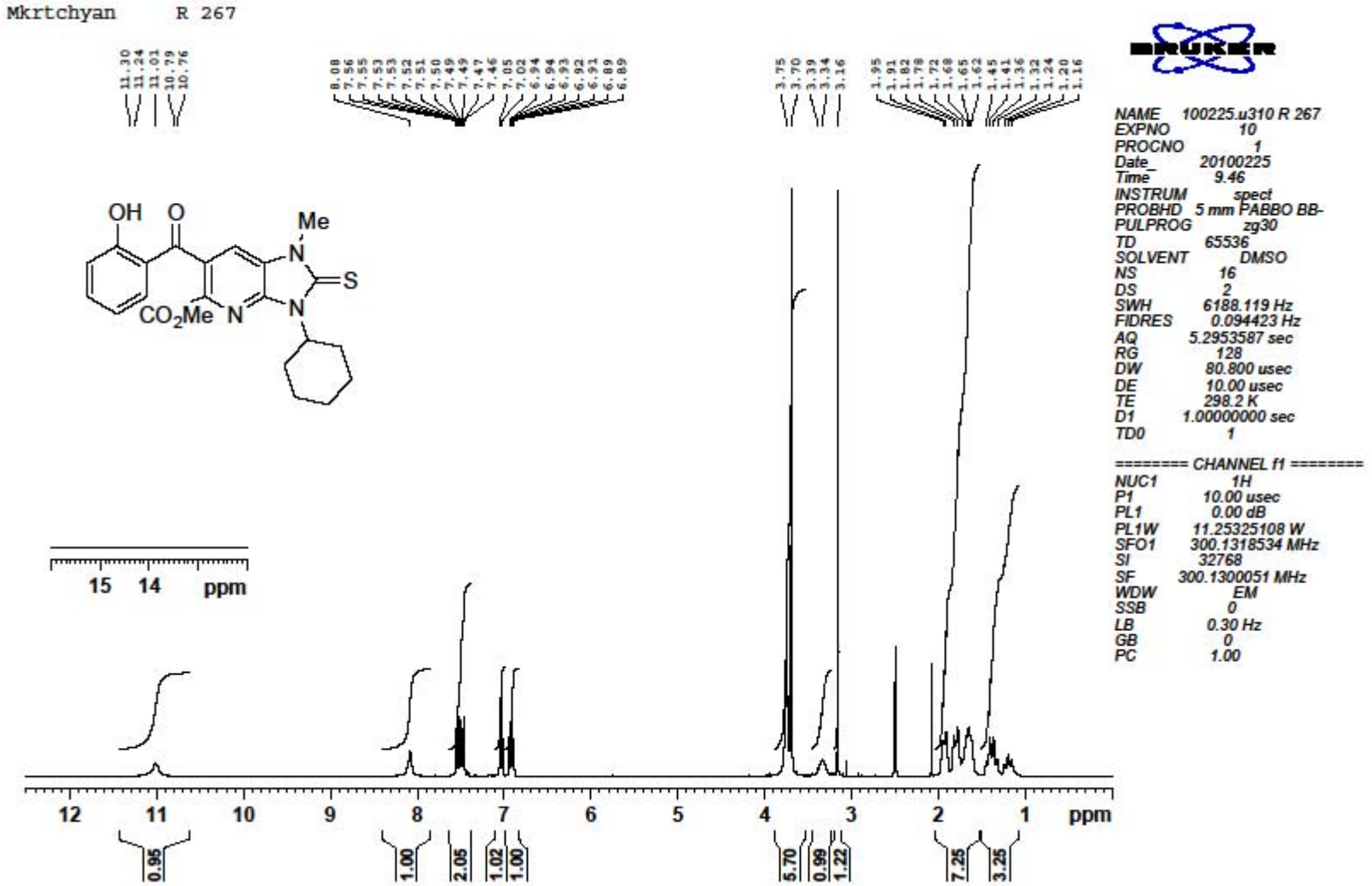
Current Data Parameters
NAME 100603.503 sm 263
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100604
Time 9.38
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3000
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 512
DW 16.650 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

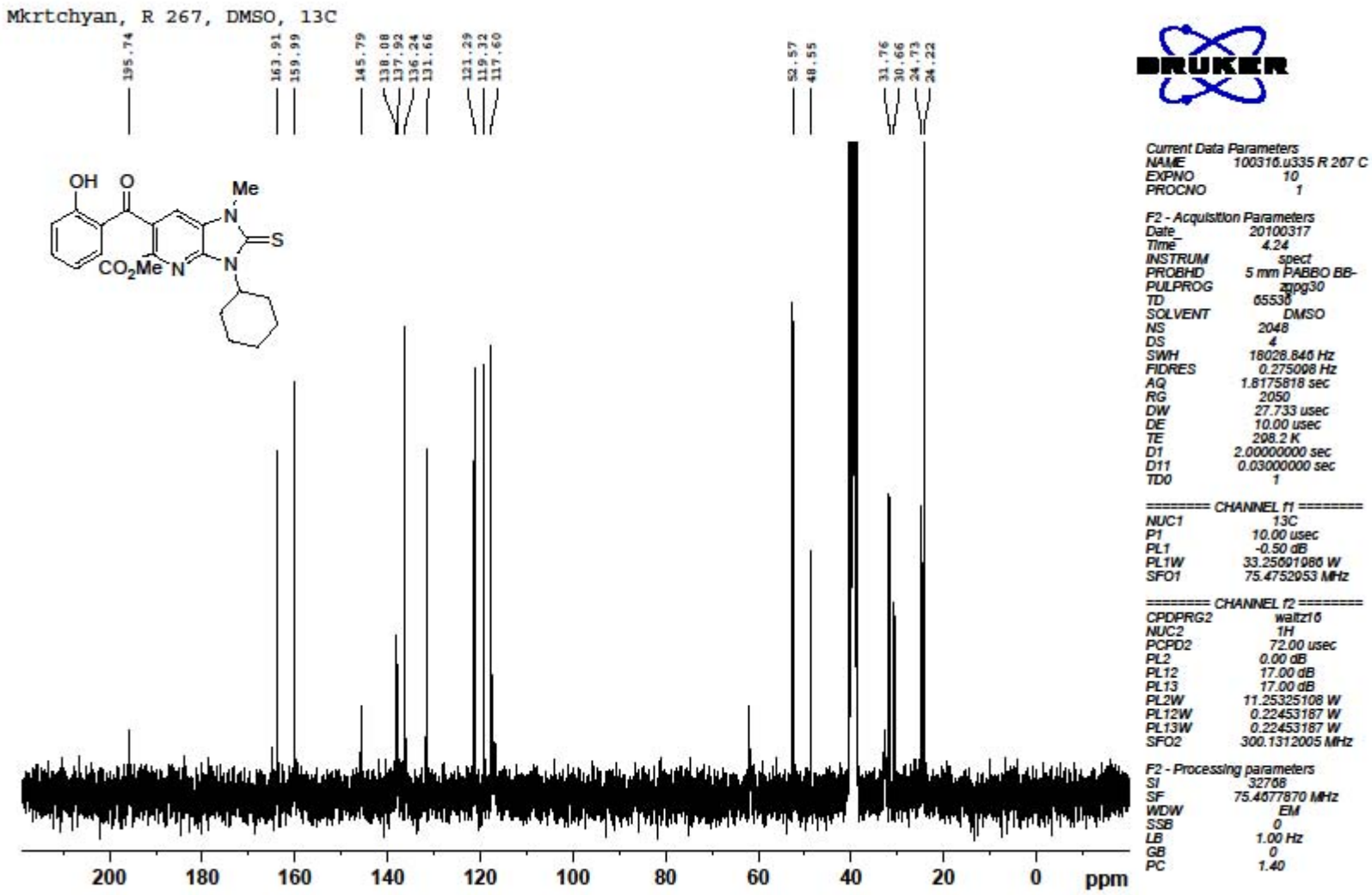
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 4.80 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.50 dB
PL13 20.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7578710 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Mkrtchyan R 267
11.30
11.24
11.01
10.79
10.76
8.08
7.56
7.55
7.53
7.53
7.52
7.51
7.50
7.49
7.49
7.47
7.46
7.05
7.02
6.94
6.94
6.93
6.92
6.91
6.89
6.89
3.75
3.70
3.39
3.34
3.16
1.95
1.91
1.82
1.78
1.72
1.68
1.65
1.62
1.45
1.41
1.36
1.32
1.24
1.20
1.16
OH
O
Me
N
S
CO2Me
N
N
15
14
ppm
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.95
1.00
2.05
1.02
1.00
5.70
0.99
1.22
7.25
3.25
NAME 100225.u310 R 267
EXPNO 10
PROCNO 1
Date_ 20100225
Time 9.46
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 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 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12 h



BRUKER

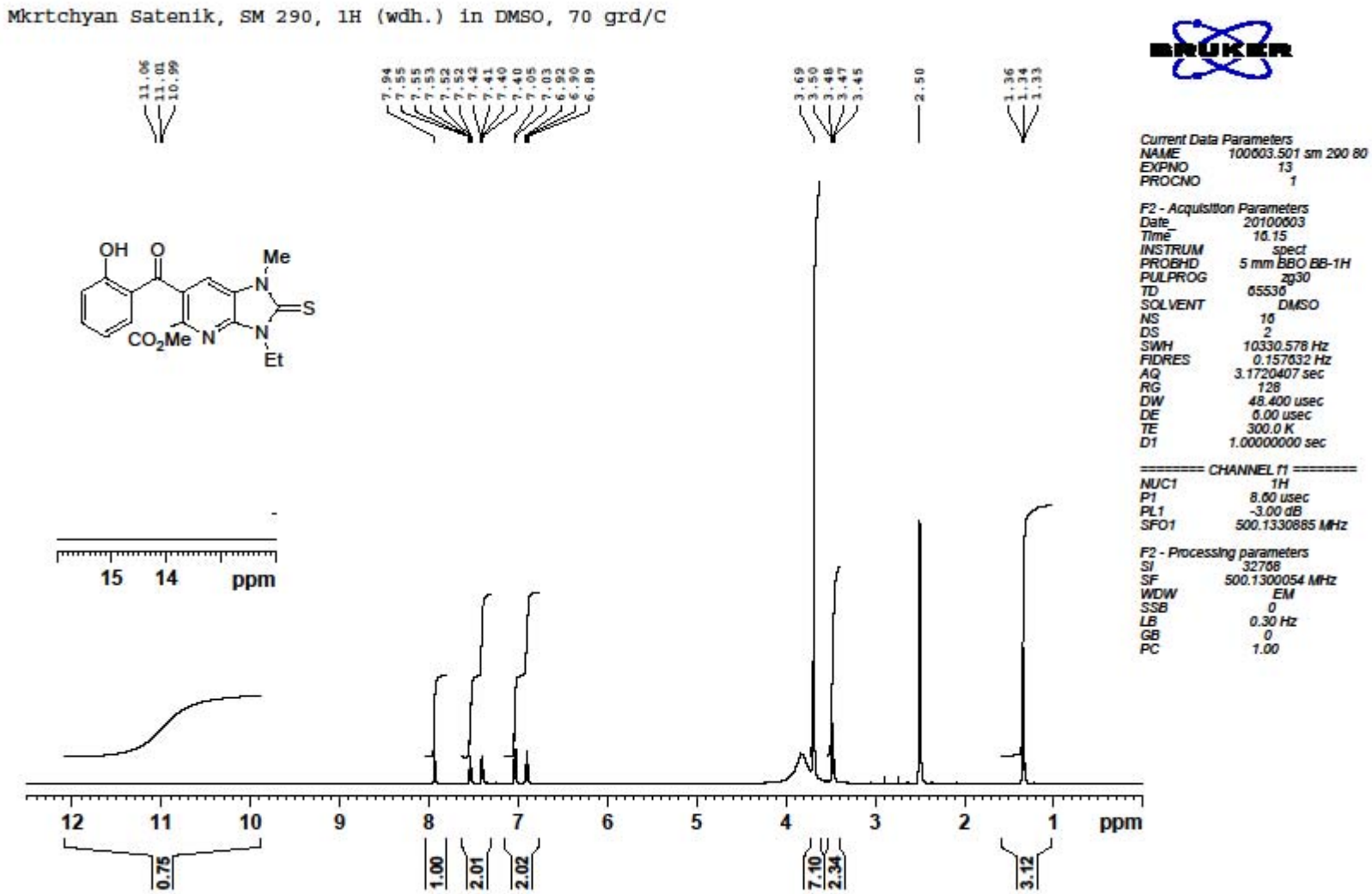
Current Data Parameters
NAME 100316.u335 R 267 C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100317
Time 4.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
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

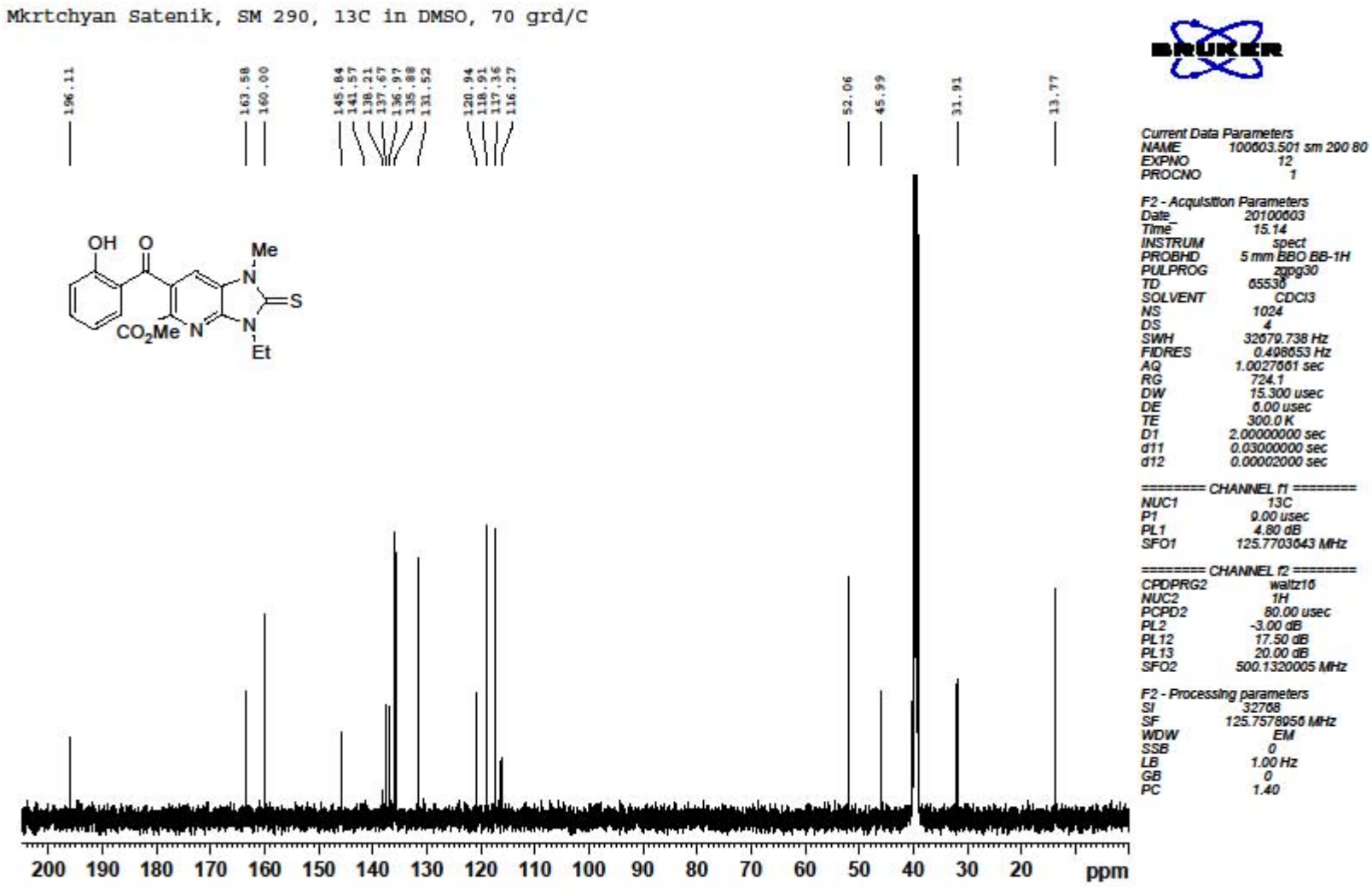
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

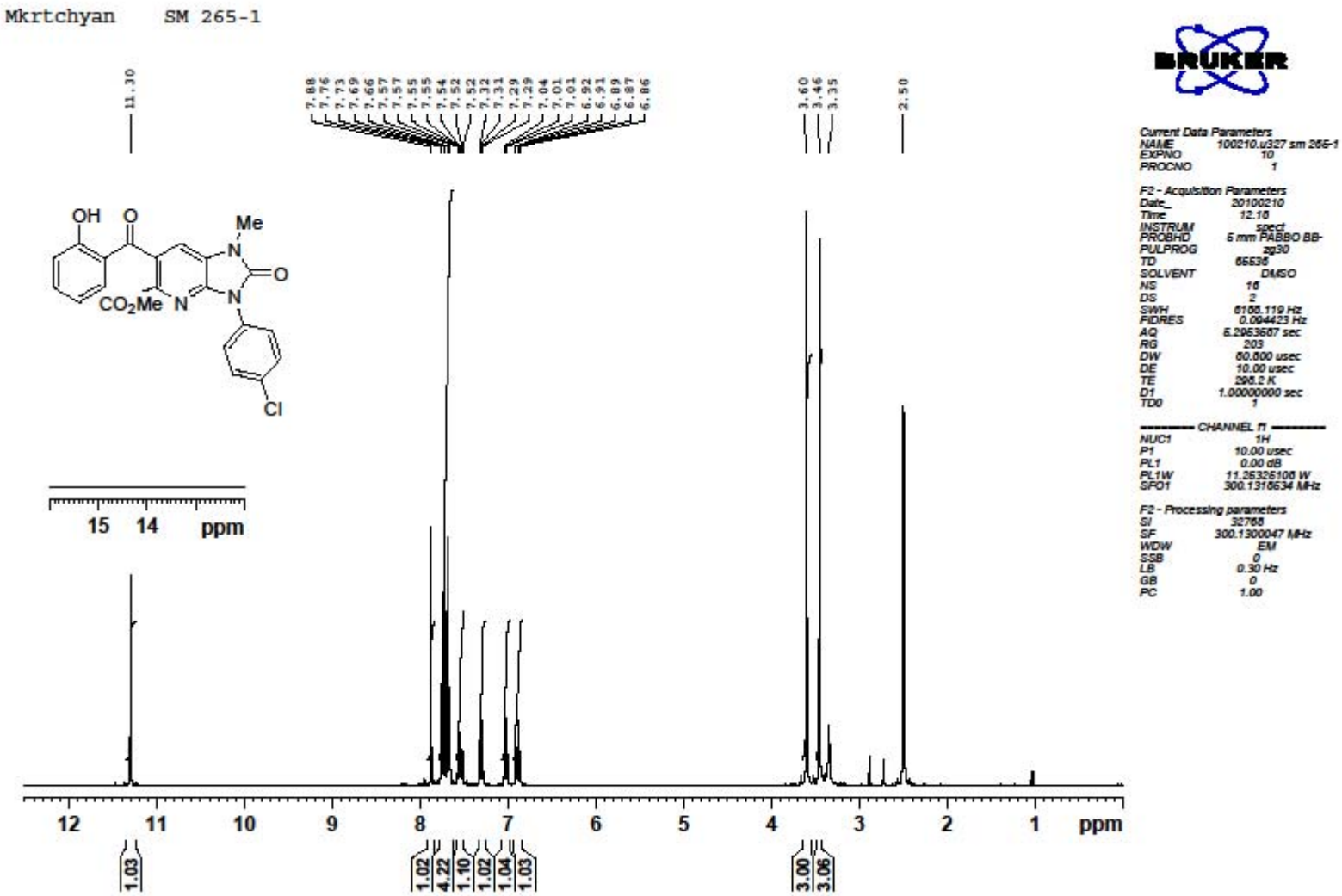
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677870 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

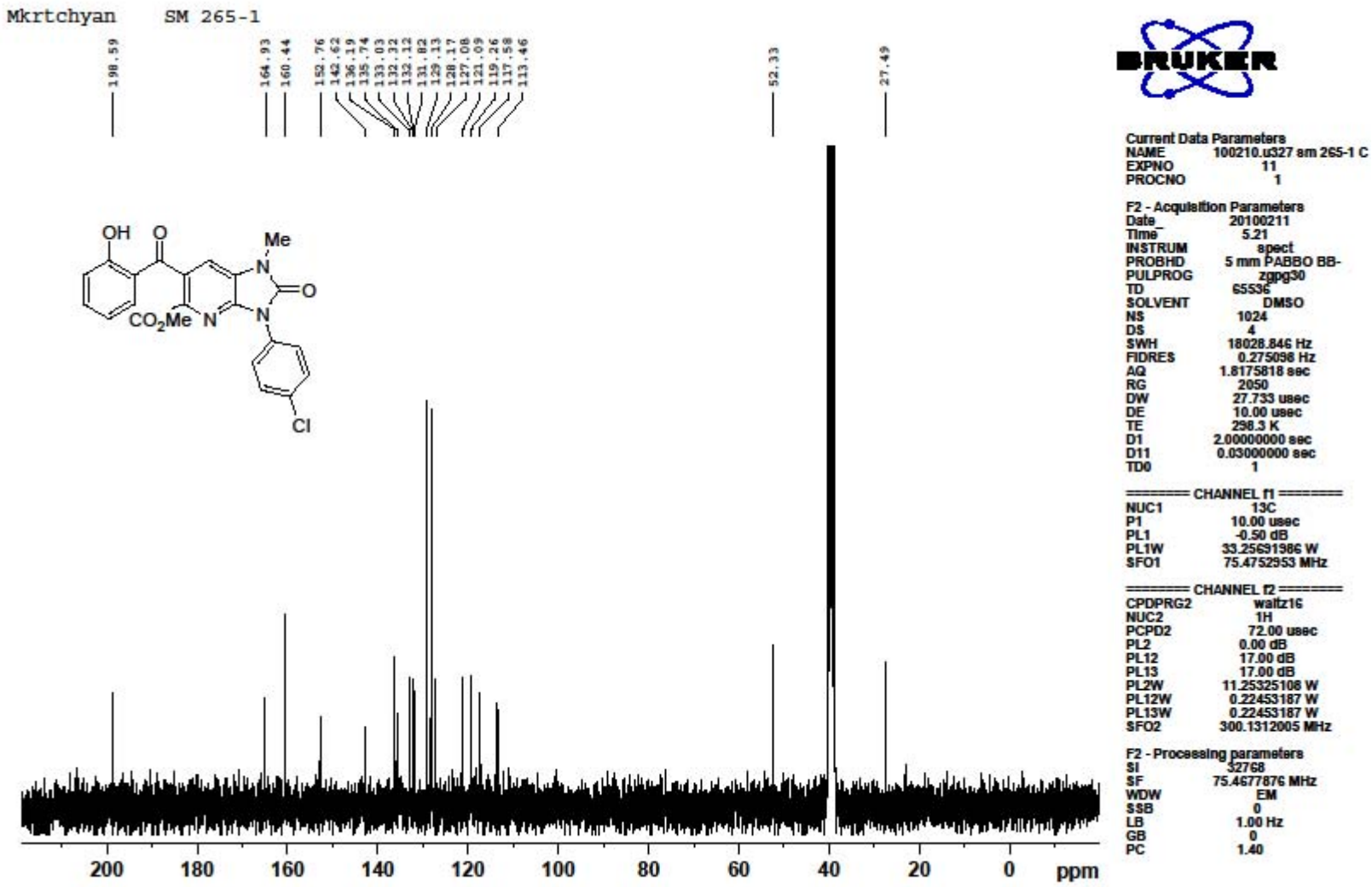

Mkrtchyan Satenik, SM 290, 1H (wdh.) in DMSO, 70 grd/C
11.06
11.01
10.99
7.94
7.55
7.55
7.53
7.52
7.52
7.42
7.41
7.40
7.40
7.05
7.03
6.92
6.90
6.89
3.69
3.50
3.48
3.47
3.45
2.50
1.36
1.34
1.33
OH
O
Me
N
S
CO2Me
N
N
Et
15
14
ppm
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.75
1.00
2.01
2.02
7.10
2.34
3.12
Current Data Parameters
NAME 100603.501 sm 290 80
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100603
Time 16.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 128
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.60 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12 i


Mkrtchyan Satenik, SM 290, 13C in DMSO, 70 grd/C
196.11
163.58
160.00
145.84
141.57
138.21
137.67
136.97
135.88
131.52
120.94
118.91
117.36
116.27
52.06
45.99
31.91
13.77
OH
O
Me
N
S
CO2Me
N
N
Et
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
Current Data Parameters
NAME 100603.501 sm 290 80
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100603
Time 15.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 724.1
DW 15.300 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 4.80 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.50 dB
PL13 20.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7578956 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Mkrtchyan SM 265-1
11.30
7.88
7.76
7.73
7.69
7.66
7.57
7.57
7.55
7.55
7.54
7.52
7.52
7.32
7.31
7.29
7.29
7.04
7.01
7.01
6.92
6.91
6.89
6.87
6.86
3.60
3.46
3.35
2.50
OH
O
Me
N
O
CO2Me
N
N
Cl
15 14 ppm
12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.03
1.02
4.22
1.10
1.02
1.04
1.03
3.00
3.06
BRUKER
Current Data Parameters
NAME 100210.u327 sm 266-1
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100210
Time 12.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6166.119 Hz
FIDRES 0.094123 Hz
AQ 5.2953687 sec
RG 203
DW 60.500 usec
DE 10.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.26326106 W
SFO1 300.1316634 MHz
F2 - Processing parameters
SI 32768
SF 300.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12 j



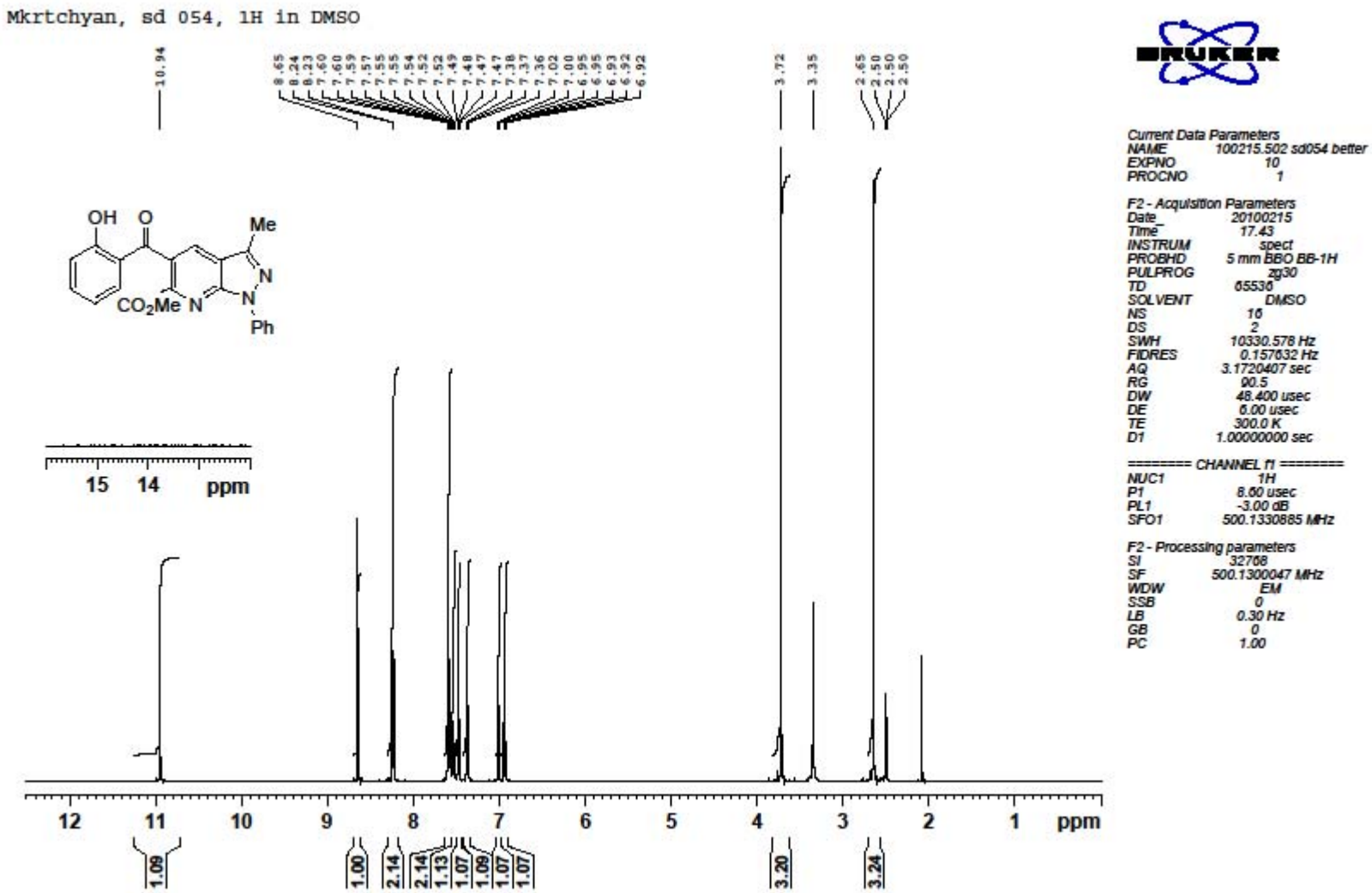
Current Data Parameters
NAME 100210.u327 sm 265-1 C
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date 20100211
Time 5.21
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 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

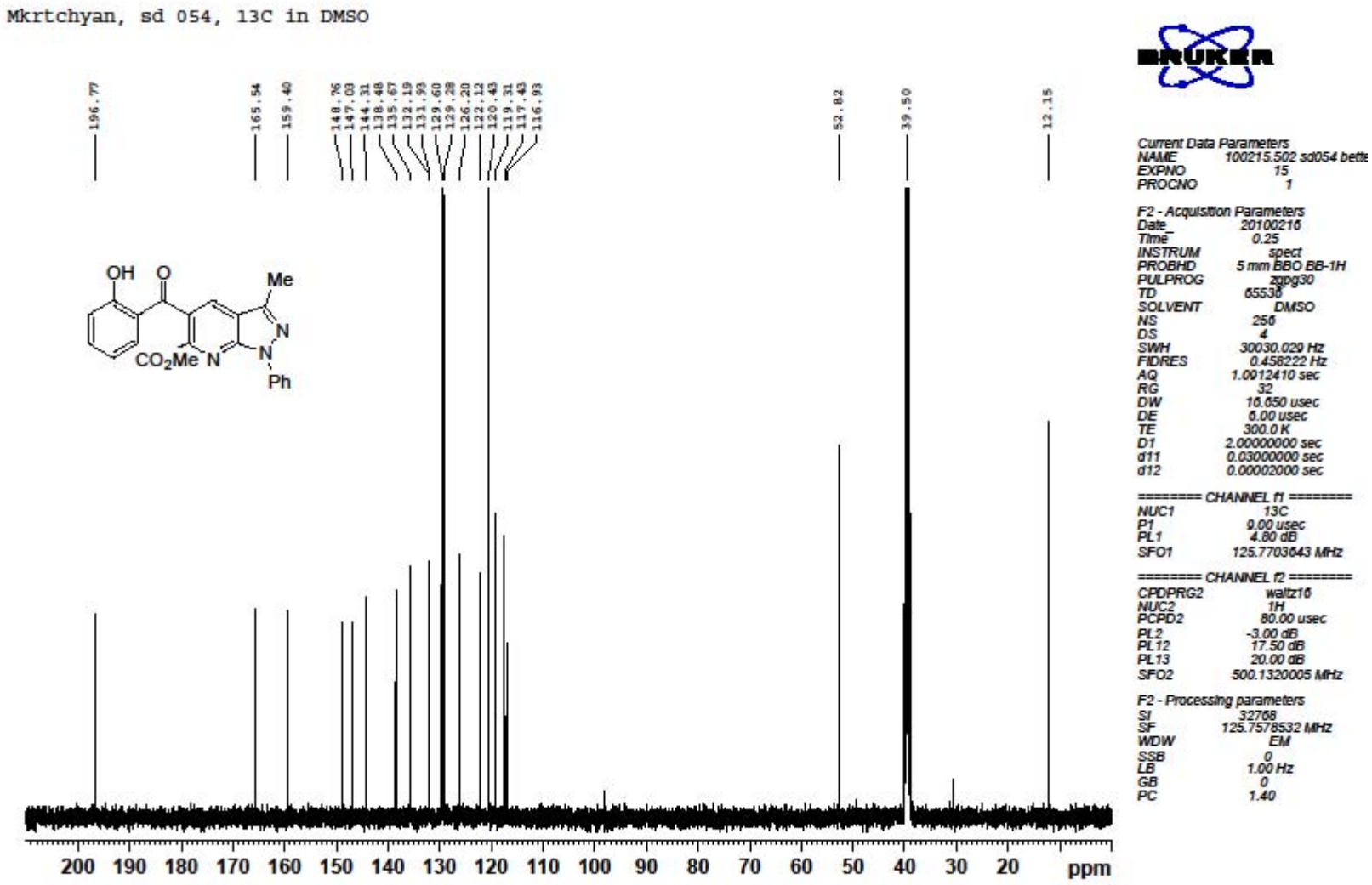
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 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 75.4677876 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Mkrtchyan, sd 054, 1H in DMSO
10.94
8.65
8.24
8.23
7.60
7.59
7.57
7.55
7.55
7.54
7.52
7.52
7.49
7.48
7.47
7.47
7.38
7.37
7.36
7.02
7.00
6.95
6.95
6.93
6.92
6.92
3.72
3.35
2.65
2.50
2.50
2.50
OH
O
Me
N
N
CO2Me
N
Ph
15
14
ppm
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.09
1.00
2.14
2.14
1.13
1.07
1.09
1.07
1.07
3.20
3.24
Current Data Parameters
NAME 100215.502 sd054 better
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100215
Time 17.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 90.5
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.60 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12k



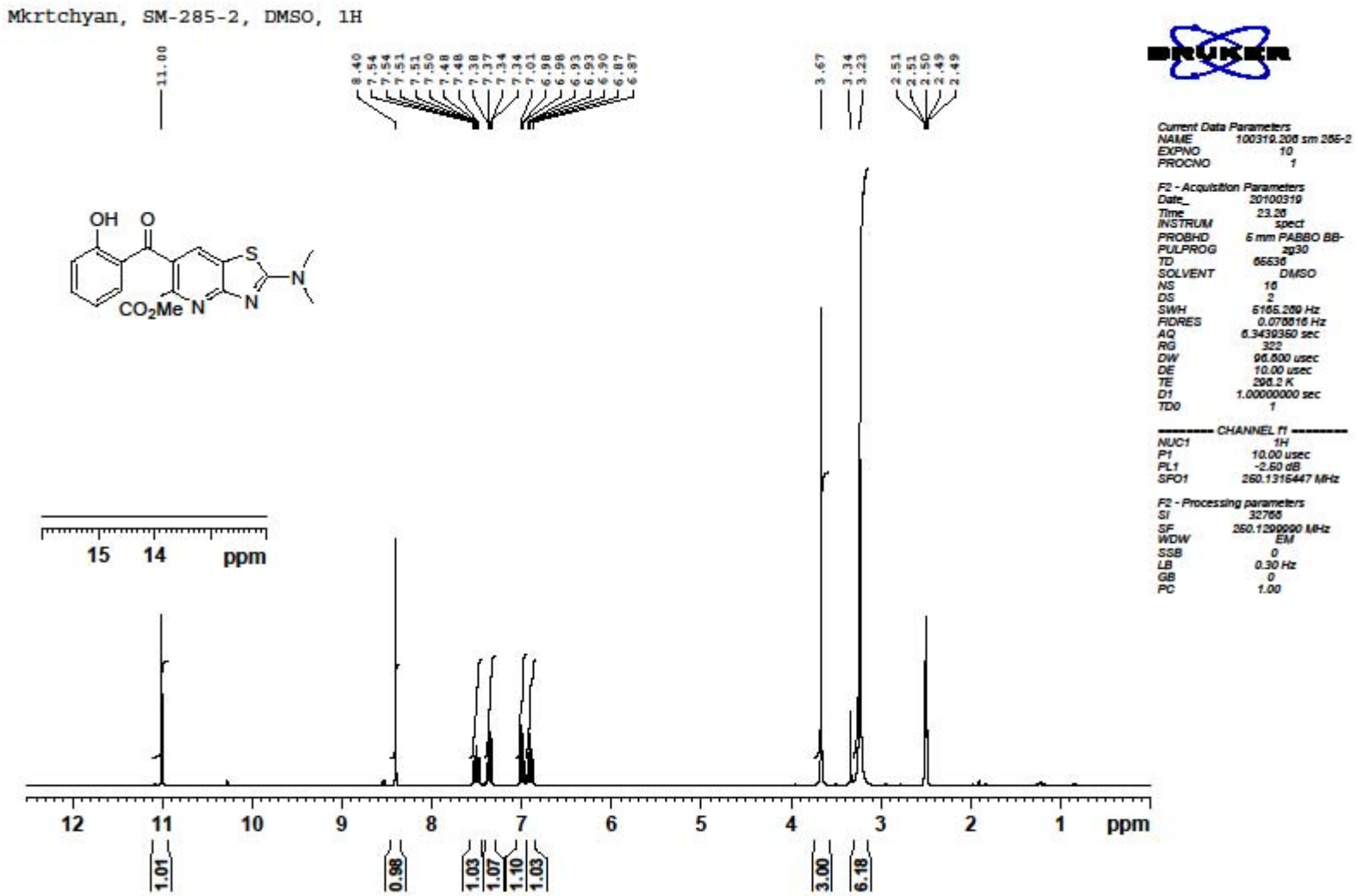
Current Data Parameters
NAME 100215.502 sd054 bett
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100216
Time 0.25
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 32
DW 16.650 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

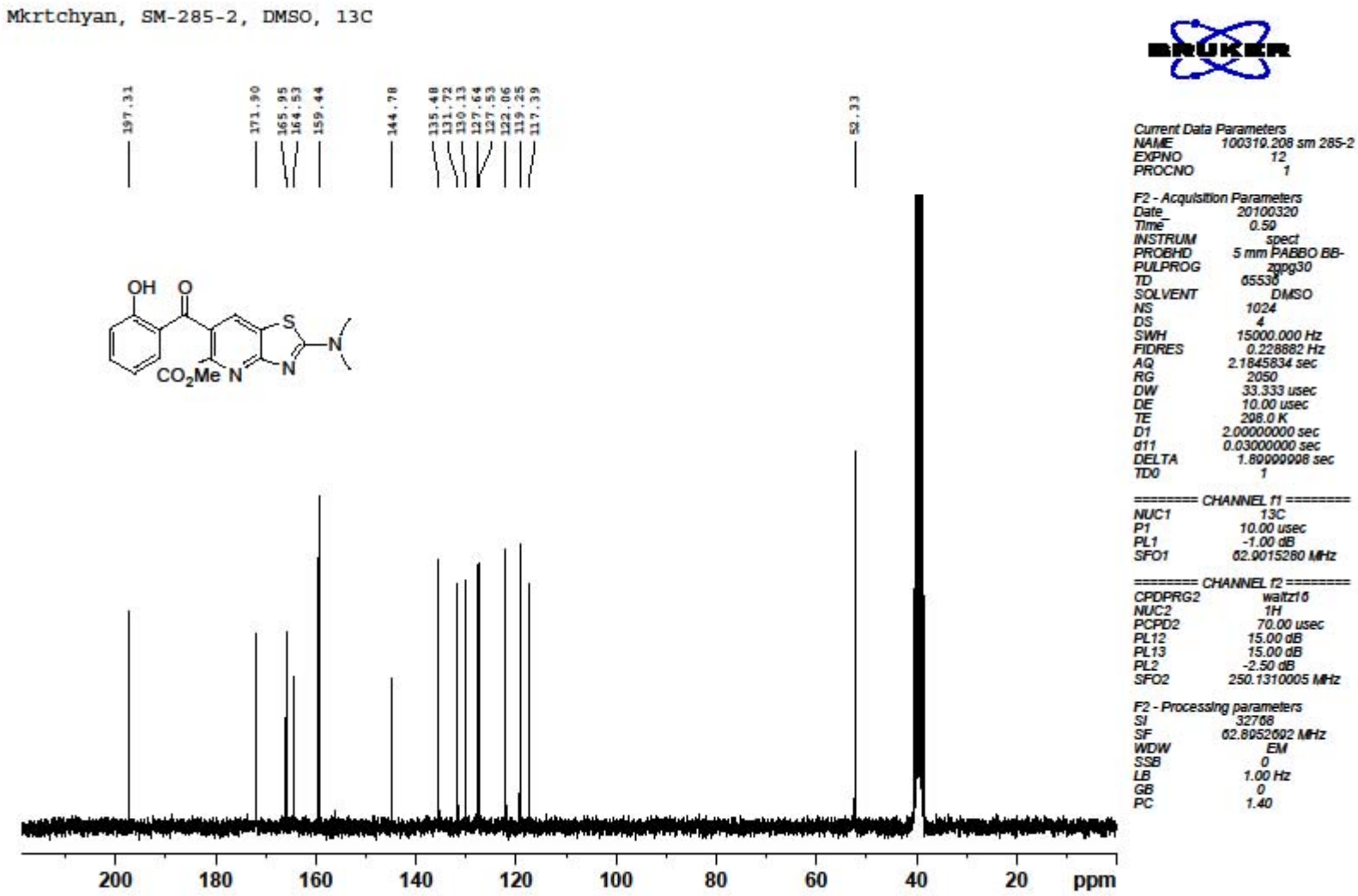
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 4.80 dB
SFO1 125.7703643 MHz

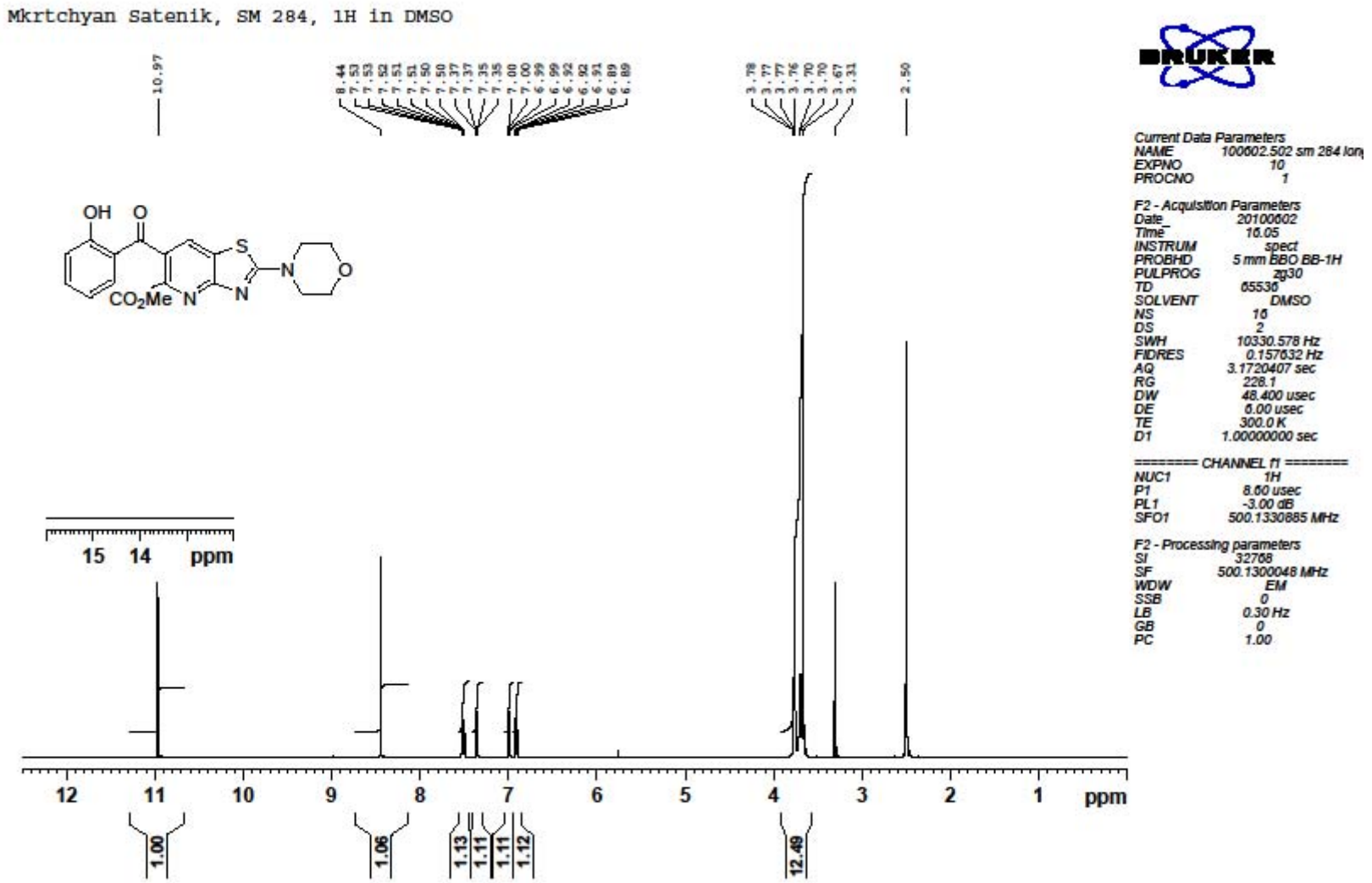
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.50 dB
PL13 20.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7578532 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

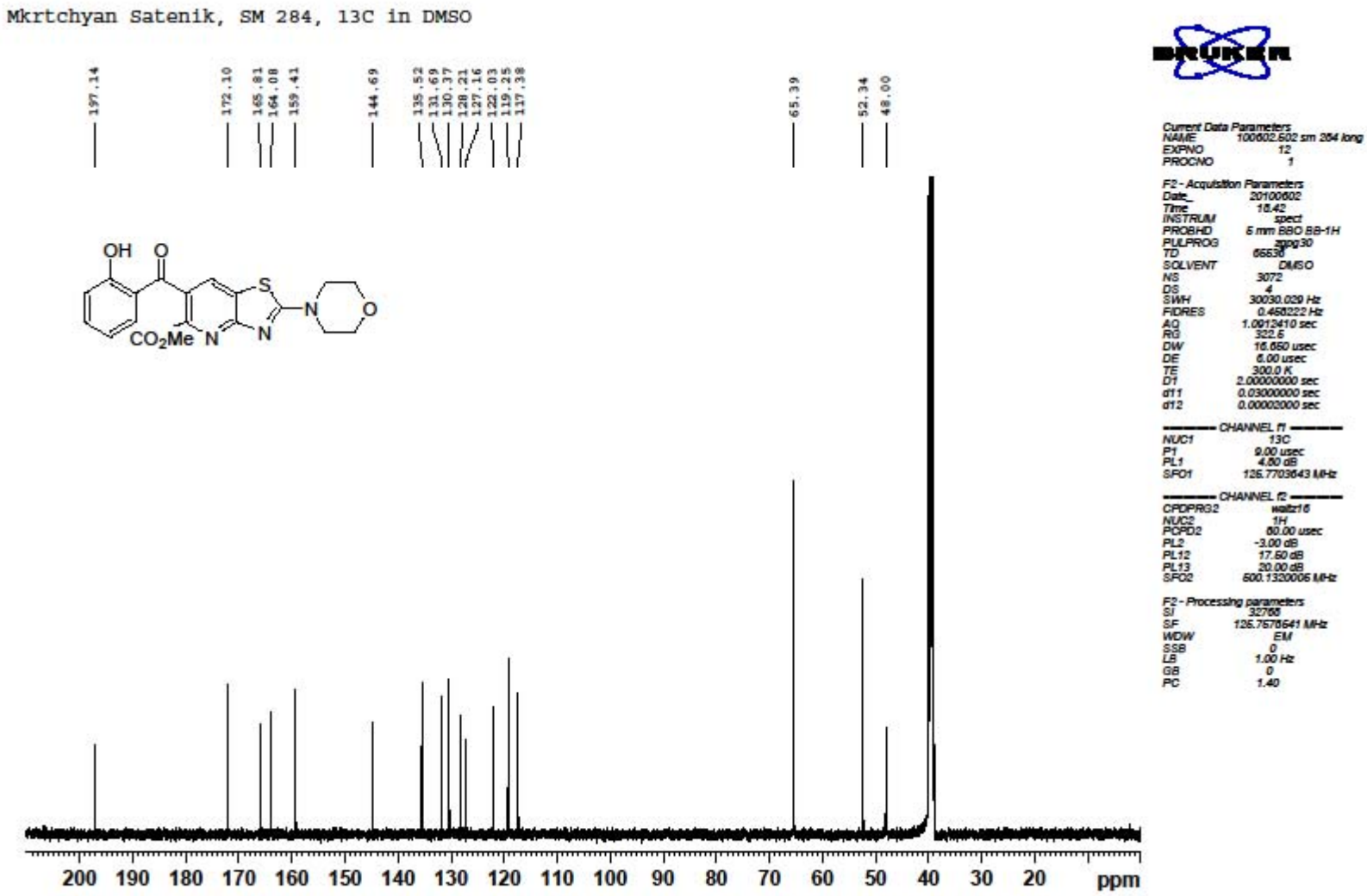

Mkrtchyan, SM-285-2, DMSO, 1H
11.00
8.40
7.54
7.54
7.51
7.51
7.50
7.48
7.48
7.38
7.37
7.34
7.34
7.01
6.98
6.98
6.93
6.90
6.87
6.87
3.67
3.34
3.23
2.51
2.51
2.50
2.49
2.49
OH
O
S
N
CO2Me
N
N
15
14
ppm
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.01
0.98
1.03
1.07
1.10
1.03
3.00
6.18
Current Data Parameters
NAME 100319.200 sm 285-2
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100319
Time 23.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6165.269 Hz
FIDRES 0.070616 Hz
AQ 6.3439360 sec
RG 322
DW 96.500 usec
DE 10.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.60 dB
SFO1 260.1316447 MHz
F2 - Processing parameters
SI 32768
SF 260.1299990 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

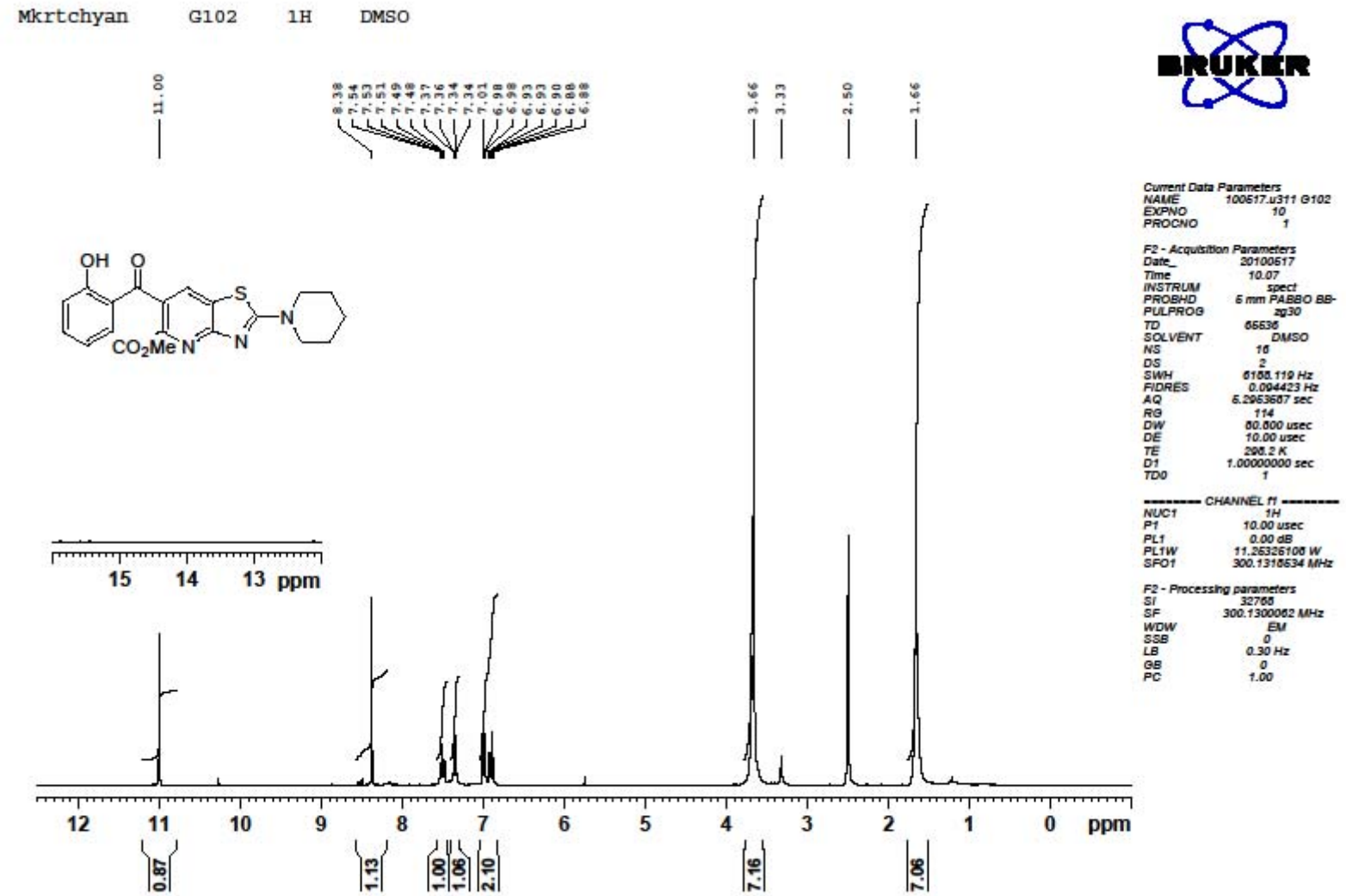
12 l


Mkrtchyan, SM-285-2, DMSO, 13C
197.31
171.90
165.95
164.53
159.44
144.78
135.48
131.72
130.13
127.64
127.53
122.06
119.25
117.39
52.33
OH
O
S
N
N
CO2Me
N
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 100319.208 sm 285-2
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100320
Time 0.59
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 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 62.8952602 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

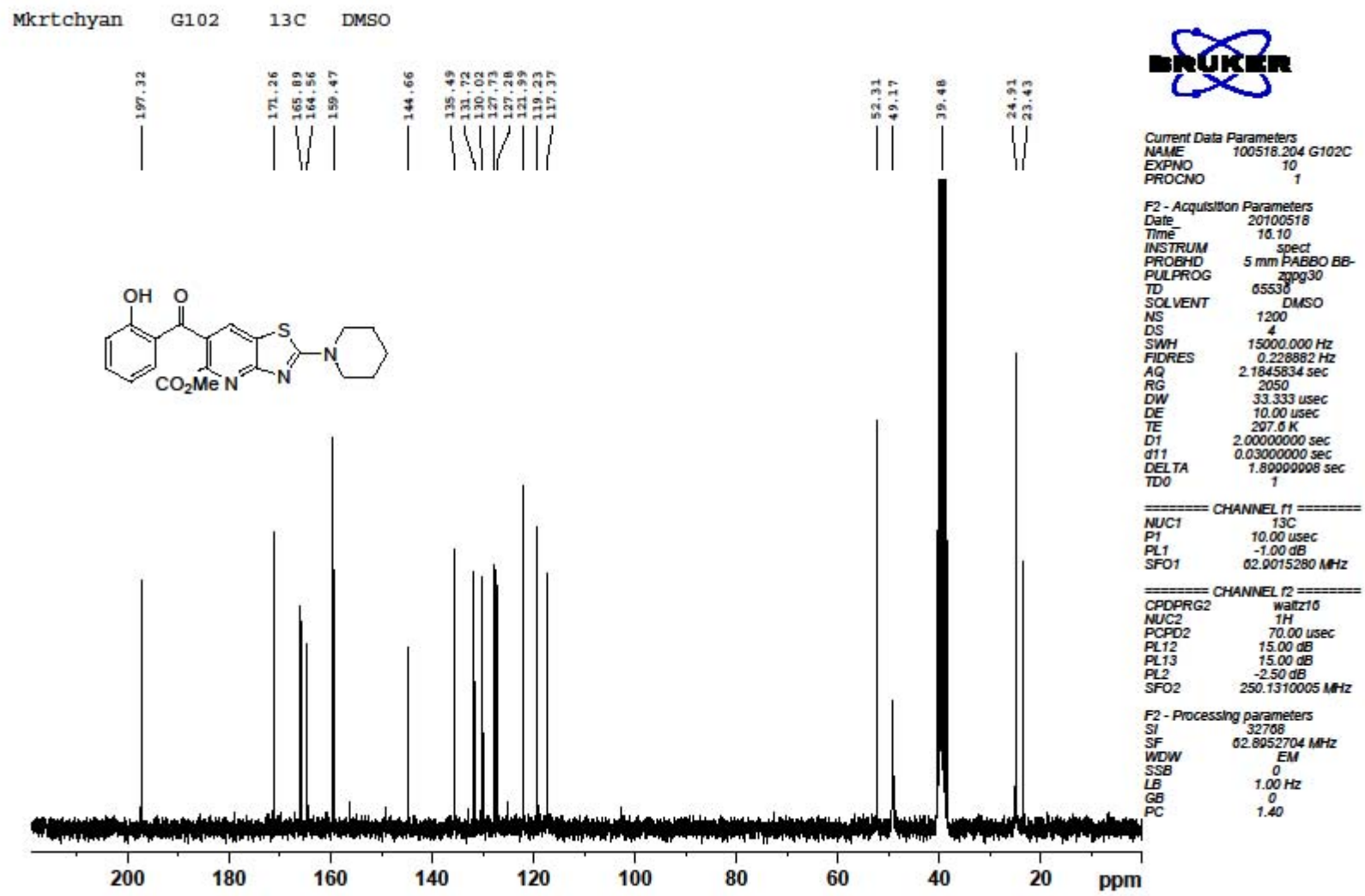

Mkrtchyan Satenik, SM 284, 1H in DMSO
10.97
8.44
7.53
7.53
7.52
7.51
7.51
7.50
7.50
7.37
7.37
7.35
7.35
7.00
7.00
6.99
6.99
6.92
6.92
6.91
6.89
6.89
3.78
3.77
3.77
3.76
3.70
3.70
3.67
3.31
2.50
OH
O
S
N
O
CO2Me
N
N
15
14
ppm
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.06
1.13
1.11
1.11
1.12
12.49
BRUKER
Current Data Parameters
NAME 100602.502 sm 284 lon
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100602
Time 16.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.60 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

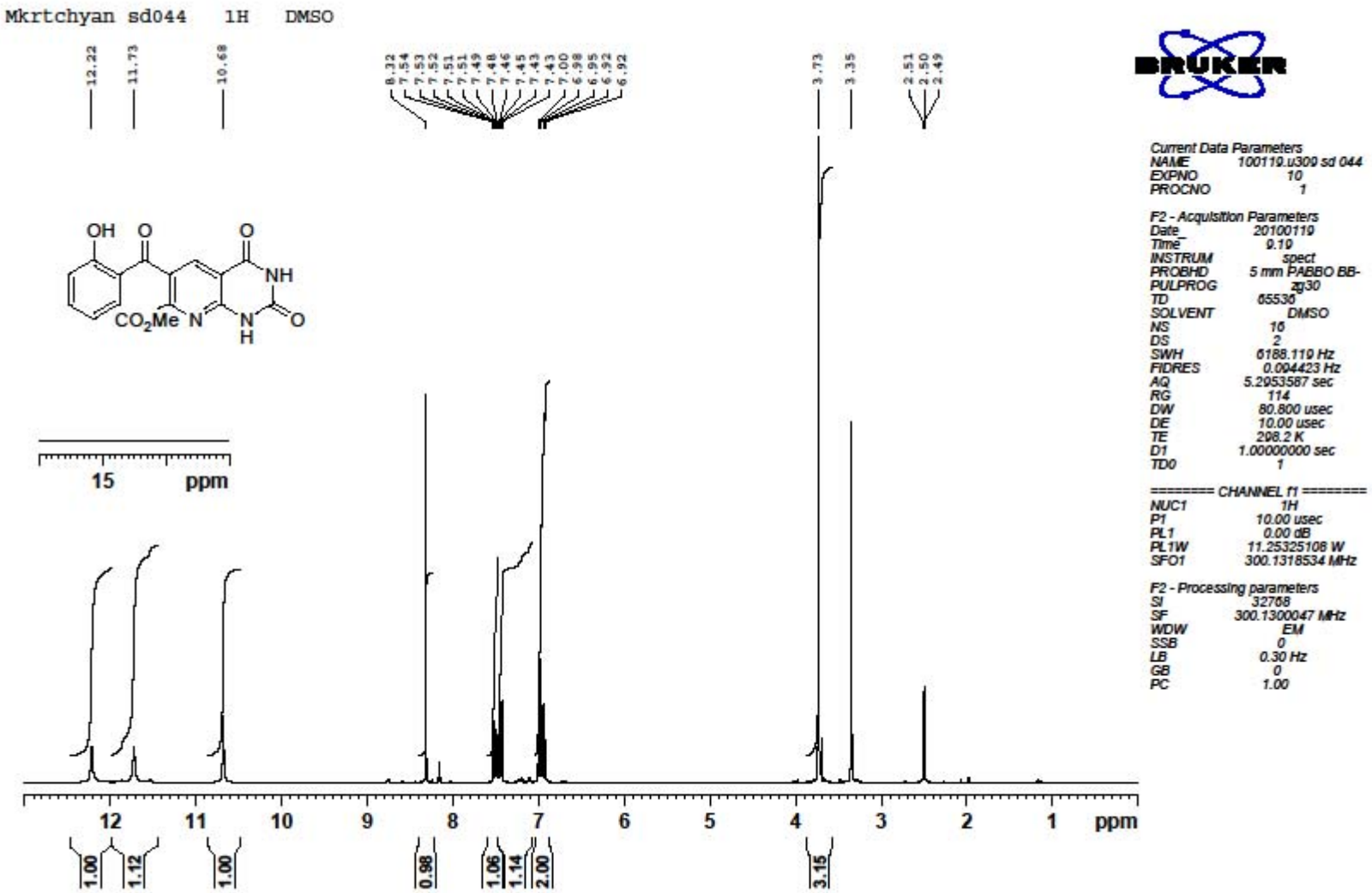
12 m


Mkrtchyan Satenik, SM 284, 13C in DMSO
197.14
172.10
165.81
164.08
159.41
144.69
135.52
131.69
130.37
128.21
127.16
122.03
119.25
117.38
65.39
52.34
48.00
OH
O
S
N
O
CO2Me
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
Current Data Parameters
NAME 100602.602 sm 284 long
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100602
Time 16.42
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 362.6
DW 16.650 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
CHANNEL f1
NUC1 13C
P1 9.00 usec
PL1 4.00 dB
SFO1 125.7703643 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 -3.00 dB
PL12 17.50 dB
PL13 20.00 dB
SFO2 500.1320006 MHz
F2 - Processing parameters
SI 32768
SF 125.7575641 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

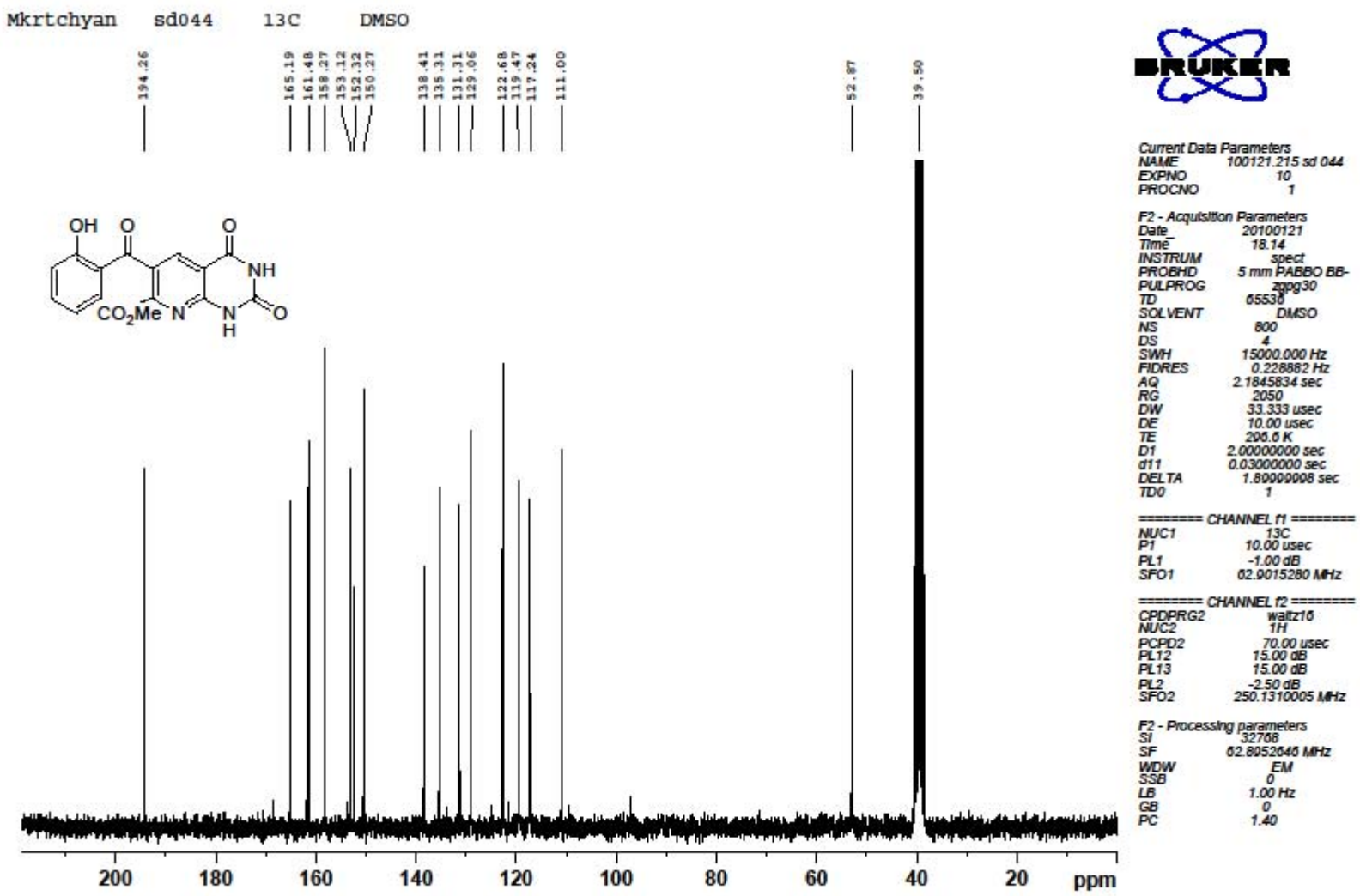

Mkrtchyan G102 1H DMSO
11.00
8.38
7.54
7.53
7.51
7.49
7.48
7.37
7.36
7.34
7.34
7.01
6.98
6.98
6.93
6.93
6.90
6.88
6.88
3.66
3.33
2.50
1.66
OH
O
S
N
N
CO2Me
N
15 14 13 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.87
1.13
1.00
1.06
2.10
7.16
7.06
Current Data Parameters
NAME 100517.u311 G102
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100517
Time 10.07
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 5.2953657 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 0.00 dB
PL1W 11.26326106 W
SFO1 300.1316634 MHz
F2 - Processing parameters
SI 32768
SF 300.1300062 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12 n


Mkrtchyan G102 13C DMSO
197.32
171.26
165.89
164.56
159.47
144.66
135.49
131.72
130.02
127.73
127.28
121.99
119.23
117.37
52.31
49.17
39.48
24.91
23.43
OH O
S
N
N
CO2Me N
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME 100518.204 G102C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100518
Time 16.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
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 297.6 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 62.8952704 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Mkrtchyan sd044 1H DMSO
12.22
11.73
10.68
8.32
7.54
7.53
7.52
7.51
7.51
7.49
7.48
7.46
7.45
7.43
7.43
7.00
6.98
6.95
6.92
6.92
3.73
3.35
2.51
2.50
2.49
OH
O
O
NH
CO2Me
N
N
H
O
15 ppm
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.12
1.00
0.98
1.06
1.14
2.00
3.15
BRUKER
Current Data Parameters
NAME 100119.u309 sd 044
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100119
Time 9.19
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 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12 o



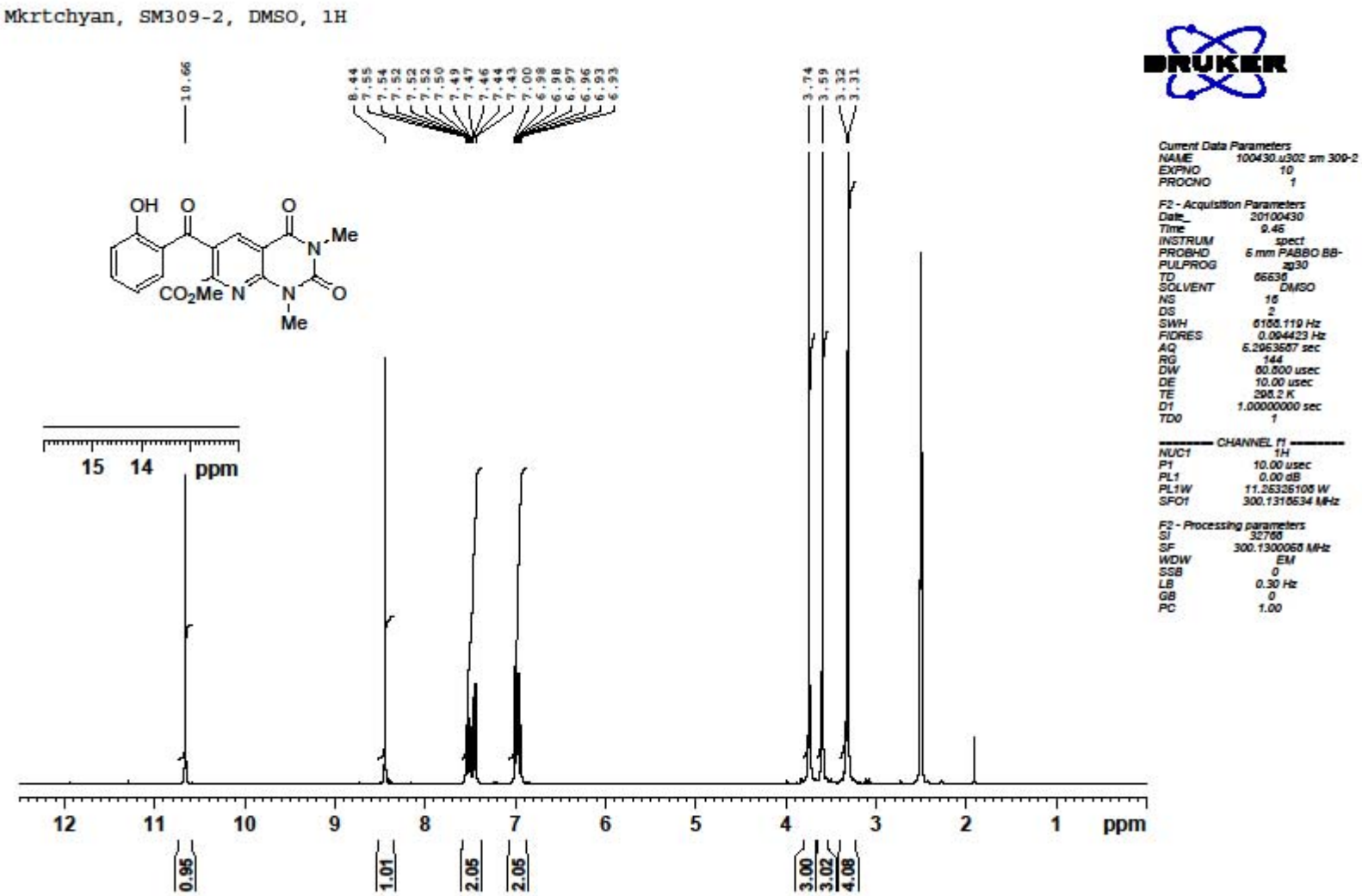
Current Data Parameters
NAME 100121.215 sd 044
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100121
Time 18.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 800
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 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

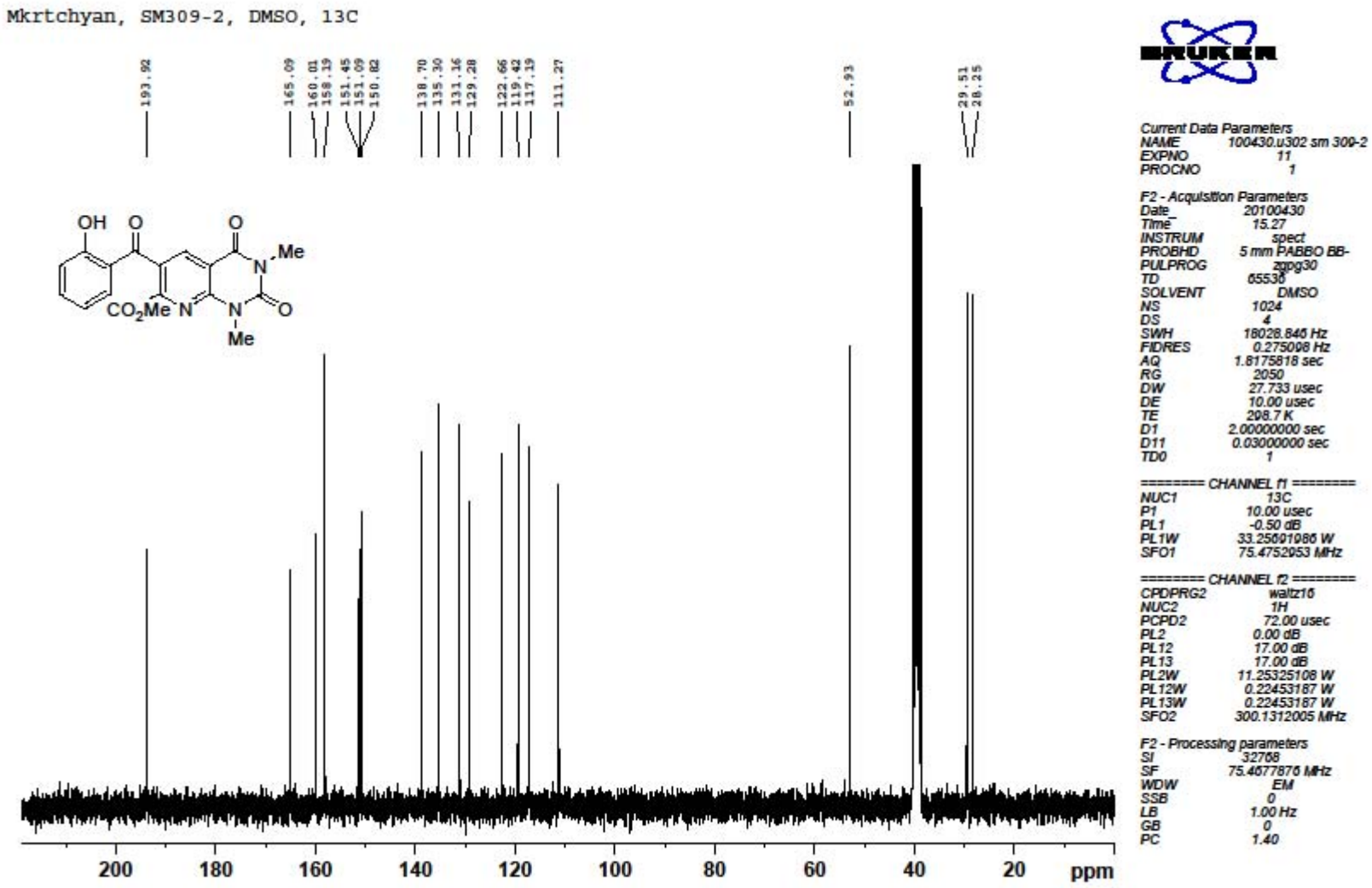
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

======== 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 62.8952640 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Mkrtchyan, SM309-2, DMSO, 1H
10.66
8.44
7.55
7.54
7.52
7.52
7.50
7.49
7.47
7.46
7.44
7.43
7.00
6.98
6.97
6.96
6.93
6.93
3.74
3.59
3.32
3.31
OH
O
O
N
Me
CO2Me
N
N
O
Me
15
14
ppm
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.95
1.01
2.05
2.05
3.00
3.02
4.08
BRUKER
Current Data Parameters
NAME 100430.u302 sm 309-2
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100430
Time 9.46
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 5.2953600 sec
RG 144
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 0.00 dB
PL1W 11.25326105 W
SFO1 300.1316534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12 p



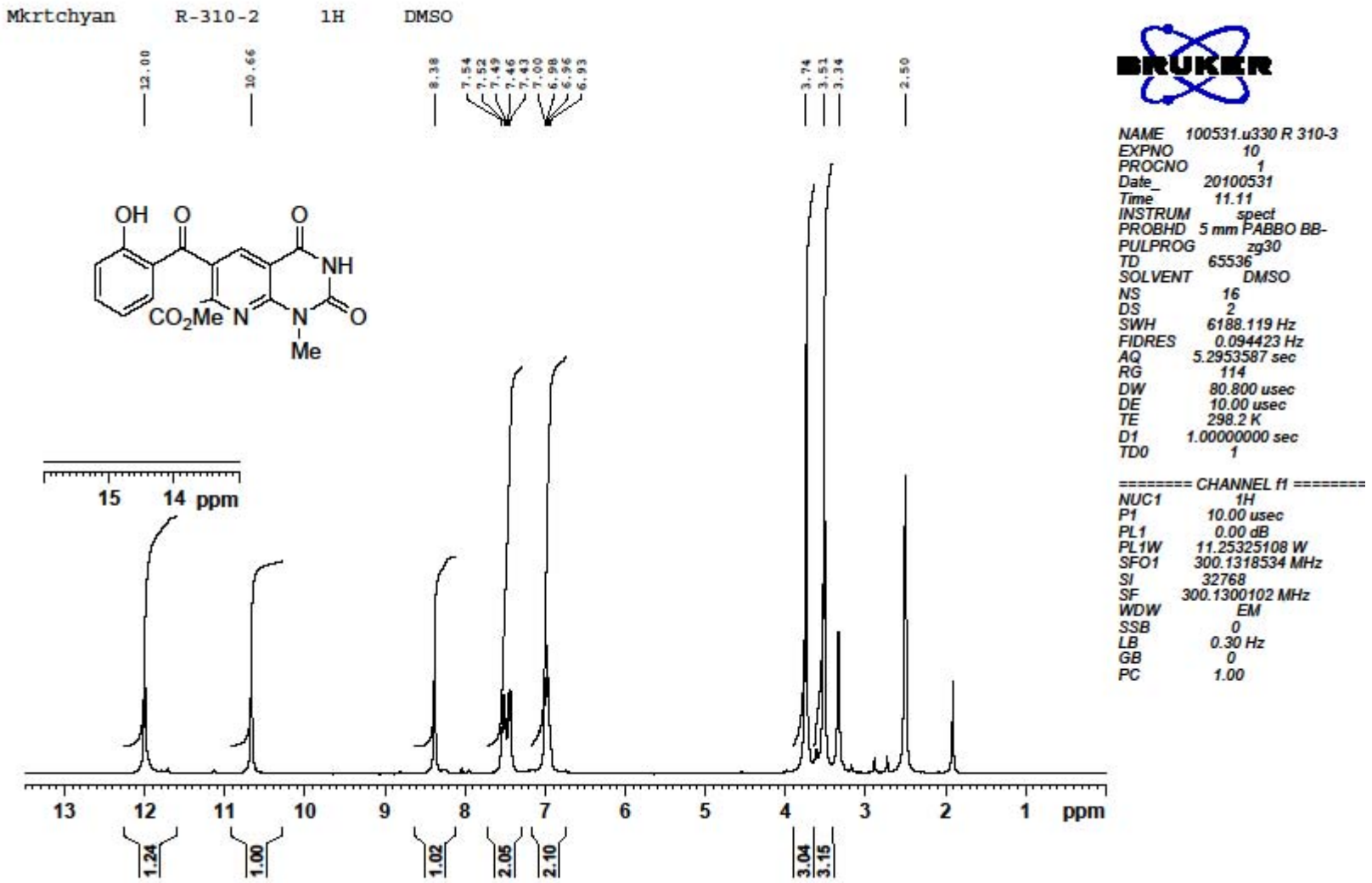
Current Data Parameters
NAME 100430.u302 sm 309-2
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date 20100430
Time 15.27
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 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

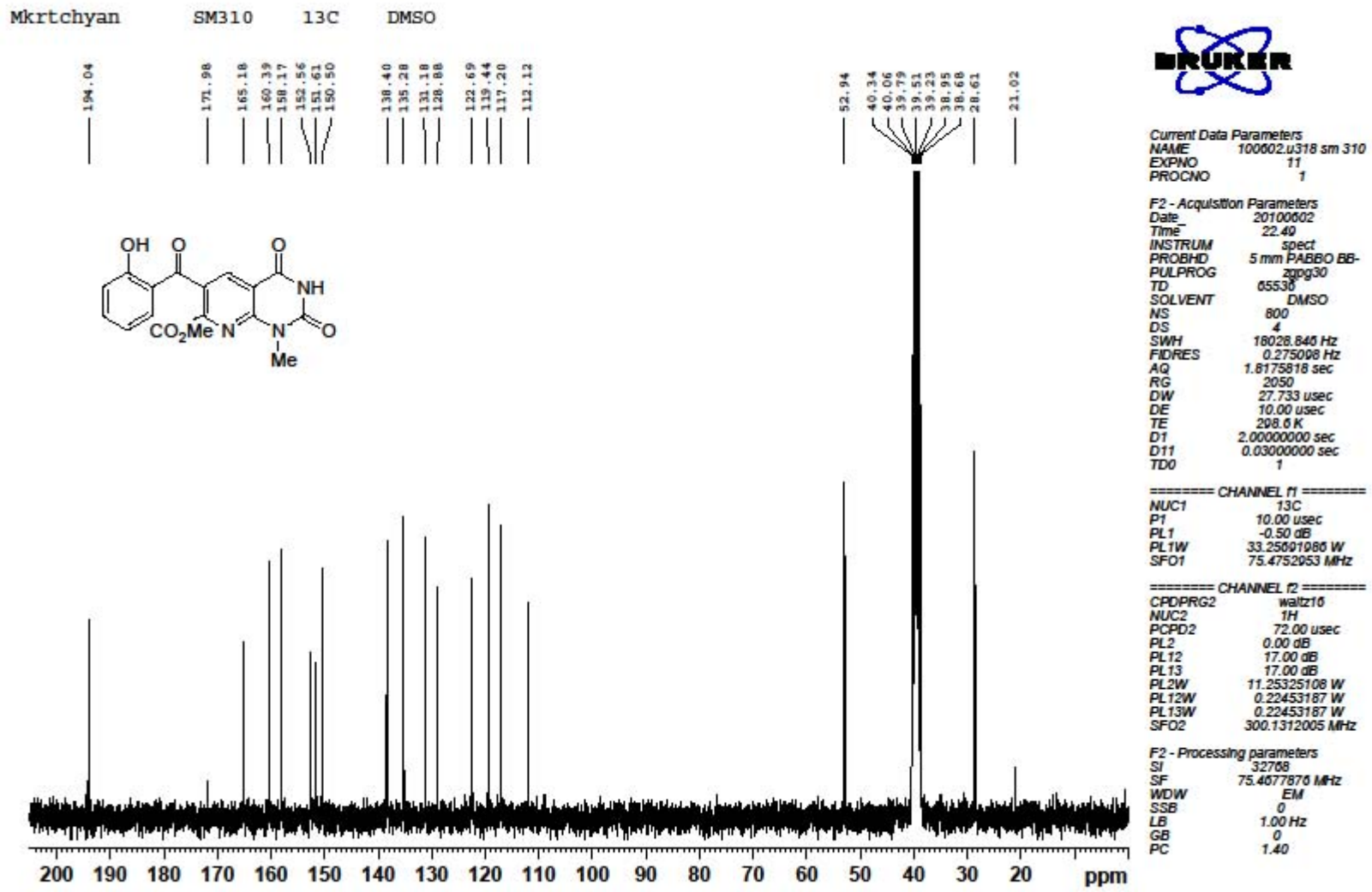
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691086 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 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 75.4677876 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Mkrtchyan R-310-2 1H DMSO
12.00
10.66
8.38
7.54
7.52
7.49
7.46
7.43
7.00
6.98
6.96
6.93
3.74
3.51
3.34
2.50
OH O O
NH
CO2Me N N O
Me
15 14 ppm
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.24
1.00
1.02
2.05
2.10
3.04
3.15
BRUKER
NAME 100531.u330 R 310-3
EXPNO 10
PROCNO 1
Date_ 20100531
Time 11.11
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 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12 q



BRUKER

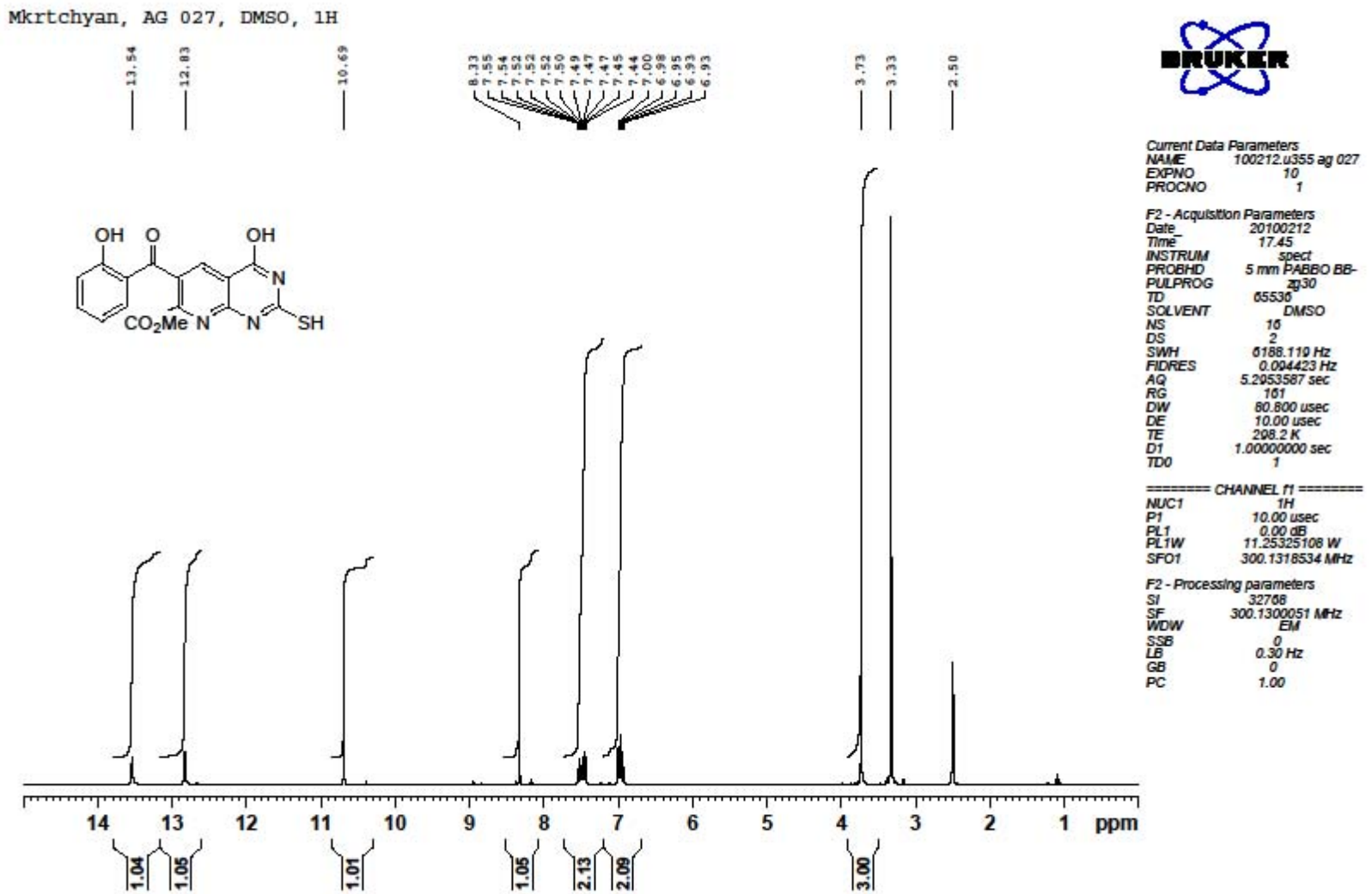
Current Data Parameters
NAME 100602.u318 sm 310
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100602
Time 22.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 800
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

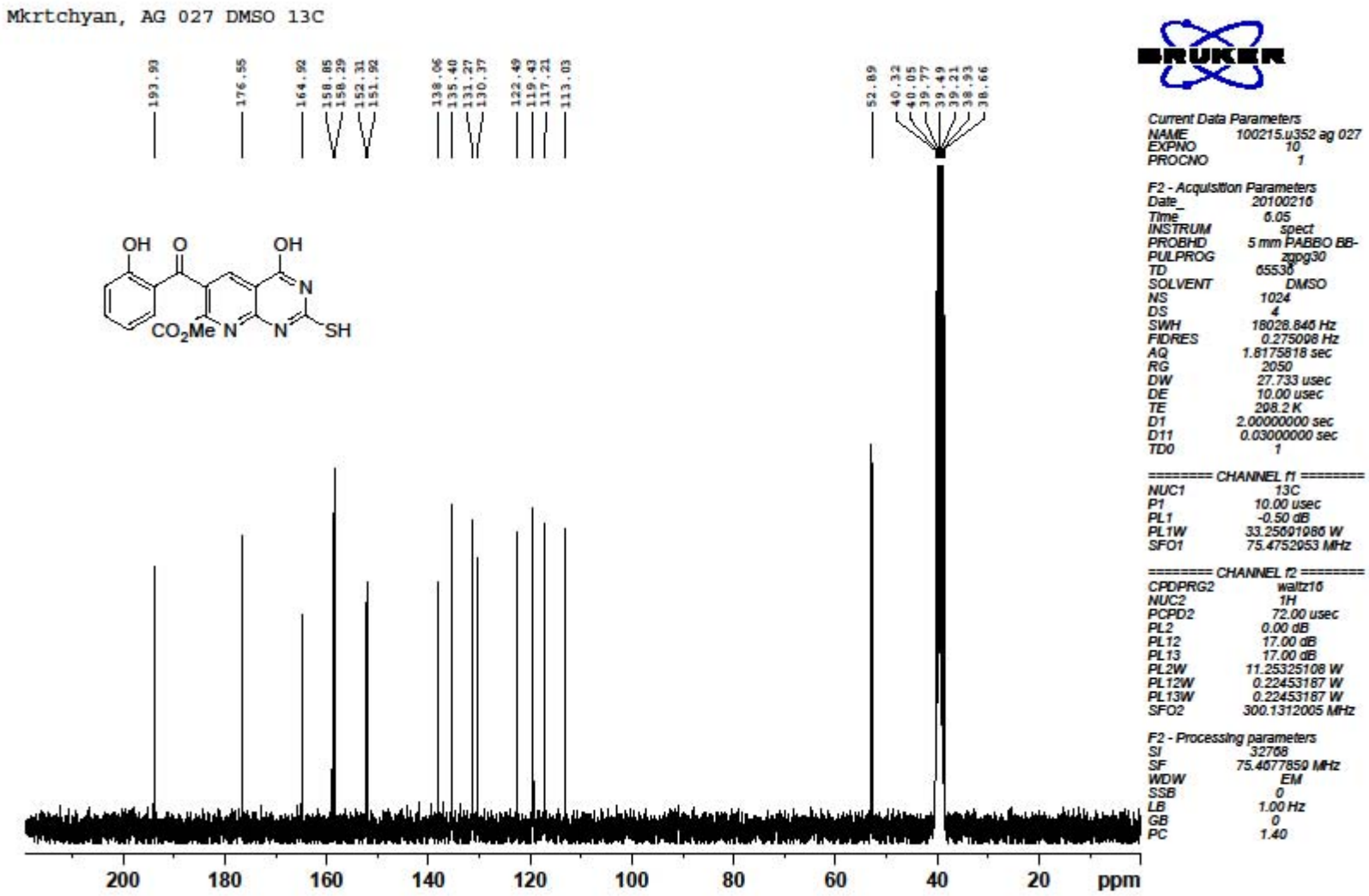
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25091986 W
SFO1 75.4752953 MHz

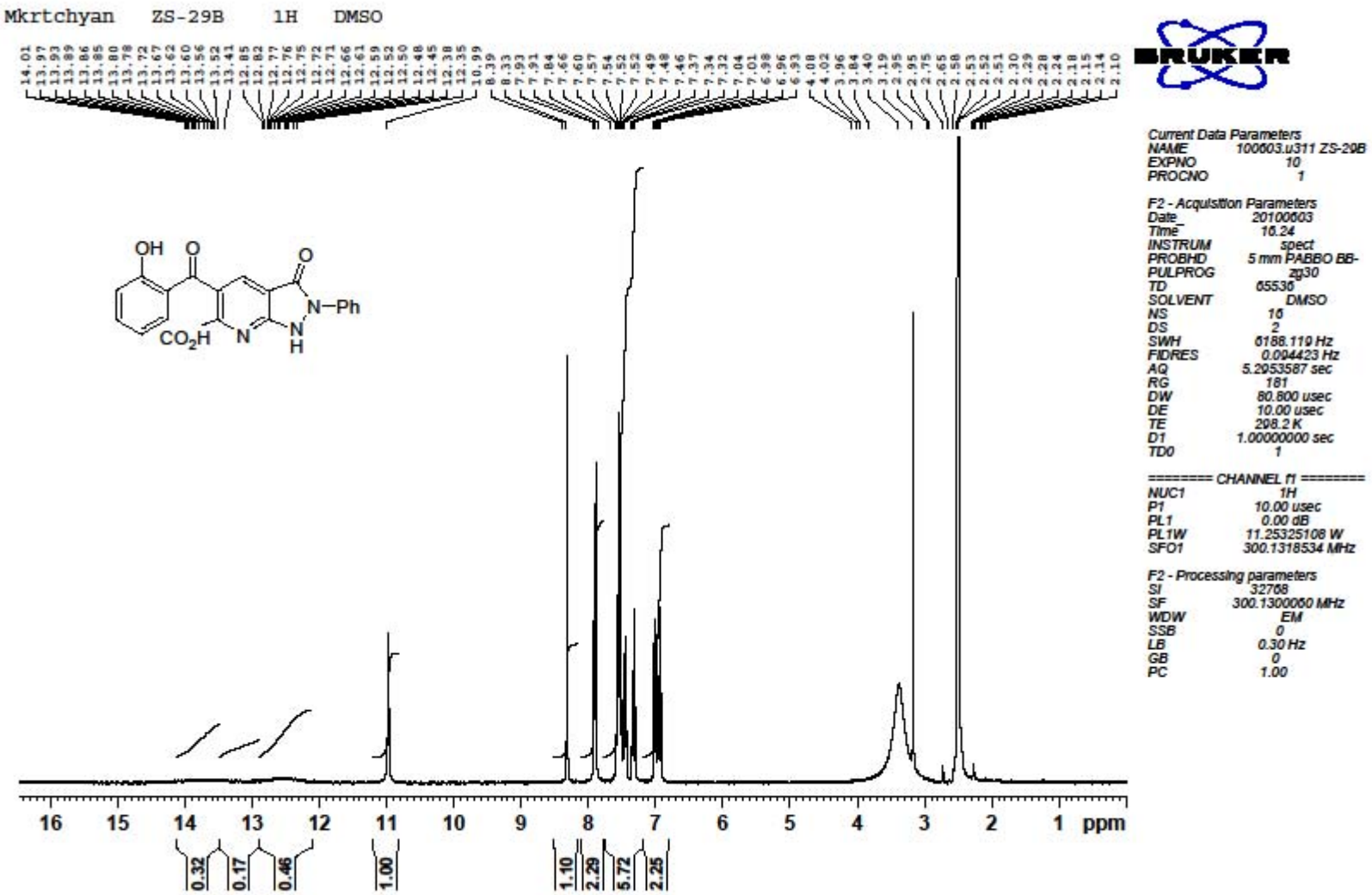
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677876 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

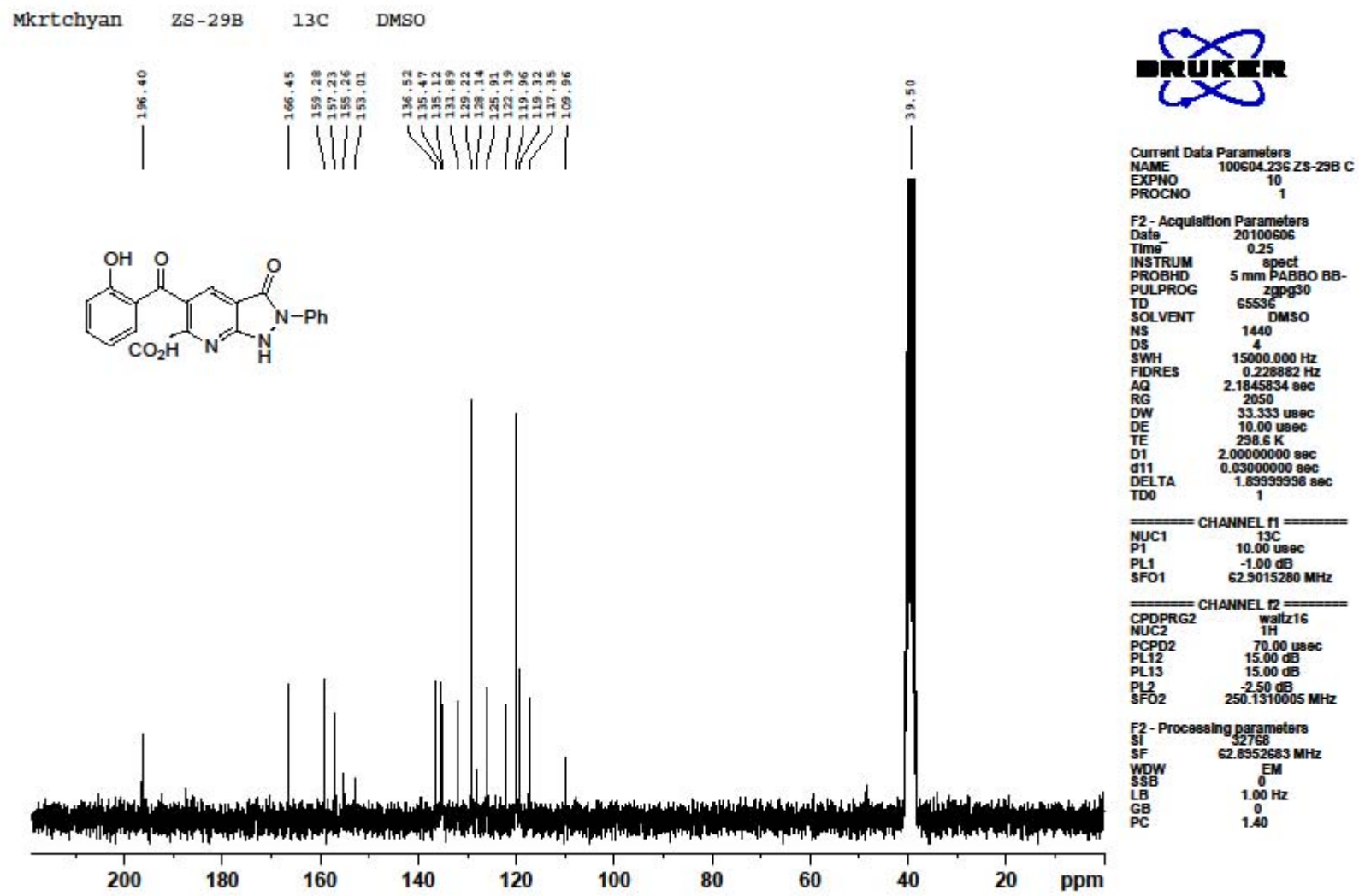

Mkrtchyan, AG 027, DMSO, 1H
13.54
12.83
10.69
8.33
7.55
7.54
7.52
7.52
7.50
7.49
7.47
7.47
7.45
7.44
7.00
6.98
6.95
6.93
6.93
3.73
3.33
2.50
OH
O
OH
N
CO2Me
N
N
SH
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.04
1.05
1.01
1.05
2.13
2.09
3.00
Current Data Parameters
NAME 100212.u355 ag 027
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100212
Time 17.45
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 0.00 dB
PL1W 11.25325108 W
SFO1 300.1316534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

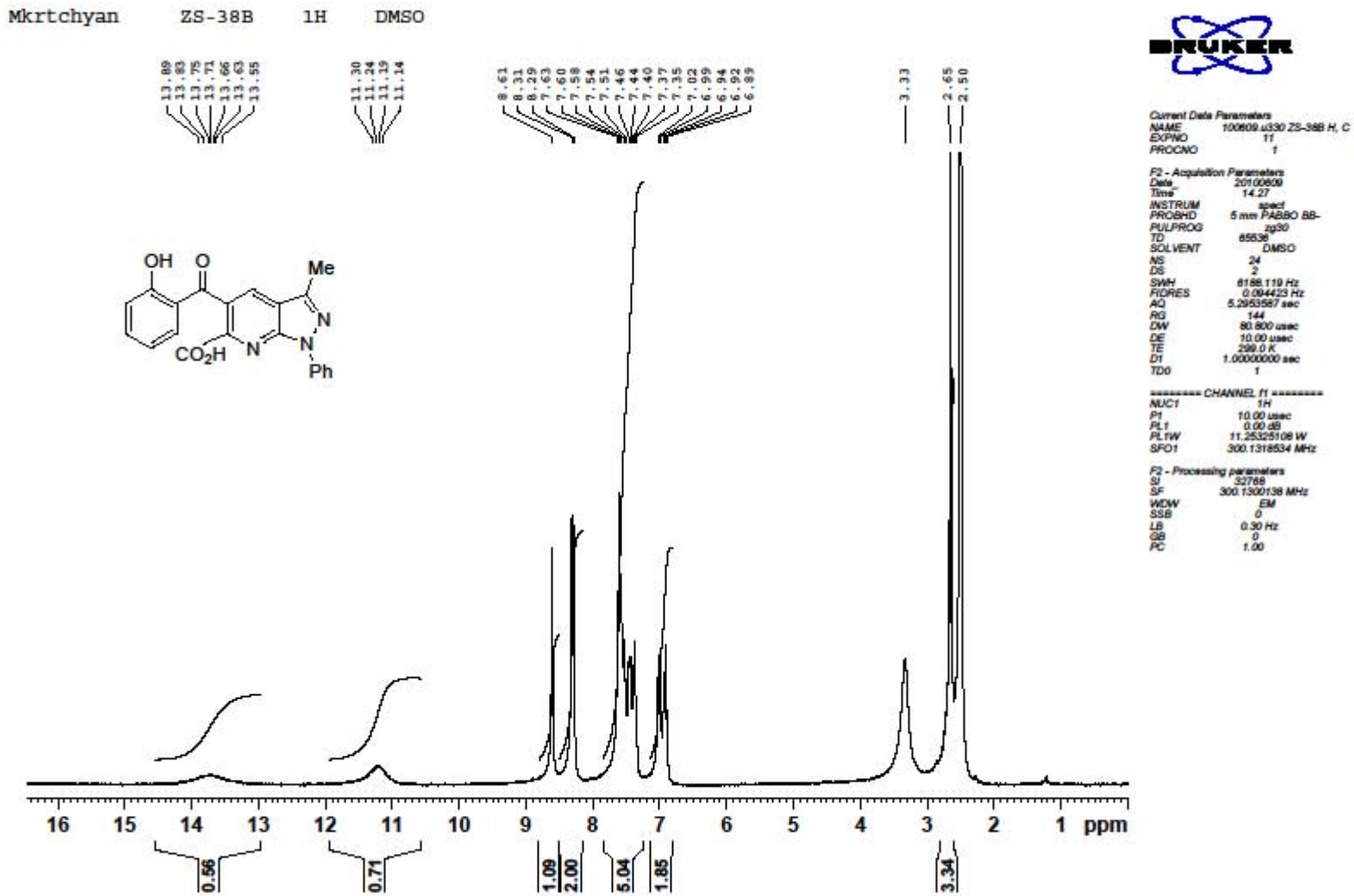
12 r



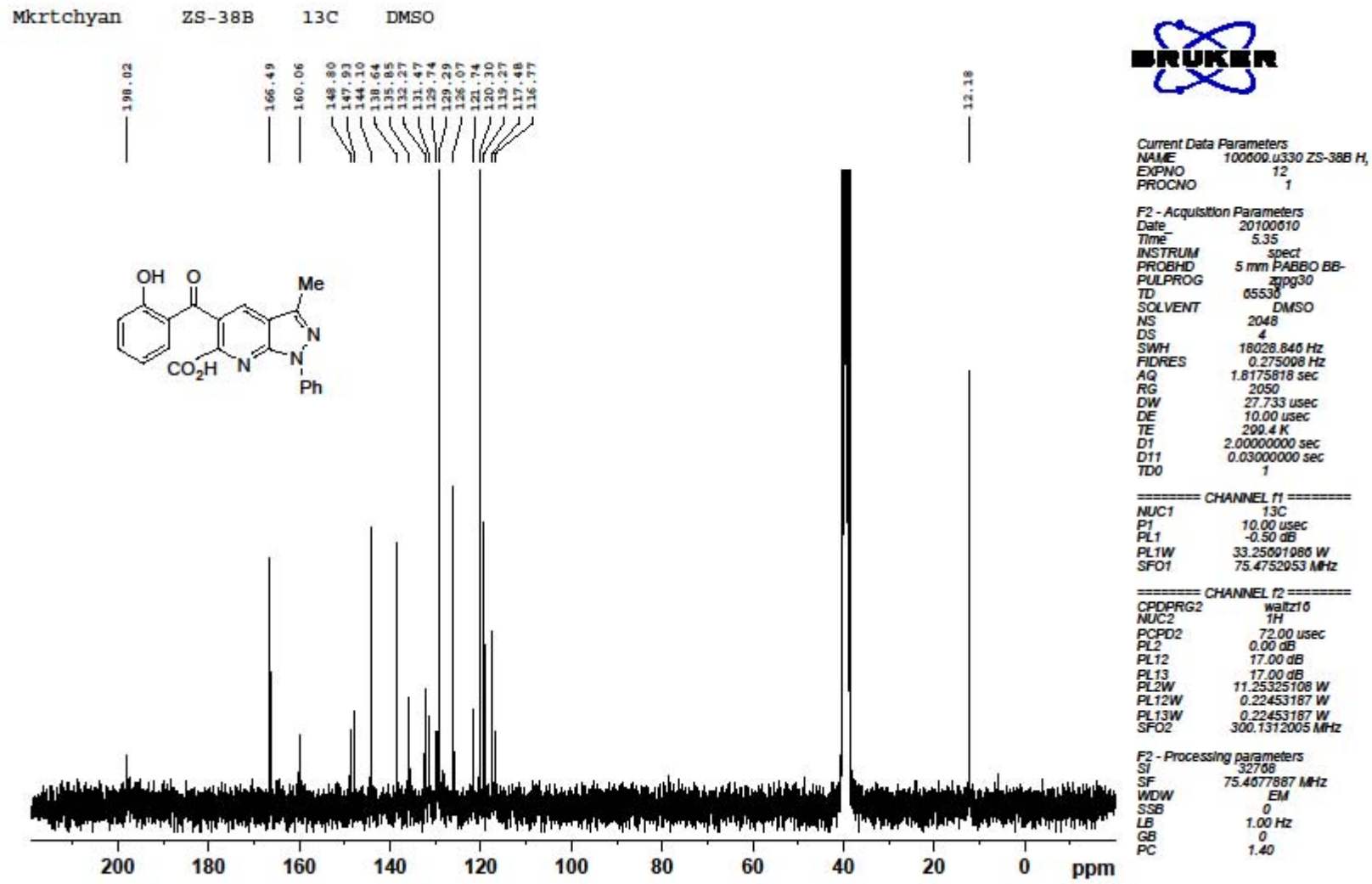

Mkrtchyan ZS-29B 1H DMSO
OH
O
O
N–Ph
N
N
H
CO2H
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.32
0.17
0.46
1.00
1.10
2.29
5.72
2.25
Current Data Parameters
NAME 100603.u311 ZS-29B
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100603
Time 16.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 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 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

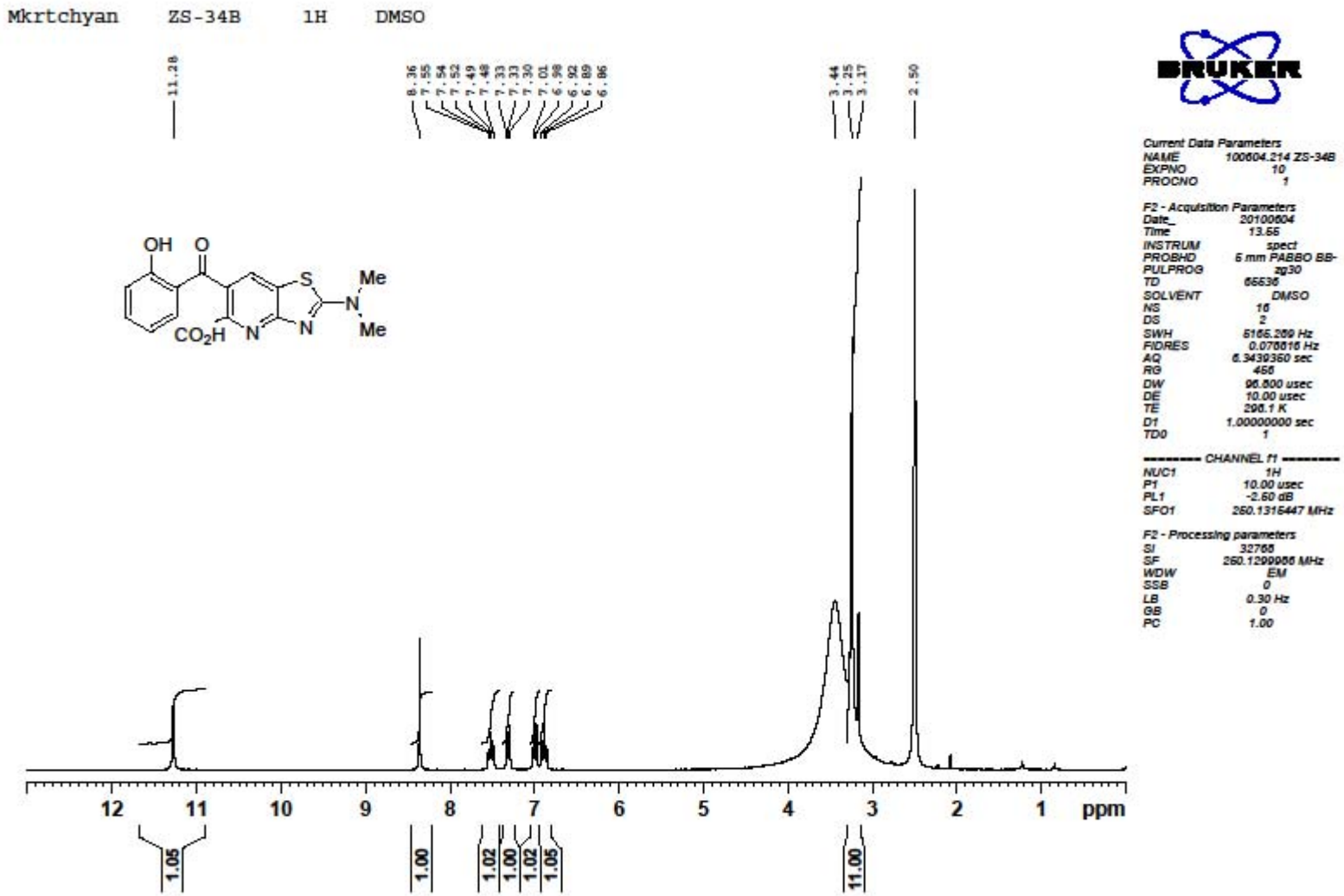
13 d


Mkrtchyan ZS-29B 13C DMSO
196.40
166.45
159.28
157.23
155.26
153.01
136.52
135.47
135.12
131.89
129.22
128.14
125.91
122.19
119.96
119.32
117.35
109.96
39.50
OH
O
O
N–Ph
N
N
H
CO2H
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME 100604.236 ZS-29B C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100606
Time 0.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1440
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 298.6 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 62.8952683 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

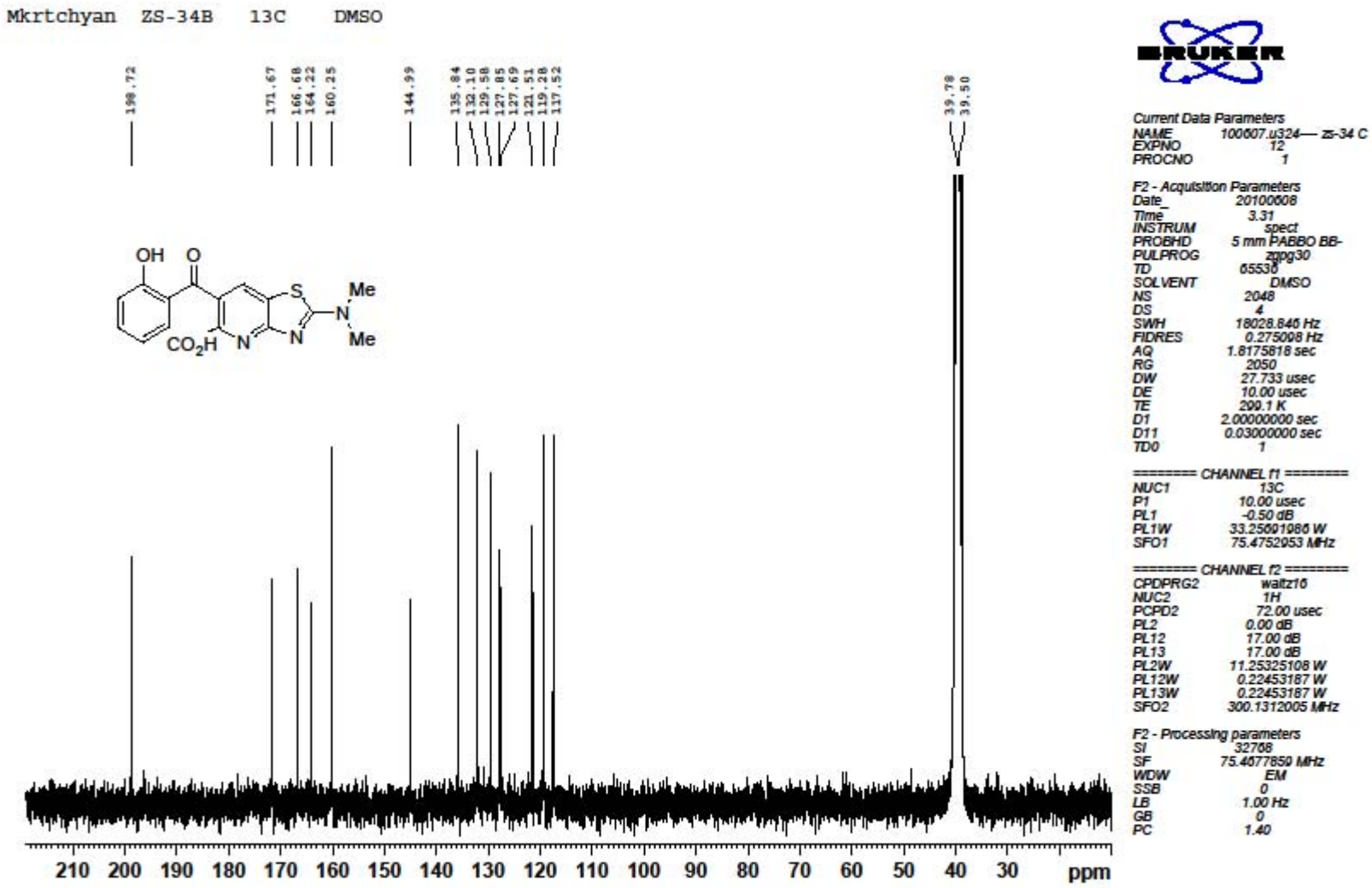

Mkrtchyan ZS-38B 1H DMSO
13.89
13.83
13.75
13.71
13.66
13.63
13.55
11.30
11.24
11.19
11.14
8.61
8.31
8.29
7.63
7.60
7.58
7.54
7.51
7.46
7.44
7.40
7.37
7.35
7.02
6.99
6.94
6.92
6.89
3.33
2.65
2.50
OH
O
Me
N
N
N
CO2H
Ph
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.56
0.71
1.09
2.00
5.04
1.85
3.34
Current Data Parameters
NAME 100809 u330 ZS-38B H, C
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100809
Time 14.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 24
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 144
DW 80.800 usec
DE 10.00 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 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

13k


Mkrtchyan ZS-38B 13C DMSO
198.02
166.49
160.06
148.80
147.93
144.10
138.64
135.85
132.27
131.47
129.74
129.29
126.07
121.74
120.30
119.27
117.48
116.77
12.18
OH
O
Me
N
N
N
CO2H
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME 100609.u330 ZS-38B H,
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100610
Time 5.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
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 33.25601986 W
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 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 75.4677887 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Mkrtchyan ZS-34B 1H DMSO
11.28
8.36
7.55
7.54
7.52
7.49
7.48
7.33
7.33
7.30
7.01
6.98
6.92
6.89
6.86
3.44
3.25
3.17
2.50
OH O
S
Me
N
Me
CO2H N
N
12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.05
1.00
1.02
1.00
1.02
1.05
11.00
BRUKER
Current Data Parameters
NAME 100604.214 ZS-34B
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100604
Time 13.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6165.269 Hz
FIDRES 0.076816 Hz
AQ 5.3439360 sec
RG 456
DW 96.800 usec
DE 10.00 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
---------- CHANNEL f1 ----------
NUC1 1H
P1 10.00 usec
PL1 -2.60 dB
SFO1 250.1316447 MHz
F2 - Processing parameters
SI 32768
SF 250.1299966 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13 l



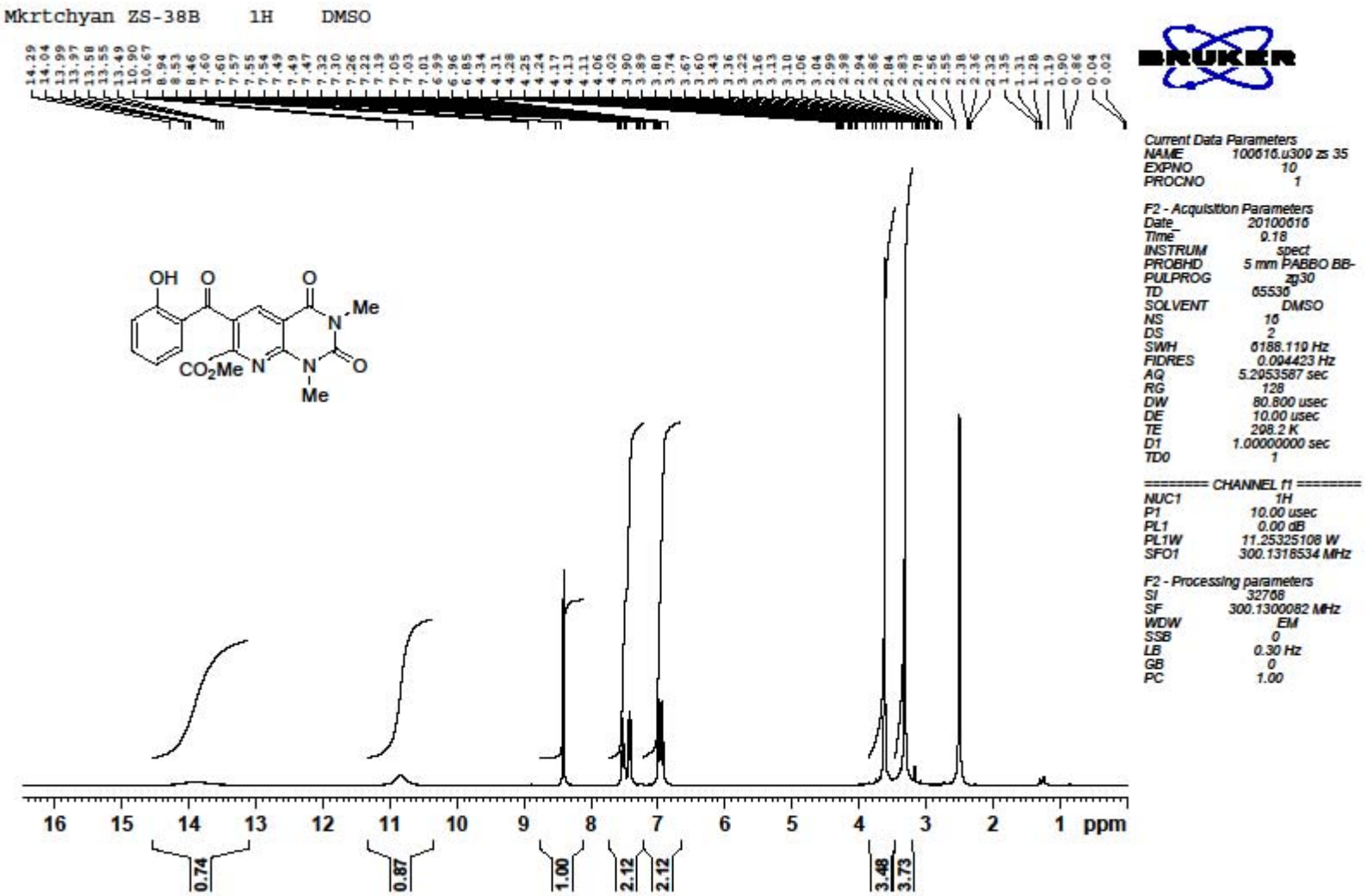
Current Data Parameters
NAME 100607.u324— zs-34 C
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100608
Time 3.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
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 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

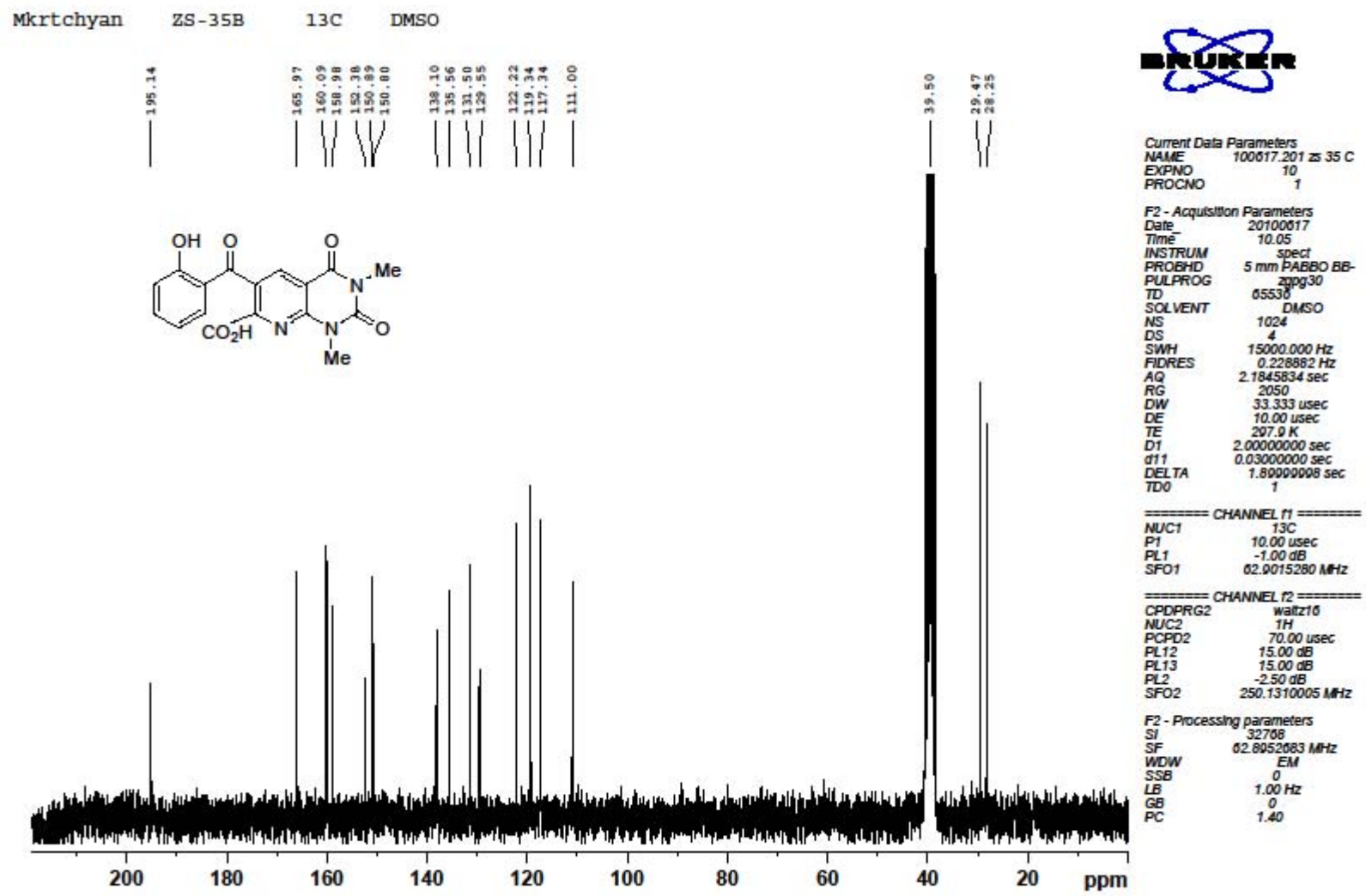
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 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 75.4677859 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Mkrtchyan ZS-38B 1H DMSO
BRUKER
Current Data Parameters
NAME 100616.u309 zs 35
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100616
Time 9.18
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 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 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OH
O
O
Me
N
CO2Me
N
N
O
Me
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.74
0.87
1.00
2.12
2.12
3.48
3.73

13 p


Mkrtchyan ZS-35B 13C DMSO
195.14
165.97
160.09
158.98
152.38
150.89
150.80
138.10
135.56
131.50
129.55
122.22
119.34
117.34
111.00
39.50
29.47
28.25
OH
O
O
Me
N
CO2H
N
N
O
Me
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME 100617.201 zs 35 C
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100617
Time 10.05
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 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 62.8952683 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40