

Supplementary Information

Synthesis of 4-Quinolones, Benzopyran Derivatives and other Fused Systems Based on the Domino ANRORC Reactions of (*Ortho*-fluoro)-3-benzoylchromones.

Viktor O. Iaroshenko,^{a,b*} Satenik Mkrtchyan,^a Ashot Gevorgyan,^a Tatevik Grigoryan,^a Alexander Villinger,^a Peter Langer^{a,c*}

^aInstitut für Chemie, Universität Rostock, Albert-Einstein-Str. 3a, 18059 Rostock, Germany;

^bNational Taras Shevchenko University, 62 Volodymyrska st., Kyiv-33, 01033, Ukraine;

^cLeibniz-Institut für Katalyse e. V. an der Universität Rostock, Albert-Einstein-Str. 29a, 18059 Rostock, Germany.

Table of Contents

(A) X-Ray data.....	2
(B) Analytical data.....	7
(C) Copies of ¹ H and ¹³ C NMR spectra.....	36

(A) X-Ray data

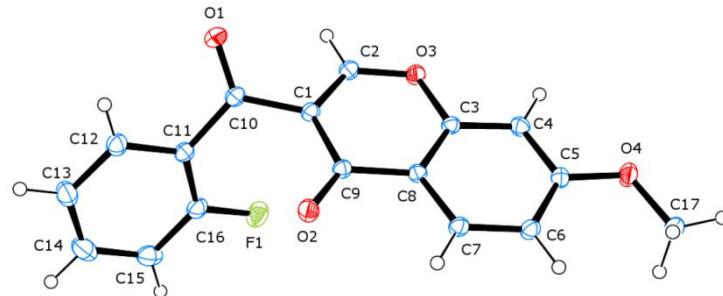


Figure 1. Crystal structure of compound 3e.

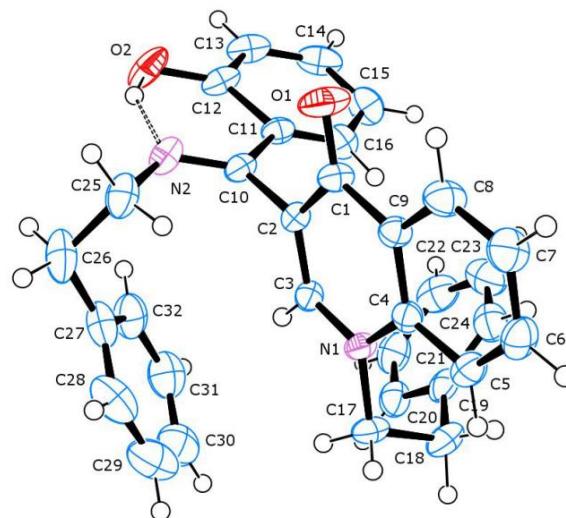


Figure 2. Crystal structure of compound 4a.

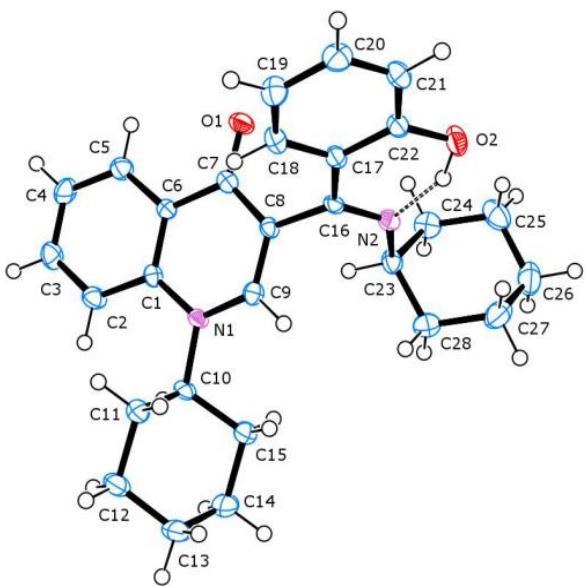


Figure 3. Crystal structure of compound 4b.

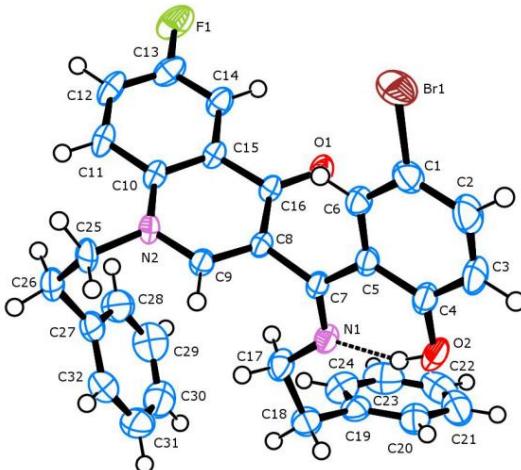


Figure 4. Crystal structure of compound 4j.

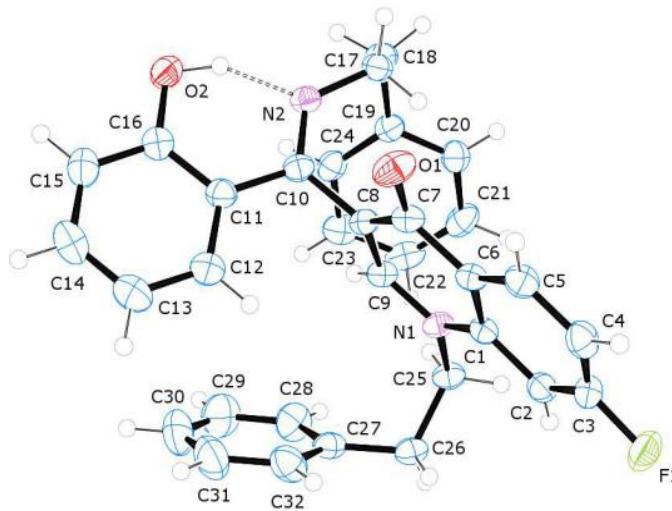


Figure 5. Crystal structure of compound 4l.

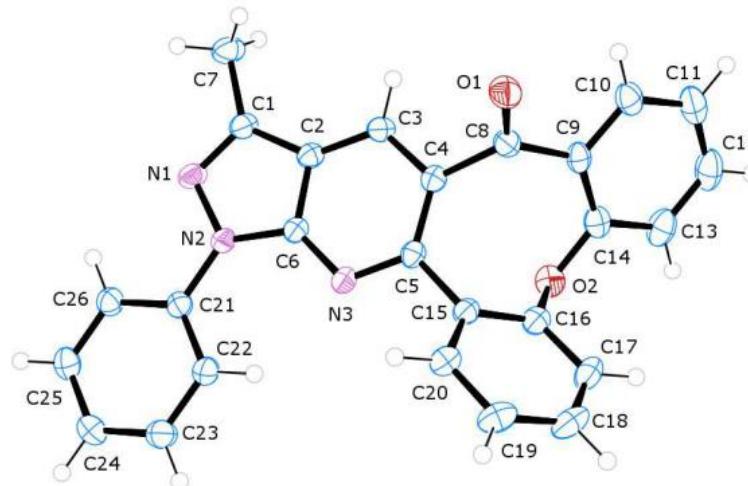


Figure 6. Crystal structure of compound 7a.

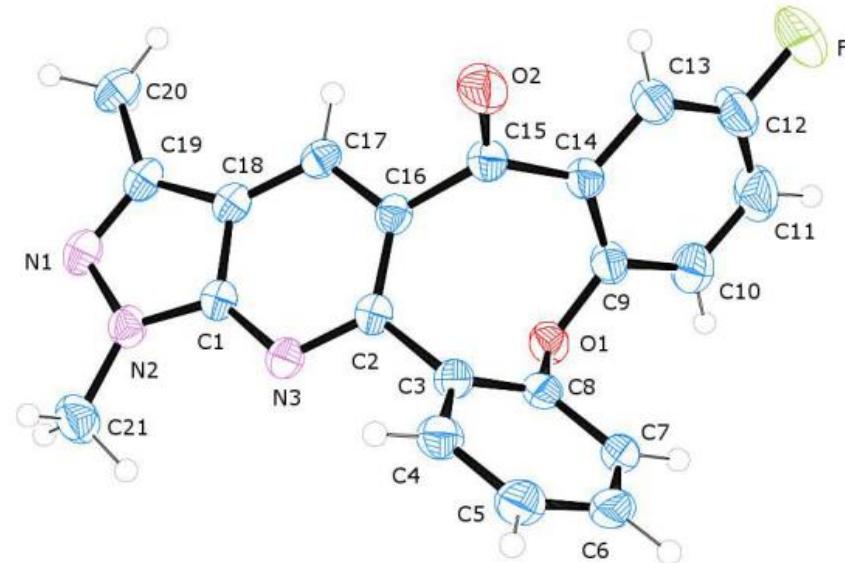


Figure 7. Crystal structure of compound 7c.

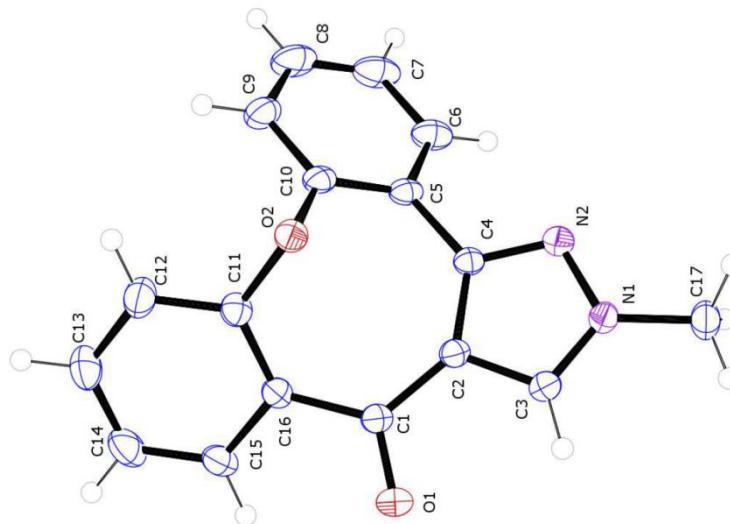


Figure 8. Crystal structure of compound 7e.

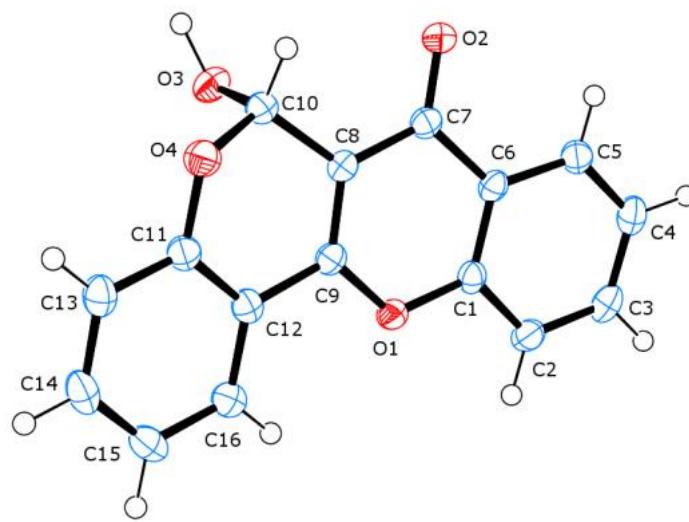
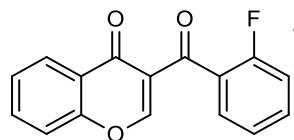


Figure 9. Crystal structure of compound 9a.

(B) Analytical data

Chromones **3a** and **3b** are known.¹

1. (a) Y. Zhao, T. F. Chow, R. S. Puckrin, S. E. Alfred, A. K. Korir, C. K. Larive, S. R. Cutler, *Nat. Chem. Biol.* **2007**, *3*, 716-721; (b) S. Yasuhara, T. Masumizu, T. Umeda, M. Kusunoki, S. Kutsuma, C. Oono, K. Iwashita, *jpn. kokai tokkyo koho* **1996**, JP 08193078 A 19960730.



3-(2-fluorobenzoyl)-4H-chromen-4-one 3c.

White solid (2.09 g, 78%), mp 130-131 °C. ¹H NMR (300 MHz, CDCl₃): δ = 7.04-7.10 (m, 1H, CH_{Ar}), 7.25 (dt, 1H, ³J = 7.6 Hz, ⁴J = 1.1 Hz, CH_{Ar}), 7.41-7.54 (m, 3H, CH_{Ar}), 7.68-7.76 (m, 2H, CH_{Ar}), 8.20 (dt, 1H, ³J = 7.8 Hz, ⁴J = 1.7 Hz, CH_{Ar}), 8.43 (s, 1H, CH_{Ar}).

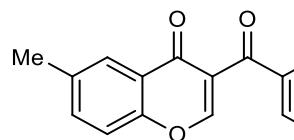
¹⁹F NMR (282 MHz, CDCl₃): δ = -111.4 (CF).

¹³C NMR (75.5 MHz, CDCl₃): δ = 115.7, 116.0, 118.3 (CH), 124.4 (d, *J* = 3.1 Hz, CH), 125.0, 125.8 (C), 126.2, 126.4 (CH), 127.4 (d, ³J = 12.6 Hz, C), 130.5 (d, *J* = 2.4 Hz, CH), 156.0, 159.5 (CH), 162.1 (d, ¹J = 253.5 Hz, CF), 174.5, 188.7 (C).

MS (GC, 70eV): *m/z* (%) = 268 (M⁺, 1), 249 (100).

HRMS (EI): Calcd for C₁₆H₉FO₃ (M⁺) 268.05302. Found 268.05297.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2922 (w), 1664 (m), 1642 (s), 1608 (s), 1563 (s), 1460 (s), 1388 (m), 1340 (m), 1300 (s), 1239 (m), 1207 (m), 1136 (m), 1099 (m), 973 (m), 864 (s), 757 (s), 706 (m), 629 (m).



3-(2-fluorobenzoyl)-6-methyl-4H-chromen-4-one 3d.

White solid (2.256 g, 80%), mp 97-99 °C. ¹H NMR (300 MHz, CDCl₃): δ = 2.27 (s, 3H, Me), 6.86-6.93 (m, 1H, CH_{Ar}), 7.06-7.11 (m, 1H, CH_{Ar}), 7.22 (s, 1H, CH_{Ar}), 7.31-7.39 (m, 2H, CH_{Ar}), 7.56 (dt, 1H, ³J = 7 Hz, ⁴J = 2 Hz,

CH_{Ar}), 7.81-7.82 (m, 1H, CH_{Ar}), 8.24 (s, 1H, CH_{Ar}).

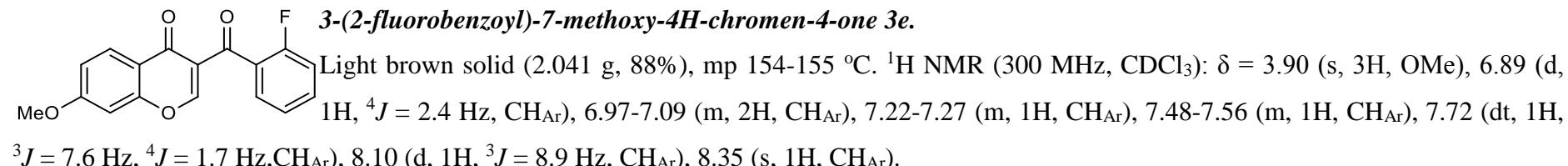
^{19}F NMR (282 MHz, CDCl_3): $\delta = -111.4$ (CF).

^{13}C NMR (75.5 MHz, CDCl_3): $\delta = 20.9$ (Me), 115.8 (d, $^2J = 22.1$ Hz, CH), 118.6 (CH), 124.4 (d, $J = 3.4$ Hz, CH), 125.3, 125.6 (C), 125.8 (CH), 127.4 (d, $^3J = 12.7$ Hz, C), 130.4 (d, $J = 1.9$ Hz, CH), 134.3 (d, $^3J = 8.8$ Hz, CH), 135.6 (CH), 136.4, 154.3 (C), 159.4 (CH), 161.2 (d, $^1J = 254.7$ Hz, CF), 174.6, 188.9 (C).

MS (GC, 70eV): m/z (%) = 282 (M^+ , 70), 263 (42), 253 (100), 235 (39), 187 (25), 135 (28), 95 (38).

HRMS (EI): Calcd for $\text{C}_{17}\text{H}_{11}\text{FO}_3$ (M^+) 282.06867. Found 282.06832.

IR (ATR, cm^{-1}): $\tilde{\nu} = 1660$ (m), 1612 (s), 1555 (m), 1478 (s), 1452 (m), 1372 (w), 1311 (S), 1216 (m), 1154 (w), 1127 (w), 1103 (m), 978 (w), 941 (w), 908 (m), 863 (m), 820 (m), 802 (m), 781 (s), 766 (s), 637 (s).



^{19}F NMR (282 MHz, CDCl_3): $\delta = -111.4$ (CF).

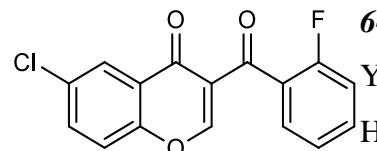
^{13}C NMR (75.5 MHz, CDCl_3): $\delta = 54.9$ (OMe), 100.6 (CH), 115.4 (d, $^2J = 22.3$ Hz, CH), 115.9 (CH), 118.4 (C), 124.2 (d, $J = 3.2$ Hz, CH), 125.7 (C), 127.4 (d, $^3J = 13.5$ Hz, C), 127.6 (CH), 130.3 (d, $J = 3.1$ Hz, CH), 134.2 (d, $^3J = 9.7$ Hz, CH), 158.1 (CH), 160.2 (d, $^1J = 254.1$ Hz, CF), 172.9, 187.9 (C).

MS (GC, 70eV): m/z (%) = 298 (M^+ , 61), 279 (35), 269 (100), 251 (28), 151 (25).

HRMS (EI): Calcd for $\text{C}_{17}\text{H}_{11}\text{FO}_4$ (M^+) 298.06359. Found 298.06287.

IR (ATR, cm^{-1}): $\tilde{\nu} = 2852$ (w), 1683 (m), 1569 (m), 1613 (s), 1454 (m), 1390 (w), 1356 (w), 1313 (m), 1278 (s), 1203 (m), 1163 (m), 1135 (m), 1089 (m), 1024 (m), 867 (m), 844 (m), 777 (s), 749 (s), 649 (m), 572 (m).

6-chloro-3-(2-fluorobenzoyl)-4H-chromen-4-one 3f.



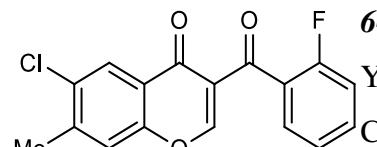
Yellow solid (2.144 g, 71%), mp 97-99 °C. ^1H NMR (300 MHz, CDCl_3): δ = 7.07 (ddd, 1H, 3J = 10.7 Hz, 4J = 8.3 Hz, 5J = 0.9 Hz, CH_{Ar}), 7.24-7.30 (m, 1H, CH_{Ar}), 7.48 (d, 1H, 3J = 8.9 Hz, CH_{Ar}), 7.50-7.58 (m, 1H, CH_{Ar}), 7.65 (dd, 1H, 3J = 8.9 Hz, 4J = 2.6 Hz, CH_{Ar}), 7.72-7.77 (m, 1H, CH_{Ar}), 8.16 (d, 1H, 4J = 2.6 Hz, CH_{Ar}), 8.41 (s, 1H, CH_{Ar}).
 ^{19}F NMR (282 MHz, CDCl_3): δ = -111.2 (CF).

^{13}C NMR (75.5 MHz, CDCl_3): δ = 115.9 (d, 2J = 21.8 Hz, CH), 120.0 (CH), 124.5 (d, J = 3.4 Hz, CH), 125.8 (CH), 128.9 (C), 127.1 (d, 3J = 10.9 Hz, C), 130.5 (CH), 132.3 (C), 134.5, 134.6 (CH), 154.3 (C), 159.4 (CH), 161.2 (d, 1J = 253.7 Hz, CF), 173.4, 188.1 (C).
MS (GC, 70eV): m/z (%) = 302 (M^+ , 69), 273 (100), 255 (35), 207 (32), 155 (31), 123 (69), 95 (51).

HRMS (EI): Calcd for $\text{C}_{16}\text{H}_8\text{ClFO}_3$ (M^+) 303.98664. Found 303.98572.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3056 (w), 1644 (s), 1608 (s), 1560 (m) 1482 (w), 1463 (s), 1436 (m), 1335 (m), 1315 (s), 1260 (m), 1211 (m), 1140 (m), 1101 (m), 1037 (w), 985 (m), 951 (m), 887 (m), 863 (m), 835 (m), 820 (s), 783 (s), 761 (s), 735 (m), 674 (m), 631 (s).

6-chloro-3-(2-fluorobenzoyl)-7-methyl-4H-chromen-4-one 3g.



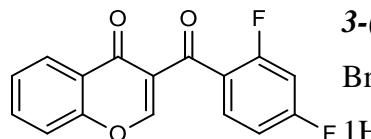
Yellow solid (2.149 g, 68%), mp 143-144 °C. ^1H NMR (300 MHz, CDCl_3): δ = 2.51 (s, 3H, Me), 7.03-7.10 (m, 1H, CH_{Ar}), 7.24-7.29 (m, 1H, CH_{Ar}), 7.40 (s, 1H, CH_{Ar}), 7.50-7.58 (m, 1H, CH_{Ar}), 7.74 (dt, 1H, 3J = 7.5 Hz, 4J = 1.8 Hz, CH_{Ar}), 8.15 (s, 1H, CH_{Ar}), 8.38 (s, 1H, CH_{Ar}).
 ^{19}F NMR (282 MHz, CDCl_3): δ = -117.3 (CF).

^{13}C NMR (75.5 MHz, CDCl_3): δ = 20.9 (Me), 100.6 (CH), 115.9 (d, 2J = 22.6 Hz, CH), 120.1 (CH), 124.0 (C), 124.4 (d, J = 2.8 Hz, CH), 125.7 (C), 126.1 (CH), 127.2 (d, 3J = 12.2 Hz, C), 130.5 (d, J = 2.0 Hz, CH), 132.9 (C), 134.5 (d, 3J = 7.9 Hz, CH), 143.9, 154.3 (C), 161.2 (d, 1J = 253.6 Hz, CF), 173.3, 188.4 (C).

MS (GC, 70eV): m/z (%) = 316 (M^+ , 65), 287 (100), 269 (34), 221 (21), 169 (25), 123 (36), 95 (39).

HRMS (EI): Calcd for $\text{C}_{17}\text{H}_{10}\text{O}_3\text{Cl}$ (M^+) 316.02970. Found 316.02908.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3040 (w), 1651 (s), 1620 (s), 1547 (m), 1486 (w), 1452 (s), 1412 (m), 1334 (m), 1308 (s), 1259 (m), 1226 (m), 1183 (m), 1145 (m), 1126 (m), 1104 (m), 1039 (w), 1003 (m), 966 (m), 934 (w), 910 (m), 871 (s), 797 (m), 768 (s), 750 (s), 704 (w), 667 (m), 638 (s).



3-(2,4-difluorobenzoyl)-4H-chromen-4-one 3h.

Brown solid (1.71 g, 60%), mp 138-140 °C. ¹H NMR (300 MHz, CDCl₃): δ = 6.78-7.03 (m, 3H, CH_{Ar}), 7.43-7.55 (m, 1H, CH_{Ar}), 7.70-7.82 (m, 1H, CH_{Ar}), 8.03-8.10 (m, 1H, CH_{Ar}), 8.20-8.23 (m, 1H, CH_{Ar}), 8.44 (s, 1H, CH_{Ar}).

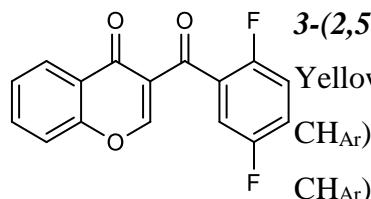
¹⁹F NMR (282 MHz, CDCl₃): δ = -106.0 (d, ³J = 13.1 Hz, CF), -102.0 (d, ³J = 13.1 Hz, CF).

¹³C NMR (75.5 MHz, CDCl₃): δ = 104.3 (t, ²J = 25.9 Hz, CH), 112.0 (dd, ²J = 21.7 Hz, J = 3.8 Hz, CH), 118.3 (CH), 124.0 (dd, ³J = 12.6 Hz, J = 3.8 Hz, C), 124.8, 125.7 (C), 126.2, 126.3 (CH), 132.3 (dd, ³J = 10.6 Hz, J = 3.8 Hz, CH), 138.4 (CH), 156.0 (C), 159.5 (CH), 161.9 (dd, ¹J = 237.8 Hz, ³J = 12.6 Hz, CF), 165.9 (dd, ¹J = 237.8 Hz, ³J = 12.6 Hz, CF), 174.4 (d, J = 2.2 Hz, C=O), 187.3 (C=O).

MS (GC, 70eV): *m/z* (%) = 286 (M⁺, 85), 267 (48), 257 (100), 239 (57), 173 (30), 141 (45).

HRMS (EI): Calcd for C₁₆H₈F₂O₃ (M⁺) 286.04360. Found 286.04384.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3080 (w), 1640 (s), 1609 (s), 1487 (w), 1464 (s), 1426 (m), 1384 (m), 1348 (m), 1294 (m), 1213 (m), 1138 (m), 1096 (s), 1028 (w), 977 (m), 855 (s), 802 (w), 757 (s), 662 (m), 302 (m).



3-(2,5-difluorobenzoyl)-4H-chromen-4-one 3i.

Yellow solid (2.29 g, 80%), mp 138-140 °C. ¹H NMR (300 MHz, CDCl₃): δ = 7.00-7.08 (m, 1H, CH_{Ar}), 7.17-7.23 (m, 1H, CH_{Ar}), 7.38-7.54 (m, 2H, CH_{Ar}), 7.70-7.75 (m, 2H, CH_{Ar}), 8.20 (dd, 1H, ³J = 8.0 Hz, ⁴J = 1.6 Hz, CH_{Ar}), 8.45 (s, 1H, CH_{Ar}).

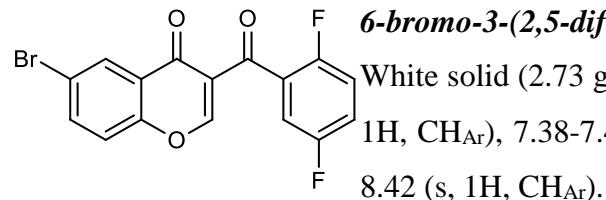
¹⁹F NMR (282 MHz, CDCl₃): δ = -117.9 (d, J = 17.7 Hz, CF), -117.2 (d, J = 17.7 Hz, CF).

¹³C NMR (75.5 MHz, CDCl₃): δ = 116.6 (dd, ²J = 25.5 Hz, J = 3.3 Hz, CH), 117.2 (dd, ²J = 25.5 Hz, J = 8.2 Hz, CH), 118.3 (CH), 120.7 (dd, ²J = 25.5 Hz, J = 9.4 Hz, CH), 124.9, 125.3 (C), 126.3 (d, J = 5.3 Hz, CH), 128.4 (dd, J = 16.7 Hz, J = 7.3 Hz, CH), 134.5 (CH), 156.0 (C), 157.1 (d, ¹J = 247.2 Hz, CF), 158.6 (d, J = 242.2 Hz, CF), 159.8 (CH), 174.4, 187.6 (C).

MS (GC, 70eV): m/z (%) = 286 (M^+ , 80), 267 (57), 257 (100), 239 (66), 173 (35), 141 (22), 121 (39).

HRMS (EI): Calcd for $C_{16}H_8F_2O_3$ (M^+) 286.04360. Found 286.043440.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3068 (w), 1636 (s), 1614 (m), 1566 (m), 1483 (m), 1461 (s), 1422 (m), 1392 (m), 1344 (m), 1316 (m), 1287 (w), 1260 (m), 1230 (m), 1186 (s), 1131 (m), 1000 (w), 961 (w), 929 (w), 891 (m), 833 (s), 773 (s), 750 (s), 700 (m), 637 (m), 591 (w), 540 (m).



6-bromo-3-(2,5-difluorobenzoyl)-4H-chromen-4-one 3j.

White solid (2.73 g, 67%), mp 153-155 °C. ^1H NMR (300 MHz, CDCl_3): δ = 7.00-7.08 (m, 1H, CH_{Ar}), 7.17-7.27 (m, 1H, CH_{Ar}), 7.38-7.44 (m, 2H, CH_{Ar}), 7.80 (dd, 1H, 3J = 8.0 Hz, 4J = 2.5 Hz, CH_{Ar}), 8.31 (d, 1H, 4J = 3 Hz, CH_{Ar}), 8.42 (s, 1H, CH_{Ar}).

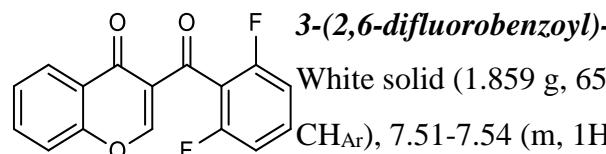
^{19}F NMR (282 MHz, CDCl_3): δ = -117.7 (d, J = 18 Hz, CF), -117.0 (d, J = 18 Hz, CF).

^{13}C NMR (75.5 MHz, CDCl_3): δ = 116.6 (dd, 2J = 25.6 Hz, J = 3.3 Hz, CH), 117.2 (dd, 2J = 25.6 Hz, J = 8.7 Hz, CH), 119.9 (C), 120.2 (CH), 121.0 (dd, 2J = 25.6 Hz, J = 8.6 Hz, CH), 125.4, 126.1 (C), 128.0 (dd, 3J = 14.3 Hz, J = 7.2 Hz, C), 129.0 (CH), 137.5 (CH), 154.8 (C), 157.2 (d, 1J = 248.4 Hz, CF), 158.6 (d, 1J = 280.1 Hz, CF), 159.7 (CH), 173.1 (d, J = 2.3 Hz, C=O), 187.0 (C=O).

MS (GC, 70eV): m/z (%) = 366 (M^+ , 91), 365 (35), 347 (69), 346 (12), 337 (100), 336 (48), 335 (95), 319 (68), 317 (64), 251 (36), 199 (32), 141 (50), 113 (62).

HRMS (EI): Calcd for $C_{16}H_7F_2O_3Br$ (M^+) 363.95411. Found 363.954477.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3067 (w), 1645 (s), 1606 (m), 1557 (m), 1488 (m), 1459 (s), 1423 (m), 1372 (w), 1329 (m), 1307 (m), 1278 (m), 1251 (m), 1192 (m), 1177 (s), 1126 (m), 1093 (m), 1062 (w), 1005 (w), 932 (w), 893 (m), 878 (m), 824 (s), 804 (s), 769 (m), 750 (s), 676 (s), 640 (m), 603 (m), 539 (m).



3-(2,6-difluorobenzoyl)-4H-chromen-4-one 3k.

White solid (1.859 g, 65%), mp 114-116 °C. ^1H NMR (300 MHz, CDCl_3): δ = 6.92-6.99 (m, 2H, CH_{Ar}), 7.37-7.48 (m, 2H, CH_{Ar}), 7.51-7.54 (m, 1H, CH_{Ar}), 7.69-7.75 (m, 1H, CH_{Ar}), 8.19 (dd, 1H, 3J = 7.9 Hz, 4J = 1.5 Hz, CH_{Ar}), 8.64 (s, 1H,

CH_{Ar}).

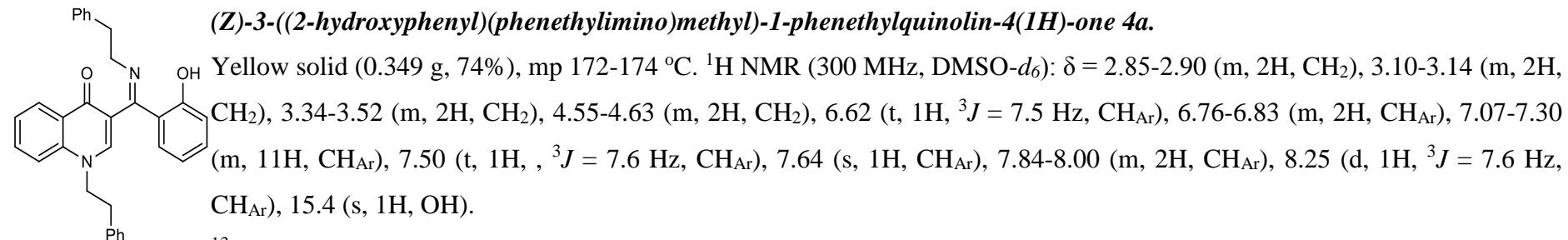
^{19}F NMR (282 MHz, CDCl_3): $\delta = -113.1$ (CF).

^{13}C NMR (75.5 MHz, CDCl_3): $\delta = 111.7$ (dd, $^2J = 22.8$ Hz, $J = 2.6$ Hz, CH), 118.3 (C), 123.8, 125.1, 126.4 (CH), 132.4 (t, $^3J = 10.4$ Hz, CH), 134.5 (CH), 155.9 (C), 160.1 (dd, $^1J = 252.6$ Hz, $J = 6.5$ Hz, CF), 161.6 (CH), 174.2, 185.1 (C).

MS (GC, 70eV): m/z (%) = 286 (M^+ , 75), 267 (44), 257 (27), 239 (100), 173 (30), 141 (28), 121 (28).

HRMS (EI): Calcd for $\text{C}_{16}\text{H}_{8}\text{F}_2\text{O}_3$ (M^+) 286.04361. Found 286.043442.

IR (ATR, cm^{-1}): $\tilde{\nu} = 3074$ (w), 1674 (m), 1656 (s), 1611 (m), 1552 (m), 1459 (s), 1384 (m), 1307 (m), 1286 (m), 1265 (m), 1232 (m), 1206 (m), 1144 (m), 994 (s), 964 (s), 865 (m), 789 (s), 760 (s), 717 (s), 680 (m), 591 (m).

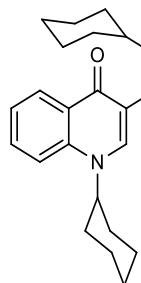


^{13}C NMR (75.5 MHz, $\text{DMSO}-d_6$): $\delta = 34.0, 36.1, 52.3, 53.4$ (CH_2), 113.1 (C), 117.1, 117.2, 117.3 (CH), 119.4 (C), 124.1, 126.0, 126.2, 126.6, 128.3, 128.4, 128.7, 128.9, 130.6, 132.0, 132.6 (CH), 137.2, 139.2, 139.7 (C), 143.5 (CH), 162.3, 169.6, 172.9 (C).

MS (GC, 70eV): m/z (%) = 472 (M^+ , 100), 455 (20), 381 (18), 367 (35), 354 (98), 262 (26), 105 (97).

HRMS (ESI): Calcd for $\text{C}_{32}\text{H}_{29}\text{N}_2\text{O}_2$ ($\text{M}+\text{H}$) 473.22336. Found 473.22235.

IR (ATR, cm^{-1}): $\tilde{\nu} = 3027$ (w), 1712 (w), 1660 (w), 1623 (m), 1605 (m), 1598 (m), 1553, 1486 (m), 1451 (m), 1375 (m), 1338 (m), 1307 (m), 1229 (m), 1183 (m), 1149 (m), 1082 (m), 1000 (m), 926 (m), 855 (m), 742 (s), 694 (s), 627 (m), 559 (m).



(Z)-1-cyclohexyl-3-((cyclohexylimino)(2-hydroxyphenyl)methyl)quinolin-4(1H)-one 4b.

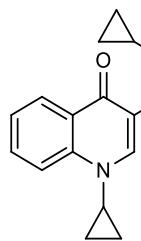
Yellow solid (0.214 g, 50%), mp 230-231 °C. ¹H NMR (300 MHz, DMSO-d₆): δ = 1.20-1.80 (m, 21H, cyclohexyl), 4.73 (br. s, 1H, cyclohexyl), 6.64 (t, 1H, ³J = 8.1 Hz, CH_{Ar}), 6.86 (d, 1H, ³J = 8.1 Hz, CH_{Ar}), 6.86 (d, 1H, ³J = 8.1 Hz, CH_{Ar}), 7.25 (t, 1H, ³J = 7.1 Hz, CH_{Ar}), 7.47 (t, 1H, ³J = 7.1 Hz, CH_{Ar}), 7.83 (t, 1H, ³J = 8.1 Hz, CH_{Ar}), 8.06 (d, 1H, ³J = 9.1 Hz, CH_{Ar}), 8.22-8.29 (m, 2H, CH_{Ar}), 16.09 (s, 1H, OH).

¹³C NMR (75.5 MHz, DMSO-d₆): δ = 23.4, 24.6, 25.1, 25.2, 31.4, 31.6, 32.9, 33.4 (cyclohexyl CH₂), 57.7, 58.8 (cyclohexyl CH), 113.9 (C), 116.4, 117.1, 117.5 (CH), 119.8 (C), 123.8, 126.2 (CH), 128.2 (C), 130.5, 131.9, 132.6, 138.9 (CH), 139.9, 163.1, 167.7, 172.9 (C).

MS (GC, 70eV): *m/z* (%) = 428 (M⁺, 90), 411 (26), 345 (27), 332 (100), 250 (35). 220 (18), 171 (14).

HRMS (EI): Calcd for C₂₈H₃₂N₂O₂ (M⁺) 428.24638. Found 428.24655.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3307 (w), 2922 (m), 2848 (w), 1626 (m), 1582 (m), 1554 (m), 1486 (m), 1445 (w), 1361 (m), 1309 (w), 1257 (w), 1216 (m), 1190 (w), 1150 (w), 1099 (w), 1002 (w), 913 (w), 889 (m), 859 (w), 838 (w), 750 (s), 709 (m), 635 (w), 575 (w), 534 (w).



(Z)-1-cyclopropyl-3-((cyclopropylimino)(2-hydroxyphenyl)methyl)quinolin-4(1H)-one 4c.

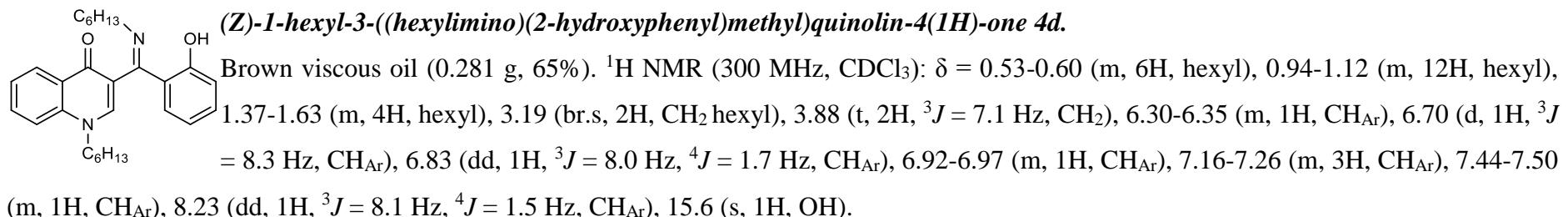
Yellow viscous oil (0.165 g, 48%). ¹H NMR (300 MHz, DMSO-d₆): δ = 0.84-1.06 (m, 4H, cyclopropyl, CH₂), 1.24-1.31 (m, 4H, cyclopropyl, CH₂), 2.84-2.94 (m, 1H, cyclopropyl CH), 3.44-3.51 (m, 1H, cyclopropyl CH), 6.64 (t, 1H, ³J = 7.2 Hz, CH_{Ar}), 6.89 (d, 1H, ³J = 7.7 Hz, CH_{Ar}), 7.04-7.07 (m, 1H, CH_{Ar}), 7.14-7.20 (m, 1H, CH_{Ar}), 7.41-7.47 (m, 1H, CH_{Ar}), 7.71-7.78 (m, 2H, CH_{Ar}), 7.99 (d, 1H, ³J = 8.6 Hz, CH_{Ar}), 8.47 (d, 1H, ³J = 8.3 Hz, CH_{Ar}), 14.51 (s, 1H, OH).

¹³C NMR (62.9 MHz, DMSO-d₆): δ = 7.8, 10.0 (cyclopropyl CH₂), 33.9, 34.0 (CH), 114.3 (C), 116.8, 117.4, 117.1 (CH), 120.1 (C), 124.1, 125.8 (CH), 125.9 (C), 130.3, 131.3, 132.3 (CH), 141.3 (C), 142.8 (CH), 161.0, 167.6, 173.4 (C).

MS (GC, 70eV): *m/z* (%) = 344 (M⁺, 4), 238 (100), 221 (18), 147 (76), 121 (43).

HRMS (ESI): Calcd for C₂₂H₂₁N₂O₂ (M+H) 345.15975. Found 345.16062.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2922 (w), 1620 (m), 1586 (s), 1480 (s), 1401 (w), 1339 (m), 1247 (m), 1166 (m), 1113 (w), 1035 (w), 943 (w), 866 (w), 752 (s), 704 (m), 644 (m).

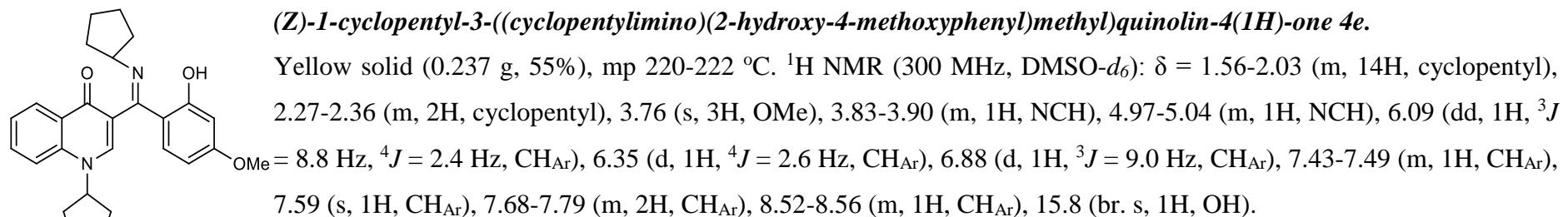


¹³C NMR (75.5 MHz, CDCl₃): δ = 13.8, 14.0 (Me), 22.4, 22.5, 26.4, 27.1, 28.8, 30.5, 31.2, 31.5, 51.2, 53.7 (CH₂), 114.8 (C), 115.6, 116.8, 118.5 (CH), 119.6 (C), 124.4 (CH), 127.1 (C), 127.7, 130.4, 132.3, 132.6 (CH), 139.3 (C), 142.6 (CH), 164.6, 168.2, 174.0 (C).

MS (GC, 70eV): *m/z* (%) = 432 (M⁺, 74), 375 (100), 334 (72), 248 (28).

HRMS (EI): Calcd for C₂₈H₃₆N₂O₂ (M⁺) 432.27713. Found 432.27756.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3038 (w), 2924 (s), 2854 (m), 1621 (s), 1603 (s), 1577 (s), 1552 (s), 1489 (s), 1451 (m), 1413 (m), 1389 (m), 1345 (m), 1311 (m), 1269 (m), 1232 (s), 1176 (m), 1152 (m), 1055 (w), 966 (w), 864 (w), 824 w, 786 (w), 753 (s), 706 (m), 660 (w), 625 (w), 529 (w).

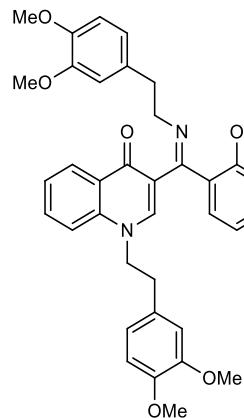


¹³C NMR (75.5 MHz, DMSO-d₆): δ = 23.8, 24.2, 24.3, 32.2, 32.3, 32.4, 34.2, 35.1 (cyclopentyl CH₂), 55.2 (OMe), 60.2, 61.0 (cyclopentyl CH), 102.3, 105.5 (CH), 112.6, 114.6 (C), 115.6, 124.4 (CH), 127.3 (C), 127.9, 131.8, 132.6, 138.1 (CH), 140.4, 164.2, 166.4, 171.6, 173.8 (C).

MS (GC, 70eV): m/z (%) = 430 (M^+ , 67), 413 (35), 399 (23), 361 (21), 348 (100), 293 (35), 251 (23), 168 (35).

HRMS (EI): Calcd for $C_{27}H_{30}N_2O_3$ (M^+) 430.22509. Found 430.22451.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2952 (w), 2859 (w), 1581 (s), 1552 (m), 1514 (w), 1485 (m), 1444 (m), 1412 (w), 1345 (m), 1281 (w), 1208 (s), 1169 (m), 1119 (m), 1100 (m), 1035 (m), 957 (m), 856 (w), 831 (m), 796 (m), 752 (s), 708 (m), 645 (w).



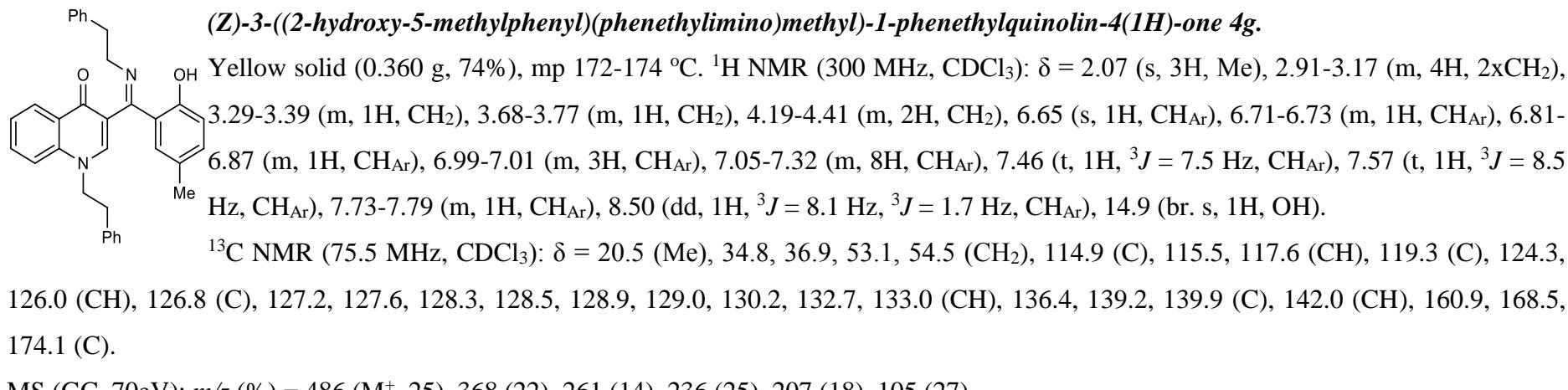
(Z)-1-(3,4-dimethoxyphenethyl)-3-((3,4-dimethoxyphenethyl)imino)(2-hydroxy-4-methoxyphenyl)methylquinolin-4(1H)-one 4f.

Yellow solid (0.473 g, 76%), mp 91-93 °C. ^1H NMR (300 MHz, CDCl_3): δ = 2.85-3.18 (m, 4H, 2x CH_2), 3.28-3.44 (m, 1H, CH_2), 3.60 (s, 3H, OMe), 3.70 (s, 3H, OMe), 3.76 (s, 3H, OMe), 3.77 (s, 3H, OMe), 3.80 (s, 3H, OMe), 3.82-3.86 (m, 1H, CH_2), 3.91-4.02 (m, 1H, CH_2), 4.36-4.50 (m, 1H, CH_2), 6.02 (dd, 1H, 3J = 8.9 Hz, 4J = 2.5 Hz, CH_{Ar}), 6.33 (d, 1H, 4J = 2.5 Hz, CH_{Ar}), 6.40-6.73 (m, 8H, CH_{Ar}), 7.45-7.61 (m, 2H, CH_{Ar}), 7.74-7.81 (m, 1H, CH_{Ar}), 8.50 (dd, 1H, 3J = 8.0 Hz, 4J = 1.5 Hz, CH_{Ar}), 16.0 (br. s, 1H, OH).
 ^{13}C NMR (75.5 MHz, CDCl_3): δ = 34.2, 36.4, 51.1, 54.8 (CH_2), 55.1, 55.5, 55.7, 55.8, 55.9 (OMe), 102.2, 105.3, 111.2, 111.7, 111.8 (CH), 112.3 (C), 112.4 (CH), 113.8 (C), 115.6, 120.6, 121.1, 124.6 (CH), 127.0 (C), 127.9 (CH), 128.6 (C), 131.8 (CH), 132.3 (C), 132.8 (CH), 139.0 (C), 143.2 (CH), 147.3, 148.7, 149.3, 164.2, 167.7, 171.0, 173.9 (C).

MS (GC, 70eV): m/z (%) = 622 (M^+ , 26), 458 (80), 444 (46), 292 (39), 165 (100).

HRMS (EI): Calcd for $C_{37}H_{38}N_2O_7$ (M^+) 622.26735. Found 622.26549.

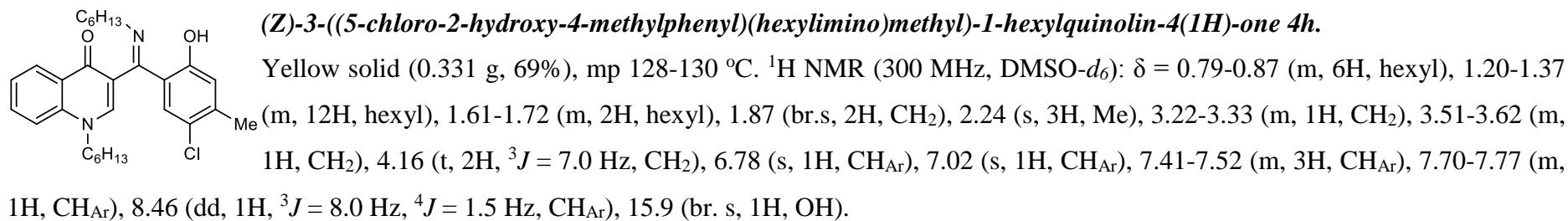
IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2934 (w), 1589 (m), 1550 (m), 1513 (s), 1488 (m), 1462 (m), 1415 (m), 1344 (w), 1260 (s), 1232 (s), 1138 (s), 1060 (w), 1024 (s), 840 (m), 808 (m), 762 (s), 707 (w), 641 (w).



MS (GC, 70eV): *m/z* (%) = 486 (M⁺, 25), 368 (22), 261 (14), 236 (25), 207 (18), 105 (27).

HRMS (EI): Calcd for C₃₃H₃₁N₂O₂ (M+H) 487.238. Found 487.23816.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2920 (w), 1621 (m), 1576 (s), 1551 (m), 1487 (s), 1454 (m), 1414 (w), 1377 (m), 1345 (m), 1284 (m), 1229 (m), 1149 (m), 1083 (w), 1029 (w), 903 (w), 821 (m), 748 (s), 698 (s).

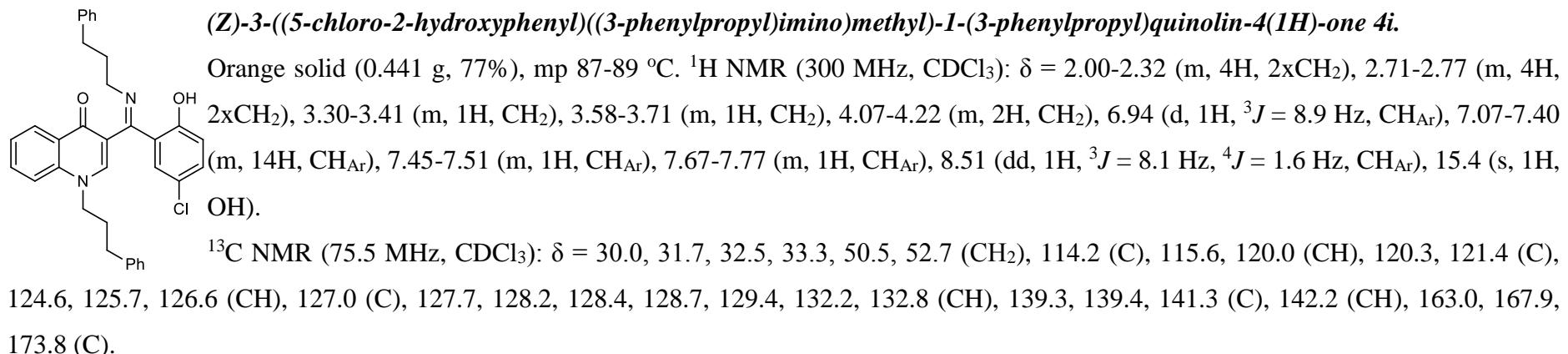


¹³C NMR (75.5 MHz, DMSO-d₆): δ = 13.8, 13.9, 20.2 (Me), 22.3, 22.4, 26.3, 27.0, 28.8, 30.3, 31.2, 31.5 (CH₂), 114.0 (C), 115.7 (CH), 118.4 (C), 120.8, 121.7, 124.5 (CH), 127.1 (C), 127.6, 129.7, 132.7 (CH), 139.3, 140.8 (C), 142.6 (CH), 163.7, 167.3, 173.9 (C).

MS (GC, 70eV): *m/z* (%) = 480 (M⁺, 69), 463 (23), 423 (100), 382 (63), 179 (16).

HRMS (ESI): Calcd for C₂₉H₃₇N₂O₂Cl (M+H) 481.26163. Found 481.26226.

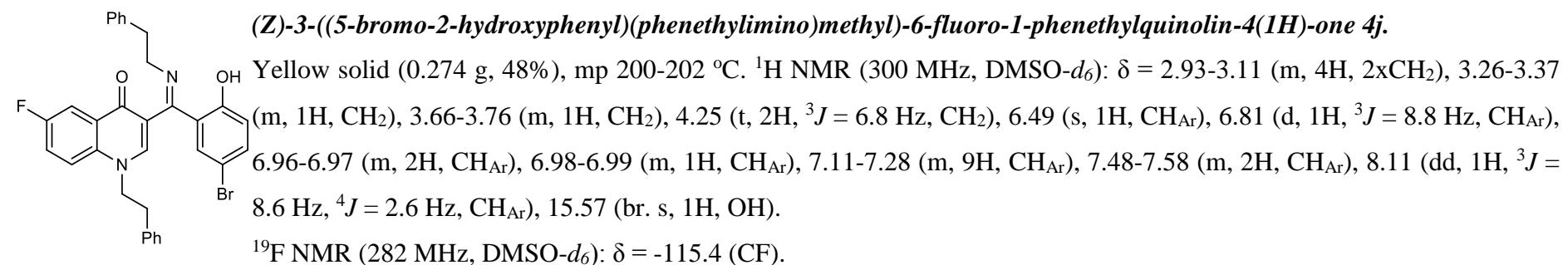
IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3041 (w), 2926 (m), 2855 (w), 1623 (m), 1599 (s), 1577 (s), 1552 (m), 1490 (s), 1461 (m), 1384 (m), 1271 (w), 1231 (s), 1168 (s), 1135 (w), 1055 (w), 1008 (w), 965 (w), 883 (w), 858 (m), 795 (w), 763 (s), 732 (w), 708 (m), 690 (m), 626 (w), 576 (w).



MS (GC, 70eV): *m/z* (%) = 534 (M⁺, 13), 443 (100), 430 (14), 91 (47).

HRMS (EI): Calcd for C₃₄H₃₁N₂O₂Cl (M+H) 535.21468. Found 535.21473.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3025 (w), 2924 (w), 1623 (s), 1600 (s), 1576 (s), 1552 (m), 1487 (s), 1415 (w), 1379 (m), 1328 (w), 1287 (m), 1226 (m), 1173 (m), 1087 (w), 1029 (w), 983 (w), 883 (w), 822 (m), 745 (s), 697 (s), 647 (m), 529 (w).

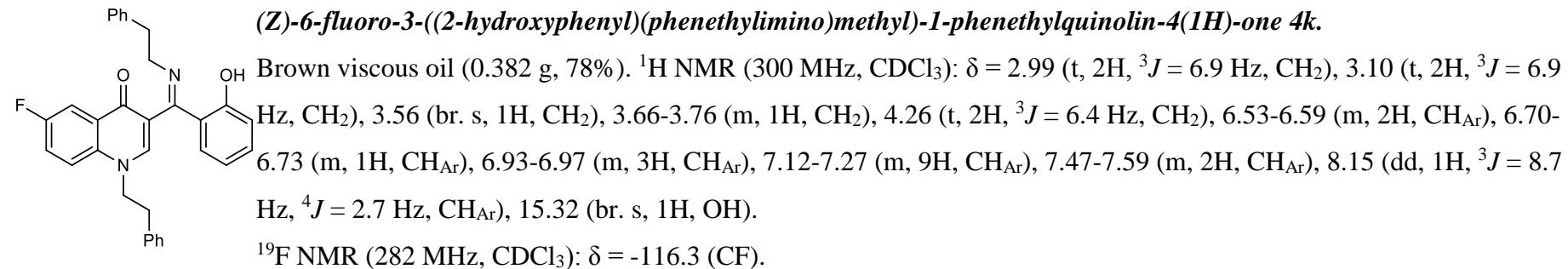


¹³C NMR (75.5 MHz, DMSO-*d*₆): δ = 34.9, 36.8, 53.2, 55.0 (CH₂), 108.7 (C), 112.5 (d, *J* = 23 Hz, CH), 113.2 (C), 117.9 (d, *J* = 8 Hz, CH), 120.2 (CH), 120.9 (C), 121.5 (d, *J* = 26 Hz, CH), 126.3, 127.5, 128.4, 128.5, 129.1, 132.3, 135.0 (CH), 135.7, 136.1, 139.5 (C), 142.0 (CH), 159.5 (d, *J* = 249 Hz, CF), 162.6, 167.5, 173.1 (C).

MS (GC, 70eV): *m/z* (%) = 570 (M⁺, 30), 568 (32), 450 (31), 360 (32), 310 (35), 105 (100).

HRMS (EI): Calcd for C₃₂H₂₆N₂O₂FBr (M⁺) 568.11562. Found 568.11507.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2919 (w), 1619 (m), 1581 (m), 1556 (m), 1489 (m), 1380 (m), 1332 (m), 1281 (m), 1226 (m), 1169 (m), 1081 (w), 1056 (w), 999 (w), 925 (w), 895 (w), 818 (m), 786 (w), 748 (m), 698 (w), 565 (m).

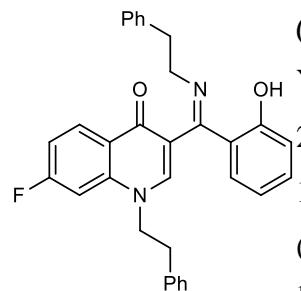


¹³C NMR (75.5 MHz, CDCl₃): δ = 34.8, 36.7, 53.2, 55.1 (CH₂), 108.7 (C), 112.6 (d, ²J = 23.4 Hz, CH), 114.0 (C), 117.4 (CH), 117.8 (d, ³J = 8 Hz, CH), 118.0 (CH), 119.5 (C), 121.3 (d, ²J = 25.6 Hz, CH), 126.1, 127.5, 128.4 (d, ³J = 11.3 Hz, CH), 129.1 (d, *J* = 3.0 Hz, CH), 130.3, 132.2 (CH), 135.6, 136.1, 139.9 (C), 142.3 (CH), 159.4 (d, ¹J = 247.7 Hz, CF), 163.3, 168.1, 173.2 (C).

MS (GC, 70eV): *m/z* (%) = 490 (M⁺, 33), 385 (13), 372 (32), 315 (19), 283 (18), 105 (28), 73 (100).

HRMS (EI): Calcd for C₃₂H₂₇N₂O₂F (M+H) 491.21293. Found 491.21309.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3388 (w), 3025 (w), 2927 (w), 1602 (m), 1560 (m), 1490 (s), 1453 (m), 1380 (m), 1335 (m), 1281 (m), 1224 (m), 1175 (m), 1151 (m), 1083 (w), 1030 (w), 895 (m), 815 (m), 748 (s), 697 (s).



(Z)-7-fluoro-3-((2-hydroxyphenyl)(phenethylimino)methyl)-1-phenethylquinolin-4(1H)-one 4l.

Yellow solid (0.196 g, 40%), mp 201-203 °C. ^1H NMR (300 MHz, CDCl_3): δ = 2.96-3.01 (m, 2H, CH_2), 3.07-3.11 (m, 2H, CH_2), 3.30-3.39 (m, 1H, CH_2), 3.73-3.82 (m, 1H, CH_2), 4.07-4.28 (m, 2H, CH_2), 6.46 (s, 1H, CH_{Ar}), 6.53-6.59 (m, 1H, CH_{Ar}), 6.72 (dd, 1H, 3J = 7.9 Hz, 4J = 1.5 Hz, CH_{Ar}), 6.90-6.98 (m, 3H, CH_{Ar}), 7.12-7.27 (m, 11H, CH_{Ar}), 8.47-8.53 (m, 1H, CH_{Ar}), 15.47 (br. s, 1H, OH).

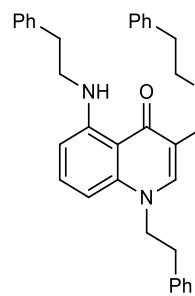
^{19}F NMR (282 MHz, CDCl_3): δ = -103.8 (CF).

^{13}C NMR (75.5 MHz, CDCl_3): δ = 34.5, 37.0, 53.3, 55.0 (CH_2), 101.7 (d, J = 25.8 Hz, CH), 113.2 (d, J = 23.2 Hz, CH), 115.2 (C), 117.7 (d, J = 38.6 Hz, CH), 119.6, 123.6 (C), 126.1, 127.5, 128.4, 128.6, 128.7, 129.1, 129.2, 130.3 (CH), 131.0 (d, J = 10.1 Hz, CH), 132.2 (CH), 139.9 (C), 140.6 (d, J = 11.7 Hz, C), 142.6, 163.2 (C), 165.4 (d, J = 251.4 Hz, CF), 168.0, 173.4 (C).

MS (GC, 70eV): m/z (%) = 490 (M^+ , 13), 434 (12), 403 (20), 373 (14), 347 (52), 315 (100), 283 (67).

HRMS (EI): Calcd for $\text{C}_{32}\text{H}_{27}\text{N}_2\text{O}_2\text{F}$ ($\text{M}+\text{H}$) 491.21293. Found 491.21247.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 1633 (m), 1608 (m), 1495 (w), 1463 (m), 1374 (w), 1330 (w), 1305 (w), 1249 (s), 1187 (w), 1148 (m), 1118 (w), 1084 (w), 1024 (w), 925 (w), 849 (m), 745 (s), 700 (s).



(Z)-3-((2-hydroxyphenyl)(phenethylimino)methyl)-1-phenethyl-5-(phenethylamino)quinolin-4(1H)-one 4m.

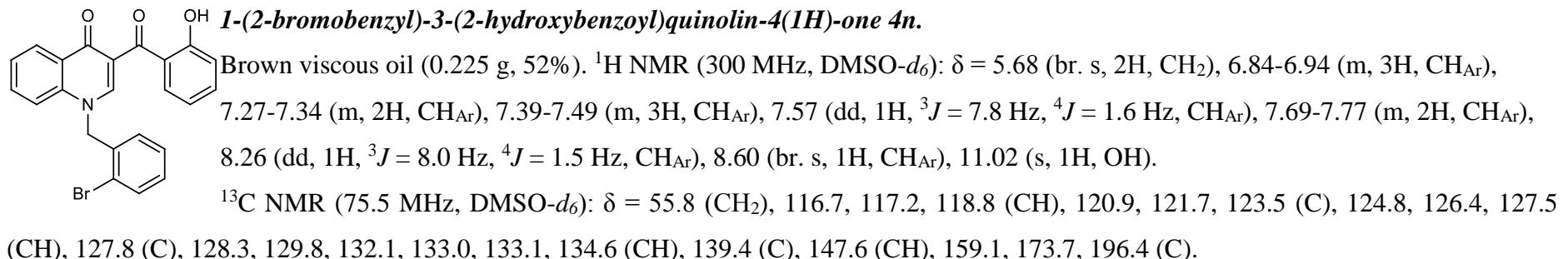
Yellow viscous oil (0.252 g, 41%). ^1H NMR (300 MHz, CDCl_3): δ = 2.96-3.13 (m, 6H, 3x CH_2), 3.37-3.46 (m, 4H, 2x CH_2), 4.09 (br. s, 1H, CH_2), 4.55-4.63 (m, 1H, CH_2), 6.28 (s, 1H, CH_{Ar}), 6.42 (d, 1H, 3J = 7.5 Hz, CH_{Ar}), 6.53-6.59 (m, 2H, CH_{Ar}), 6.78-6.81 (m, 1H, CH_{Ar}), 6.90-7.00 (m, 3H, CH_{Ar}), 7.12-7.31 (s, 14H, CH_{Ar}), 7.46 (t, 1H, 3J = 8.4 Hz, CH_{Ar}), 10.32 (t, 1H, 3J = 4.6 Hz, NH), 15.57 (br. s, 1H, OH).

^{13}C NMR (75.5 MHz, CDCl_3): δ = 34.1, 35.3, 37.0, 44.9, 53.0, 55.5 (CH_2), 99.5, 103.0 (CH), 111.9, 114.7 (C), 117.2, 118.0 (CH), 119.6 (C), 126.1, 126.3, 127.2, 128.3, 128.4, 128.6, 128.7, 129.0, 129.2, 130.5, 132.1, 133.9, 136.6 (CH), 139.4, 139.9 (C), 140.9 (CH), 141.7, 152.3, 163.5, 168.7, 177.8 (C).

MS (GC, 70eV): m/z (%) = 591 (M^+ , 16), 500 (15), 396 (18), 105 (15), 43 (100).

HRMS (ESI): Calcd for $C_{40}H_{38}N_3O_2$ ($M+H$) 592.29585. Found 592.29622.

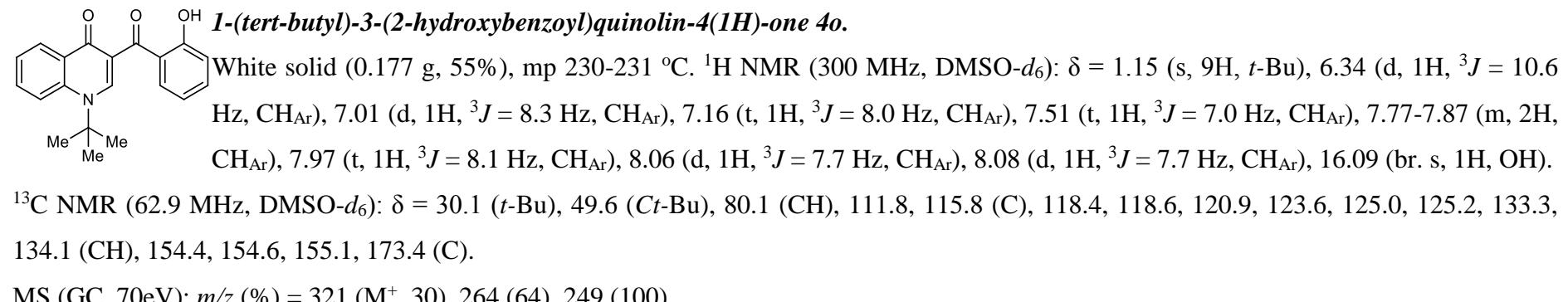
IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3207 (w), 3026 (w), 2922 (w), 2851 (w), 1631 (m), 1596 (m), 1570 (m), 1513 (m), 1469 (m), 1452 (m), 1303 (m), 1268 (m), 1186 (m), 1152 (m), 1080 (w), 908 (w), 850 (w), 796 (w), 746 (s), 697 (s).



MS (GC, 70eV): m/z (%) = 433 (M^+ , 33), 385 (13).

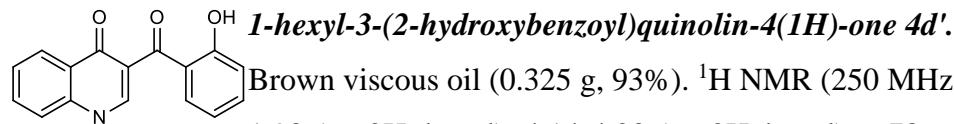
HRMS (EI): Calcd for $C_{23}H_{16}\text{BrNO}_3$ (M^+) 433.03136. Found 433.03158.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3029 (w), 1615 (m), 1484 (m), 1384 (w), 1347 (m), 1271 (s), 1233 (m), 1145 (m), 1025 (w), 948 (w), 860 (w), 812 (m), 752 (s), 702 (m), 627 (m), 586 (m), 546 (m).



HRMS (EI): Calcd for C₂₀H₁₉NO₃ (M⁺) 321.13594. Found 321.136189.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3303 (w), 2965 (w), 1638 (s), 1604 (m), 1561 (m), 1514 (w), 1465 (s), 1419 (s), 1360 (w), 1327 (w), 1311 (w), 1258 (m), 1205 (m), 1142 (m), 1099 (m), 1023 (w), 949 (w), 900 (w), 869 (m), 840 (m), 755 (s), 709 (s), 673 (m), 614 (m), 555 (m).



Brown viscous oil (0.325 g, 93%). ¹H NMR (250 MHz, CDCl₃): δ = 0.84-0.90 (m, 3H, hexyl), 1.23-1.36 (m, 6H, hexyl), 1.86-

1.90 (m, 2H, hexyl), 4.14-4.20 (m, 2H, hexyl), 6.78-6.84 (m, 1H, CH_{Ar}), 6.94-6.97 (m, 1H, CH_{Ar}), 7.40-7.50 (m, 3H, CH_{Ar}),

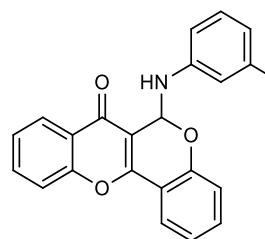
7.66-7.73 (m, 2H, CH_{Ar}), 8.00 (s, 1H, CH_{Ar}), 8.50 (d, 1H, ³J = 7.9 Hz, CH_{Ar}), 12.05 (s, 1H, OH).

¹³C NMR (62.9 MHz, CDCl₃): δ = 13.8 (Me), 22.4, 26.3, 28.8, 31.2, 54.0 (CH₂), 115.8, 117.7 (CH), 118.5 (C), 119.9, 120.6, 124.9 (CH), 127.8 (C), 128.6 (CH), 132.8 (C), 133.5, 136.2, 139.0, 146.2 (CH), 162.4, 174.2, 198.7 (C).

MS (GC, 70eV): *m/z* (%) = 349 (M⁺, 76), 350 (100).

HRMS (EI): Calcd for C₂₂H₂₃NO₃ (M⁺) 349.16779. Found 349.16793.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2927 (w), 2856 (w), 1625 (s), 1596 (s), 1548 (m), 1484 (m), 1460 (m), 1418 (w), 1345 (m), 1269 (m), 1227 (m), 1150 (m), 1122 (w), 1033 (w), 979 (w), 907 (m), 866 (w), 755 (m), 724 (s), 643 (m), 595 (w), 563 (w).



6-((3-(trifluoromethyl)phenyl)amino)chromeno[4,3-b]chromen-7(6H)-one 5a.

Yellow solid (0.303 g, 74%), mp 277-279 °C. ¹H NMR (300 MHz, DMSO-*d*₆): δ = 6.83 (d, 1H, ³J = 7.7 Hz, CHNH), 7.04-7.07 (m, 2H, CHNH, CH_{Ar}), 7.14-7.27 (m, 3H, CH_{Ar}), 7.40-7.45 (m, 1H, CH_{Ar}), 7.49-7.58 (m, 3H, CH_{Ar}), 7.84-7.91 (m, 2H, CH_{Ar}), 8.05-8.13 (m, 2H, CH_{Ar}).

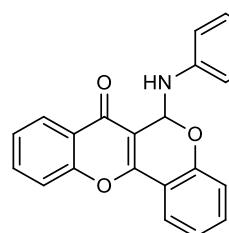
¹⁹F NMR (282 MHz, DMSO-*d*₆): δ = -61.3 (CF₃).

¹³C NMR (75.5 MHz, DMSO-*d*₆): δ = 76.9 (CHNH), 109.4 (q, *J* = 4 Hz, CH), 110.0 (C), 114.5 (q, *J* = 4 Hz, CH), 115.4 (C), 117.0, 118.3, 122.1 (CH), 123.6 (C), 123.9 (CH), 124.3 (q, ¹J = 272 Hz, CF₃), 125.0, 125.7 (CH), 129.9 (q, ²J = 31 Hz, CCF₃), 130.2, 133.9, 134.6 (CH), 145.9, 154.3, 155.1, 155.2, 173.5 (C).

MS (GC, 70eV): m/z (%) = 409 (M^+ , 1), 249 (100).

HRMS (ESI): Calcd for $C_{23}H_{14}NNaO_3F_3$ ($M+Na$) 432.0818. Found 432.08149.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3297 (w), 1634 (m), 1601 (m), 1563 (m), 1539 (m), 1489 (m), 1466 (m), 1425 (s), 1342 (s), 1312 (m), 1263 (m), 1214 (m), 1166 (m), 1136 (m), 1089 (s), 1068 (s), 1025 (m), 996 (w), 927 (m), 868 (m), 856 (m), 760 (s), 695 (s), 564 (m).



F 6-((4-fluorophenyl)amino)chromeno[4,3-b]chromen-7(6H)-one 5b.

Yellow solid (0.309 g, 84%), mp 274-276 °C. ^1H NMR (300 MHz, DMSO- d_6): δ = 6.71 (d, 1H, 3J = 8.0 Hz, CHNH), 6.86-6.91 (m, 2H, CH_{Ar}), 6.99-7.07 (m, 4H, CHNH, CH_{Ar}), 7.23 (t, 1H, 3J = 8.0 Hz, CH_{Ar}), 7.48-7.58 (m, 2H, CH_{Ar}), 7.83-7.93 (m, 2H, CH_{Ar}), 8.03-8.12 (m, 2H, CH_{Ar}).

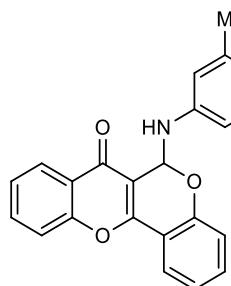
^{19}F NMR (282 MHz, DMSO- d_6): δ = -126.5 (CF).

^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 77.8 (CHNH), 110.3 (C), 114.4 (d, 3J = 8.0 Hz, CH), 115.3 (CH), 115.5 (C), 115.6 (CH), 118.4 (d, 3J = 8.0 Hz, CH), 121.7 (CH), 123.7 (C), 123.8, 125.0, 125.6, 133.8, 134.5 (CH), 140.1 (d, 2J = 50.8 Hz, C), 141.9, 154.5, 155.2 (C), 155.6 (d, 1J = 232.8 Hz, CF), 173.5 (C=O).

MS (GC, 70eV): m/z (%) = 359 (M^+ , 1), 249 (100).

HRMS (ESI): Calcd for $C_{22}H_{15}FNO_3$ ($M+H$) 360.10305. Found 360.1038.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3312 (m), 2958 (w), 1636 (s), 1603 (m), 1563 (w), 1530 (m), 1506 (s), 1464 (s), 1426 (s), 1347 (w), 1306 (m), 1253 (w), 1207 (m), 1149 (m), 1130 (m), 1088 (m), 1027 (w), 921 (s), 867 (m), 825 (s), 760 (s), 700 (m), 658 (m), 603 (m), 554 (m).



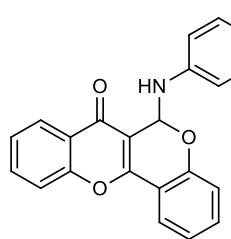
6-((3,5-dimethylphenyl)amino)chromeno[4,3-b]chromen-7(6H)-one 5c.

Yellow solid (0.203 g, 55%), mp 278-280 °C. ^1H NMR (300 MHz, DMSO- d_6): δ = 2.19 (s, 6H, Me), 6.39 (s, 1H, CH_{Ar}), 6.50 (s, 2H, CH_{Ar}), 6.72 (d, 1H, 3J = 7.7 Hz, CHNH), 6.91 (d, 1H, 3J = 8.1 Hz, CH_{Ar}), 7.04 (d, 1H, 3J = 7.7 Hz, CHNH), 7.22 (t, 1H, 3J = 7.7 Hz, CH_{Ar}), 7.47-7.57 (m, 2H, CH_{Ar}), 7.84-7.90 (m, 2H, CH_{Ar}), 8.02-8.12 (m, 2H, CH_{Ar}). ^{13}C NMR data not obtained due to poor solubility.

MS (GC, 70eV): m/z (%) = 369 (M $^+$, 10), 249 (100).

HRMS (ESI): Calcd for C₂₄H₂₀NO₃ (M+H) 370.14377. Found 370.14331.

IR (ATR, cm $^{-1}$): $\tilde{\nu}$ = 3311 (m), 1631 (s), 1601 (s), 1559 (m), 1464 (m), 1424 (s), 1356 (w), 1336 (m), 1309 (m), 1256 (m), 1215 (w), 1185 (m), 1139 (m), 1097 (m), 1025 (w), 994 (w), 917 (m), 866 (m), 851 (m), 820 (m), 756 (s), 690 (m), 624 (w), 535 (m).



6-((4-ethylphenyl)amino)chromeno[4,3-b]chromen-7(6H)-one 5d.

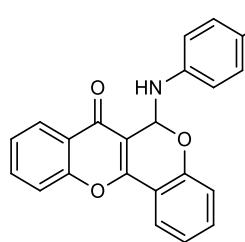
Yellow solid (0.306 g, 83%), mp 248-249 °C. ^1H NMR (300 MHz, DMSO- d_6): δ = 1.14 (t, 3H, 3J = 7.6 Hz, Me), 2.44-2.54 (m, 2H, CH₂), 6.70 (d, 1H, 3J = 8.0 Hz, CHNH), 6.80 (d, 2H, 3J = 8.4 Hz, CH_{Ar}), 6.92 (m, 1H, 3J = 7.8 Hz, CH_{Ar}), 7.01 (d, 3H, 3J = 8.4 Hz, CHNH, CH_{Ar}), 7.22 (t, 1H, 3J = 7.5 Hz, CH_{Ar}), 7.47-7.56 (m, 2H, CH_{Ar}), 7.82-7.91 (m, 2H, CH_{Ar}), 8.02-8.11 (m, 2H, CH_{Ar}).

^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 16.0 (Me), 27.4 (CH₂), 77.7 (CHNH), 110.3 (C), 113.4 (CH), 115.6 (C), 118.4, 118.5, 121.7 (CH), 123.7 (C), 123.8, 125.0, 125.5, 128.2 (CH), 133.5 (C), 133.7, 134.4 (CH), 143.1, 154.5, 154.9, 155.1, 173.5 (C).

MS (GC, 70eV): m/z (%) = 369 (M $^+$, 2), 249 (100).

HRMS (ESI): Calcd for C₂₄H₂₀NO₃ (M+H) 370.14377. Found 370.14351.

IR (ATR, cm $^{-1}$): $\tilde{\nu}$ = 3318 (m), 2958 (w), 1626 (s), 1559 (m), 1520 (m), 1465 (m), 1428 (s), 1358 (w), 1300 (m), 1254 (m), 1186 (w), 1137 (m), 1097 (m), 947 (w), 920 (m), 866 (m), 823 (m), 759 (s), 700 (m), 601 (m), 534 (m).



6-((4-methoxyphenyl)amino)chromeno[4,3-b]chromen-7(6H)-one 5e.

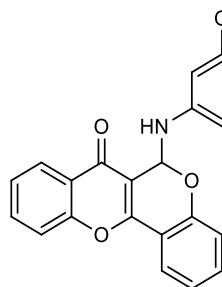
Yellow solid (0.211 g, 57%), mp 238-240 °C. ^1H NMR (300 MHz, DMSO- d_6): δ = 3.68 (s, 3H, OMe), 6.66-6.83 (m, 5H, CHNH, CH_{Ar}), 7.01-7.04 (m, 1H, CHNH), 7.20-7.24 (m, 2H, CH_{Ar}), 7.50-7.54 (m, 2H, CH_{Ar}), 7.86 (br. s, 2H, CH_{Ar}), 8.02-8.11 (m, 2H, CH_{Ar}).

^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 55.2 (OMe), 78.3 (CHNH), 114.4, 114.5 (CH), 115.6 (C), 118.3, 118.4, 121.7 (CH), 123.7 (C), 123.8, 125.0, 125.5, 133.7, 134.4 (CH), 139.1, 152.3, 154.6, 154.8, 155.1, 173.5 (C).

MS (GC, 70eV): m/z (%) = 371 (M⁺, 3), 249 (100).

HRMS (ESI): Calcd for C₂₃H₁₈NO₄ (M+H) 372.12303. Found 372.12293.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3328 (m), 1637 (s), 1601 (m), 1552 (w), 1509 (s), 1462 (m), 1424 (s), 1342 (w), 1292 (m) 1230 (s), 1209 (m), 1136 (m), 1097 (m), 1036 (m), 922 (m), 852 (m), 814 (s), 759 (s), 700 (s), 655 (m), 551 (m).



6-((3-methoxyphenyl)amino)chromeno[4,3-b]chromen-7(6H)-one 5f.

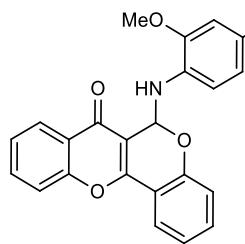
Yellow solid (0.226 g, 61%), mp 239-241 °C. ^1H NMR (300 MHz, DMSO- d_6): δ = 3.70 (s, 3H, OMe), 6.31-6.35 (m, 1H, CH_{Ar}), 6.43-6.50 (m, 2H, CH_{Ar}), 6.72 (d, 1H, 3J = 7.7 Hz, CHNH), 7.03-7.12 (m, 3H, CHNH, CH_{Ar}), 7.23 (t, 1H, 3J = 7.5 Hz, CH_{Ar}), 7.48-7.58 (m, 2H, CH_{Ar}), 7.83-7.93 (m, 2H, CH_{Ar}), 8.03-8.13 (m, 2H, CH_{Ar}).

^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 54.7 (OMe), 77.4 (CHNH), 99.3, 103.9, 106.1 (CH), 110.2, 115.5 (C), 118.4, 118.5, 121.8 (CH), 123.9 (C), 123.9, 125.0, 125.6, 129.8, 133.7, 134.5 (CH), 146.6, 154.5, 155.0, 155.1, 160.2, 173.5 (C).

MS (GC, 70eV): m/z (%) = 371 (M⁺, 3), 249 (100).

HRMS (ESI): Calcd for C₂₃H₁₈NO₄ (M+H) 372.12303. Found 372.12329.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3309 (m), 1632 (s), 1598 (s), 1559 (m), 1487 (m), 1464 (m), 1429 (s), 1359 (w), 1313 (m), 1255 (m), 1227 (w), 1203 (m), 1161 (m), 1099 (m), 1044 (m), 925 (m), 858 (m), 829 (m), 756 (s), 686 (s), 662 (m), 532 (m).



6-((2,4-dimethoxyphenyl)amino)chromeno[4,3-b]chromen-7(6H)-one 5g.

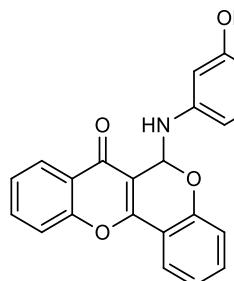
Black solid (0.120 g, 30%), mp 214-216 °C. ^1H NMR (300 MHz, DMSO-*d*₆): δ = 3.62 (s, 3H, OMe), 3.71 (s, 3H, OMe), 5.93 (d, 1H, 3J = 8.2 Hz, CH_{Ar}), 6.49-6.52 (m, 2H, CH_{Ar}), 6.69 (d, 1H, 3J = 8.0 Hz, CHNH), 6.99 (d, 1H, 3J = 8.0 Hz, CHNH), 7.15-7.23 (m, 2H, CH_{Ar}), 7.46-7.55 (m, 2H, CH_{Ar}), 7.81-7.87 (m, 2H, CH_{Ar}), 8.00-8.11 (m, 2H, CH_{Ar}).

^{13}C NMR (62.9 MHz, DMSO-*d*₆): δ = 55.2, 55.2 (OMe), 78.1 (CHNH), 99.2, 104.2 (CH), 110.1 (C), 112.2 (CH), 115.9 (C), 118.2, 121.7, 123.9, 125.3 (CH), 128.3, 133.5, 134.2, 147.5, 152.7, 154.4, 155.2, 173.8 (C).

MS (GC, 70eV): *m/z* (%) = 401 (M⁺, 4), 249 (100).

HRMS (ESI): Calcd for C₂₄H₂₀NO₅ (M+H) 402.1336. Found 402.13361.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3352 (s), 1637 (s), 1606 (m), 1564 (w), 1524 (m), 1465 (m), 1425 (s), 1312 (w), 1259 (m), 1205 (s), 1144 (m), 1095 (m), 1033 (m), 921 (m), 830 (m), 754 (s), 698 (m), 617 (w).



6-((3,4,5-trimethoxyphenyl)amino)chromeno[4,3-b]chromen-7(6H)-one 5h.

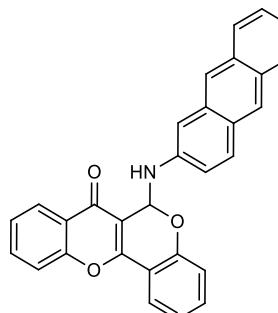
Yellow solid (0.302 g, 70%), mp 265-267 °C. ^1H NMR (300 MHz, DMSO-*d*₆): δ = 3.57 (s, 3H, OMe), 3.74 (s, 6H, 2xOMe), 6.18 (s, 2H, CH_{Ar}), 6.74 (d, 1H, 3J = 7.4 Hz, CHNH), 6.95 (d, 1H, 3J = 7.4 Hz, CH_{Ar}), 7.08 (d, 1H, 3J = 8.2 Hz, CHNH), 7.22 (t, 1H, 3J = 7.4 Hz, CH_{Ar}), 7.50-7.57 (m, 2H, CH_{Ar}), 7.84-7.92 (m, 2H, CH_{Ar}), 8.03-8.12 (m, 2H, CH_{Ar}).

^{13}C NMR data not obtained due to poor solubility.

MS (GC, 70eV): *m/z* (%) = 431 (M⁺, 3), 249 (100).

HRMS (ESI): Calcd for C₂₅H₂₂NO₆ (M+H) 432.14416. Found 432.14418.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3322 (m), 2938 (w), 1638 (s), 1600 (s), 1563 (m), 1530 (m), 1509 (m), 1456 (s), 1422 (s), 1348 (w), 1310 (w), 1236 (s), 1196 (s), 1121 (s), 1101 (s), 1010 (m), 912 (m), 883 (m), 850 (m), 804 (m), 757 (s), 705 (m), 651 (m).



6-(anthracen-2-ylamino)chromeno[4,3-b]chromen-7(6H)-one 5i.

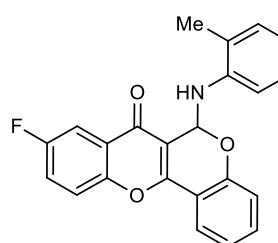
Yellow solid (0.238 g, 54%), mp 297-298 °C. ^1H NMR (300 MHz, DMSO- d_6): δ = 6.99 (d, 1H, 3J = 7.7 Hz, CHNH), 7.07-7.13 (m, 2H, CHNH, CH_{Ar}), 7.25-7.30 (m, 1H, CH_{Ar}), 7.37-7.61 (m, 6H, CH_{Ar}), 7.91-8.02 (m, 5H, CH_{Ar}), 8.10-8.16 (m, 2H, CH_{Ar}), 8.38 (d, 2H, 3J = 14.9 Hz, CH_{Ar}).

^{13}C NMR data not obtained due to poor solubility.

MS (GC, 70eV): m/z (%) = 441 (M $^+$, 1), 249 (100), 193 (47), 165 (25).

HRMS (ESI): Calcd for C₃₀H₂₀NO₃ (M+H) 442.14377. Found 442.14405.

IR (ATR, cm $^{-1}$): $\tilde{\nu}$ = 3329 (m), 1623 (s), 1602 (m), 1548 (m), 1462 (m), 1422 (s), 1353 (m), 1323 (m), 1272 (w), 1229 (m), 1204 (m), 1183 (m), 1124 (m), 1092 (m), 998 (w), 946 (w), 913 (m), 867 (s), 812 (m), 776 (m), 760 (s), 741 (s), 686 (m), 609 (m), 584 (m), 566 (m), 538 (m).



6-((2,4-dimethylphenyl)amino)-9-fluorochromeno[4,3-b]chromen-7(6H)-one 5j.

Yellow solid (0.143 g, 37%), mp 240-242 °C. ^1H NMR (300 MHz, DMSO- d_6): δ = 1.89 (s, 3H, Me), 2.19 (s, 3H, Me), 6.00 (t, 1H, 3J = 8.2 Hz, CH_{Ar}), 6.67 (d, 1H, 3J = 7.8 Hz, CHNH), 6.82 (br. s, 1H, CH_{Ar}), 6.95-7.06 (m, 2H, CHNH, CH_{Ar}), 7.17-7.24 (m, 2H, CH_{Ar}), 7.47-7.56 (m, 1H, CH_{Ar}), 7.75-8.05 (m, 4H, CH_{Ar}).

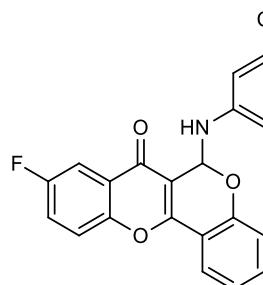
^{19}F NMR (282 MHz, DMSO- d_6): δ = -115.5 (CF).

^{13}C NMR data not obtained due to poor solubility.

MS (GC, 70eV): m/z (%) = 387 (M $^+$, 3), 267 (100), 121 (19).

HRMS (ESI): Calcd for C₂₄H₁₉NFO₃ (M+H) 388.13435. Found 388.13504.

IR (ATR, cm $^{-1}$): $\tilde{\nu}$ = 3353 (w), 1633 (s), 1603 (s), 1565 (m), 1515 (m), 1478 (s), 1454 (s), 1410 (s), 1367 (m), 1318 (m), 1247 (m), 1212 (m), 1187 (m), 1134 (m), 1088 (m), 1010 (w), 954 (w), 918 (m), 861 (m), 823 (m), 807 (m), 774 (s), 757 (s), 744 (s), 700 (m), 659 (m).



6-((3,5-dichlorophenyl)amino)-9-fluorochromeno[4,3-b]chromen-7(6H)-one 5k.

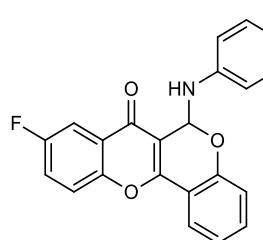
White solid (0.304 g, 71%), mp 285-286 °C. ^1H NMR (300 MHz, DMSO- d_6): δ = 6.83 (d, 1H, 3J = 7.6 Hz, CHNH), 6.90 (br. s, 3H, CH_{Ar}), 7.10 (d, 1H, 3J = 8.1 Hz, CHNH), 7.25 (t, 1H, 3J = 7.2 Hz, CH_{Ar}), 7.51-7.60 (m, 2H, CH_{Ar}), 7.78-7.83 (m, 2H, CH_{Ar}), 7.96-8.00 (m, 1H, CH_{Ar}), 8.06 (m, 1H, CH_{Ar}). ^{19}F NMR (282 MHz, DMSO- d_6): δ = -114.9 (CF).

^{13}C NMR data not obtained due to poor solubility.

MS (GC, 70eV): m/z (%) = 427 (M^+ , 1), 267 (100).

HRMS (ESI): Calcd for C₂₂H₁₁NCl₂FO₃ (M+H) 426.01055. Found 426.01175.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3290 (m), 1626 (m), 1580 (s), 1556 (s), 1479 (m), 1446 (m), 1409 (m), 1356 (m), 1272 (w), 1253 (m), 1209 (m), 1129 (m), 1105 (m), 1088 (m), 1014 (w), 989 (w), 961 (m), 923 (m), 872 (m), 824 (m), 773 (m), 763 (s), 746 (m), 668 (m), 611 (m).



9-fluoro-6-((4-methoxyphenyl)amino)chromeno[4,3-b]chromen-7(6H)-one 5l.

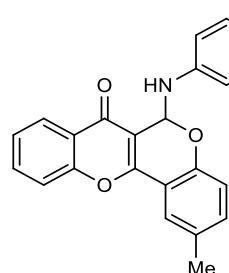
Yellow solid (0.187 g, 48%), mp 249-251 °C. ^1H NMR (300 MHz, DMSO- d_6): δ = 3.68 (s, 3H, OMe), 6.66 (d, 1H, 3J = 7.6 Hz, CHNH), 6.77-6.86 (m, 5H, CH_{Ar}), 7.02 (d, 1H, 3J = 8.2 Hz, CHNH), 7.22 (m, 1H, 3J = 7.6 Hz, CH_{Ar}), 7.51 (t, 1H, 3J = 7.0 Hz, CH_{Ar}), 7.76-7.90 (m, 2H, CH_{Ar}), 7.95-8.09 (m, 2H, CH_{Ar}). ^{19}F NMR (282 MHz, DMSO- d_6): δ = -115.2 (CF).

^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 55.2 (OMe), 77.2 (CHNH), 109.7 (d, J = 24 Hz, CH), 109.8 (C), 114.5, 114.6 (CH), 115.4 (C), 118.4 (CH), 121.2 (d, J = 9 Hz, CH), 121.7 (CH), 122.4 (d, J = 25 Hz, CH), 123.8 (CH), 124.9 (d, J = 7 Hz, C), 133.8 (CH), 139.1, 151.6, 152.3, 154.6, 155.2 (C), 159.0 (d, J = 245 Hz, CF), 172.8 (C).

MS (GC, 70eV): m/z (%) = 389 (M^+ , 3), 267 (100).

HRMS (ESI): Calcd for C₂₃H₁₇FNO₄ (M+H) 390.11361. Found 390.11406.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3310 (m), 1626 (s), 1614 (s), 1599 (s), 1581 (m), 1558 (s), 1510 (s), 1479 (s), 1462 (s), 1410 (s), 1347 (w), 1313 (w), 1273 (m), 1232 (s), 1208 (s), 1178 (m), 1135 (s), 1092 (m), 1026 (m), 955 (w), 880 (m), 818 (s), 774 (s), 761 (s), 747 (s), 650 (w), 583 (m), 555 (m).



6-((3,4-dimethoxyphenyl)amino)-2-methylchromeno[4,3-b]chromen-7(6H)-one 5m.

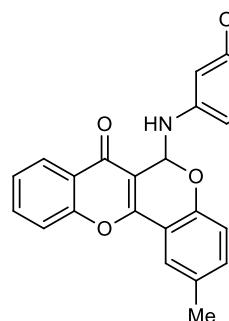
Yellow solid (0.249 g, 60%), mp 258-260 °C. ¹H NMR (300 MHz, DMSO-*d*₆): δ = 2.38 (s, 3H, Me), 3.67 (s, 3H, OMe), 3.69 (s, 3H, OMe), 6.44-6.46 (m, 2H, CH_{Ar}), 6.64 (d, 1H, ³J = 7.8 Hz, CHNH), 6.74 (d, 1H, ³J = 7.8 Hz, CH_{Ar}), 6.81 (d, 1H, ³J = 7.8 Hz, CH_{Ar}), 6.94 (d, 1H, ³J = 7.8 Hz, CHNH), 7.29-7.33 (m, 1H, CH_{Ar}), 7.51-7.56 (m, 1H, CH_{Ar}), 7.83-7.79 (m, 3H, CH_{Ar}), 8.09 (d, 1H, ³J = 7.4 Hz, CH_{Ar}).

¹³C NMR data not obtained due to poor solubility.

MS (GC, 70eV): *m/z* (%) = 415 (M⁺, 3), 263 (100).

HRMS (ESI): Calcd for C₂₅H₂₂NO₅ (M+H) 416.14925. Found 416.14892.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3312 (m), 1635 (s), 101 (m), 1515 (m), 1463 (s), 1429 (s), 1355 (w), 1318 (m), 1296 (w), 1257 (m), 1227 (s), 1202 (s), 1168 (m), 1134 (s), 1106 (s), 1028 (m), 928 (m), 910 (m), 859 (m), 828 (s), 786 (m), 757 (s), 702 (m), 670 (m).



6-((3,5-dimethoxyphenyl)amino)-2-methylchromeno[4,3-b]chromen-7(6H)-one 5n.

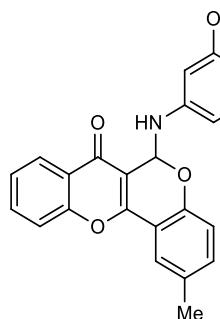
Yellow solid (0.203 g, 49%), mp 268-270 °C. ¹H NMR (300 MHz, DMSO-*d*₆): δ = 2.38 (s, 3H, Me), 3.68 (s, 6H, 2xOMe), 5.92 (t, 1H, ⁴J = 2.0 Hz, CH_{Ar}), 6.04 (d, 2H, ⁴J = 2.0 Hz, CH_{Ar}), 6.67 (d, 1H, ³J = 7.7 Hz, CHNH), 6.96 (d, 1H, ³J = 8.3 Hz, CH_{Ar}), 7.02 (d, 1H, ³J = 7.7 Hz, CHNH), 7.30-7.34 (m, 1H, CH_{Ar}), 7.51-7.57 (m, 1H, CH_{Ar}), 7.83-7.79 (m, 3H, CH_{Ar}), 8.10 (d, 1H, ³J = 8.1 Hz, CH_{Ar}).

¹³C NMR (62.9 MHz, DMSO-*d*₆): δ = 20.2 (Me), 54.8 (OMe), 77.1, 90.8, 92.2 (CH), 110.3, 115.3 (C), 118.2, 118.4, 123.5 (CH), 123.7 (C), 125.0, 125.6 (CH), 130.9 (C), 134.5 (CH), 147.2, 152.4, 155.2, 161.1, 173.5 (C).

MS (GC, 70eV): *m/z* (%) = 415 (M⁺, 3), 263 (100).

HRMS (ESI): Calcd for C₂₅H₂₂NO₅ (M+H) 416.14925. Found 416.14974.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3317 (m), 1634 (m), 1596 (s), 1564 (s), 1540 (m), 1465 (s), 1429 (s), 1343 (w), 1296 (w), 1224 (w), 1195 (s), 1175 (m), 1144 (s), 1109 (s), 1059 (m), 1001 (m), 928 (m), 910 (m), 860 (s), 812 (s), 786 (m), 758 (s), 705 (m), 677 (s), 621 (m), 560 (m).



2-methyl-6-((3,4,5-trimethoxyphenyl)amino)chromeno[4,3-b]chromen-7(6H)-one 5o.

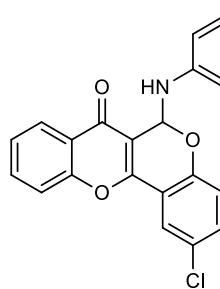
Yellow solid (0.174 g, 39%), mp 271-272 °C. ¹H NMR (300 MHz, DMSO-d₆): δ = 2.38 (s, 3H, Me), 3.57 (s, 3H, OMe), 3.73 (s, 6H, 2xOMe), 6.17 (s, 2H, CH_{Ar}), 6.69 (d, 1H, ³J = 7.6 Hz, CH_{Ar}), 6.89 (d, 1H, ³J = 7.6 Hz, CHNH), 6.97 (d, 1H, ³J = 7.8 Hz, CHNH), 7.31-7.33 (m, 1H, CH_{Ar}), 7.52-7.57 (m, 1H, CH_{Ar}), 7.84-7.791 (m, 3H, CH_{Ar}), 8.09 (d, 1H, ³J = 7.6 Hz, CH_{Ar}).

¹³C NMR data not obtained due to poor solubility.

MS (GC, 70eV): *m/z* (%) = 445 (M⁺, 21), 263 (100), 168 (19).

HRMS (ESI): Calcd for C₂₆H₂₄NO₆ (M+H) 446.15981. Found 446.16022.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3323 (m), 1636 (m), 1602 (m), 1566 (m), 1510 (m), 1465 (m), 1429 (s), 1341 (w), 1239 (m), 1192 (m), 1129 (s), 1110 (s), 1013 (m), 909 (m), 856 (m), 807 (m), 776 (m), 760 (s), 706 (m), 665 (m), 630 (m), 605 (m), 545 (m).



4-((2-chloro-7-oxo-6,7-dihydrochromeno[4,3-b]chromen-6-yl)amino)benzonitrile 5p.

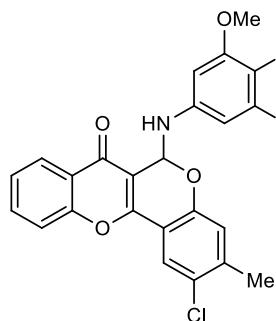
Yellow solid (0.196 g, 49%), mp 288-289 °C. ¹H NMR (300 MHz, DMSO-d₆): δ = 6.90 (d, 1H, ³J = 8.2 Hz, CHNH), 7.01 (d, 2H, ³J = 8.6 Hz, CHNH), 7.10 (d, 1H, ³J = 8.6 Hz, CH_{Ar}), 7.53-7.64 (m, 4H, CH_{Ar}), 7.85-7.94 (m, 3H, CH_{Ar}), 8.09-8.12 (m, 2H, CH_{Ar}).

¹³C NMR data not obtained due to poor solubility.

MS (GC, 70eV): *m/z* (%) = 398 (M⁺, 4), 402 (100), 400 (26).

HRMS (ESI): Calcd for C₂₃H₁₃ClN₂O₃ (M-H) 399.05488. Found 399.05419.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3279 (w), 2919 (w), 2220 (m), 1603 (m), 1531 (m), 1463 (m), 1428 (s), 1318 (m), 1255 (m), 1212 (m), 1170 (m), 1089 (m), 1011 (m), 943 (m), 866 (m), 815 (s), 762 (s), 644 (m).



2-chloro-3-methyl-6-((3,4,5-trimethoxyphenyl)amino)chromeno[4,3-b]chromen-7(6H)-one 5q.

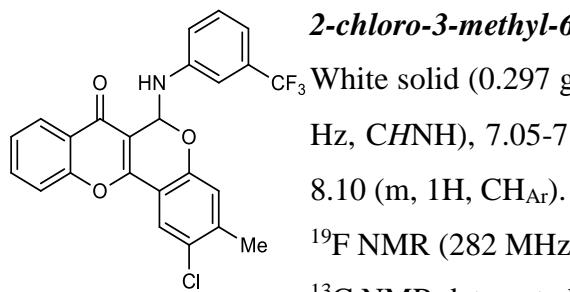
Yellow solid (0.187 g, 39%), mp 289-291 °C. ^1H NMR (300 MHz, DMSO- d_6): δ = 2.35 (s, 3H, Me), 3.57 (s, 3H, OMe), 3.74 (s, 6H, 2xOMe), 6.17 (s, 2H, CH_{Ar}), 6.77 (br. s, 1H, CHNH), 6.96 (br. s, 1H, CH_{Ar}), 7.14 (br. s, 1H, CHNH), 7.55 (br. s, 1H, CH_{Ar}), 7.90-8.09 (m, 4H, CH_{Ar}).

^{13}C NMR data not obtained due to poor solubility.

MS (GC, 70eV): m/z (%) = 479 (M $^+$, 4), 297 (100).

HRMS (ESI): Calcd for C₂₆H₂₂NClO₆ (M+H) 480.12084. Found 480.12112.

IR (ATR, cm $^{-1}$): $\tilde{\nu}$ = 3317 (w), 1637 (m), 1605 (s), 1533 (m), 1510 (m), 1461 (m), 1424 (s), 1341 (w), 1288 (w), 1247 (m), 1209 (m), 1124 (s), 998 (m), 914 (m), 847 (m), 802 (m), 762 (s), 679 (m), 565 (m).



2-chloro-3-methyl-6-((3-(trifluoromethyl)phenyl)amino)chromeno[4,3-b]chromen-7(6H)-one 5r.

White solid (0.297 g, 65%), mp 297-299 °C. ^1H NMR (300 MHz, DMSO- d_6): δ = 2.33 (s, 3H, Me), 6.83 (d, 1H, 3J = 7.9 Hz, CHNH), 7.05-7.21 (m, 4H, CHNH, CH_{Ar}), 7.39-7.58 (m, 3H, CH_{Ar}), 7.90-7.93 (m, 2H, CH_{Ar}), 8.04 (s, 1H, CH_{Ar}), 8.10 (m, 1H, CH_{Ar}).

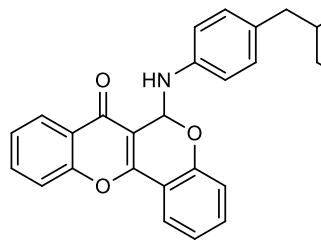
^{19}F NMR (282 MHz, DMSO- d_6): δ = -61.2 (CF₃).

^{13}C NMR data not obtained due to poor solubility.

MS (GC, 70eV): m/z (%) = 457 (M $^+$, 1), 297 (100), 161 (26).

HRMS (ESI): Calcd for C₂₄H₁₅NClF₃NaO₃ (M+Na) 480.05848. Found 480.05841.

IR (ATR, cm $^{-1}$): $\tilde{\nu}$ = 3307 (w), 1614 (m), 1573 (w), 1540 (m), 1477 (m), 1427 (m), 1337 (s), 1294 (w), 1270 (w), 1246 (w), 1165 (m), 1111 (s), 1068 (s), 1005 (w), 974 (w), 921 (m), 893 (s), 876 (m), 856 (m), 838 (m), 783 (m), 764 (s), 695 (m), 675 (m), 554 (m).



6,6'-(methylenebis(4,1-phenylene))bis(azanediyl)bis(chromeno[4,3-b]chromen-7(6H)-one) 5s.

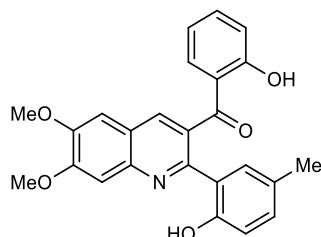
Yellow solid (0.555 g, 80%), mp more than 375 °C. ^1H NMR (300 MHz, DMSO- d_6): δ = 3.76 (s, 2H, CH₂), 6.75 (d, 2H, 3J = 8.0 Hz, CH_{Ar}), 6.85 (d, 4H, 3J = 8.3 Hz, CH_{Ar}), 7.00-7.09 (m, 8H, CH_{Ar}), 7.23-7.28 (m, 2H, CH_{Ar}), 7.51-7.61 (m, 4H, CH_{Ar}), 7.87-7.93 (m, 4H, CH_{Ar}), 8.06-8.10 (m, 2H, CH_{Ar}), 8.13-8.16 (m, 2H, CH_{Ar}).

^{13}C NMR data not obtained due to poor solubility.

MS (GC, 70eV): m/z (%) = 694 (M $^+$, 21), 263 (100).

HRMS (ESI): Calcd for C₄₅H₃₀N₂O₆ (M+H) 695.21766. Found 695.21771.

IR (ATR, cm $^{-1}$): $\tilde{\nu}$ = 3305 (m), 1626 (s), 1559 (s), 1517 (m), 1466 (m), 1427 (s), 1297 (m), 1249 (m), 1212 (m), 1137 (m), 1095 (m), 849 (m), 812 (m), 754 (s), 701 (m), 663 (m), 599 (m), 558 (m).



(2-(2-hydroxy-5-methylphenyl)-6,7-dimethoxyquinolin-3-yl)(2-hydroxymethyl)methanone 6a.

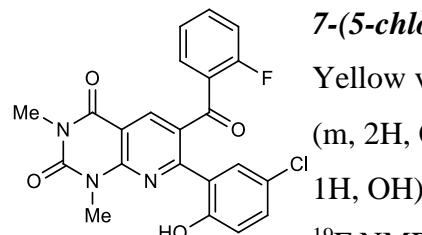
Yellow solid (0.042 g, 10%), mp 173-174 °C. ^1H NMR (300 MHz, CDCl₃): δ = 2.08 (s, 3H, Me), 4.04 (s, 3H, OMe), 4.10 (s, 3H, OMe), 6.62-6.69 (m, 1H, CH_{Ar}), 6.92 (d, 1H, 3J = 8.4 Hz, CH_{Ar}), 7.00-7.05 (m, 2H, CH_{Ar}), 7.11 (s, 1H, CH_{Ar}), 7.14-7.24 (m, 3H, CH_{Ar}), 7.42 (s, 1H, CH_{Ar}), 8.15 (s, 1H, Py), 11.84 (s, 1H, OH), 12.72 (br. s, 1H, OH).

^{13}C NMR (62.9 MHz, CDCl₃): δ = 20.2 (Me), 56.3, 56.5 (OMe), 105.3, 106.5, 117.9, 118.2, 119.0 (CH), 119.1, 120.1, 121.1, 128.4, 129.4 (C), 130.1, 131.2, 132.4, 136.9, 138.1 (CH), 142.9, 150.9, 153.7, 154.6, 158.2, 161.3, 201.8 (C).

MS (GC, 70eV): m/z (%) = 415 (M $^+$, 3), 263 (100).

HRMS (ESI): Calcd for C₂₅H₂₂NO₅ (M+H) 416.14925. Found 416.14892.

IR (ATR, cm $^{-1}$): $\tilde{\nu}$ = 3305 (s), 1619 (w), 1580 (w), 1499 (m), 1474 (m), 1372 (w), 1282 (w), 1243 (m), 1195 (m), 1155 (m), 1009 (m), 953 (w), 910 (w), 886 (w), 851 (m), 827 (m), 777 (m), 757 (m), 711 (m), 689 (m), 656 (m).



7-(5-chloro-2-hydroxyphenyl)-6-(2-fluorobenzoyl)-1,3-dimethylpyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione 6b.

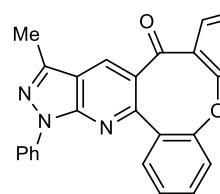
Yellow viscous oil (0.290 g, 66%). ^1H NMR (300 MHz, DMSO- d_6): δ = 3.47 (s, 3H, Me), 3.75 (s, 3H, Me), 6.88-6.96 (m, 2H, CH_{Ar}), 7.18-7.28 (m, 2H, CH_{Ar}), 7.31-7.37 (m, 2H, CH_{Ar}), 7.58-7.64 (m, 1H, CH_{Ar}), 8.53 (s, 1H, Py), 11.34 (s, 1H, OH). ^{19}F NMR (282 MHz, DMSO- d_6): δ = -114.5 (CF).

^{13}C NMR data not obtained due to poor solubility.

MS (GC, 70eV): m/z (%) = 439 (M^+ , 27), 419 (19), 285 (100), 257 (16), 154 (21).

HRMS (ESI): Calcd for C₂₂H₁₄N₃O₄FCl (M+H) 440.10077. Found 440.08074.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 1716 (w), 1657 (m), 1631 (m), 1596 (s), 1568 (m), 1464 (m), 1413 (m), 1368 (m), 1344 (m), 1285 (m), 1199 (m), 1110 (m), 1019 (w), 938 (w), 913 (w), 830 (m), 806 (w), 750 (m), 685 (m), 645 (m), 600 (w).



13-methyl-11-phenyldibenzo[2,3:7,8]oxocino[4,5-b]pyrazolo[4,3-e]pyridin-15(11H)-one 7a.

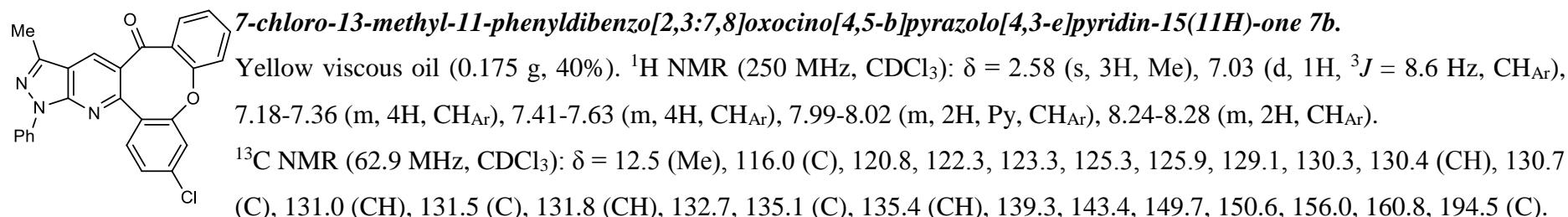
Yellow solid (0.214 g, 53%), mp 250-251 °C. ^1H NMR (250 MHz, CDCl₃): δ = 2.40 (s, 3H, Me), 6.07-7.10 (m, 1H, CH_{Ar}), 7.17-7.45 (m, 7H, CH_{Ar}), 7.51-7.57 (m, 1H, CH_{Ar}), 7.66 (dd, 1H, 3J = 7.4 Hz, 3J = 1.7 Hz, CH_{Ar}), 7.98-8.01 (m, 2H, CH_{Ar}), 8.28-8.31 (m, 2H, CH_{Ar}).

^{13}C NMR (62.9 MHz, CDCl₃): δ = 12.5 (Me), 115.7 (C), 120.6, 121.7, 122.4, 125.0, 125.6, 126.1, 129.0, 130.1, 130.6, 130.8, 130.9, 131.6 (CH), 132.8, 133.7 (C), 135.2 (CH), 139.4, 143.3, 150.7, 151.1, 127.5, 161.1, 194.9 (C).

MS (GC, 70eV): m/z (%) = 403 (M^+ , 100).

HRMS (ESI): Calcd for C₂₆H₁₈N₃O₂ (M+H) 404.13935. Found 404.1389.

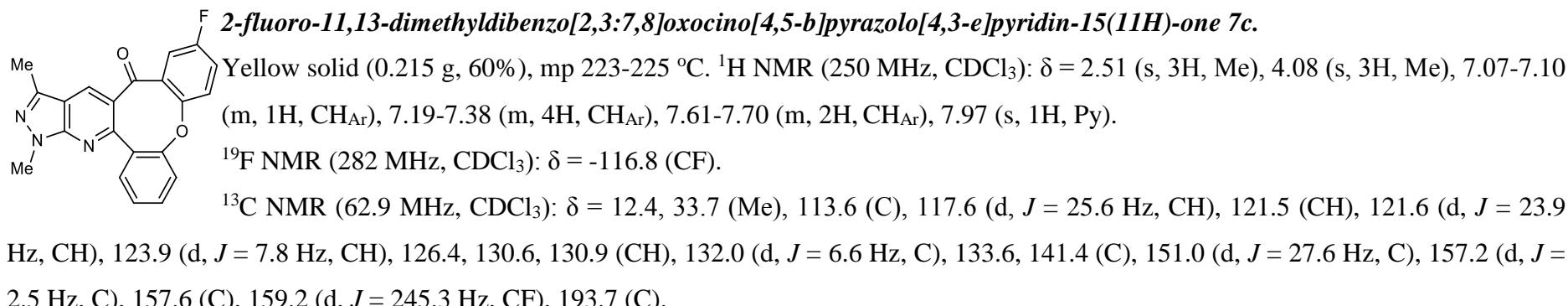
IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3064 (s), 1645 (w), 1594 (s), 1495 (m), 1446 (m), 1382 (m), 1340 (w), 1308 (m), 1280 (s), 1210 (m), 1120 (m), 1102 (m), 1080 (m), 998 (w), 908 (w), 781 (m), 754 (s), 711 (m), 689 (s), 661 (m), 626 (m), 607 (m).



MS (GC, 70eV): m/z (%) = 437 (M^+ , 100).

HRMS (ESI): Calcd for $\text{C}_{26}\text{H}_{16}\text{N}_3\text{O}_2\text{Cl}$ (M^+) 437.09256. Found 437.09255.

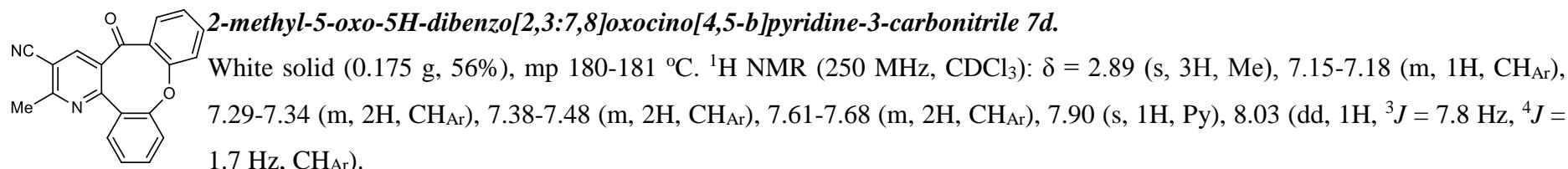
IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3068 (w), 1632 (m), 1596 (m), 1507 (m), 1468 (m), 1413 (m), 1377 (m), 1340 (w), 1303 (m), 1278 (m), 1243 (m), 1210 (m), 1158 (m), 1120 (m), 1088 (m), 1000 (w), 945 (m), 876 (m), 812 (m), 768 (s), 711 (m), 683 (m), 626 (m).



MS (GC, 70eV): m/z (%) = 359 (M^+ , 100).

HRMS (ESI): Calcd for $\text{C}_{21}\text{H}_{14}\text{N}_3\text{O}_2\text{F}$ ($\text{M}+\text{H}$) 360.11453. Found 360.11428.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3070 (w), 1654 (m), 1597 (m), 1554 (w), 1480 (m), 1450 (m), 1412 (m), 1330 (w), 1259 (m), 1213 (m), 1181 (s), 1121 (m), 1016 (m), 914 (m), 891 (m), 848 (m), 835 (m), 781 (m), 765 (s), 744 (m), 708 (m), 637 (m), 594 (m).

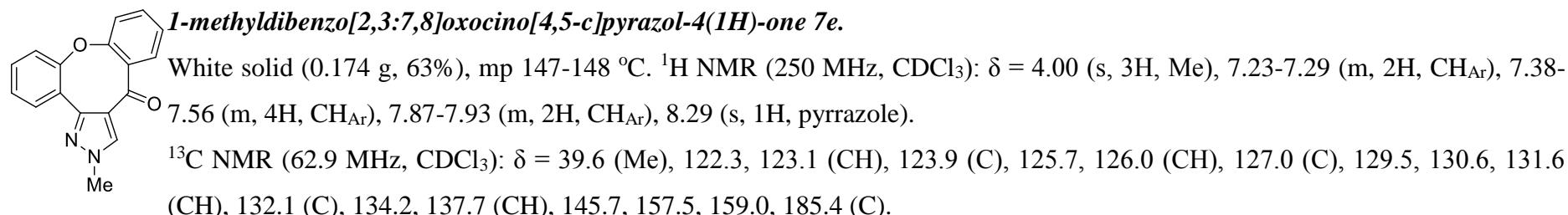


White solid (0.175 g, 56%), mp 180-181 °C. ^1H NMR (250 MHz, CDCl_3): δ = 2.89 (s, 3H, Me), 7.15-7.18 (m, 1H, CH_{Ar}), 7.29-7.34 (m, 2H, CH_{Ar}), 7.38-7.48 (m, 2H, CH_{Ar}), 7.61-7.68 (m, 2H, CH_{Ar}), 7.90 (s, 1H, Py), 8.03 (dd, 1H, 3J = 7.8 Hz, 4J = 1.7 Hz, CH_{Ar}).
 ^{13}C NMR (62.9 MHz, CDCl_3): δ = 23.8 (Me), 108.3, 116.3 (C), 121.9, 122.8, 125.4, 126.5 (CH), 129.9 (C), 130.1, 131.8, 131.9 (CH), 132.3, 135.7 (C), 136.2, 140.5 (CH), 153.4, 157.1, 161.2, 162.7, 192.1 (C).

MS (GC, 70eV): m/z (%) = 312 (M^+ , 100), 283 (60), 271 (27), 258 (43).

HRMS (EI): Calcd for $\text{C}_{20}\text{H}_{12}\text{N}_2\text{O}_2$ (M^+) 312.08933. Found 312.08883.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2229 (w), 1636 (m), 1582 (m), 1537 (w), 1474 (m), 1452 (m), 1429 (m), 1310 (m), 1281 (m), 1222 (s), 1160 (m), 1099 (m), 992 (w), 931 (w), 887 (m), 854 (m), 770 (s), 746 (s), 706 (s), 674 (m), 658 (m).



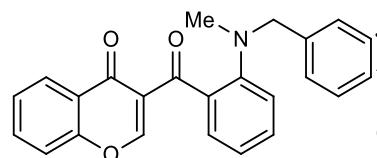
White solid (0.174 g, 63%), mp 147-148 °C. ^1H NMR (250 MHz, CDCl_3): δ = 4.00 (s, 3H, Me), 7.23-7.29 (m, 2H, CH_{Ar}), 7.38-7.56 (m, 4H, CH_{Ar}), 7.87-7.93 (m, 2H, CH_{Ar}), 8.29 (s, 1H, pyrazole).

^{13}C NMR (62.9 MHz, CDCl_3): δ = 39.6 (Me), 122.3, 123.1 (CH), 123.9 (C), 125.7, 126.0 (CH), 127.0 (C), 129.5, 130.6, 131.6 (CH), 132.1 (C), 134.2, 137.7 (CH), 145.7, 157.5, 159.0, 185.4 (C).

MS (GC, 70eV): m/z (%) = 276 (M^+ , 100), 248 (24).

HRMS (EI): Calcd for $\text{C}_{17}\text{H}_{12}\text{N}_2\text{O}_2$ (M^+) 276.08933. Found 276.08903.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3132 (w), 1619 (m), 1593 (m), 1519 (m), 1456 (m), 1311 (m), 1256 (m), 1202 (m), 1186 (s), 1107 (m), 1007 (w), 918 (s), 859 (m), 816 (m), 777 (m), 748 (m), 716 (s), 665 (m).



3-(2-(benzyl(methyl)amino)benzoyl)-4H-chromen-4-one 8a.

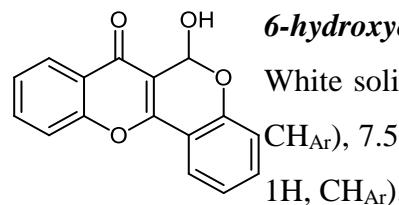
White solid (0.336 g, 91%), mp 149-150 °C. ^1H NMR (300 MHz, CDCl_3): δ = 2.28 (s, 3H, Me), 3.90 (q, 2H, 3J = 9.7 Hz, CH_2), 6.48 (s, 1H, chromone), 7.04-7.11 (m, 2H, CH_{Ar}), 7.15-7.33 (m, 5H, CH_{Ar}), 7.38-7.49 (m, 2H, CH_{Ar}), 7.53-7.56 (m, 1H, CH_{Ar}), 7.65-7.72 (m, 1H, CH_{Ar}), 7.89 (dd, 1H, 3J = 8.2 Hz, 4J = 1.8 Hz, CH_{Ar}), 8.27 (dd, 1H, 3J = 8.0 Hz, 4J = 1.5 Hz, CH_{Ar}).

^{13}C NMR (75.5 MHz, CDCl_3): δ = 35.5 (Me), 56.6 (CH_2), 88.4, 109.2, 114.8 (C), 116.36, 117.9, 120.8, 123.6 (CH), 124.4 (C), 125.1, 126.0, 127.0, 128.2, 128.6, 133.6, 133.9 (CH), 155.5, 156.5, 157.7, 175.1 (C).

MS (GC, 70eV): m/z (%) = 369 (M^+ , 1), 249 (100), 120 (27).

HRMS (ESI): Calcd for $\text{C}_{24}\text{H}_{20}\text{NO}_3$ ($\text{M}+\text{H}$) 370.14377. Found 370.14384.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2997 (w), 1640 (m), 1601 (m), 1563 (m), 1485 (w), 1463 (m), 1416 (s), 1350 (m), 1330 (m), 1258 (m), 1209 (m), 1164 (m), 1148 (m), 1107 (w), 1047 (s), 994 (w), 964 (m), 906 (m), 882 (m), 840 (m), 790 (w), 758 (s), 744 (s), 698 (s), 663 (m), 638 (m).



6-hydroxychromeno[4,3-b]chromen-7(6H)-one 9a.

White solid (0.021 g, 8%), mp 240-241 °C. ^1H NMR (300 MHz, $\text{DMSO}-d_6$): δ = 6.55 (s, 1H, CHOH), 7.16-7.27 (m, 2H, CH_{Ar}), 7.50-7.61 (m, 2H, CH_{Ar}), 7.64 (br. s, 1H, CHOH), 7.79-7.90 (m, 2H, CH_{Ar}), 8.01-8.04 (m, 1H, CH_{Ar}), 8.09-8.12 (m, 1H, CH_{Ar}).

^{13}C NMR (62.9 MHz, $\text{DMSO}-d_6$): δ = 87.3 (CHOH), 111.5, 114.6 (C), 117.9, 118.5, 122.0, 123.6 (CH), 123.7 (C), 125.0, 125.6, 133.8, 134.5 (CH), 154.1, 154.6, 155.1, 173.8 (C).

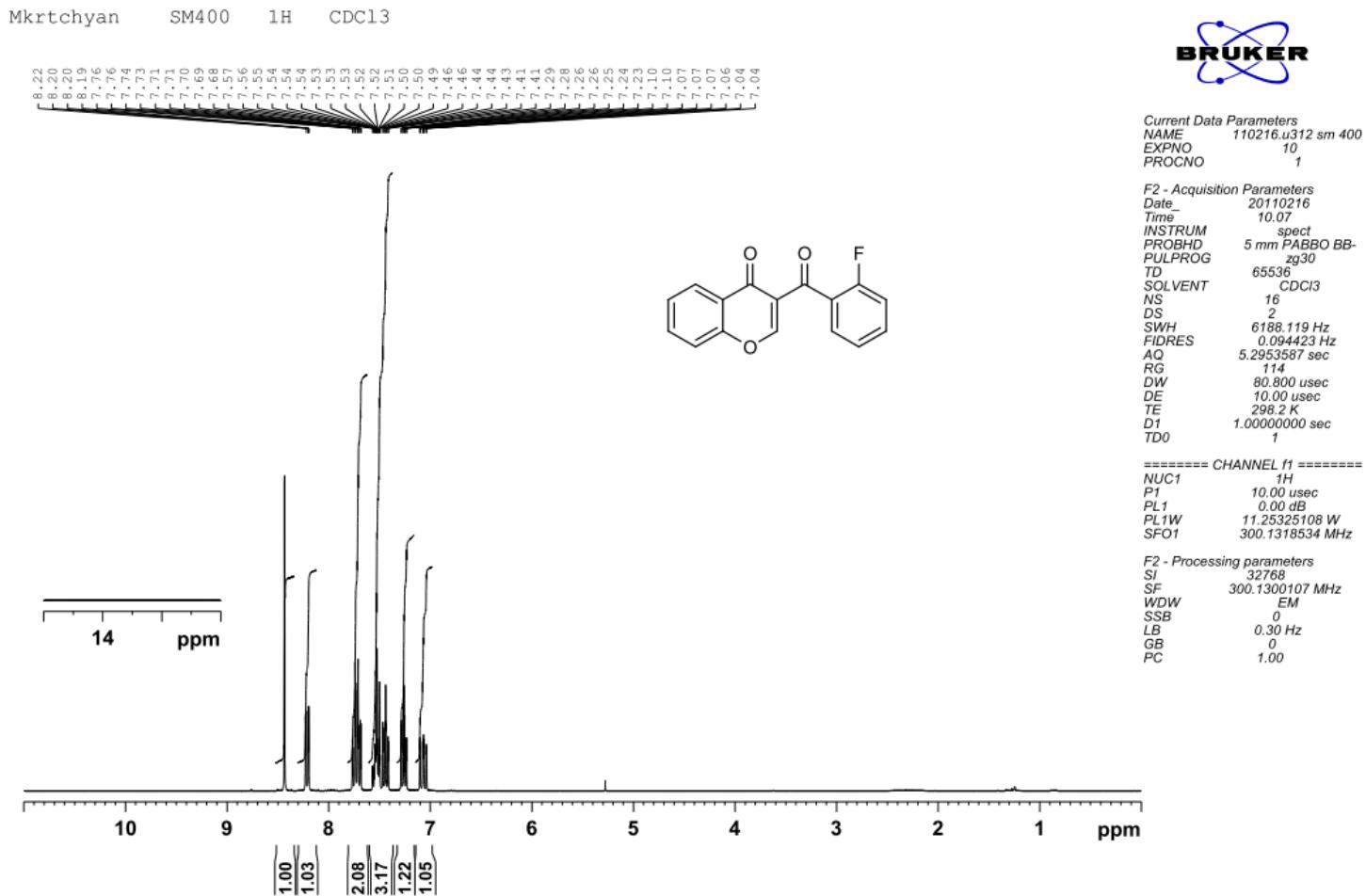
MS (GC, 70eV): m/z (%) = 266 (M^+ , 100).

HRMS (EI): Calcd for $\text{C}_{16}\text{H}_{10}\text{O}_4$ ($\text{M}+\text{Na}$) 289.04713. Found 289.04668.

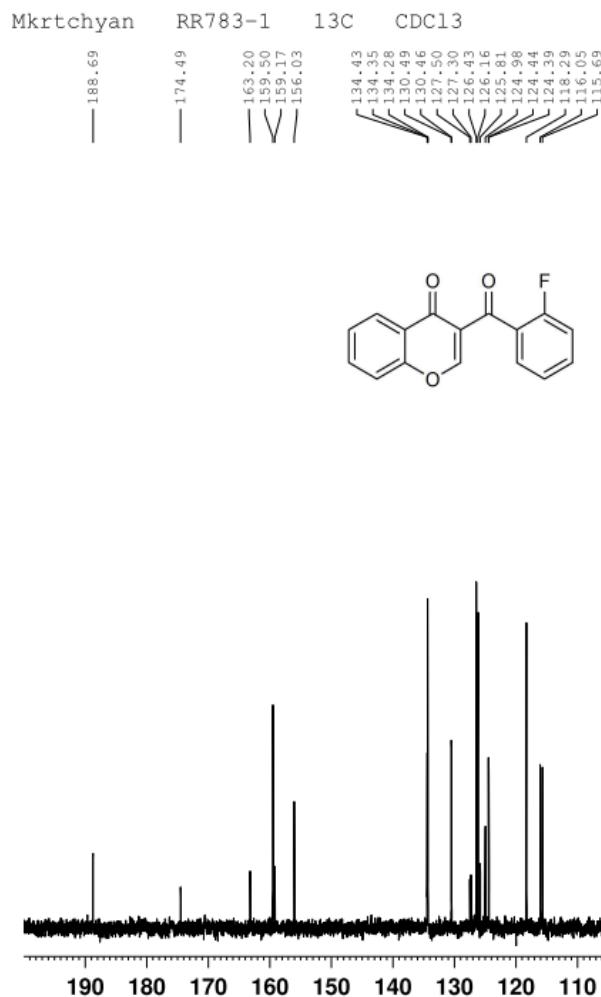
IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3024 (w), 1641 (m), 1600 (m), 1557 (m), 1477 (w), 1416 (s), 1351 (m), 1331 (m), 1258 (m), 1210 (m), 1164 (m), 1100 (w), 1051 (s), 994 (w), 906 (m), 882 (m), 840 (m), 790 (w), 758 (s), 698 (s), 650 (m).

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

Compound 3c



Compound 3c



Current Data Parameters
NAME 130718.205 sm:
EXPNO 10
PROCNO 1

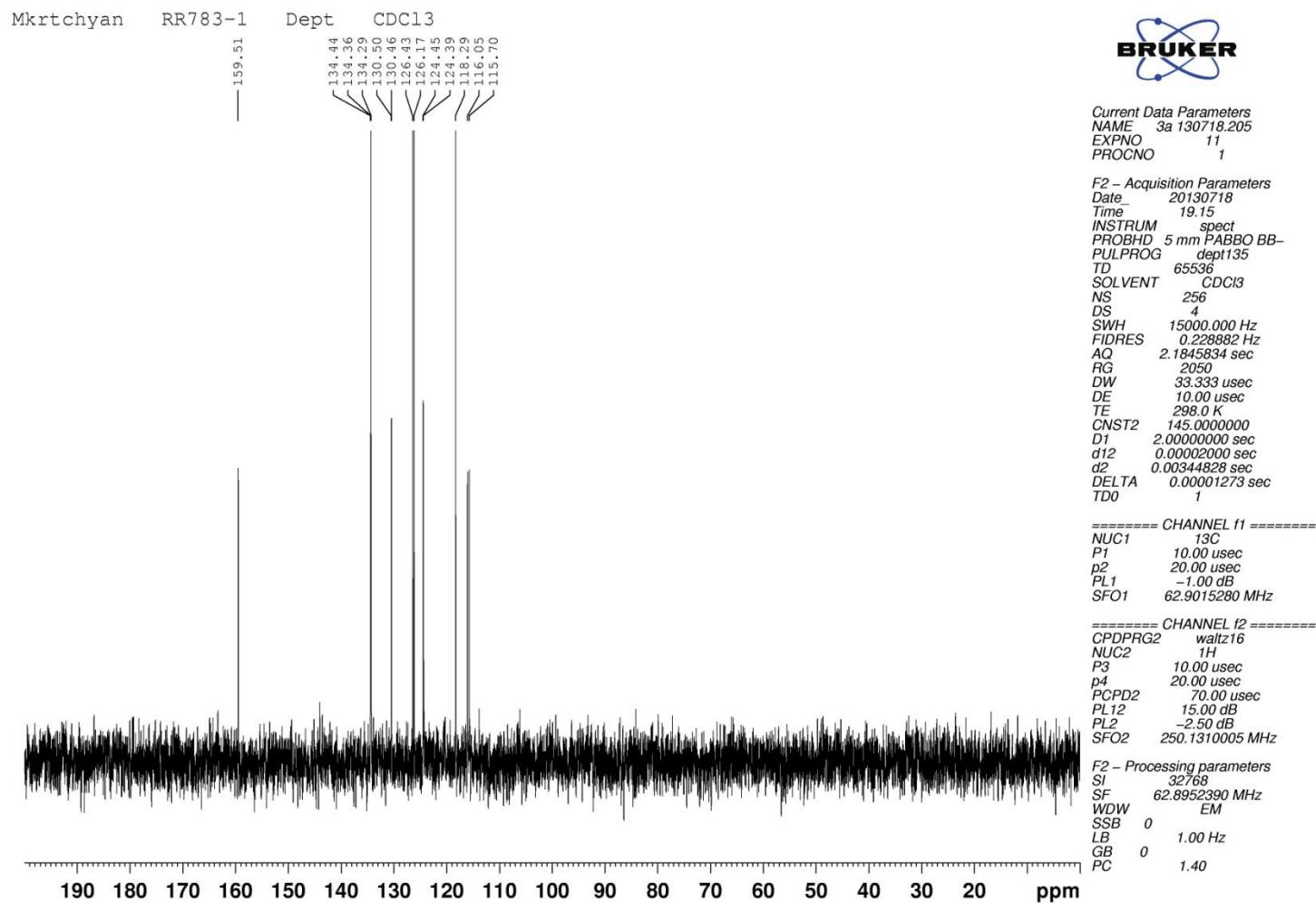
F2 - Acquisition Parameters
Date 20130718
Time 18.56
INSTRUM spect
PROBHD 5 mm PABBC
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 t
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.3 K
D1 2.0000000 se
d11 0.03000000 se
DELTA 1.89999998
TD0 1

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

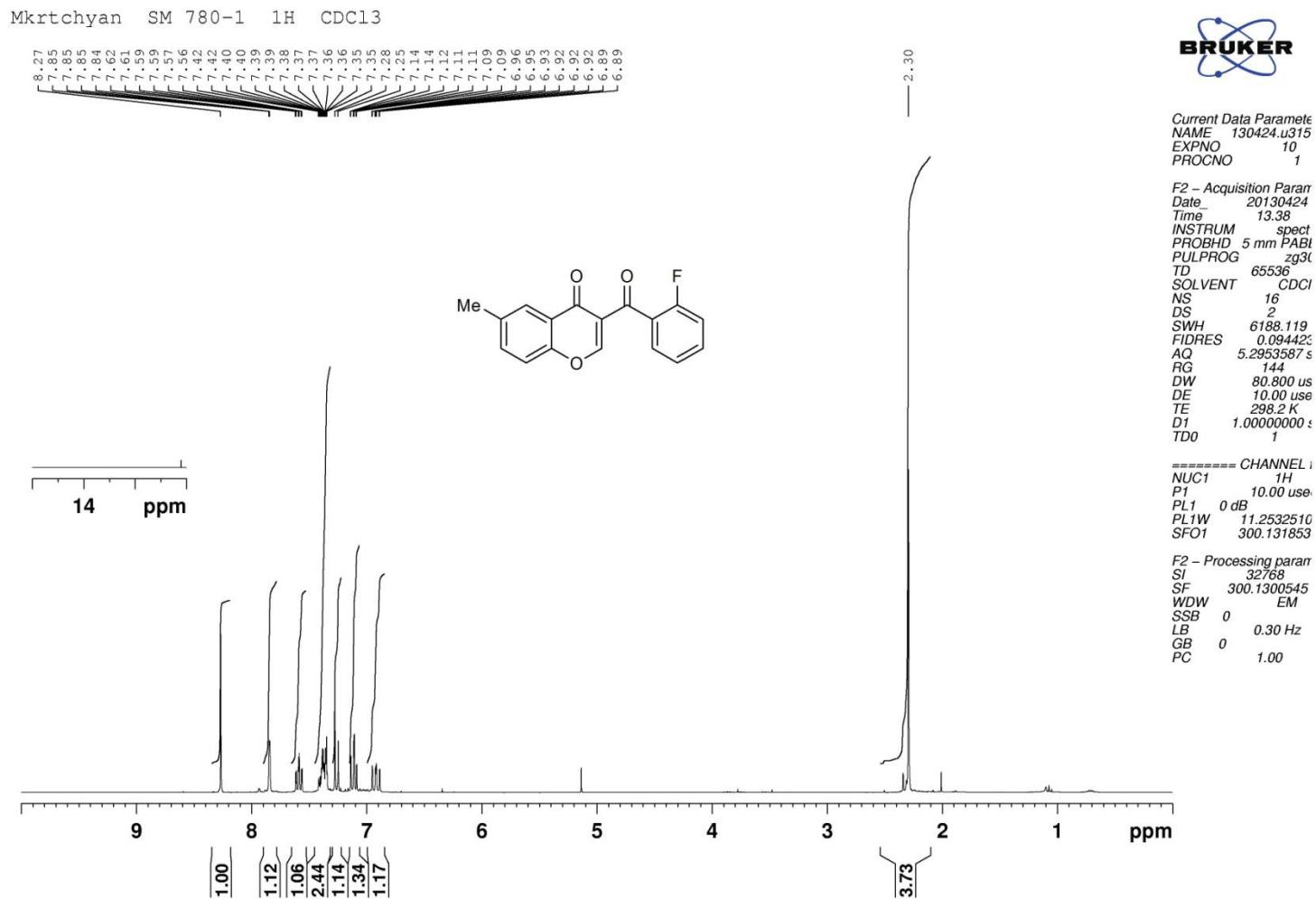
===== CHANNEL f2
CPDPG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005

F2 - Processing parameters
SI 32768
SF 62.8952393 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

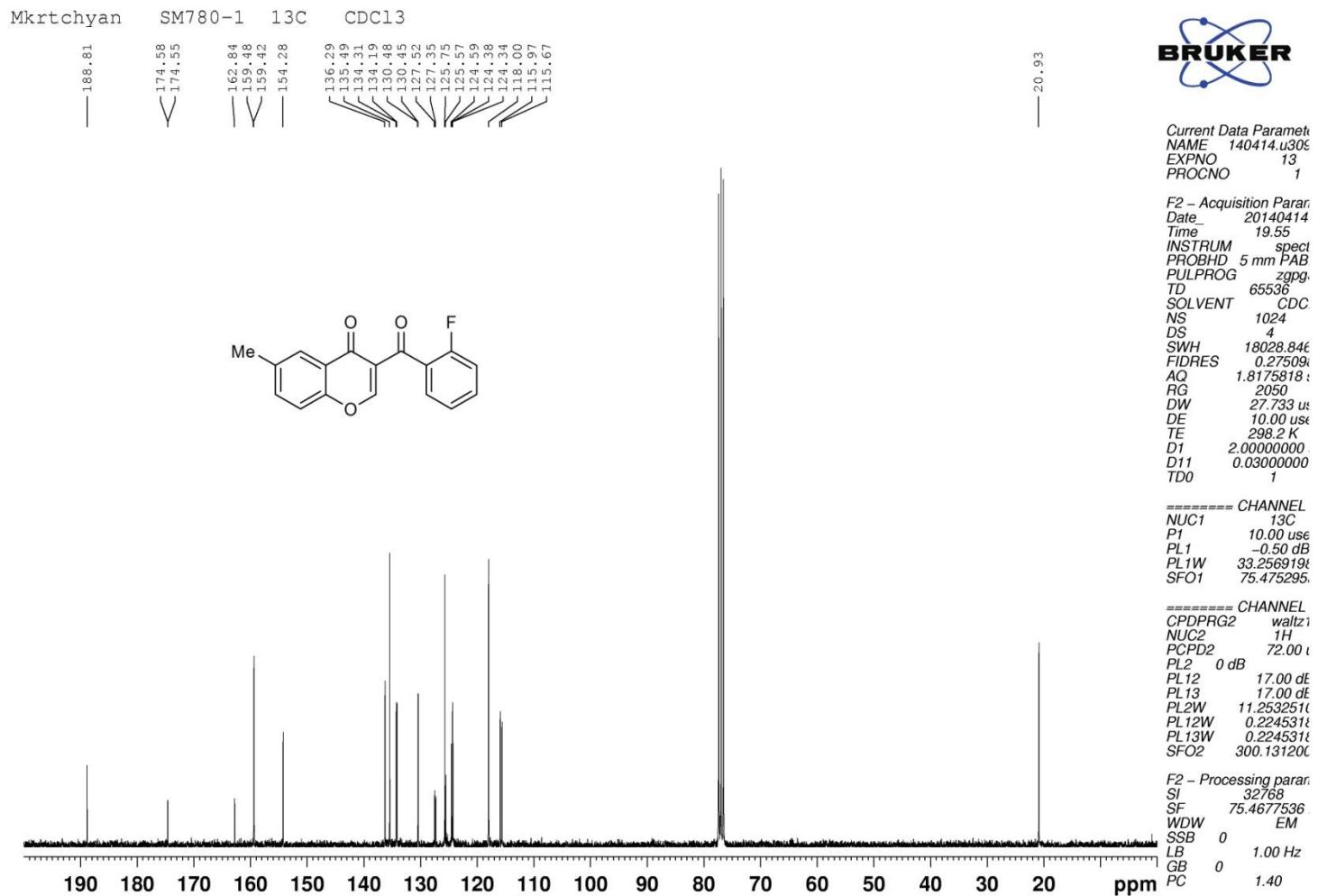
Compound 3c



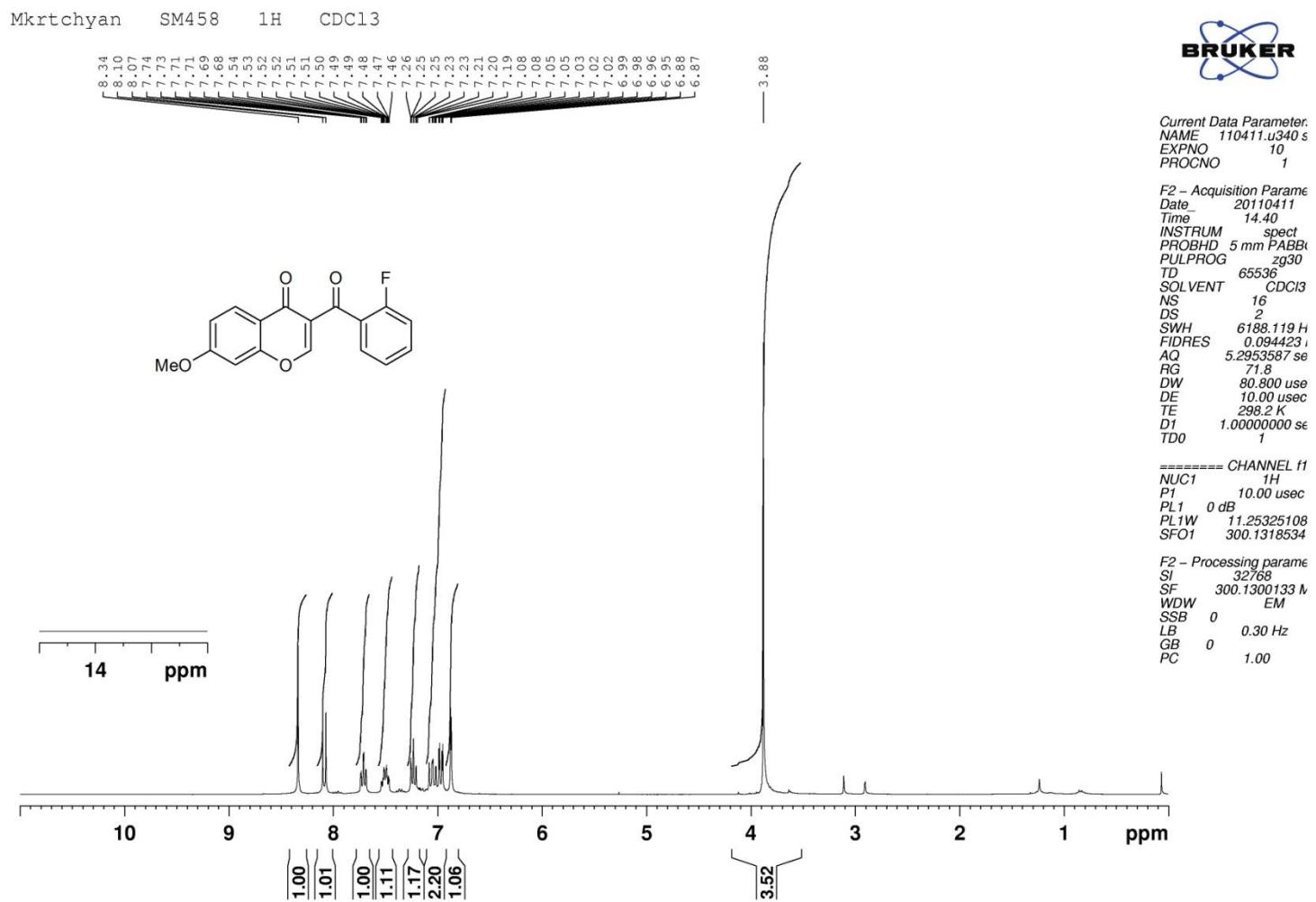
Compound 3d



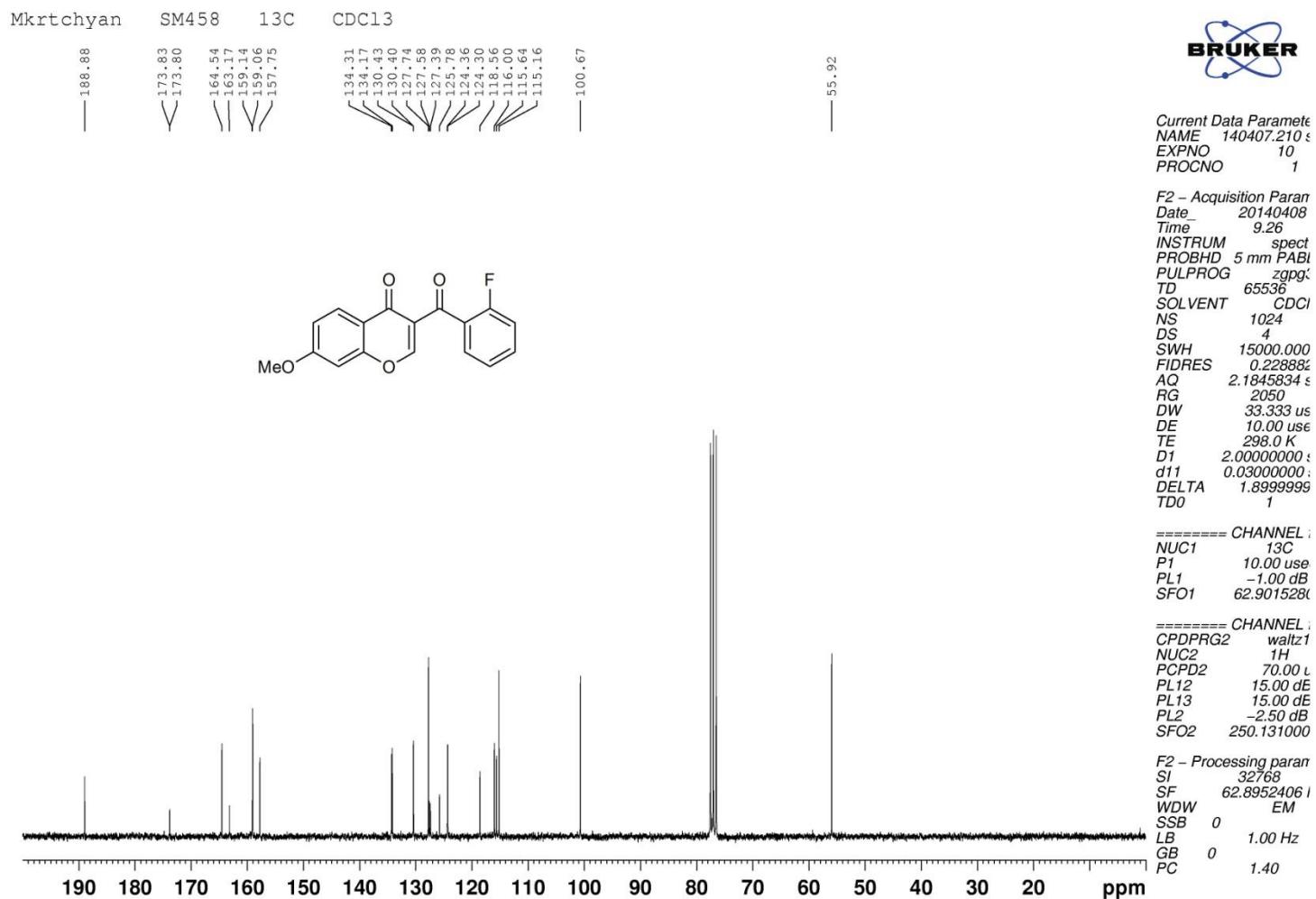
Compound 3d



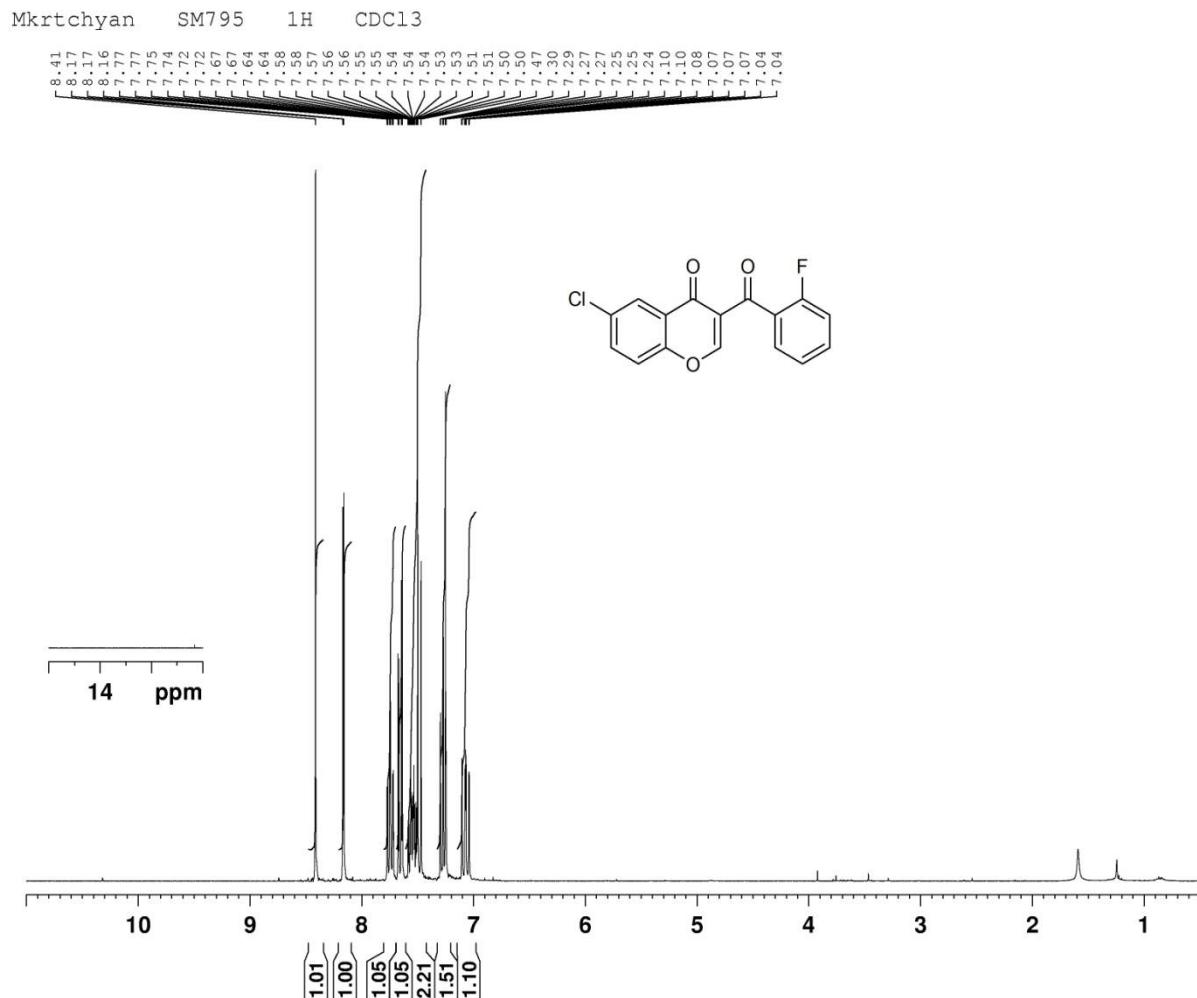
Compound 3e



Compound 3e



Compound 3f



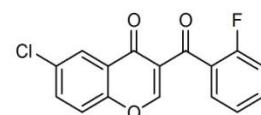
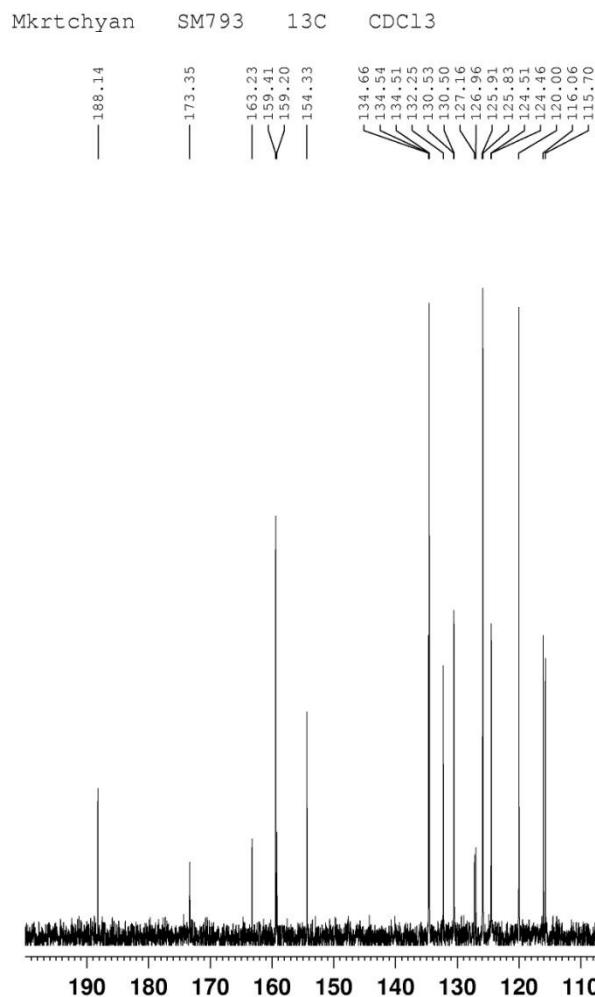
Current Data Parameters
NAME 130614.u303 sm
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20130614
Time 8.03
INSTRUM spect
PROBHD 5 mm PABBO,
PULPROG zg30
TD 65536
SOLVENT CDCl3
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 1.0000000 sec
TDO 1

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

F2 - Processing parameters
SI 32768
SF 300.1300132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 3f



Current Data Parameters
NAME 140407.211 sm
EXPNO 10
PROCNO 1

F2 - Acquisition Paramet
Date 20140408
Time 10.34
INSTRUM spect
PROBHD 5 mm PABBC
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 627
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 2.0000000 sec
d11 0.03000000 sec
DELTA 1.89999998 s
TDO 1

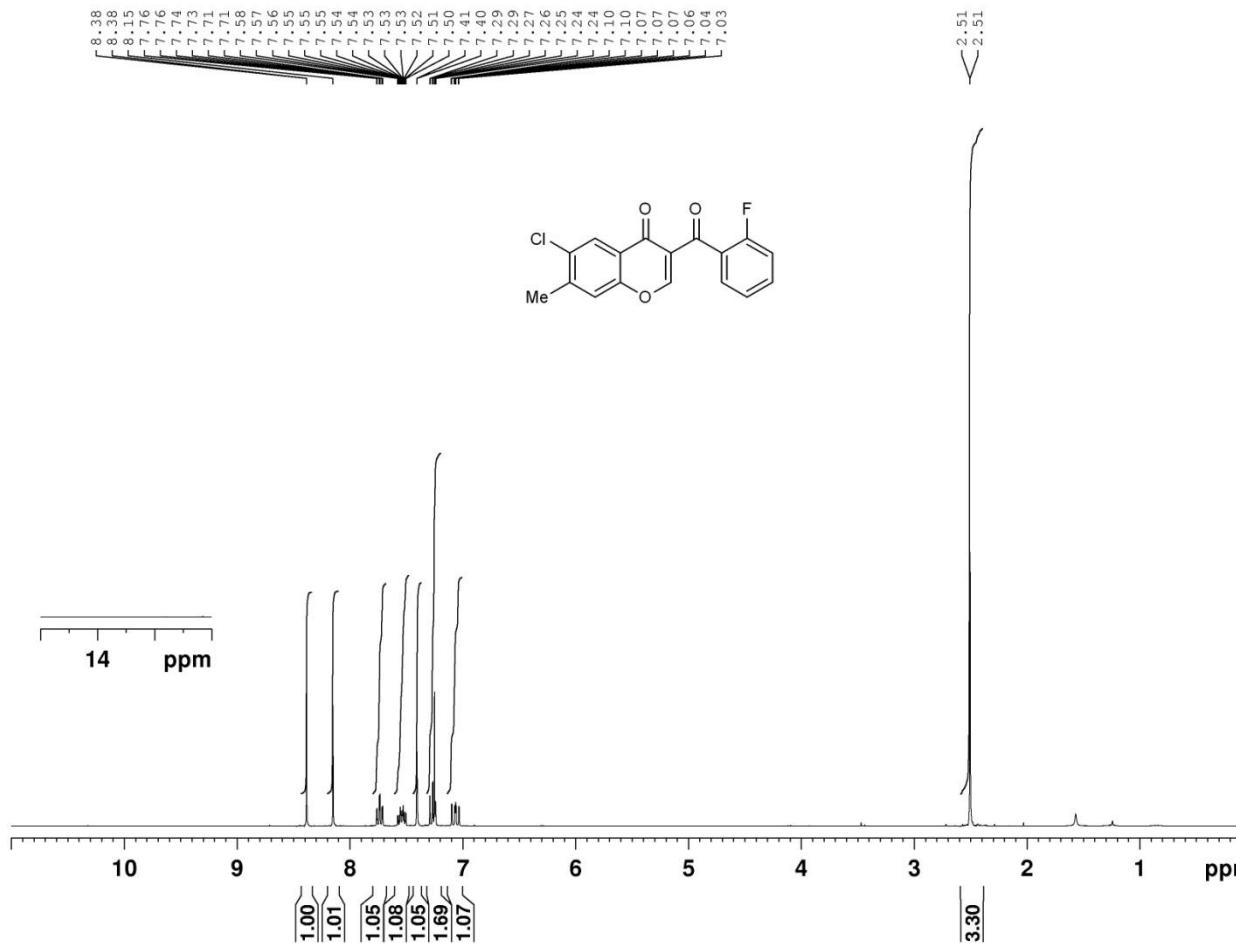
===== CHANNEL f1 :
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

===== CHANNEL f2 :
CPDPG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 Hz

F2 - Processing param
SI 32768
SF 62.8952402 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 3g

Mkrtchyan SM796 1H CDCl₃



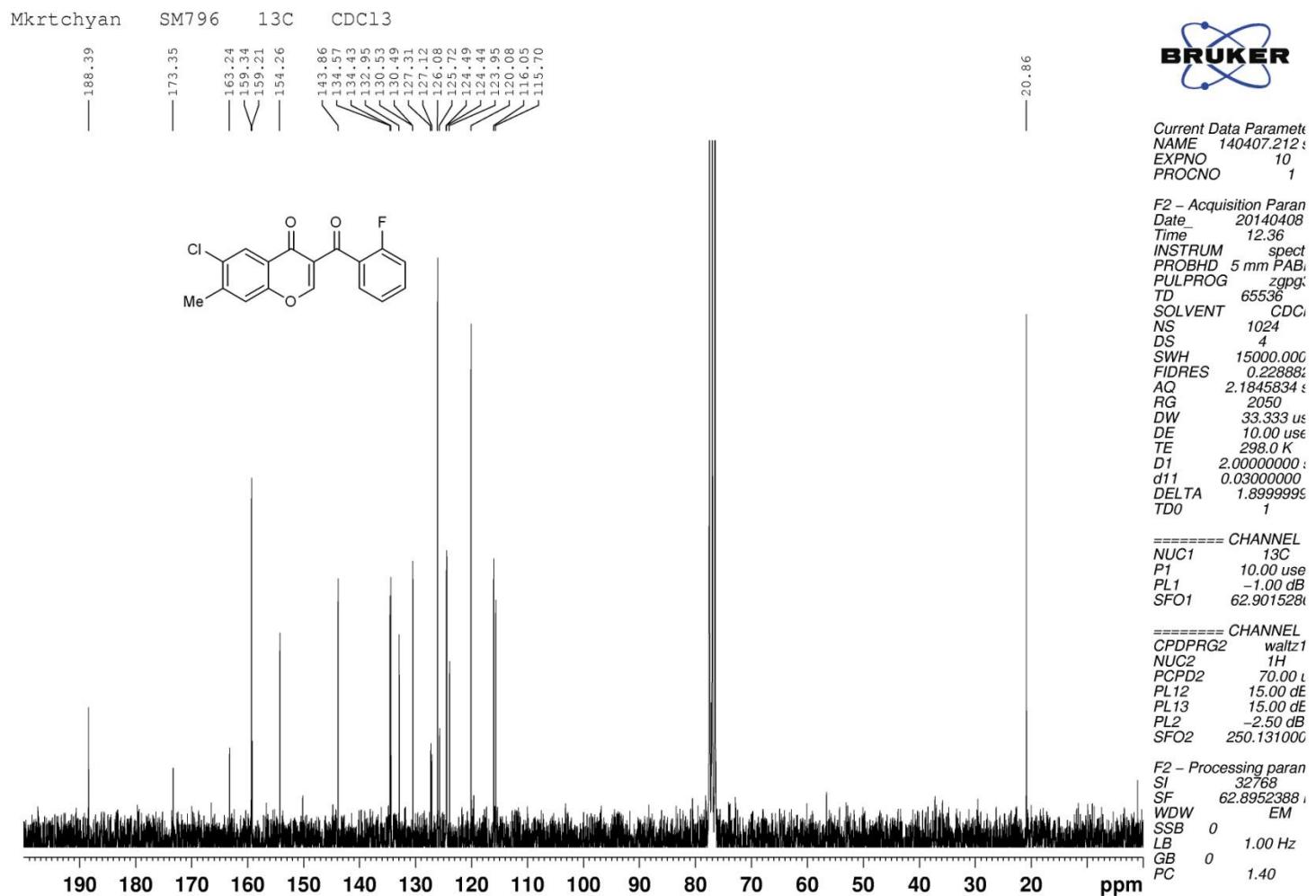
Current Data Parameters
NAME 130614.u304
EXPNO 10
PROCNO 1

F2 - Acquisition Param
Date 20130614
Time 8.13
INSTRUM spect
PROBHD 5 mm PABE
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 6188.119 f
FIDRES 0.094423
AQ 5.2953587 s
RG 287
DW 80.800 us
DE 10.00 us
TE 298.2 K
D1 1.0000000 s
TDO 1

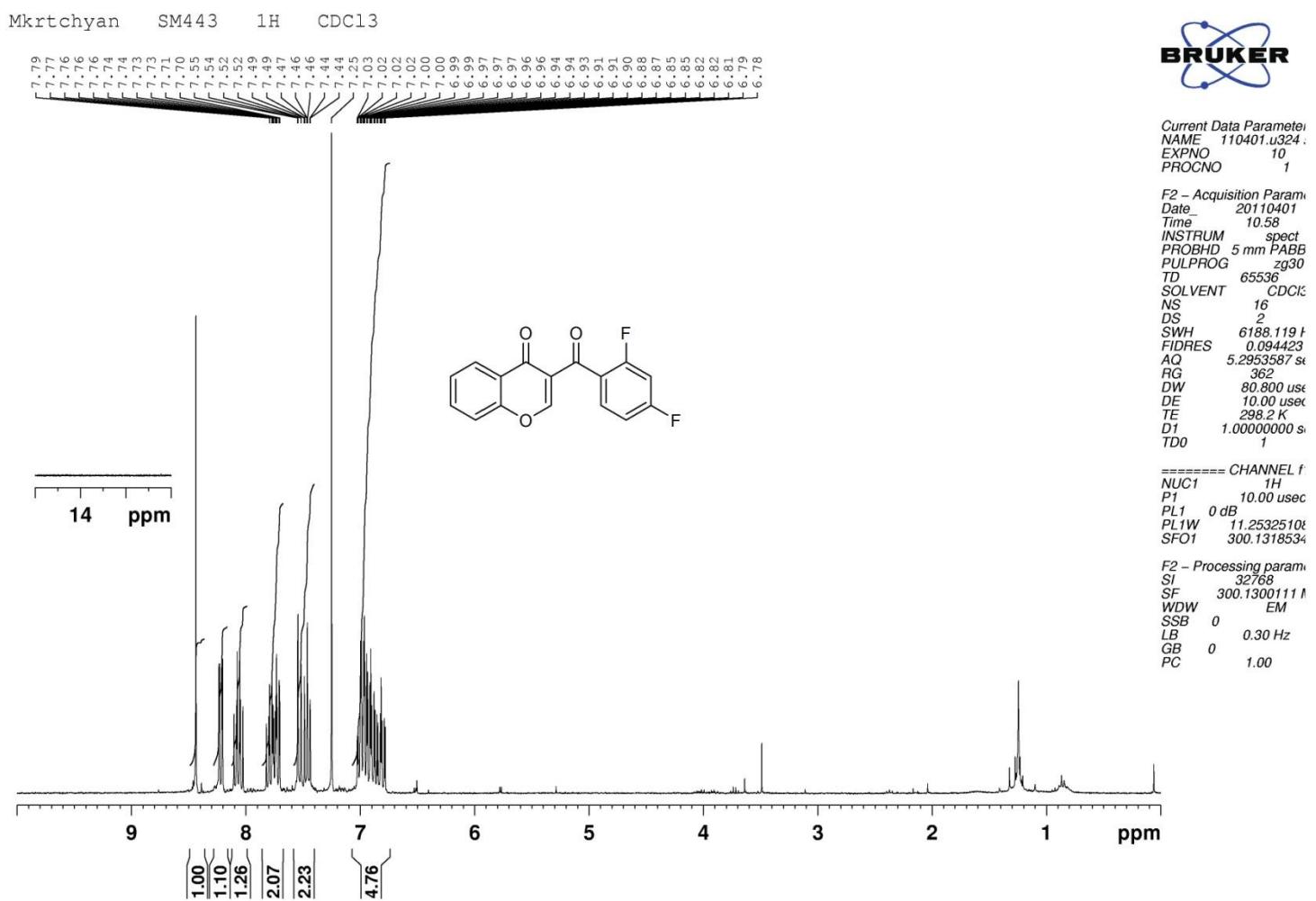
===== CHANNEL f
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.2532510*i*
SF01 300.131853*c*

F2 - Processing param
SI 32768
SF 300.1300130*l*
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

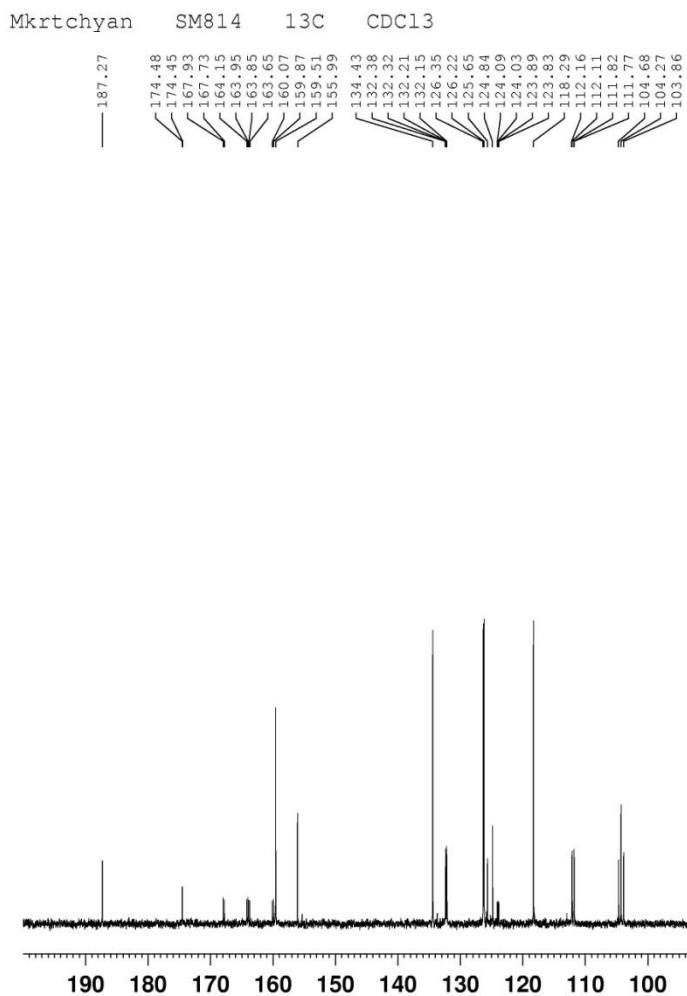
Compound 3g



Compound 3h



Compound 3h



Current Data Parameters
NAME 130718.206.s
EXPNO 10
PROCNO 1

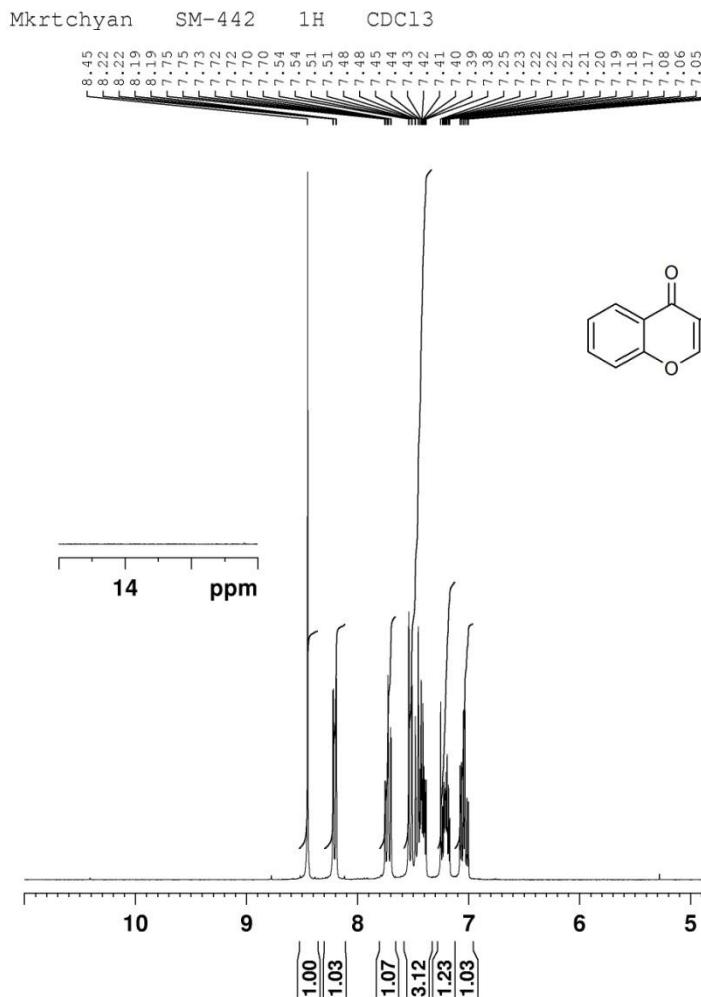
F2 - Acquisition Parameters
Date 20130718
Time 20.32
INSTRUM spect
PROBHD 5 mm PABt
PULPROG zgpg3
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000
FIDRES 0.228882
AQ 2.1845834 s
RG 2050
DW 33.333 us
DE 10.00 use
TE 298.1 K
D1 2.0000000 s
d11 0.03000000 s
DELTA 1.8999999
TD0 1

===== CHANNEL 1
NUC1 13C
P1 10.00 use
PL1 -1.00 dB
SFO1 62.9015280

===== CHANNEL 1
CPDPGR2 waltz1
NUC2 1H
PCPD2 70.00 u
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.131000

F2 - Processing parameters
SI 32768
SF 62.89524061
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 3i



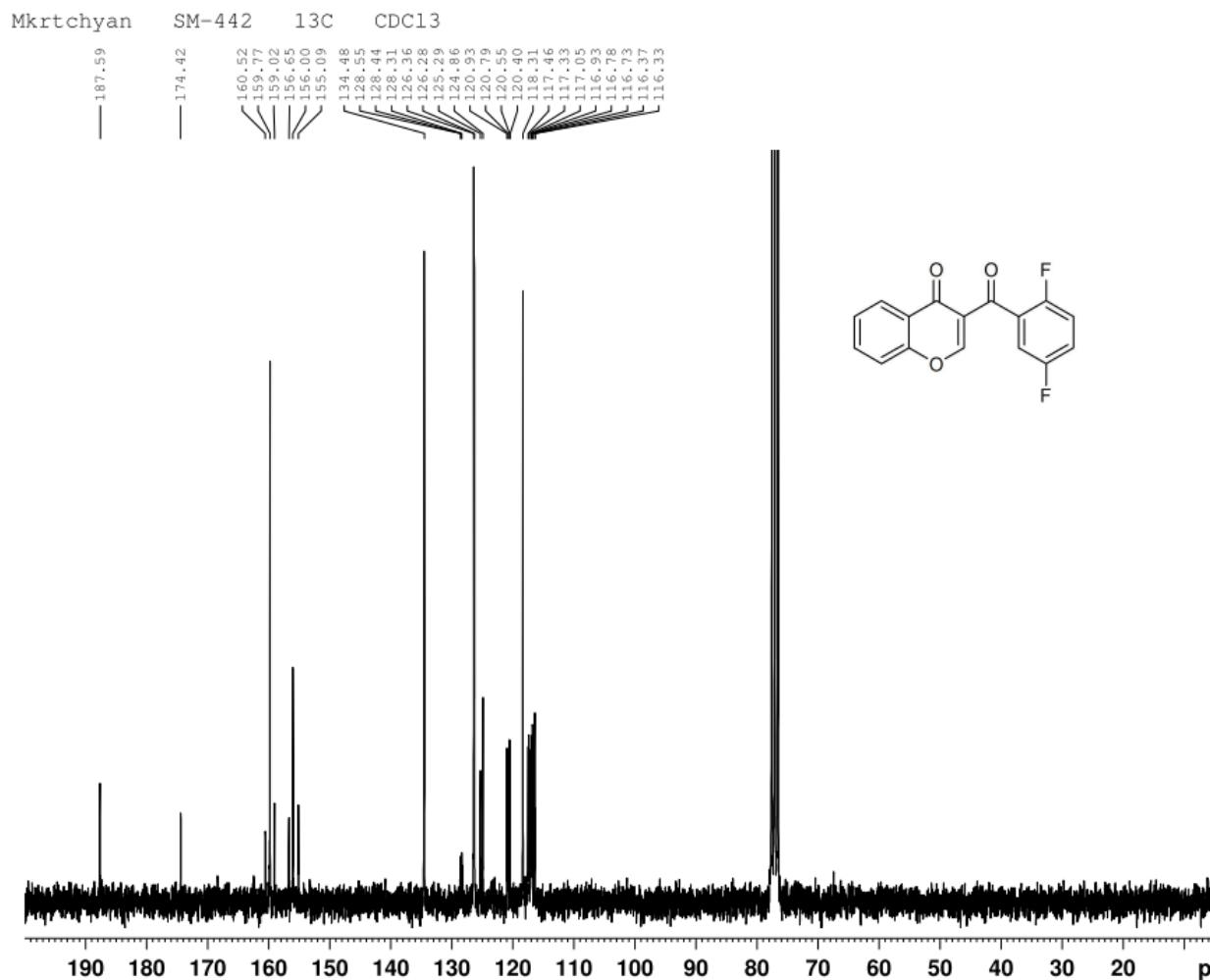
Current Data Parameters
NAME 110328.u313 sm 4
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20110328
Time 10.38
INSTRUM spect
PROBHD 5 mm PABBO Bl
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 1.0000000 sec
TD0 1

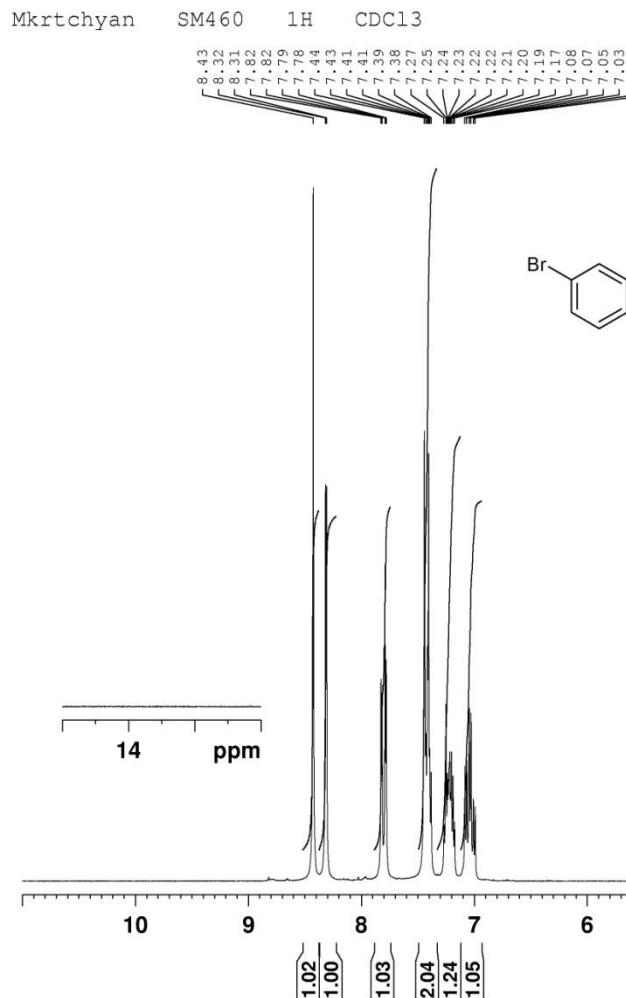
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 3i



Compound 3j



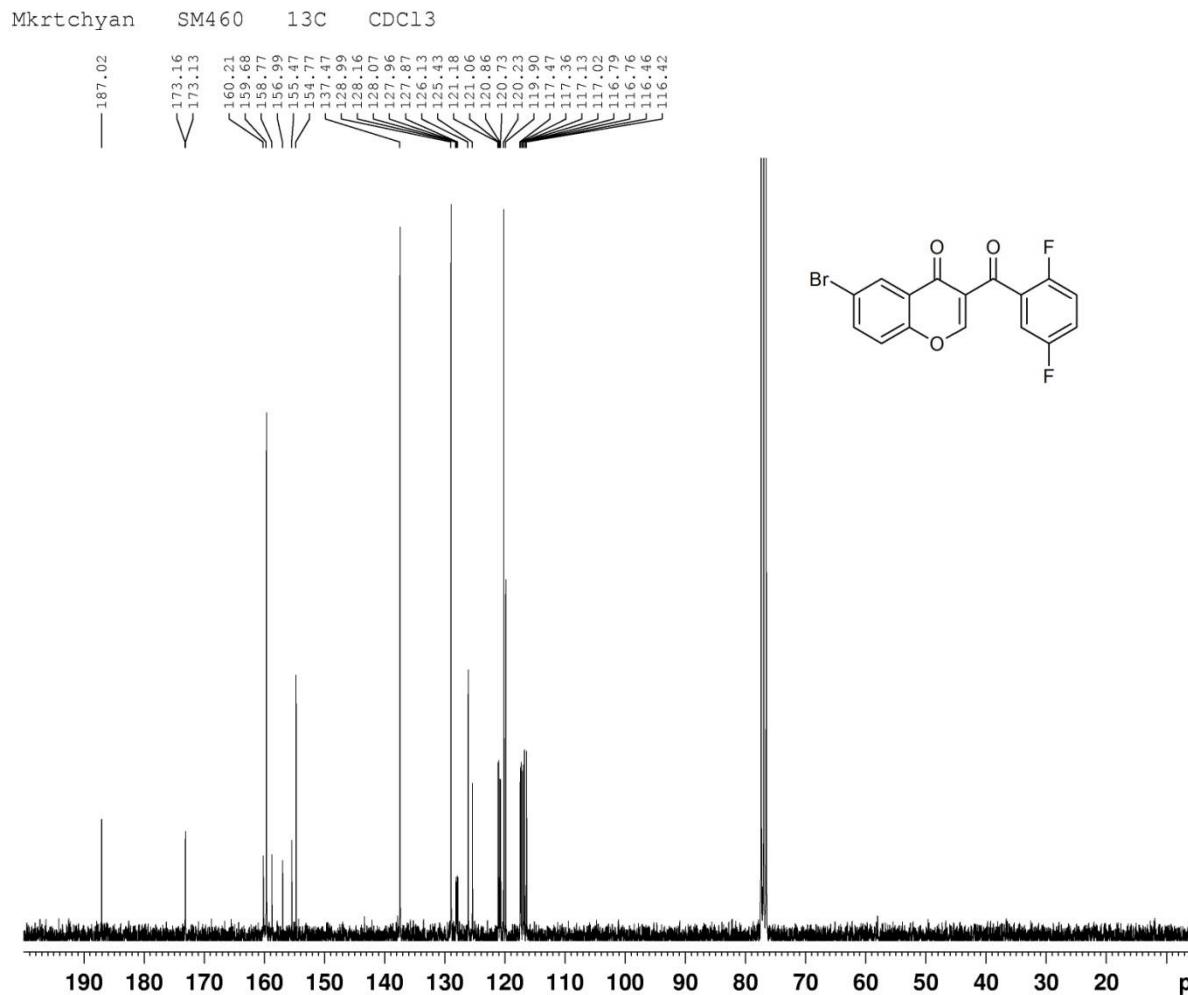
Current Data Parameters
 NAME 110406.213
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date 20110406
 Time 11.54
 INSTRUM spect
 PROBHD 5 mm PAB
 PULPROG zg3t
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5165.289
 FIDRES 0.07881t
 AQ 6.3439350s
 RG 575
 DW 96.800 us
 DE 10.00 us
 TE 298.0 K
 D1 1.0000000s
 TDO 1

===== CHANNEL
 NUC1 1H
 P1 10.00 use
 PL1 -2.50 dB
 SFO1 250.131544

F2 - Processing parameters
 SI 32768
 SF 250.130029
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Compound 3j



Current Data Parameters
NAME 110407.u344 sm 46
EXPNO 11
PROCNO 1

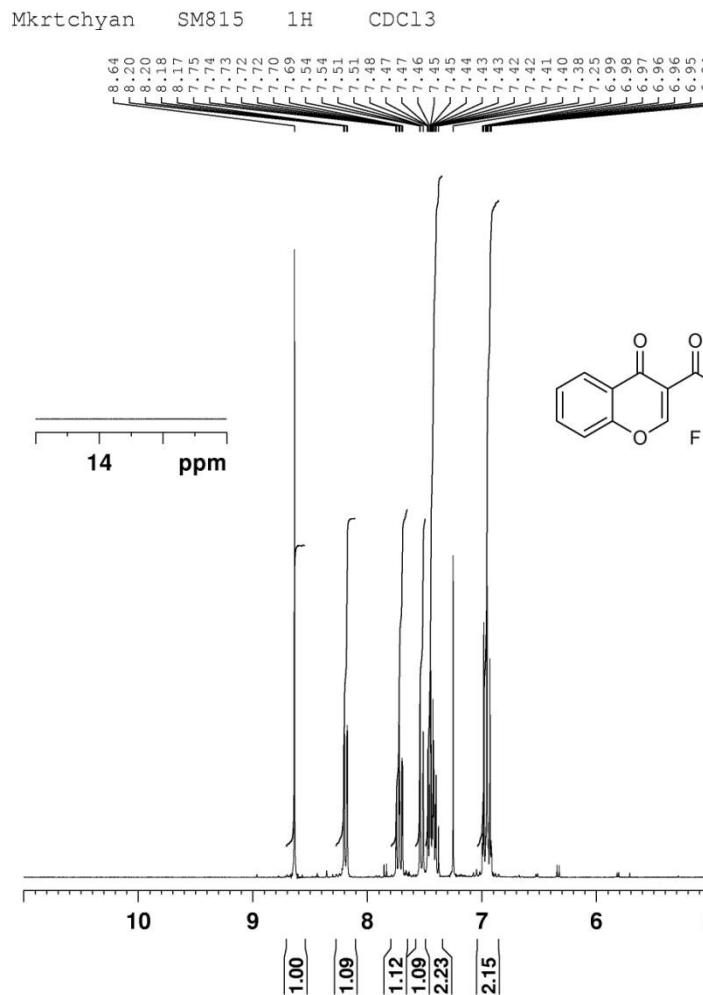
F2 - Acquisition Parameters
Date 20110408
Time 12:10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.4 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== 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 75.4677525 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 3k



Current Data Parameters
NAME 130717.u330 sn
EXPNO 10
PROCNO 1

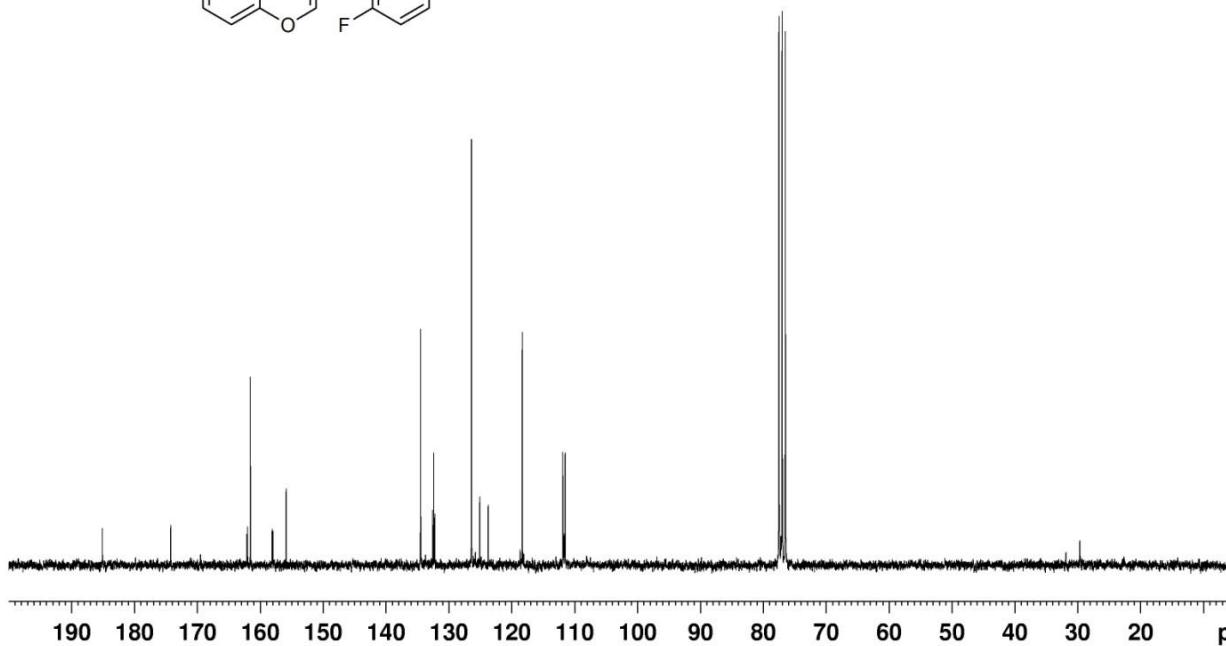
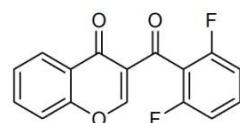
F2 - Acquisition Parameters
Date 20130717
Time 15.46
INSTRUM spect
PROBHD 5 mm PABBO
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 256
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 3k

Mkrtchyan SM815 13C CDC13



BRUKER

Current Data Parameters
NAME 130718.207 sr
EXPNO 10
PROCNO 1

F2 – Acquisition Param
Date 20130718
Time 22.09
INSTRUM spect
PROBHD 5 mm PABC
PULPROG zpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 15000.000 h
FIDRES 0.228882 f
AO 2.184583 se
RG 2050
DW 33.333 usec
DE 10.000 usec
TE 298.1 K
D1 2.0000000 se
d11 0.03000000 se
DELTA 1.89999998
TDO 1

===== CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SE01 62.90152801

```

===== CHANNEL f2
CPDPRG2      waltz16
NUC2          1H
PCPD2         70.00 us
PL12          15.00 dB
PL13          15.00 dB
PL2           -2.50 dB
SFO2          250,1310005

```

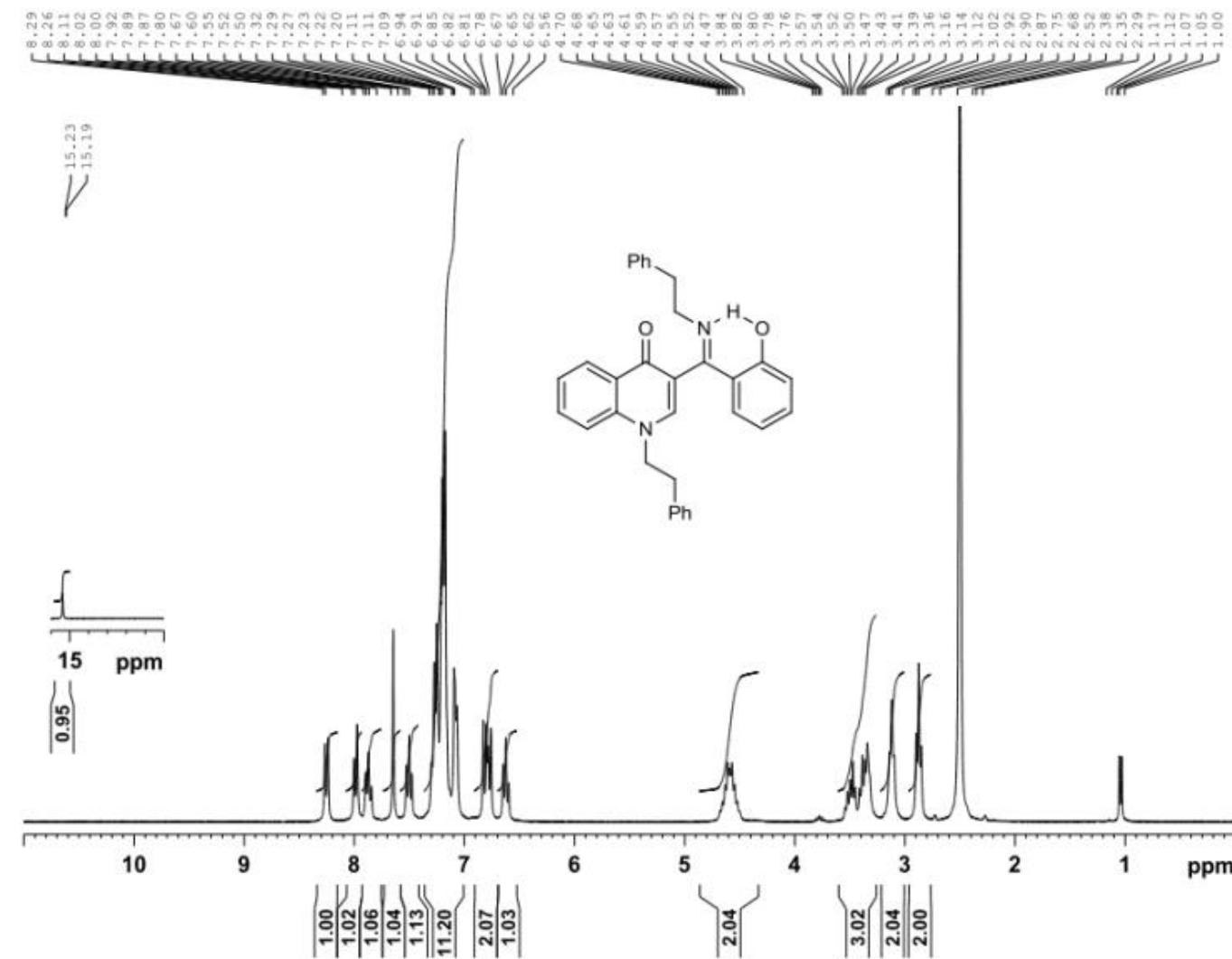
```

F2 - Processing parameters
SI           32768
SF          62.8952402 MI
WDW          EM
SSB          0
LB           1.00 Hz
GB          0
PC          1.40

```

Compound 4a

Mkrtchyan SM395 1H DMSO



BRUKER

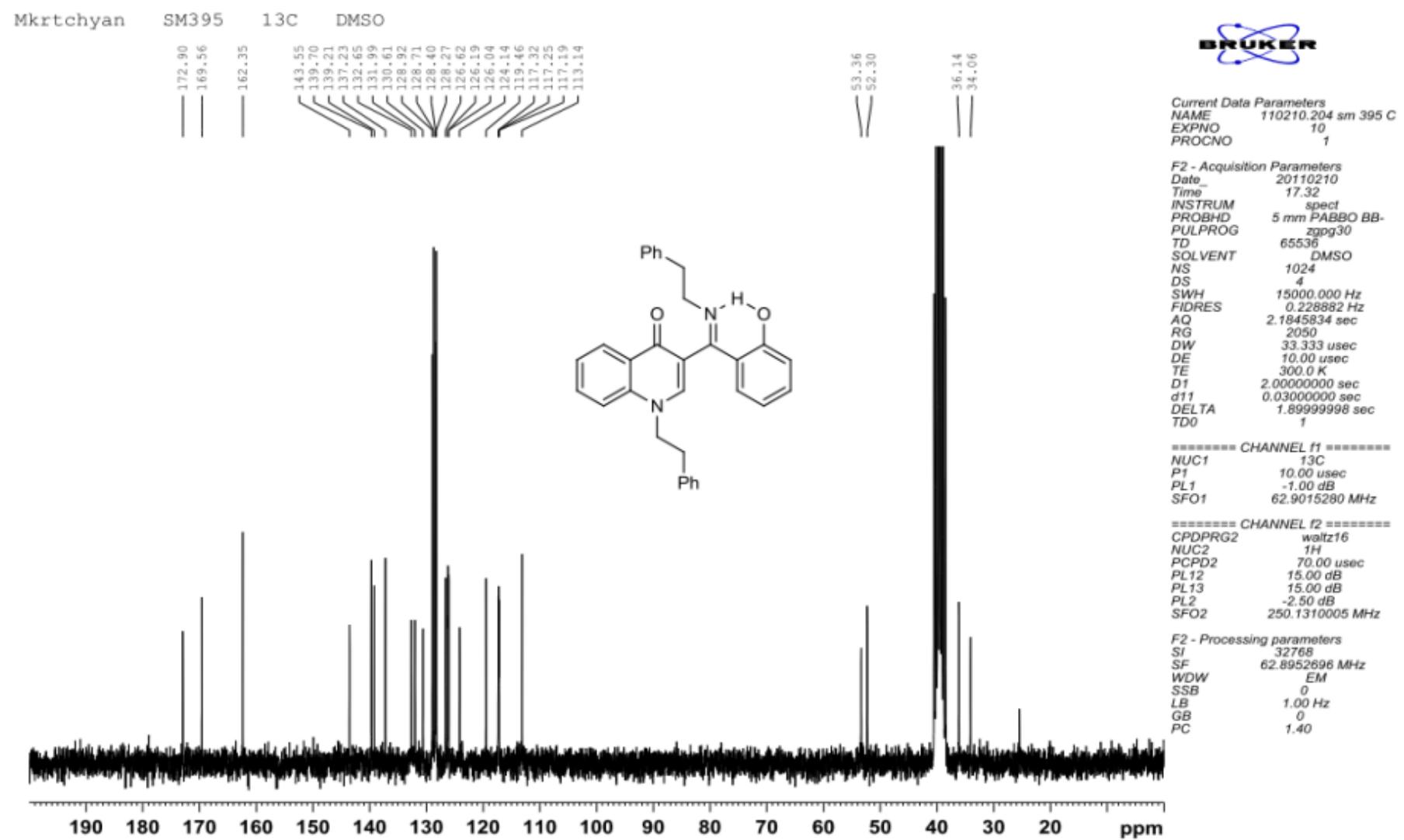
Current Data Parameters
NAME 110208.u334 sm 395
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
 Date 20110208
 Time 15.26
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 1.0000000 sec
TD0 1

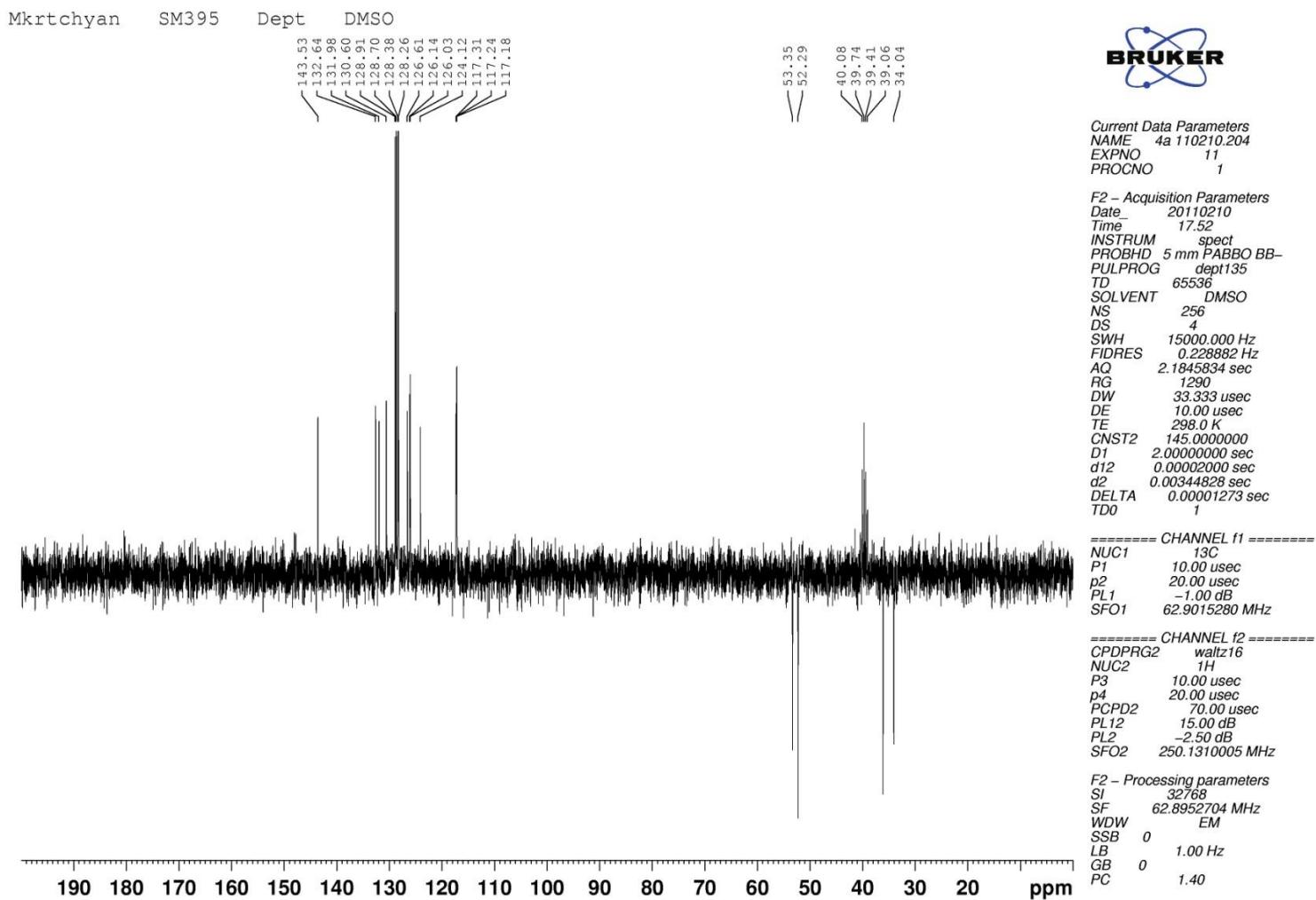
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHZ

F2 - Processing parameters
 SI 32768
 SF 300.1300071 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

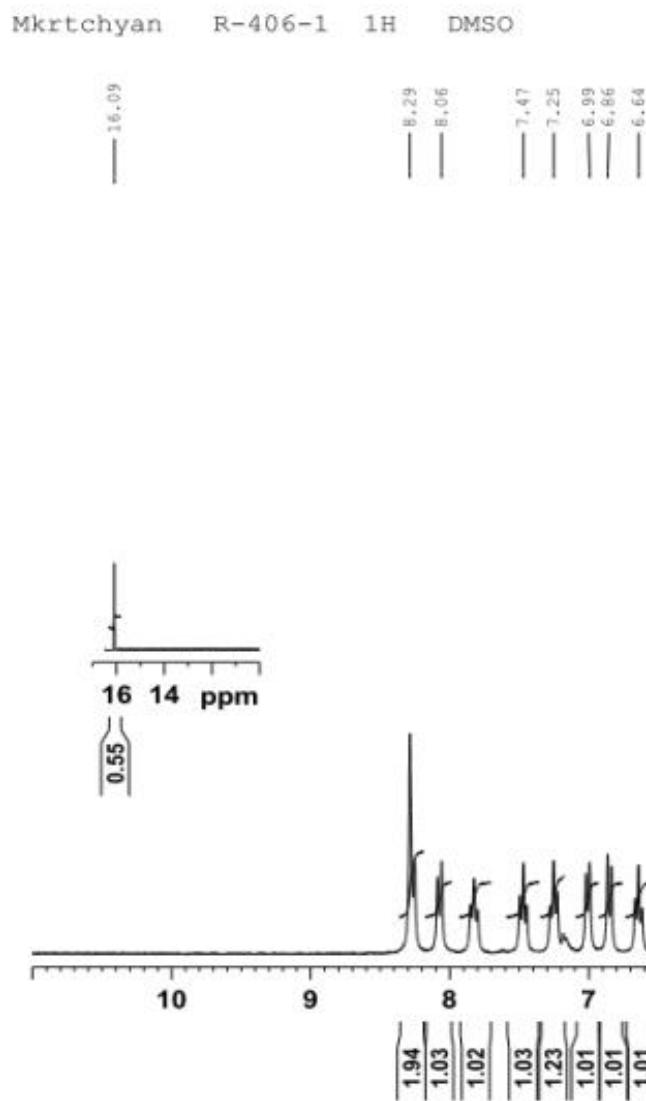
Compound 4a



Compound 4a



Compound 4b



Compound 4b



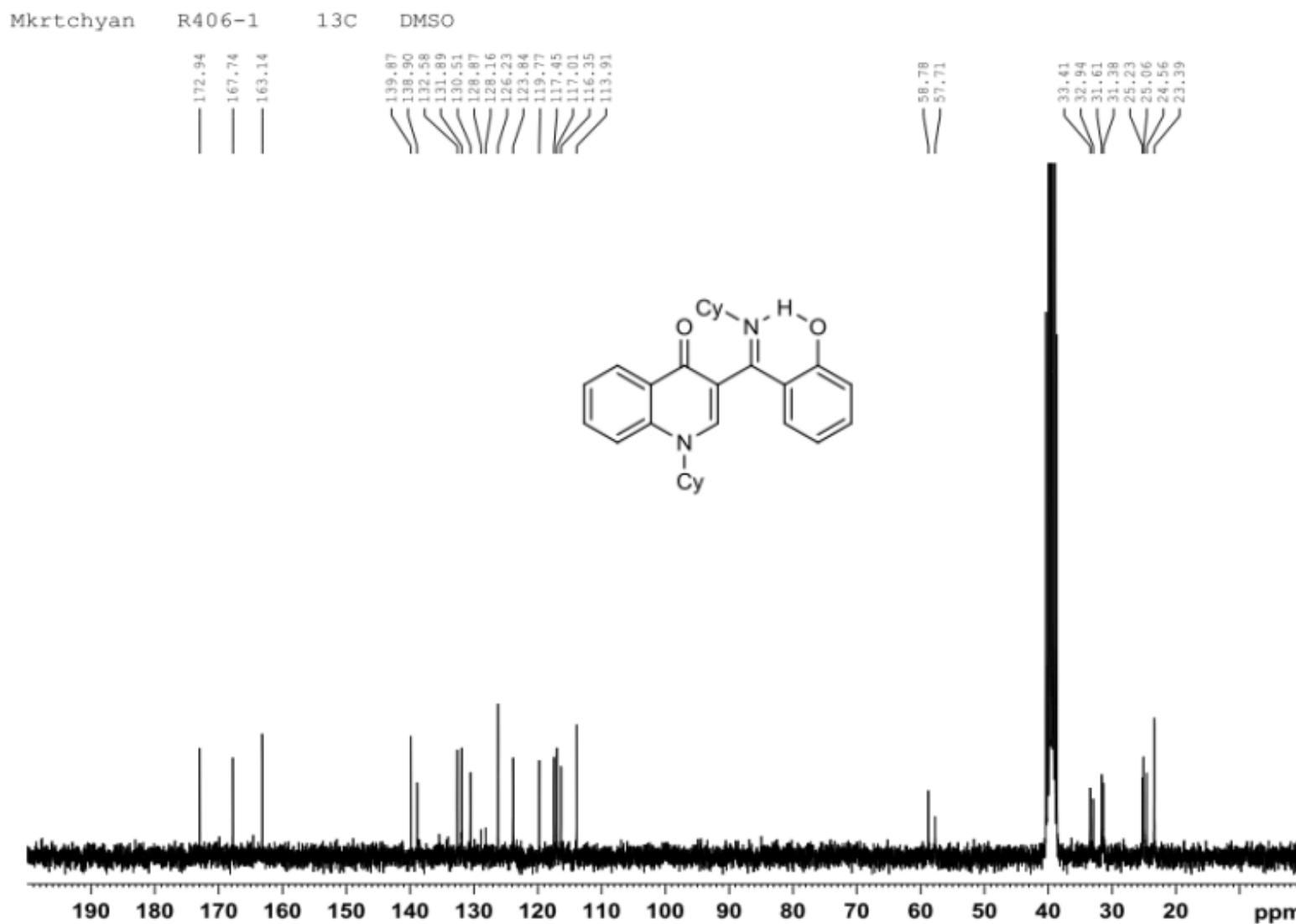
Current Data Parameters
NAME 110307.u332 sm 406
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110307
Time_ 14.13
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 80.000 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 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

Compound 4b



Current Data Parameters
 NAME 110309.u315 sm 406 C
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110309
 Time 18.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1280
 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
 TDO 1

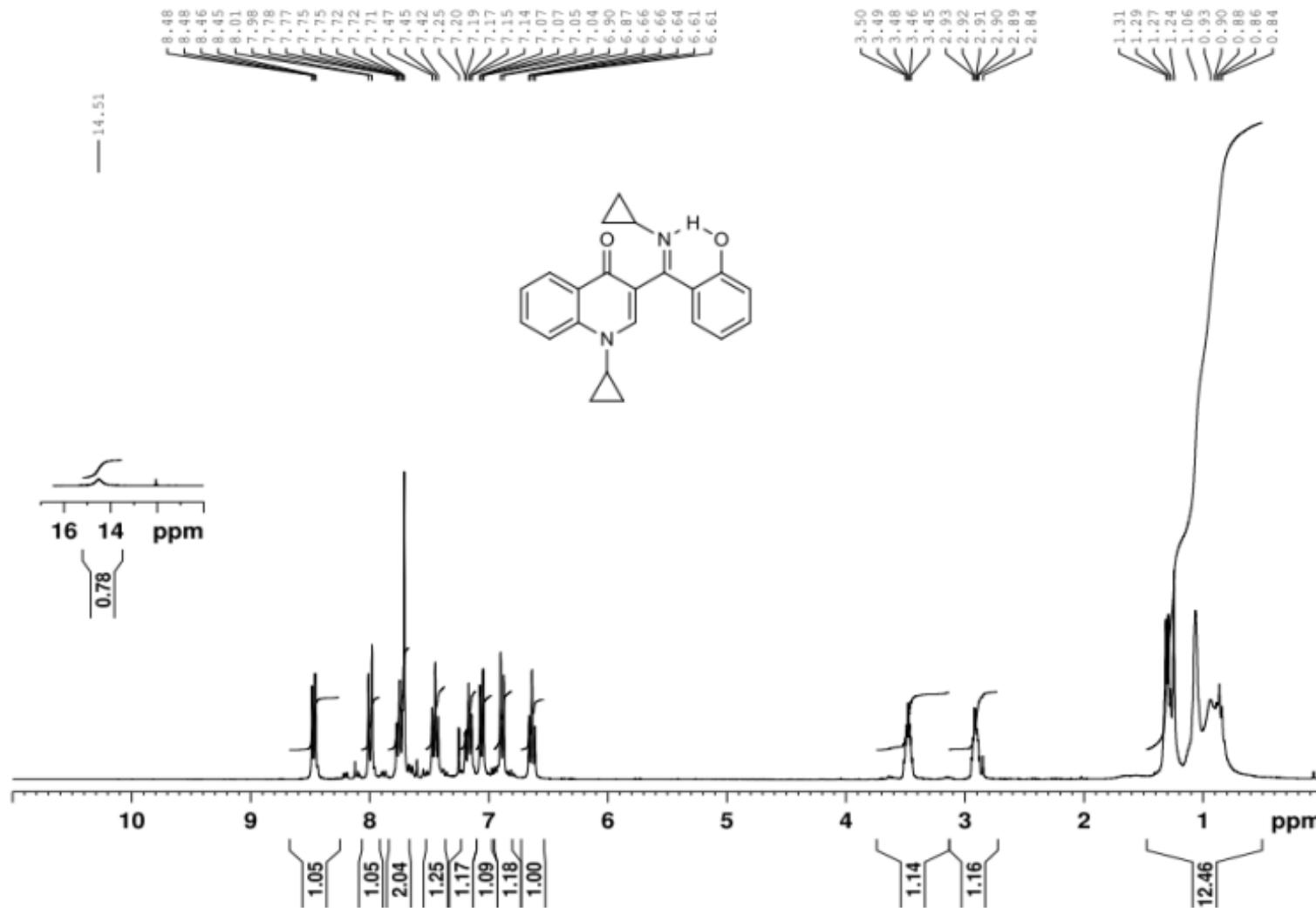
===== CHANNEL f1 ======
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 PL1W 33.25691986 W
 SFO1 75.4752953 MHz

===== CHANNEL f2 ======
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 72.00 usec
 PL2 0.00 dB
 PL12 17.00 dB
 PL13 17.00 dB
 PL2W 11.22453187 W
 PL12W 0.22453187 W
 PL13W 0.22453187 W
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4681463 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Compound 4c

Mkrtchyan SM-412-R 1H CDCl_3



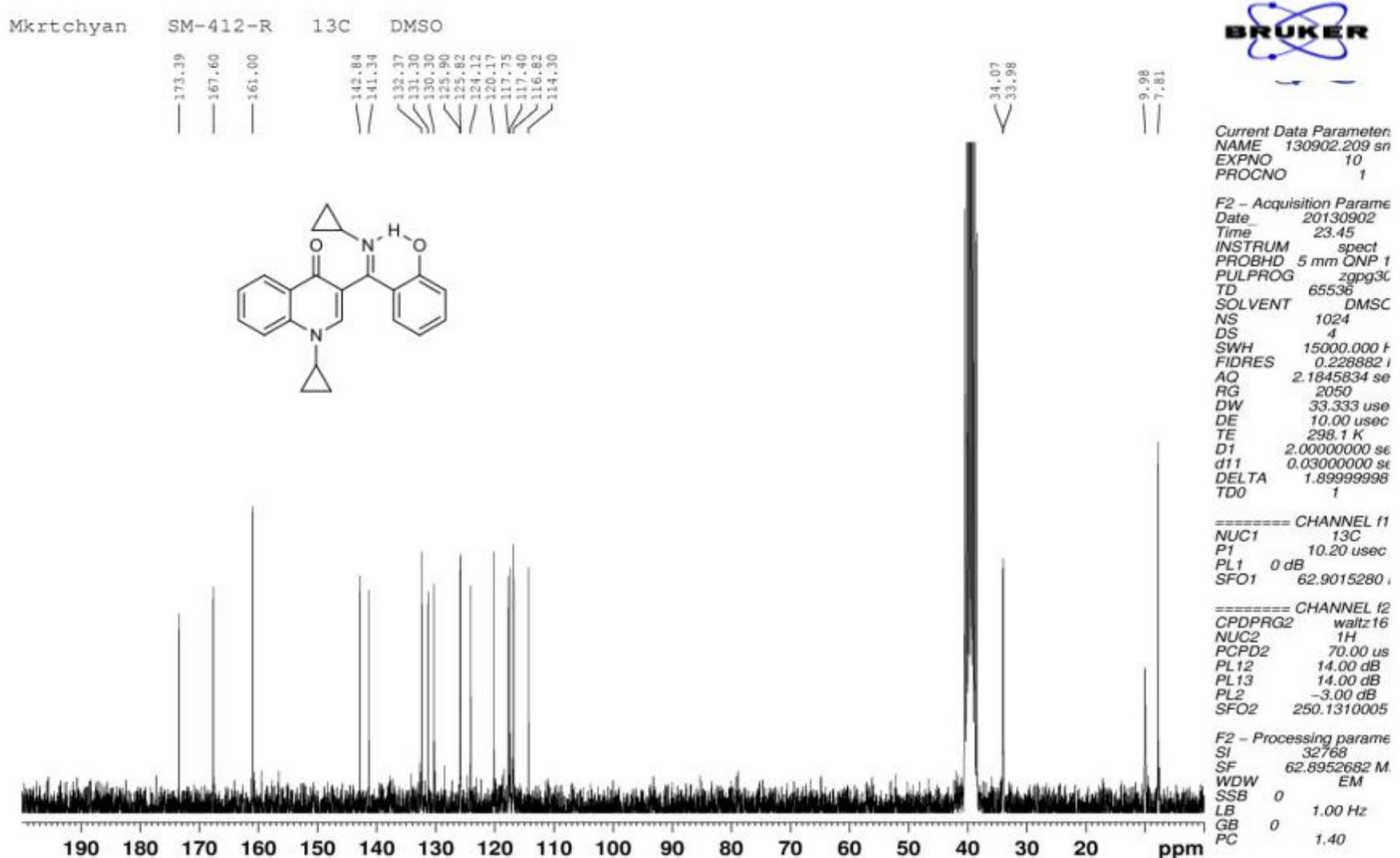
Current Data Parameters
NAME 110307.u333 sm
EXPNO 10
PROCNO 1

F2 - Acquisition Parameter
Date 20110307
Time 14.19
INSTRUM spect
PROBHD 5 mm PABBO.
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 50.8
DW 80.000 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

----- CHANNEL f1 =
NUC1 ^1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 V
SFO1 300.1318534 M

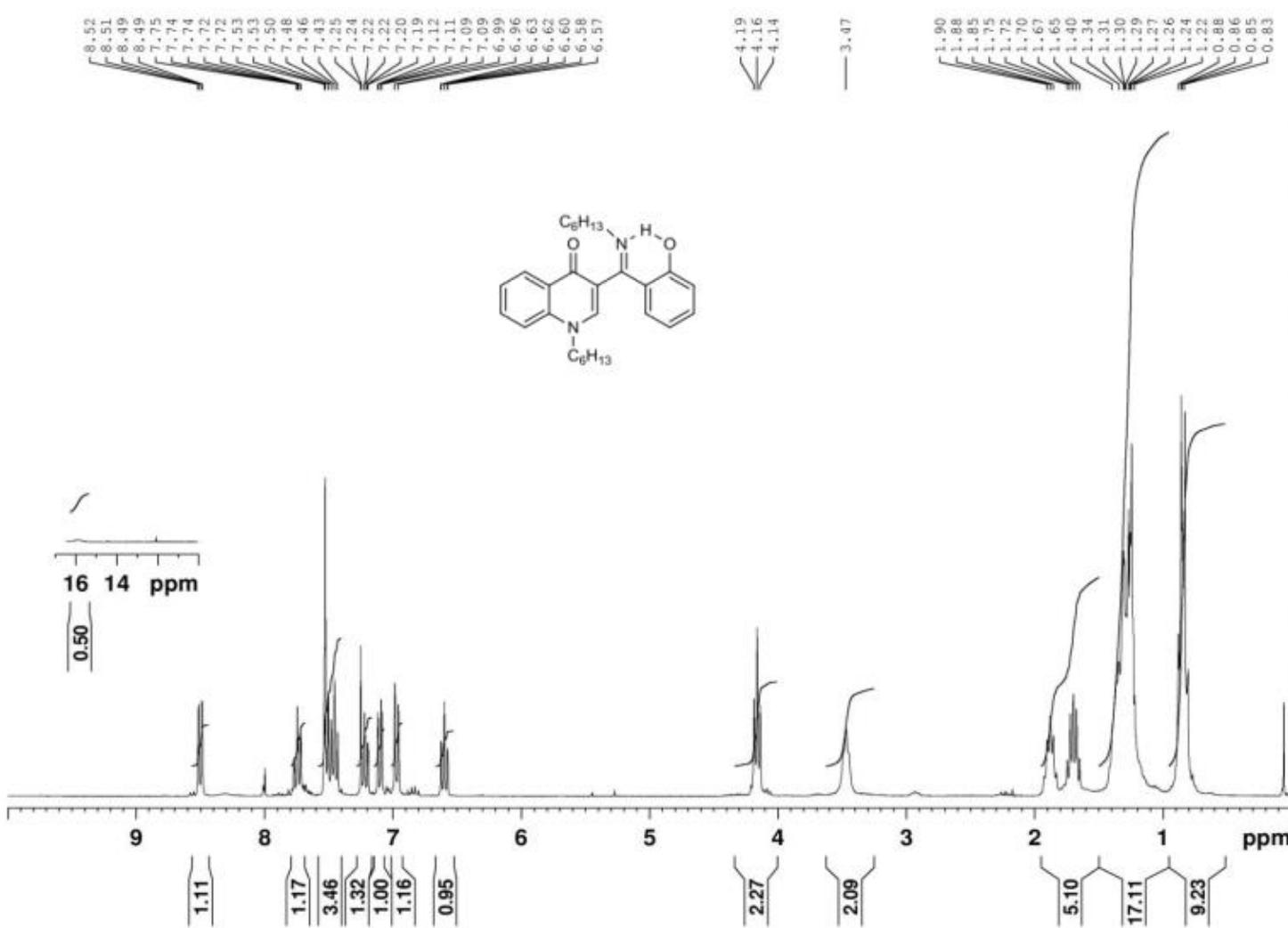
F2 - Processing parameter
SI 32768
SF 300.1300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 4c



Compound 4d

Mkrtchyan SM784 1H CDC13



Current Data Parameters
NAME_ 130523_u301.
EXPNO_ 10
PROCNO_ 1

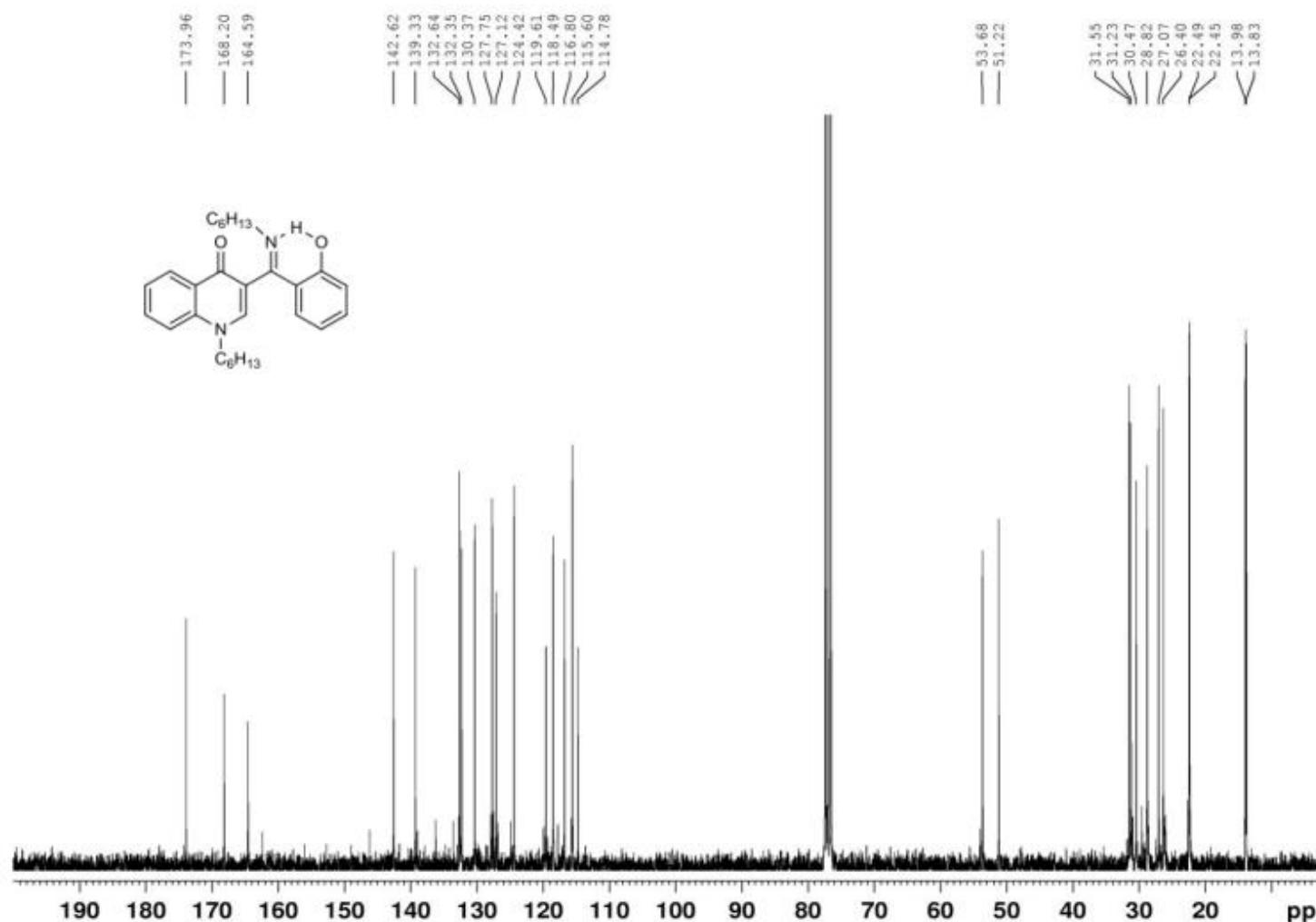
F2 - Acquisition Parameters
Date_ 20130523
Time_ 8.56
INSTRUM spect
PROBHD 5 mm PABP
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 6188.119 F
FIDRES 0.094423
AQ 5.2953587 s
RG 50.8
DW 80.000 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 s
TD0 1

===== CHANNEL f
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.2532510 t
SF01 300.1318534

F2 - Processing parameters
SI 32768
SF 300.1300131 f
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 4d

Mkrtchyan SM784 13C CDC13



Current Data Parameter
NAME 130523.u301:
EXPNO 12
PROCNO 1

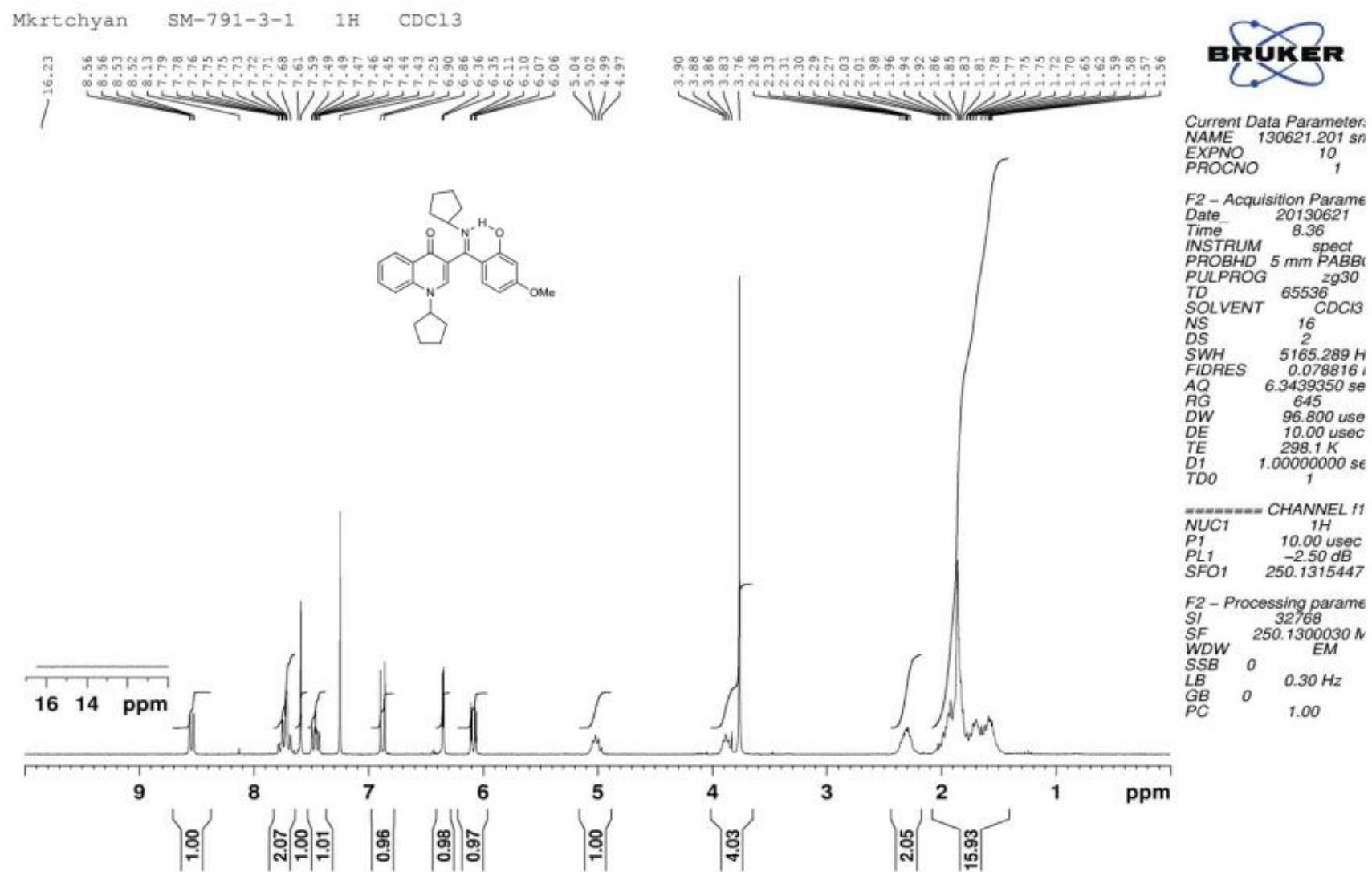
F2 - Acquisition Param:
Date 20130523
Time 18.56
INSTRUM spect
PROBHD 5 mm PABB
PULPROG zgpg3t
TD 65536
SOLVENT CDCl3
NS 800
DS 4
SWH 18028.846 Hz
FIDRES 0.275098
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 st
D11 0.03000000 s
TDO 1

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

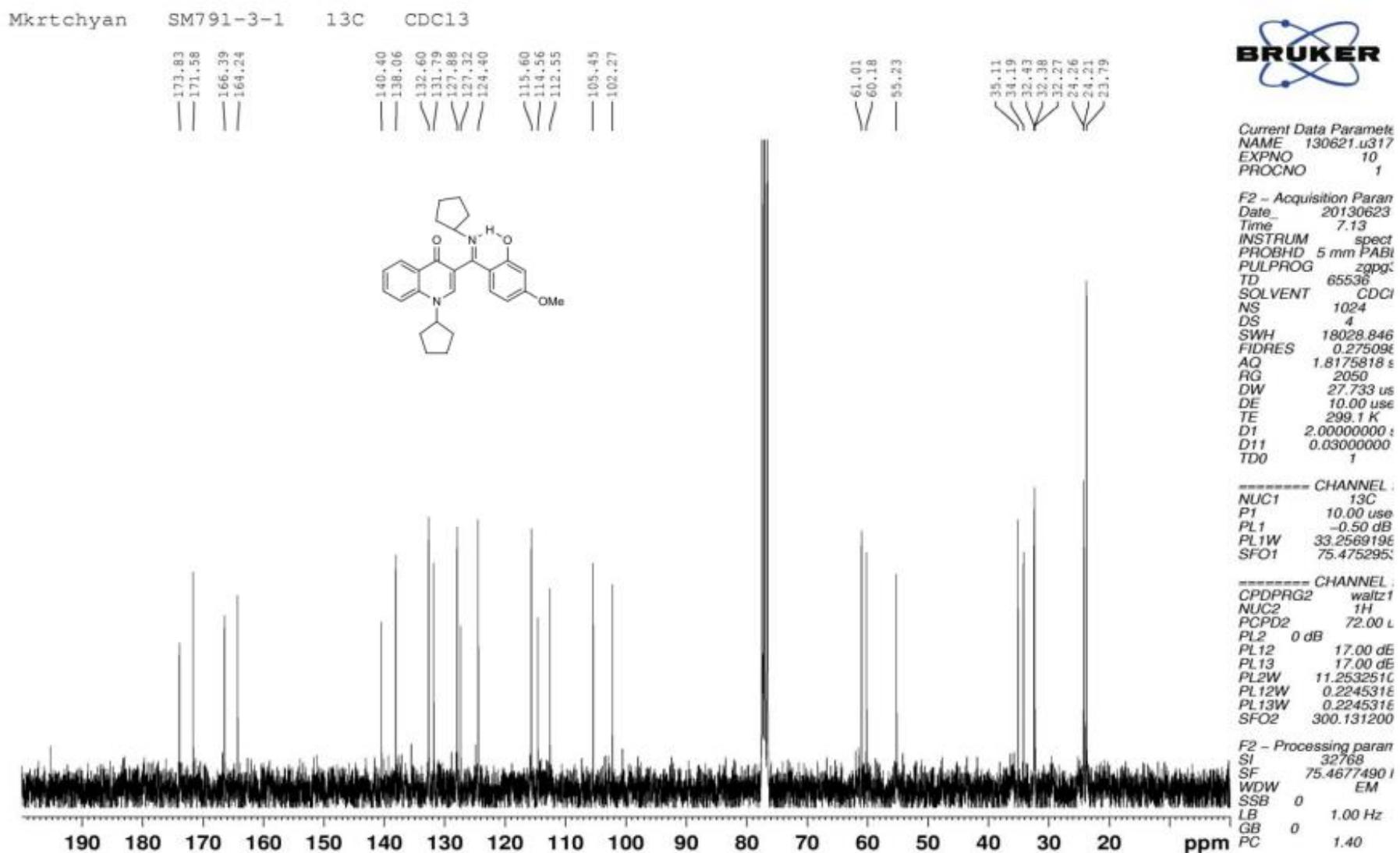
----- CHANNEL f2:
CPDPGR2 waltz16
NUC2 1H
PCPD2 72.00 us
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325106
PL12W 0.22453187
PL13W 0.22453187
SFO2 300.1312005

F2 - Processing param:
SI 32768
SF 75.4677542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 4e

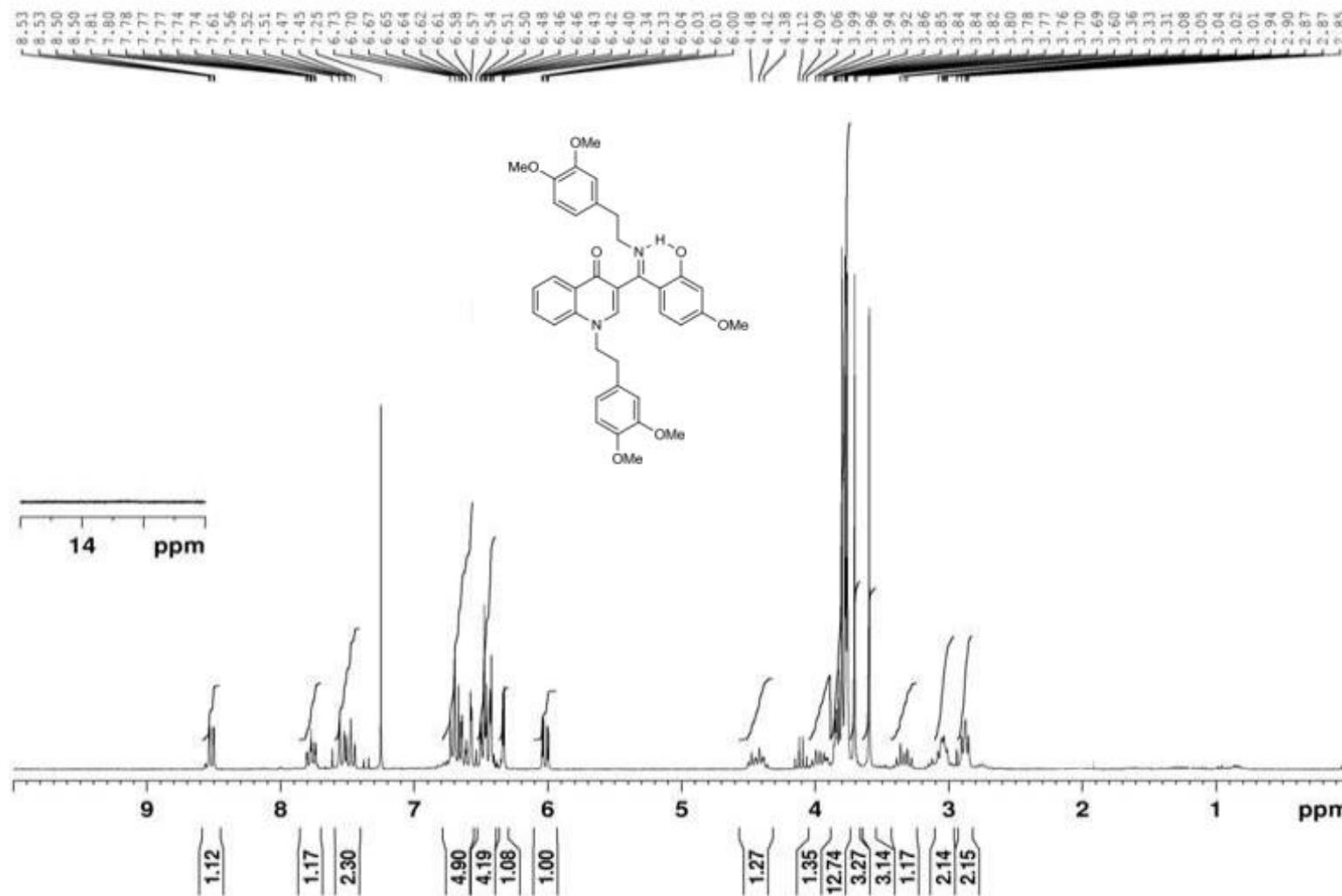


Compound 4e



Compound 4f

Mkrtchyan SM792-3 1H CDCl₃



Current Data Parameters
NAME 130619.2011
EXPNO 10
PROCNO 1

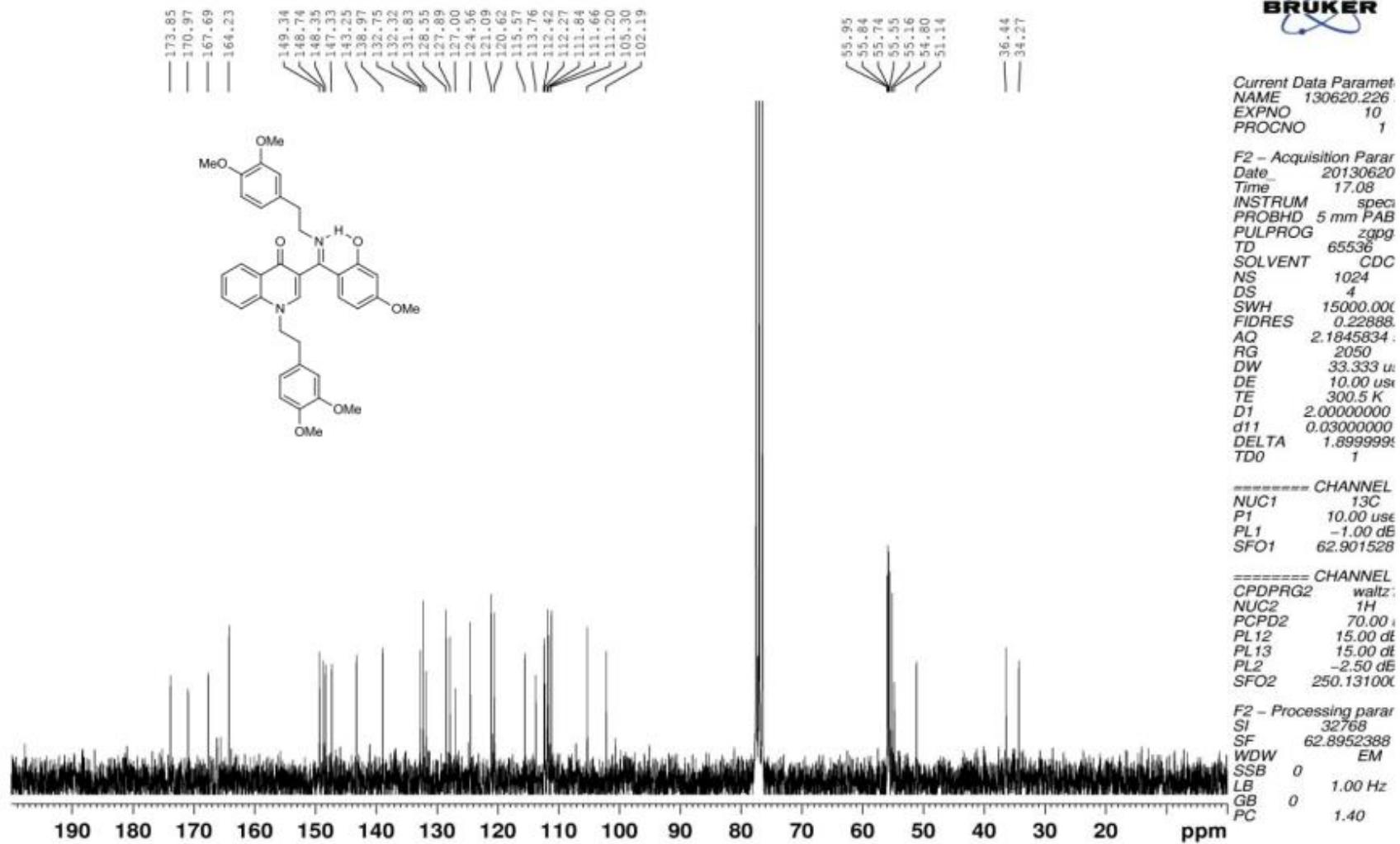
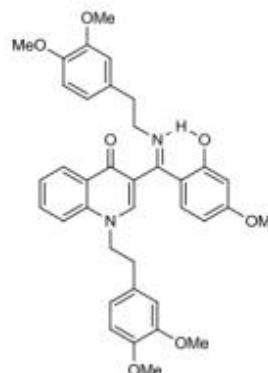
F2 - Acquisition Parans
Date 20130619
Time 9.56
INSTRUM spect
PROBHD 5 mm PAB�
PULPROG zg3t
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 5165.289
FIDRES 0.07881t
AQ 6.3439350 :
RG 645
DW 96.800 us
DE 10.00 us
TE 298.1 K
D1 1.0000000 :
TD0 1

===== CHANNEL
NUC1 1H
P1 10.00 us
PL1 -2.50 dB
SFO1 250.131544

F2 - Processing parans
SI 32768
SF 250.1300030
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

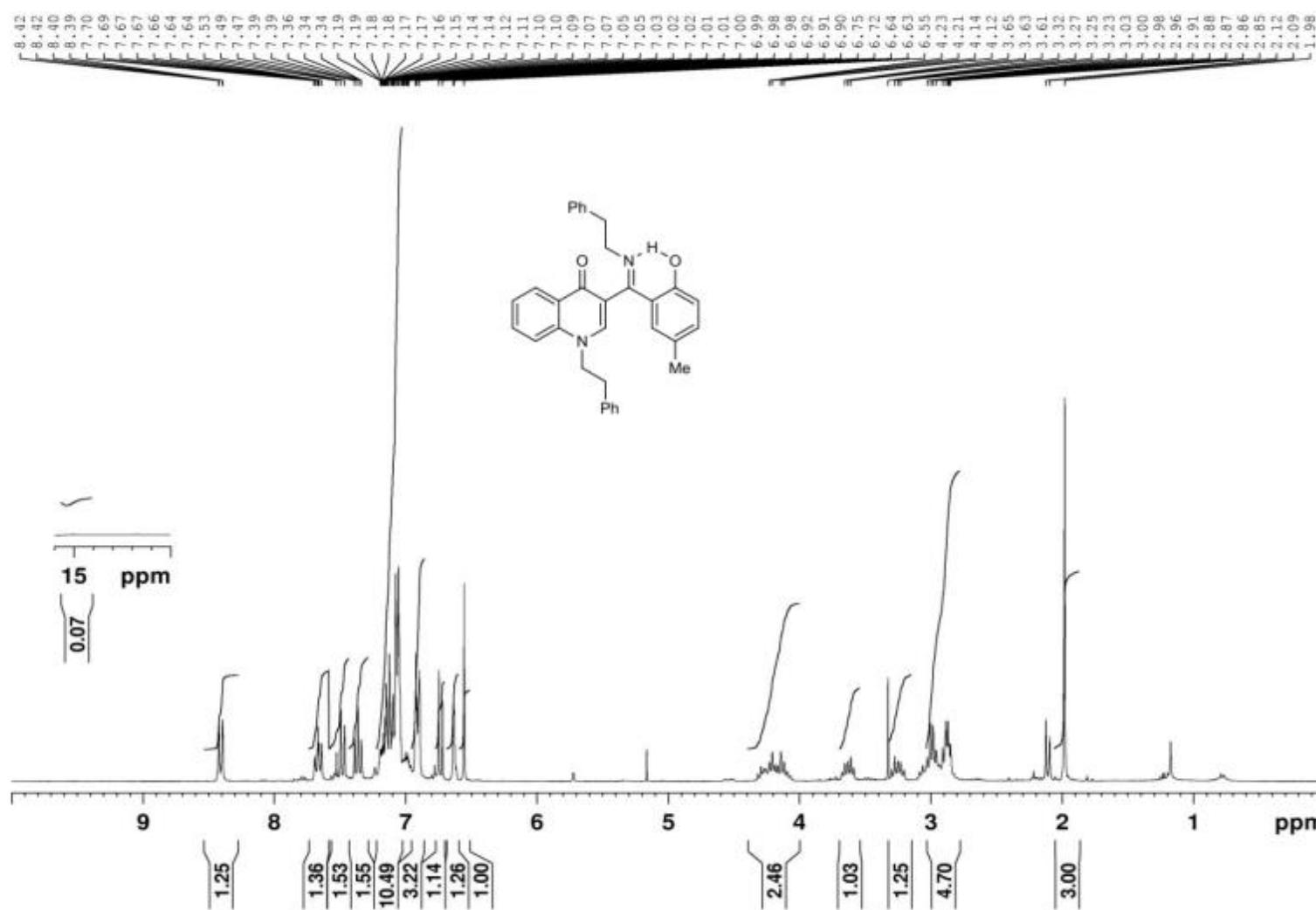
Compound 4f

Mkrtchyan SM792-3 13C CDC13



Compound 4g

Mkrtyan SM781 1H CDC13



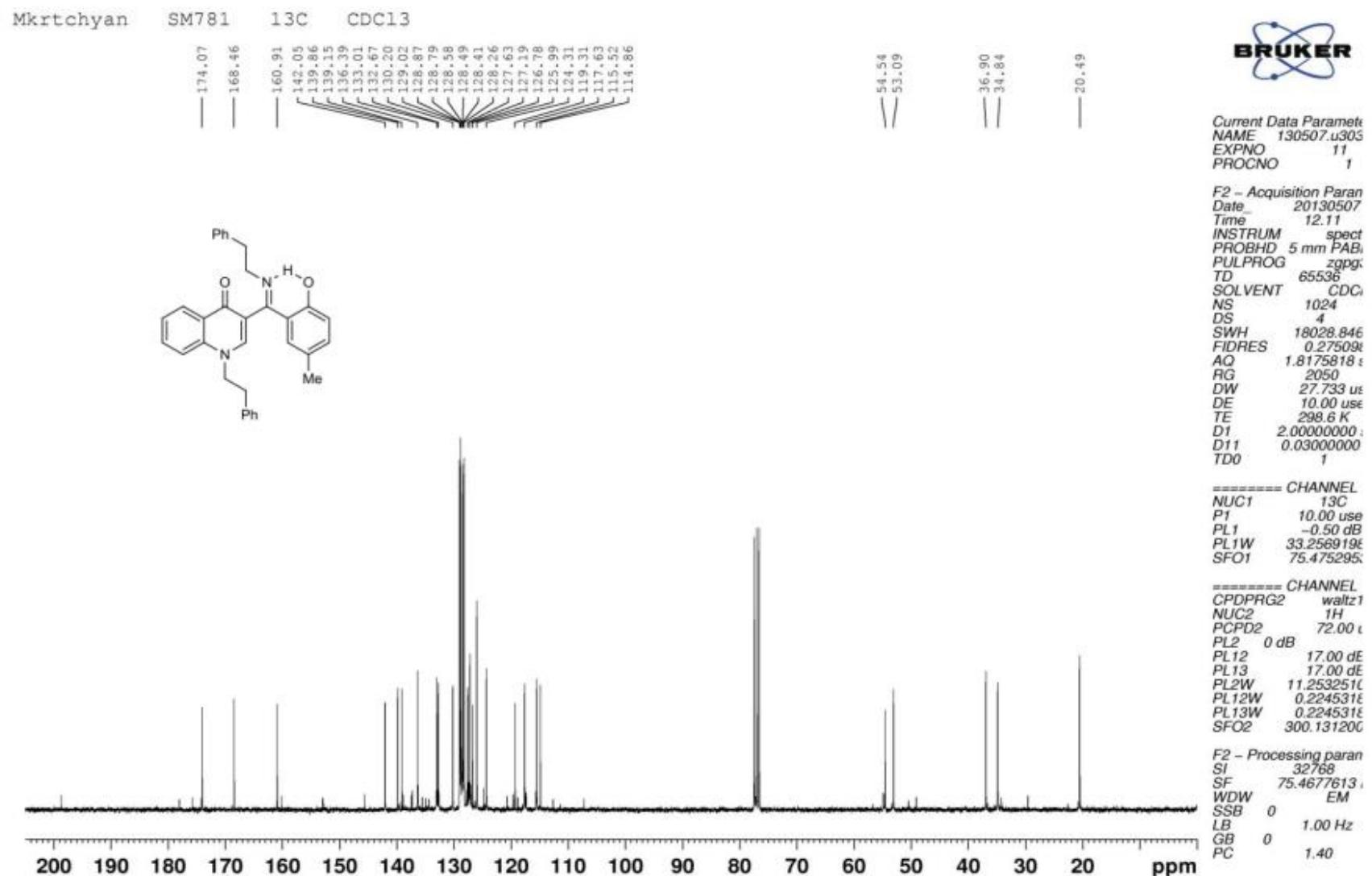
Current Data Parameters
NAME 130507.u303 :
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20130507
Time 8.42
INSTRUM spect
PROBHD 5 mm PABBA
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423
AQ 5.2953587 sec
RG 32
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 s
TDO 1

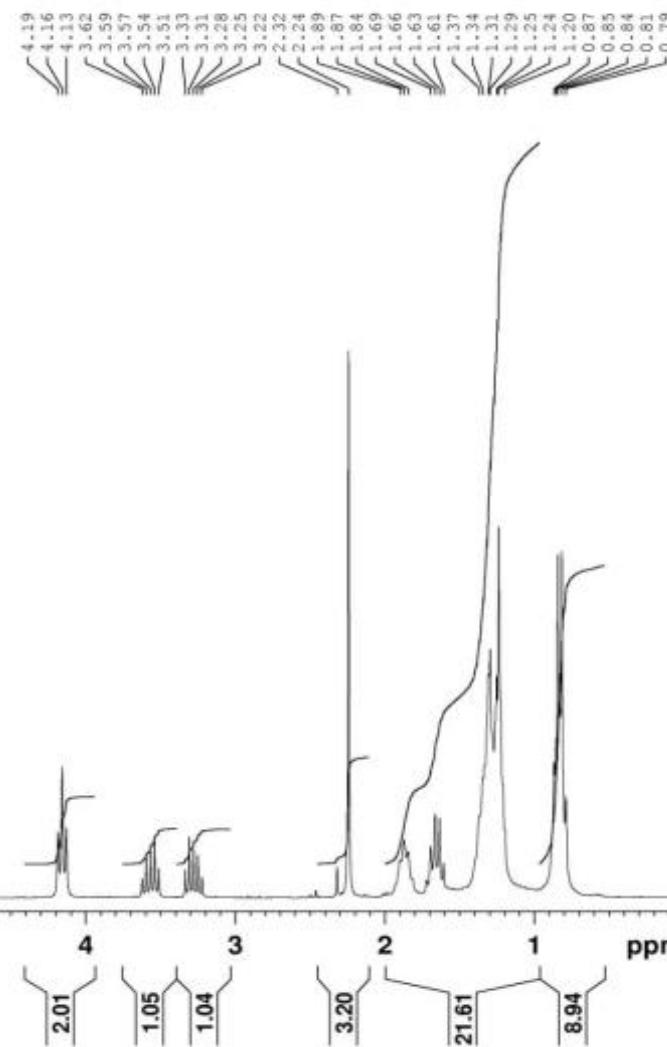
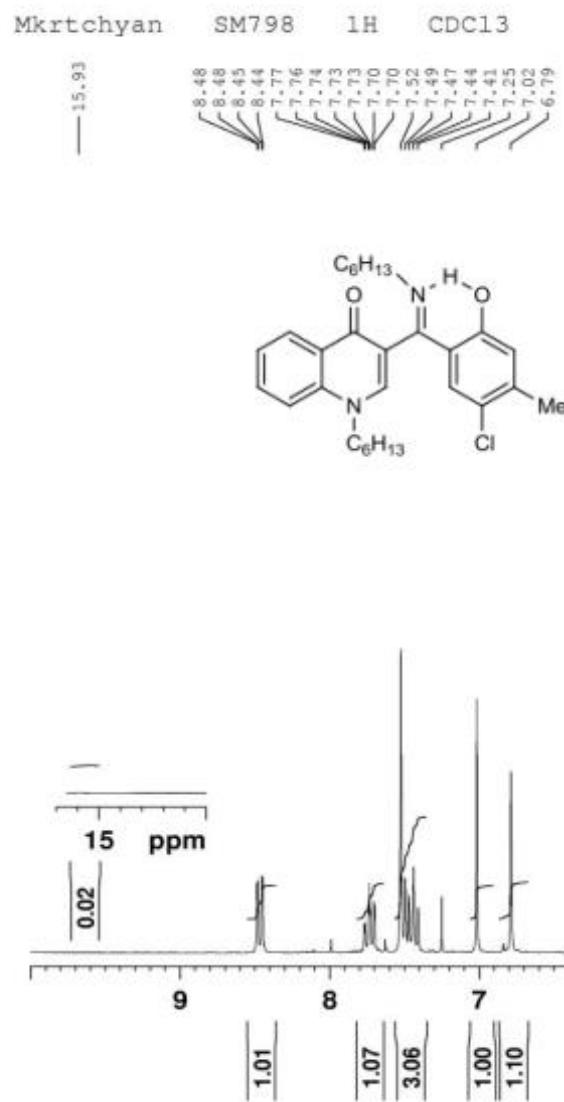
CHANNEL f
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108
SFO1 300.1318534

F2 - Processing parameters
SI 32768
SF 300.1300412 Hz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 4g



Compound 4h



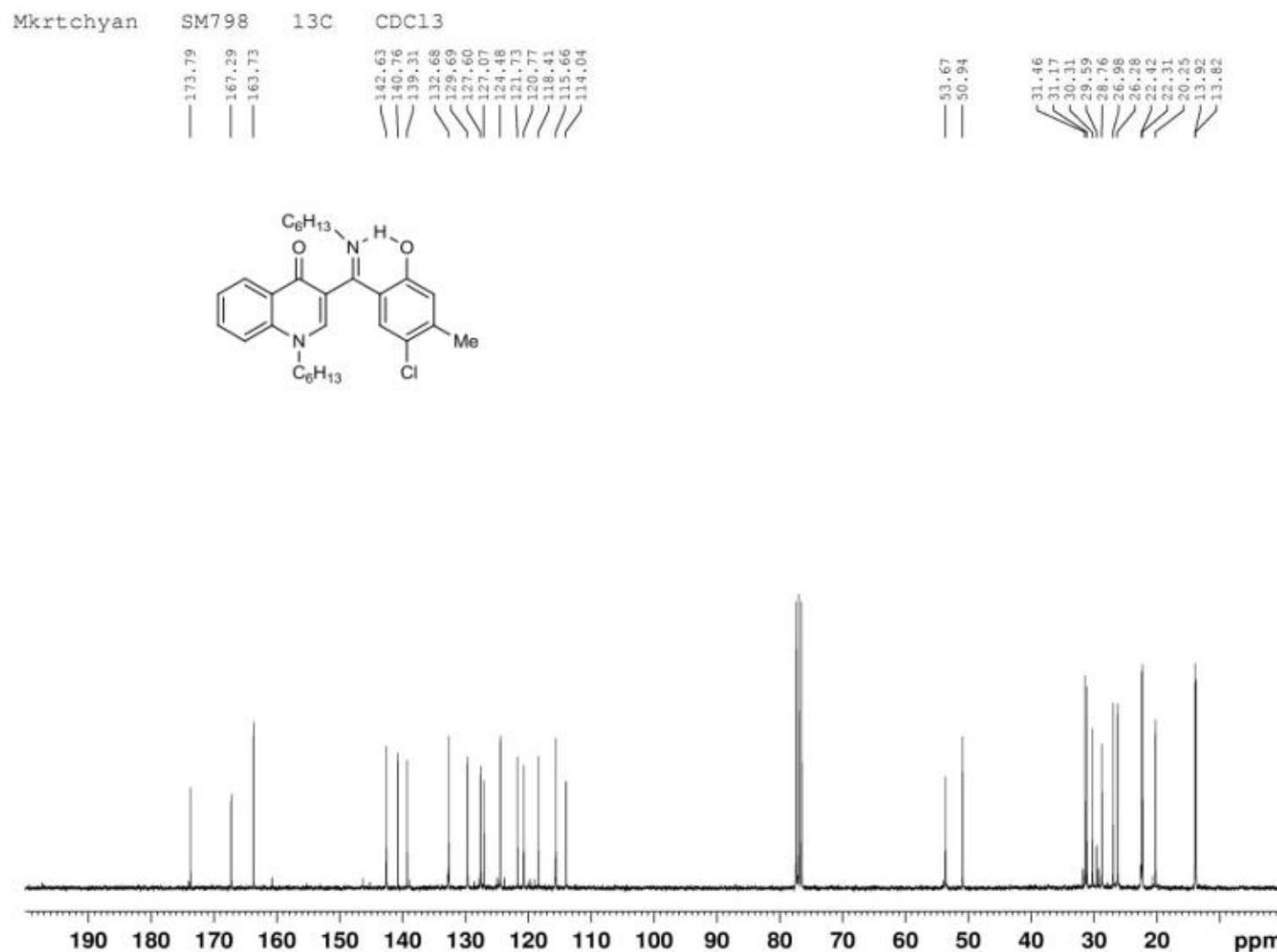
Current Data Param
NAME 130620.212
EXPNO 10
PROCNO 1

F2 - Acquisition Para
Date 2013062
Time 12.34
INSTRUM spect
PROBHD 5 mm PAI
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5165.28
FIDRES 0.0788
AQ 6.343935C
RG 161
DW 96.800 μ s
DE 10.00 μ s
TE 298.2 K
D1 1.0000000C
TD0 1

===== CHANNEL
NUC1 1H
P1 10.00 us
PL1 -2.50 d
SFO1 250.13154

F2 - Processing para
SI 32768
SF 250.130002
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 4h



Current Data Parameters
NAME 130621.u316.s
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20130623
Time 5.44
INSTRUM spect
PROBHD 5 mm PABBC
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 t
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 299.1 K
D1 2.00000000 se
D11 0.03000000 se
TD0 1

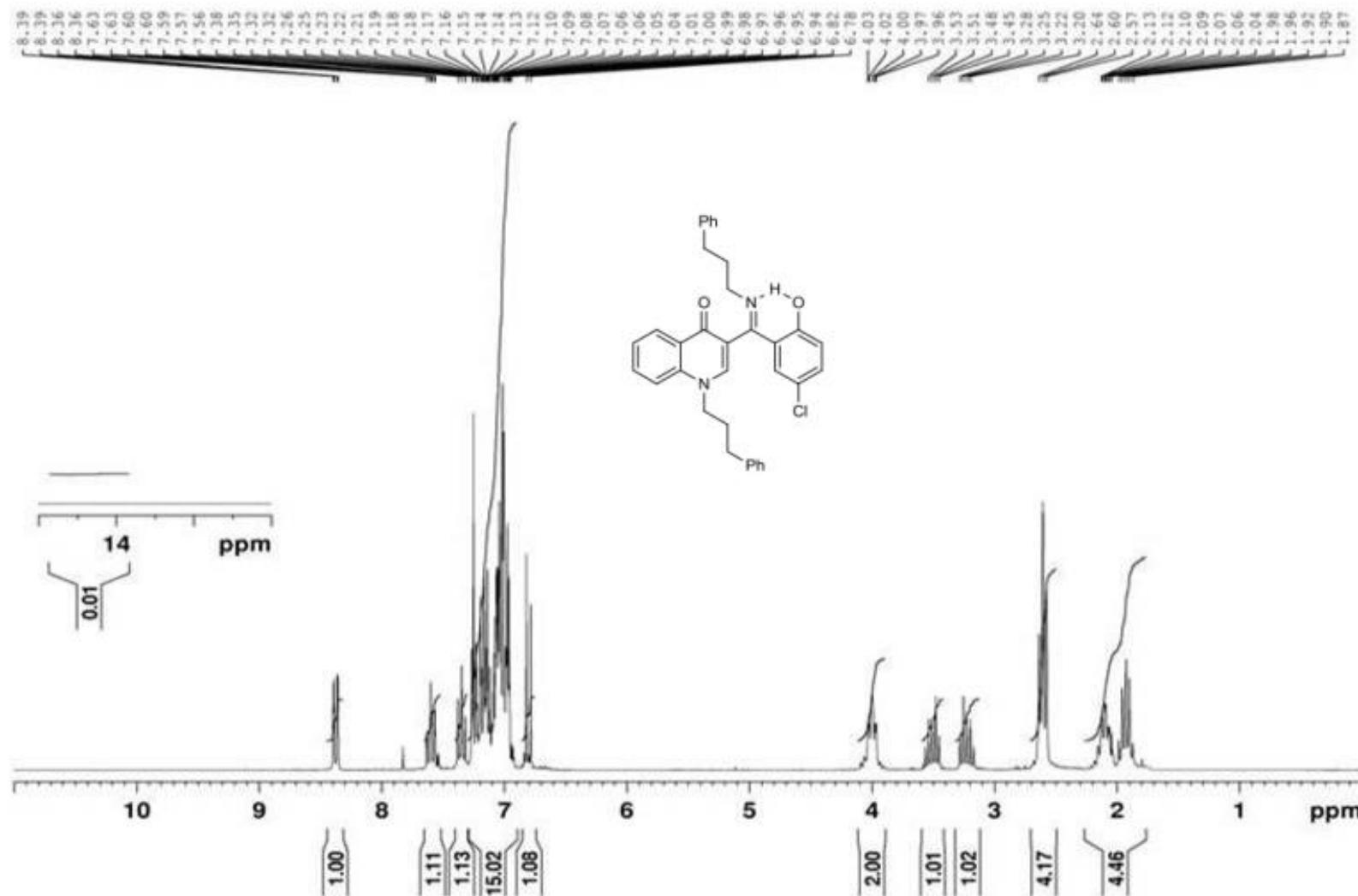
CHANNEL H1
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986
SFO1 75.47529531

CHANNEL I2
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 us
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108
PL12W 0.22453187
PL13W 0.22453187
SFO2 300.1312005

F2 - Processing parameters
SI 32768
SF 75.4677569 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 4i

Mkrtchyan SM800 1H CDC13



BRUKER

Current Data Parameters
NAME 130620.213
EXPNO 10
PROCNO 1

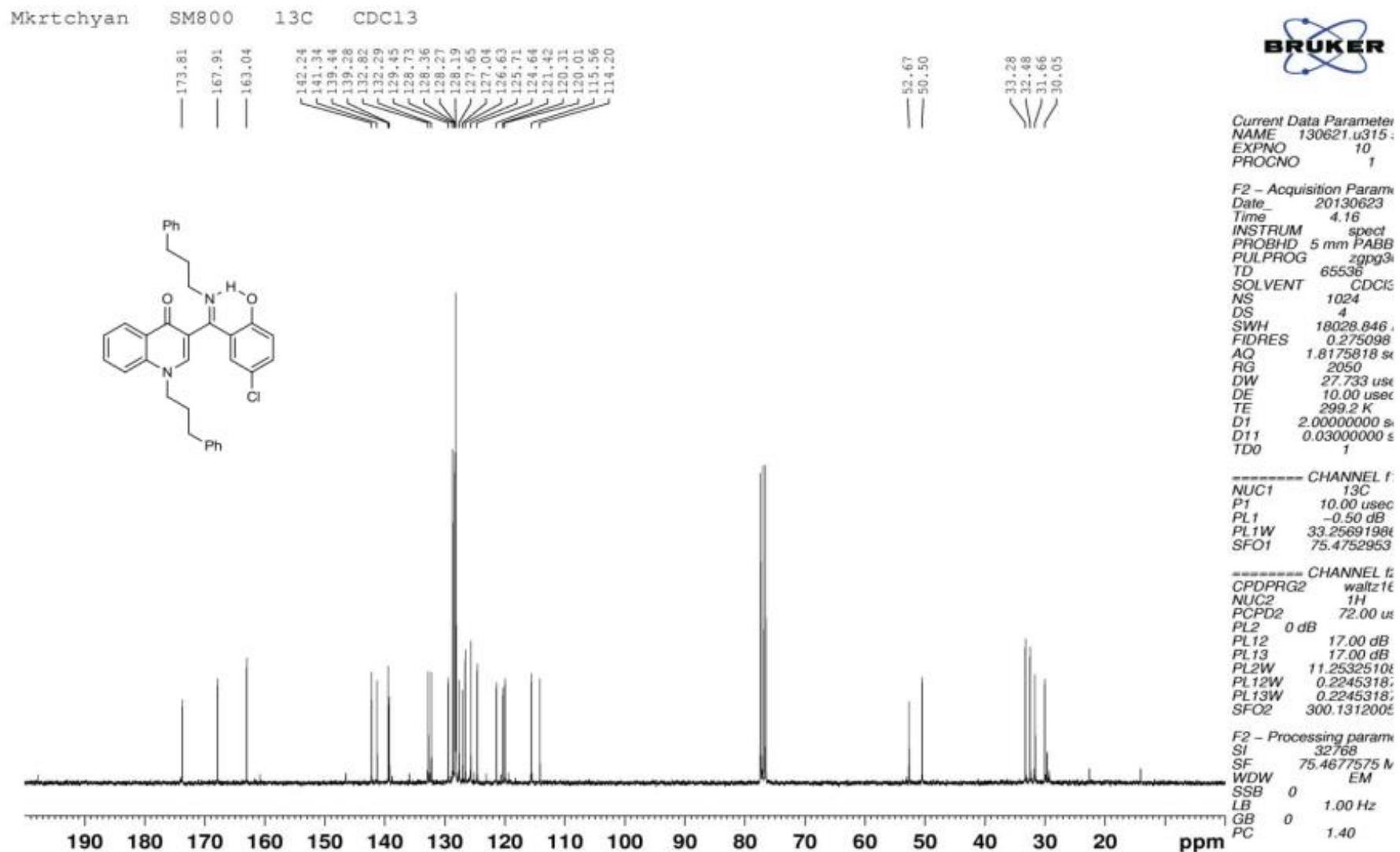
F2 - Acquisition Param
 Date 20130620
 Time 12.41
INSTRUM spect
PROBHD 5 mm PABl
PULPROG zg3t
TD 65536
SOLVENT CDCl
NS 16
DS 2
SWH 5165.289
FIDRES 0.07881t
AO 6.3439350 ±
RG 228
DW 96.800 us
DE 10.00 us
TE 298.2 K
D1 1.00000000 :
TDO 1

----- CHANNEL .
NUC1 1H
P1 10.00 use
PL1 -2.50 dB
SFO1 250.131544

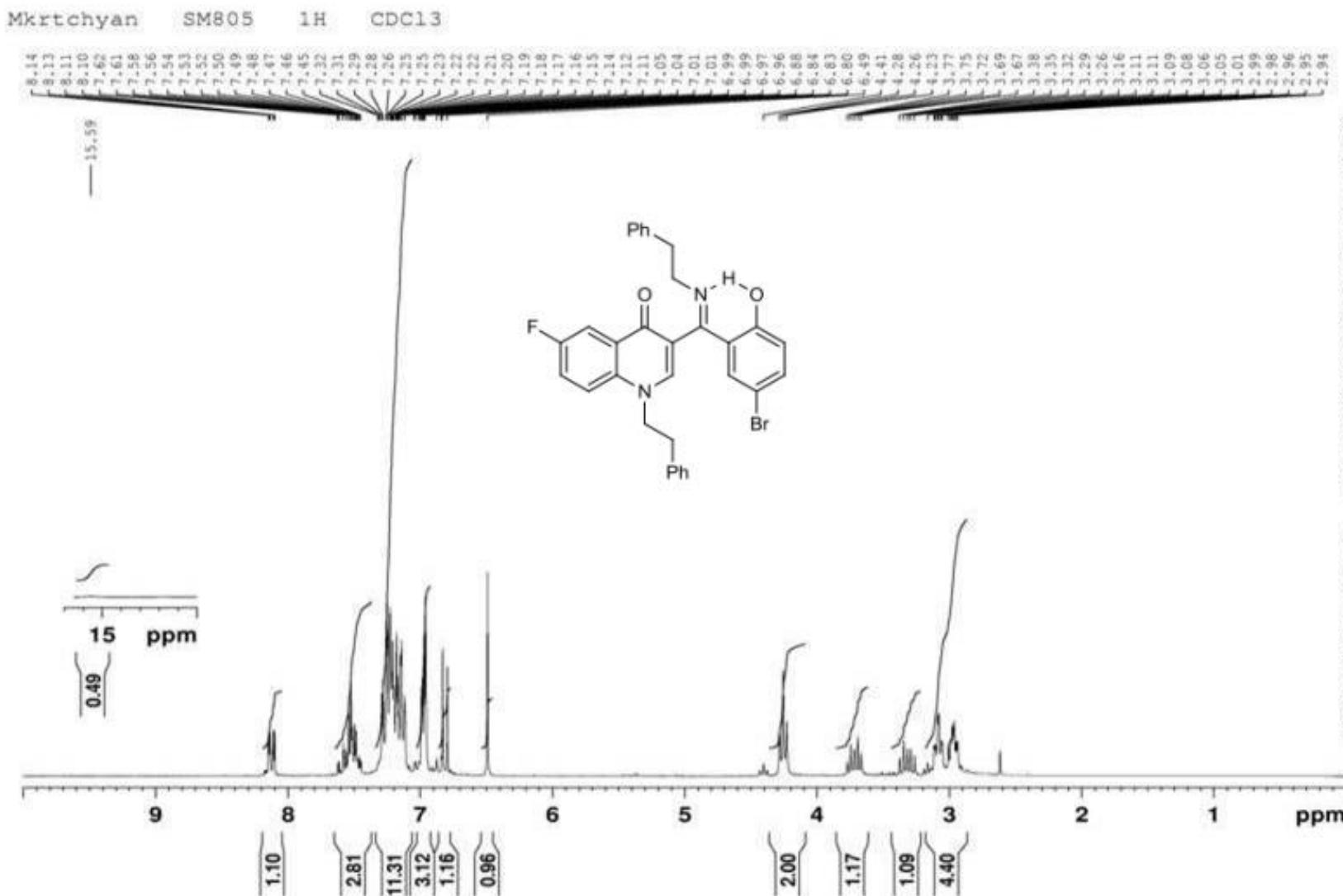
F2 – Processing parameters

<i>SI</i>	32768
<i>SF</i>	250.1300316
<i>WDW</i>	EM
<i>SSB</i>	0
<i>LB</i>	0.30 Hz
<i>GB</i>	0
<i>PC</i>	1.00

Compound 4i

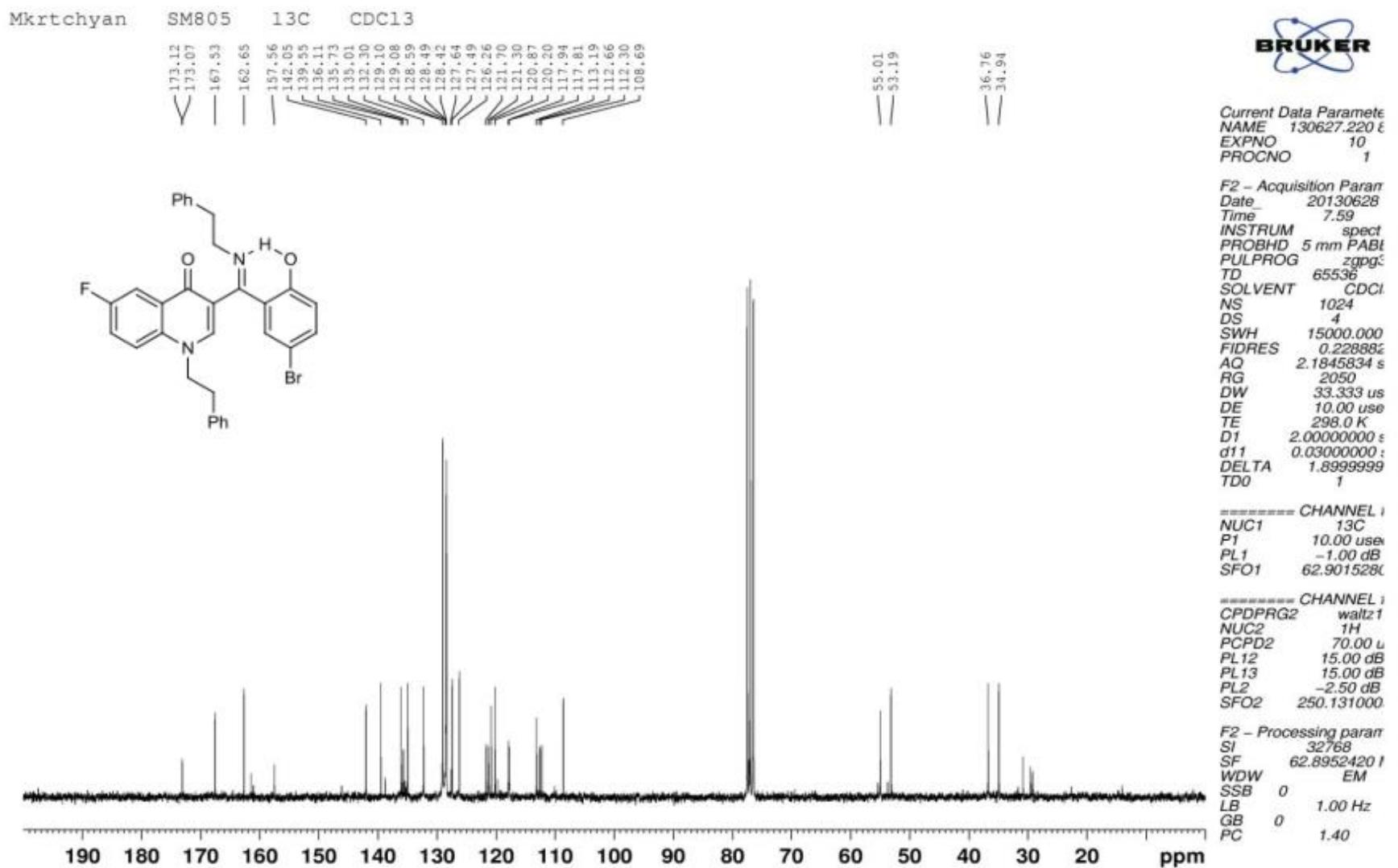


Compound 4j

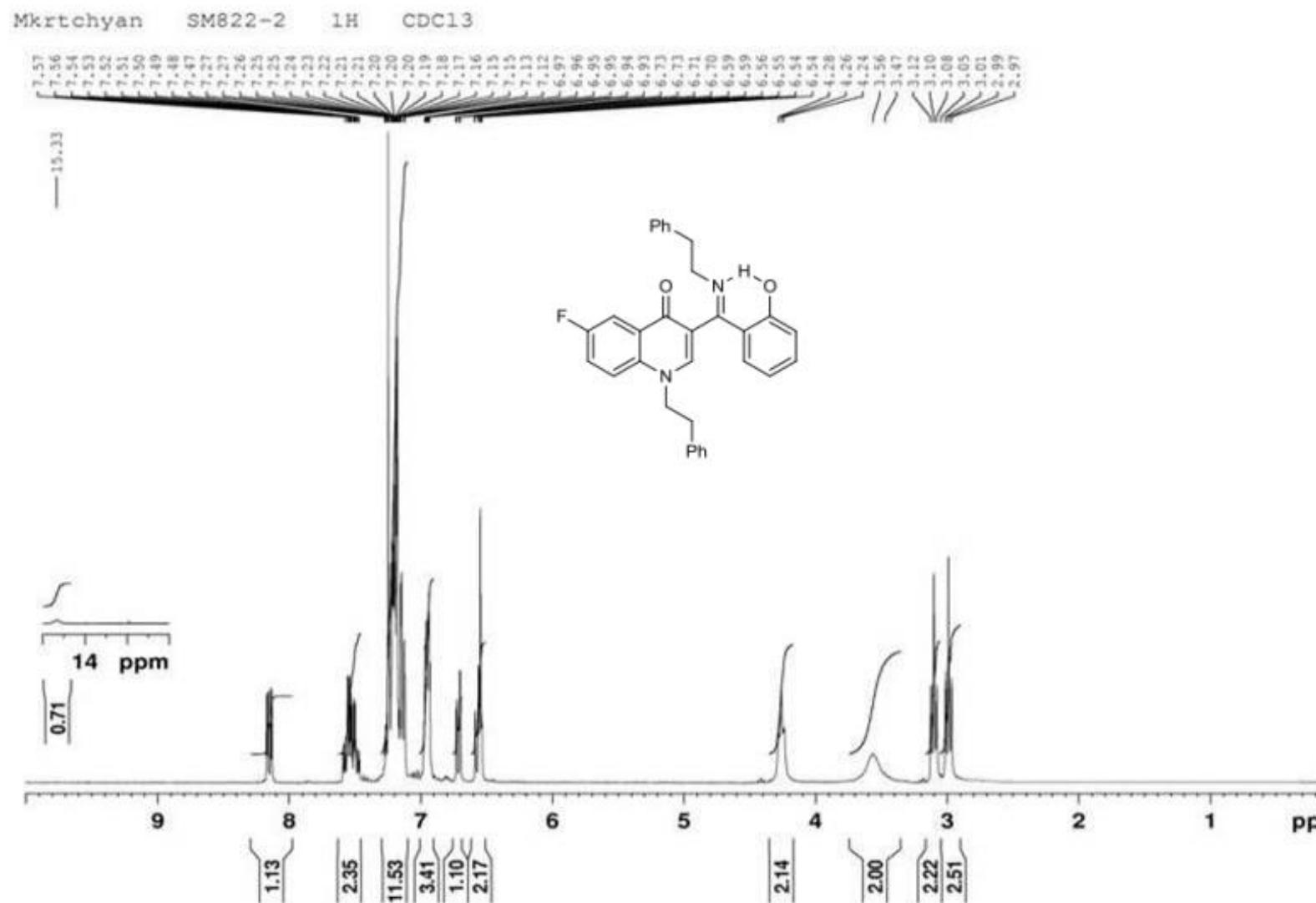


BRUKER

Compound 4j



Compound 4k



Current Data Param
NAME 130830.u3
EXPNO 10
PROCNO

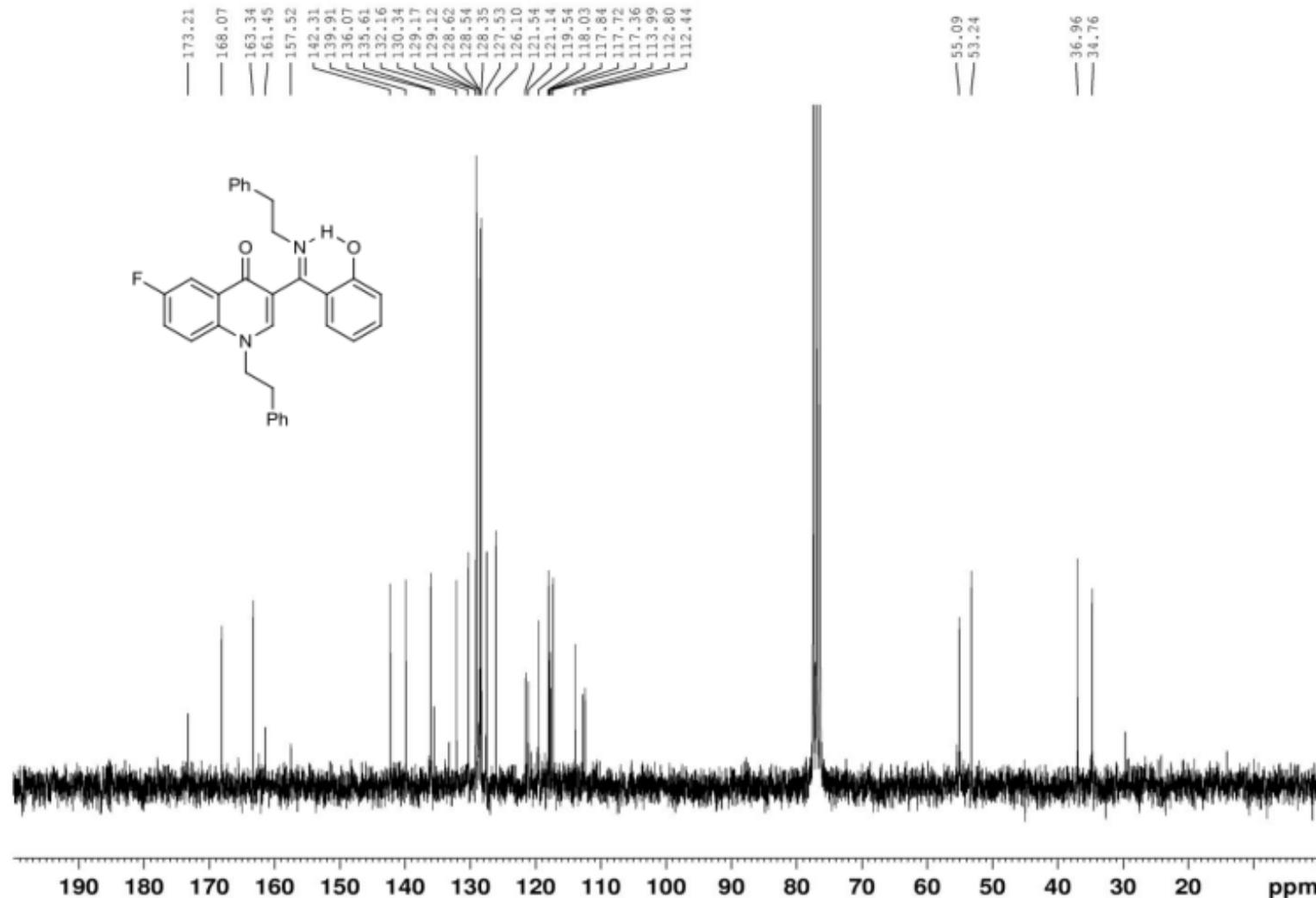
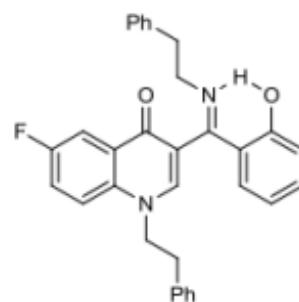
F2 - Acquisition Par
Date 201308:
Time 13.36
INSTRUM sp6
PROBHD 5 mm PA
PULPROG zg3
TD 65536
SOLVENT CD
NS 16
DS 2
SWH 6188.1
FIDRES 0.0944
AQ 5.295358
RG 128
DW 80.000
DE 10.00 L
TE 298.2 K
D1 1.000000 G
TD0 1

----- CHANNEL
NUC1 1H
P1 10.00 u
PL1 0 dB
PL1W 11.25326
SFO1 300.1318

F2 - Processing par
SI 32768
SF 300.13001-
WDW EM
SSB 0
LB 0.30 H.
GB 0
PC 1.00

Compound 4k

Mkrtchyan SM-822-2 13C CDC13



BRUKER

Current Data Parameter
NAME 130902.208 sr
EXPNO 10
PROCNO 1

F2 - Acquisition Param
 Date 20130902
 Time 22.10
INSTRUM spect
PROBHD 5 mm QNP 1
PULPROG zgpg3k
TD 65536
SOLVENT CDCI3
NS 1024
DS 4
SWH 15000.000 I
FIDRES 0.228882
AQ 2.1845834 SE
RG 2050
DW 33.333 USEC
DE 10.00 USEC
TE 298.2 K
D1 2.00000000 SE
d11 0.03000000 SE
DELTA 1.89999996
TDO 1

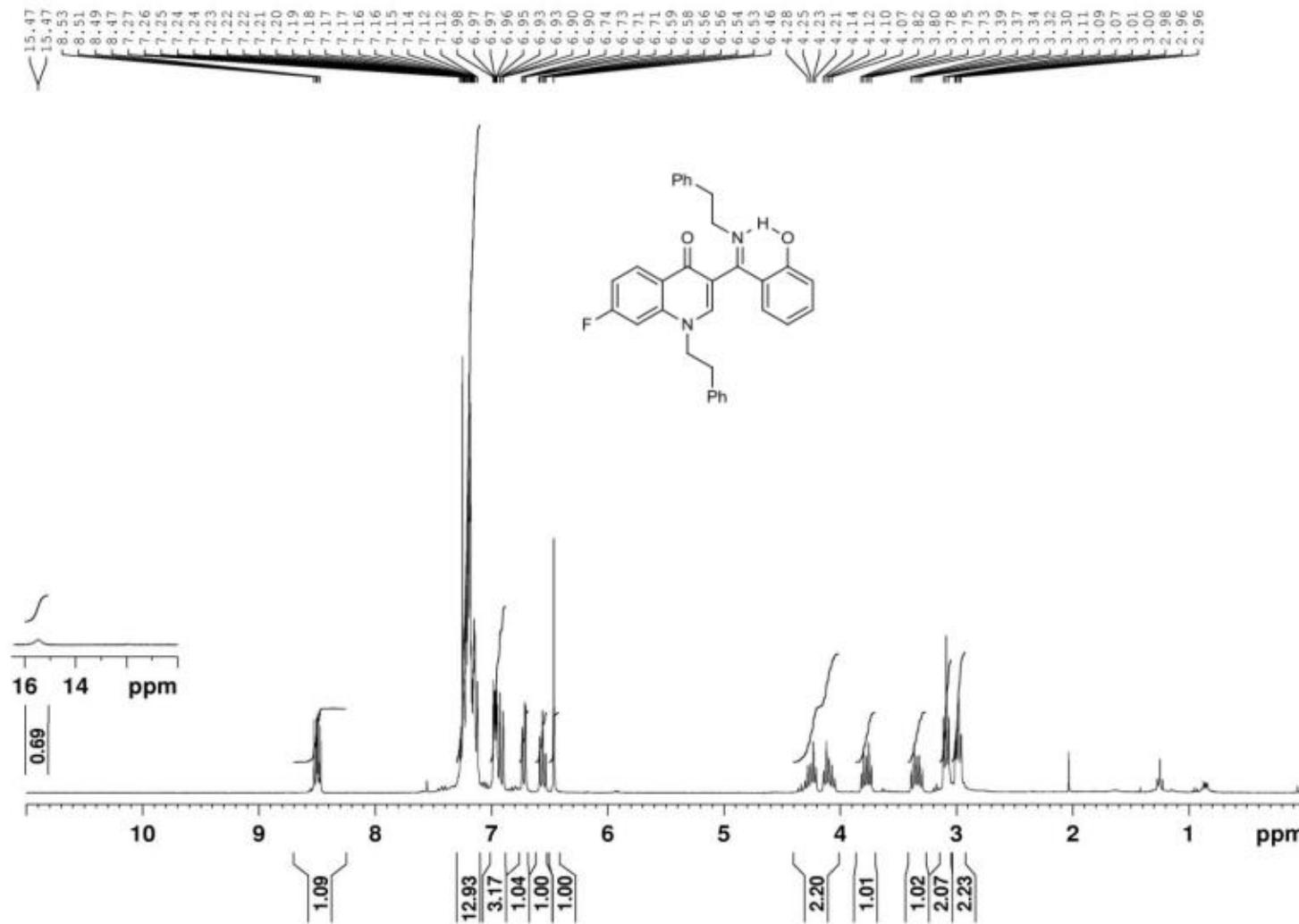
----- CHANNEL f1
NUC1 13C
P1 10.20 usec
PL1 0 dB
SFO1 62.9015280

```
----- CHANNEL 12
CPDPRG2    waltz16
NUC2        1H
PCPD2      70.00 us
PL12       14.00 dB
PL13       14.00 dB
PL2        -3.00 dB
SFO2      250.1310005
```

F2 - Processing parameters
 SI 32768
 SF 62.8952397 M
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Compound 4l

Mkrtchyan SM817-2cr 1H CDC13



BRUKER

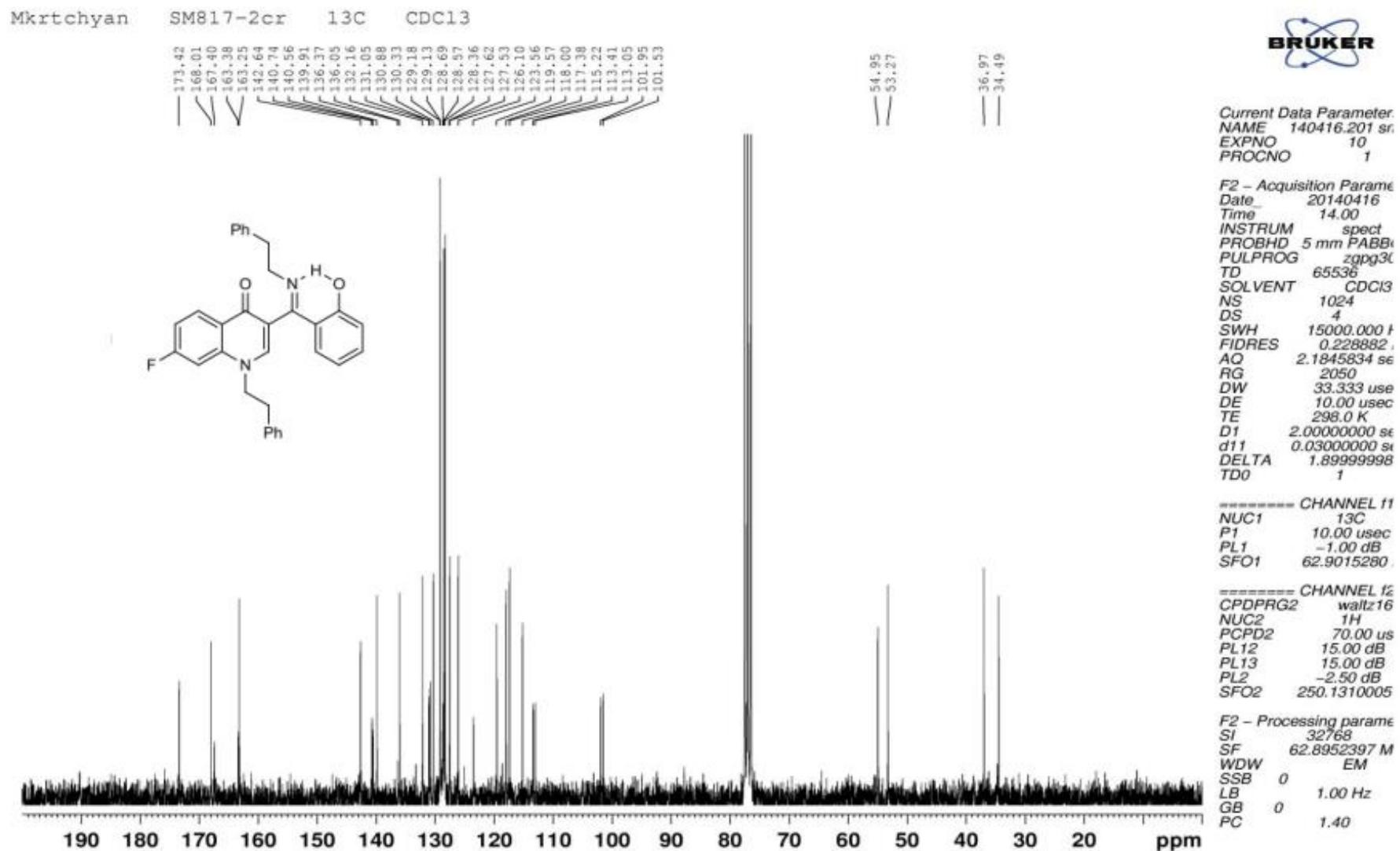
Current Data Parameter:
NAME 140414.u305.s
EXPNO 10
PROCNO 1

F2 - Acquisition Param
 Date 20140414
 Time 10.54
 INSTRUM spec
 PROBHD 5 mm PABBr
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 s
 AQ 5.2953587 se
 RG 128
 DW 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 se
 TDO 1

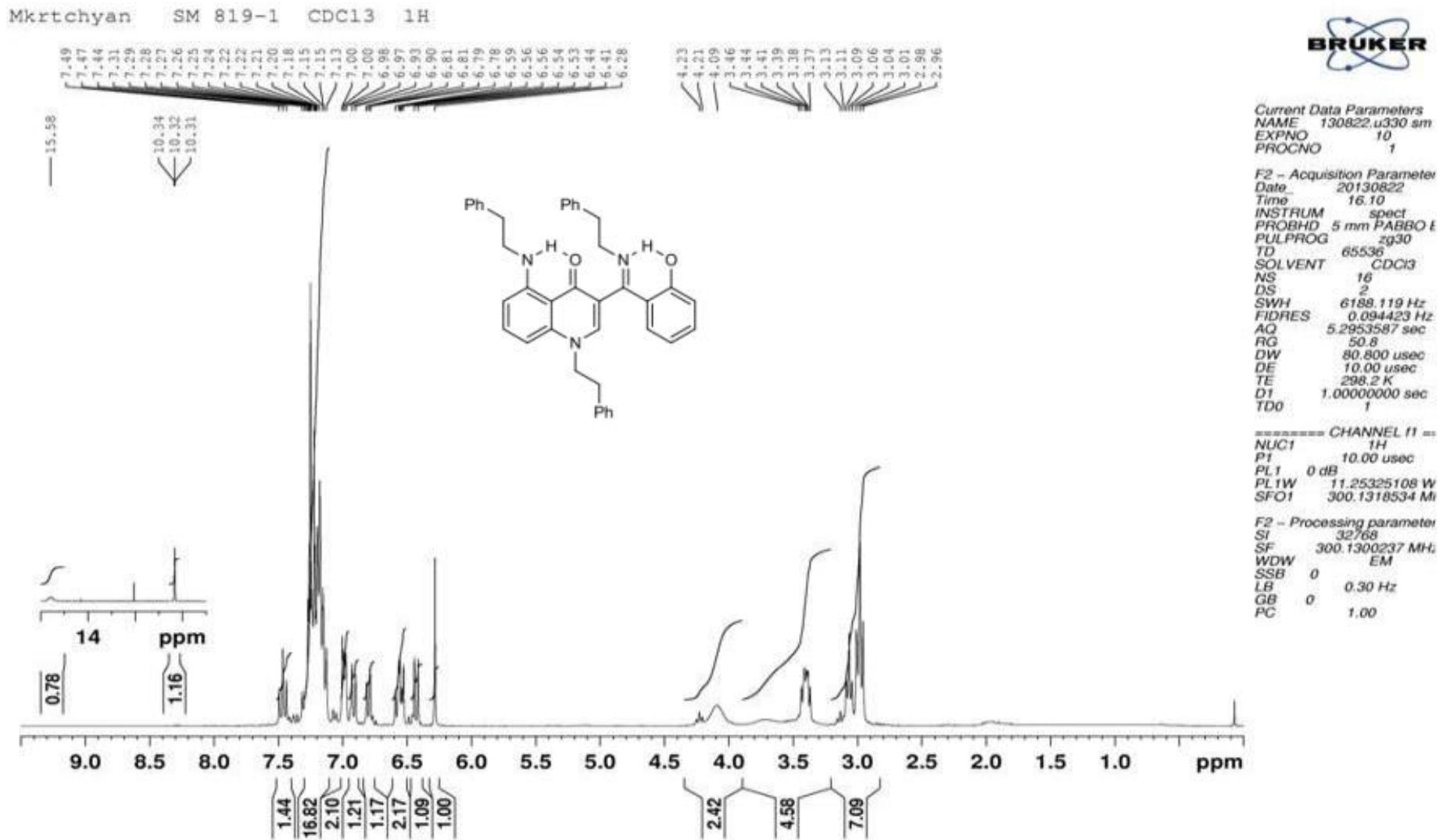
----- CHANNEL H
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108
SFO1 300.1318534

$F2$ - Processing parameters
 SI 32768
 SF 300.1300141 Hz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Compound 4l

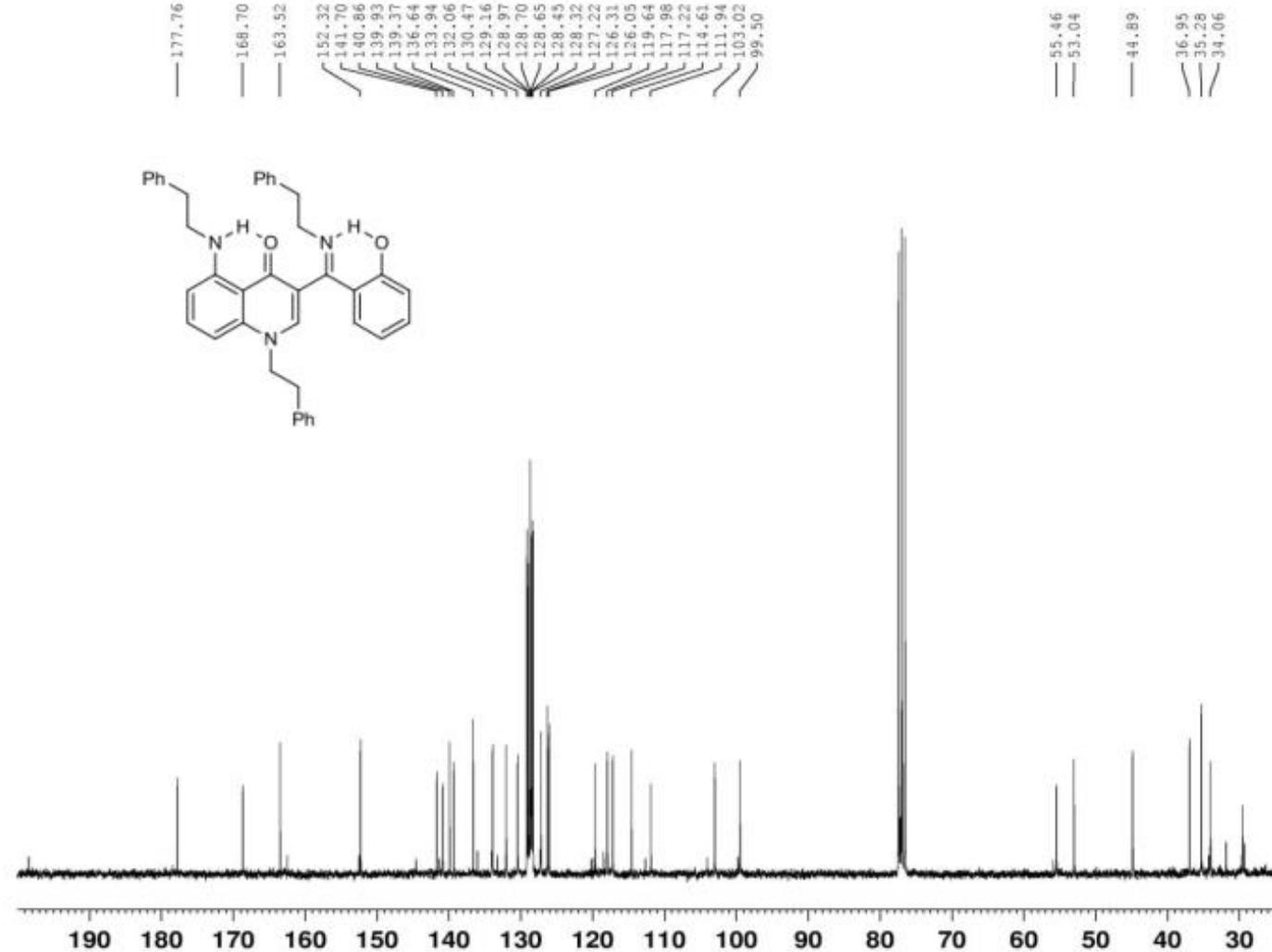
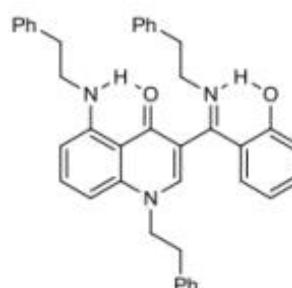


Compound 4m



Compound 4m

Mkrtschyan SM819-1 CDC13 13C



Current Data Param
NAME 130823.u3E
EXPNO 10
PROCNO 1

F2 - Acquisition Para
 Date 2013082
 Time 18.50
 INSTRUM spect
 PROBHD 5 mm PAI
 PULPROG zgpp
 TD 65536
 SOLVENT CDI
 NS 1024
 DS 4
 SWH 18028.84
 FIDRES 0.2750:
 AQ 1.8175818
 RG 2050
 DW 27.733 us
 DE 10.00 us
 TE 298.4 K
 D1 2.00000000
 D11 0.03000000
 TDD 1

----- CHANNEL
 NUC1 13C
 P1 10.00 us
 PL1 -0.50 d.
 PL1W 33.25691E
 SFQ1 75.47529

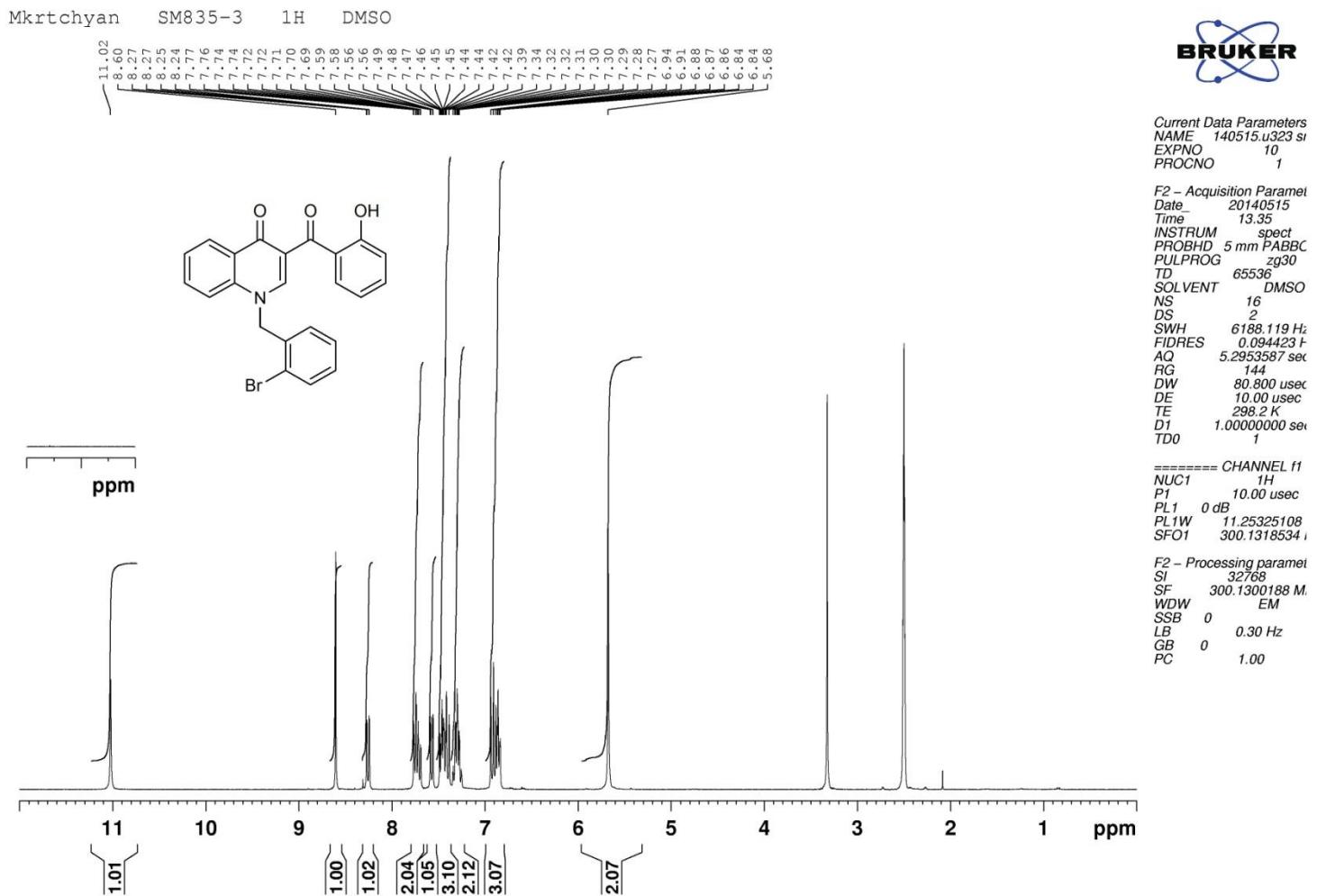
```
===== CHANNEL
CPDPRG2    waltz
NUC2        1H
PCPD2       72.00
PL2         0 dB
PL12        17.00 c
PL13        17.00 c
PL2W        11.253251
PL12W       0.224531
PL13W       0.224531
SEO2        300.11120
```

```

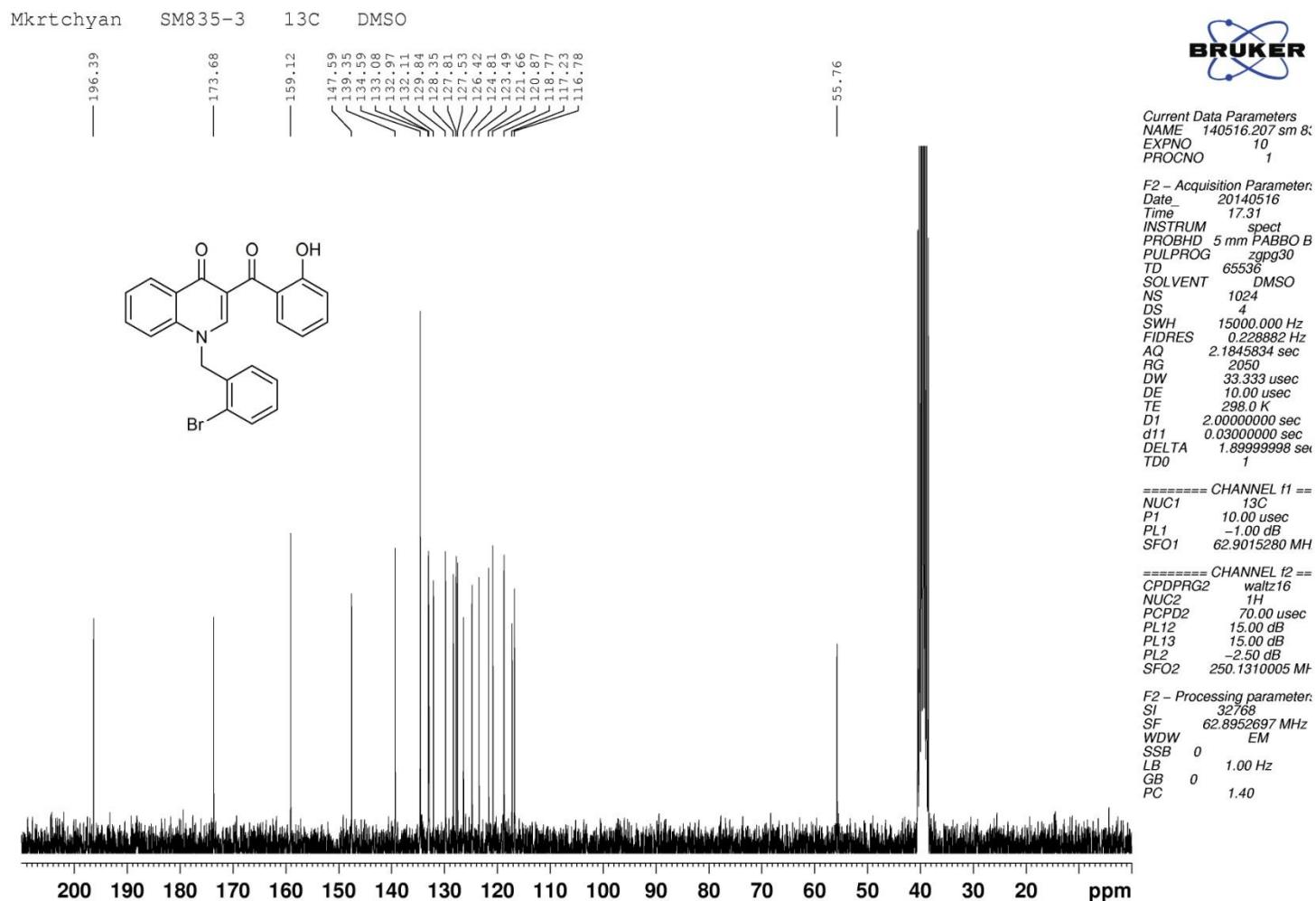
F2 - Processing para
SI      32768
SF      75.4677565
WDW      EM
SSB      0
LB      1.00 Hz
GB      0
PC      1.40

```

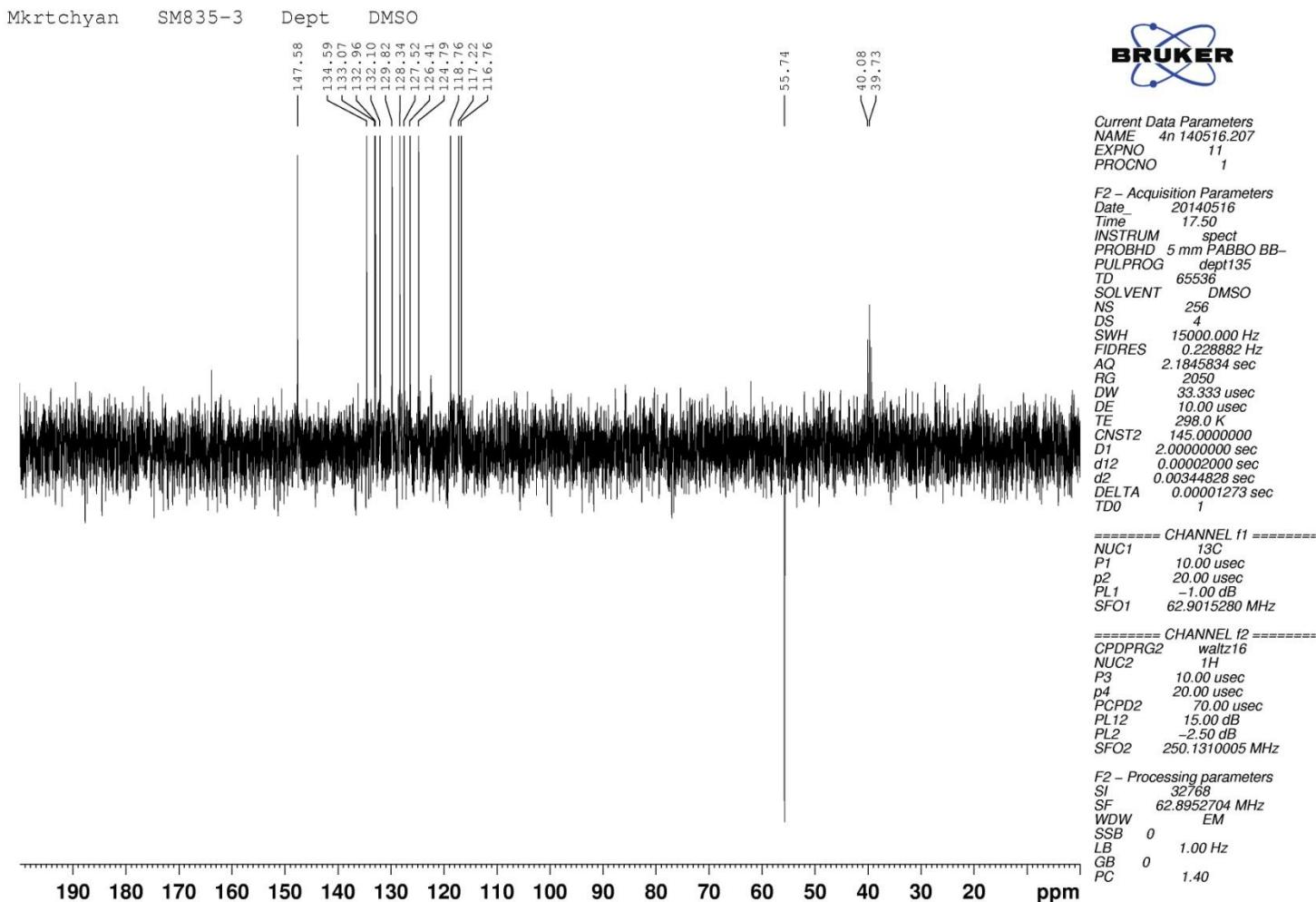
Compound 4n



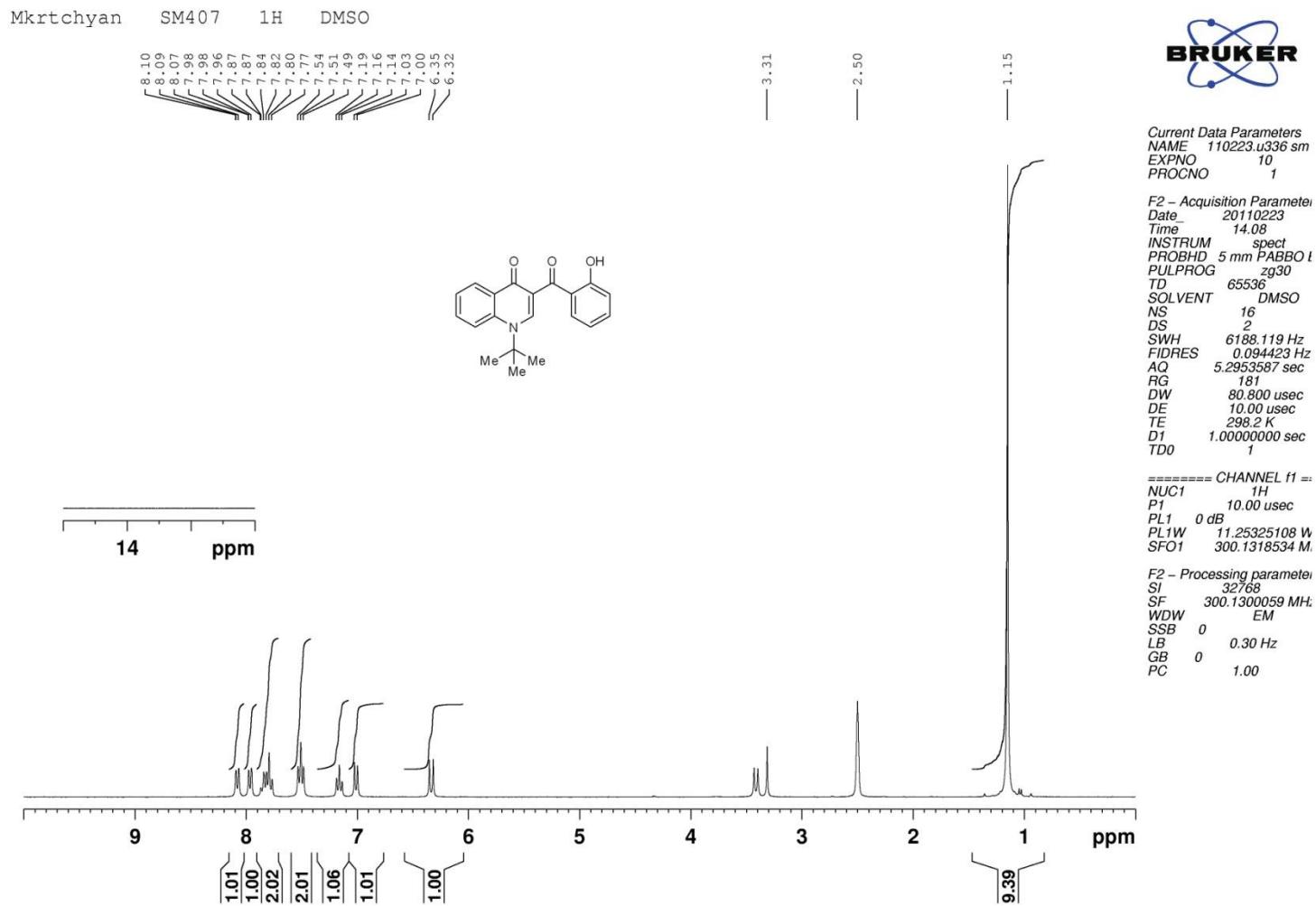
Compound 4n



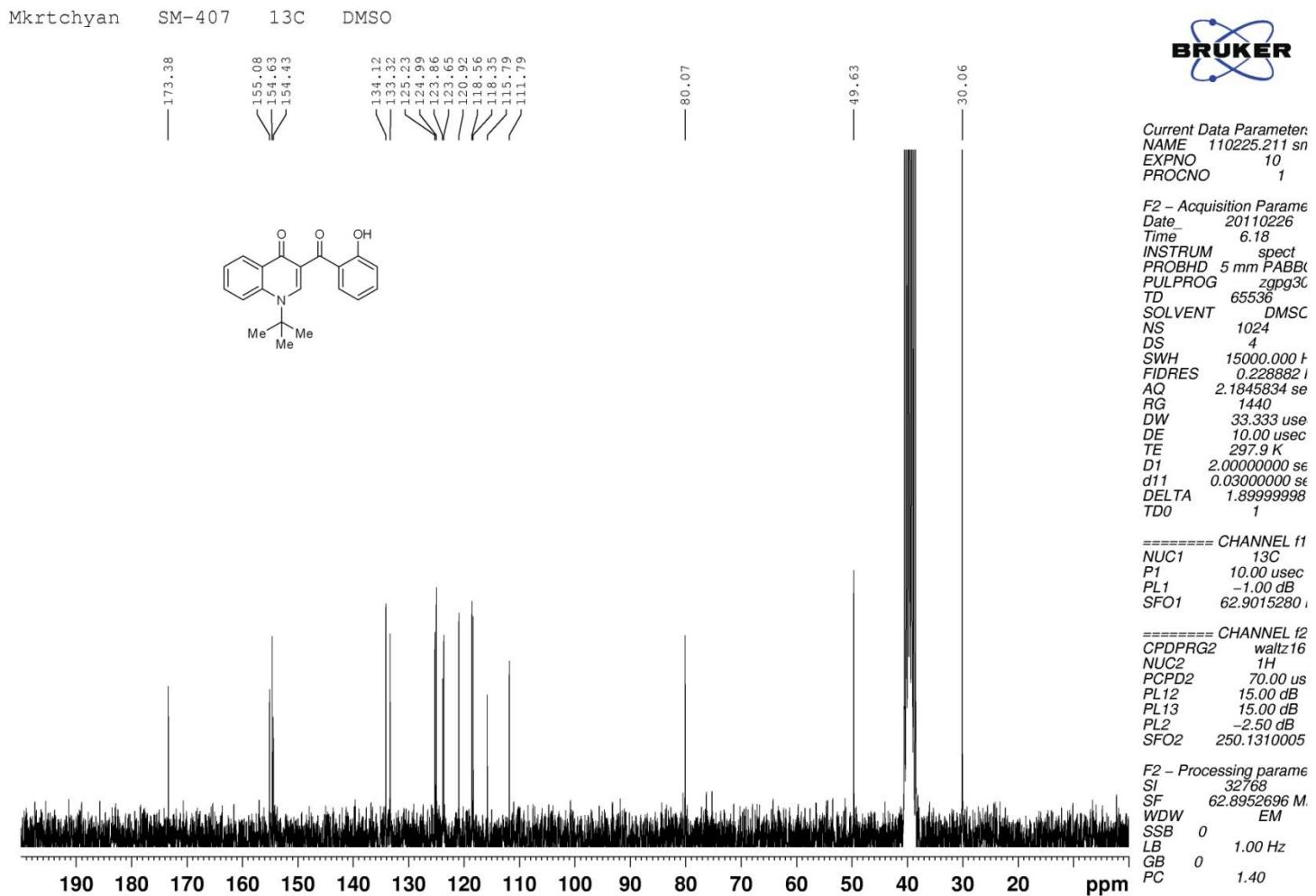
Compound 4n



Compound 4o

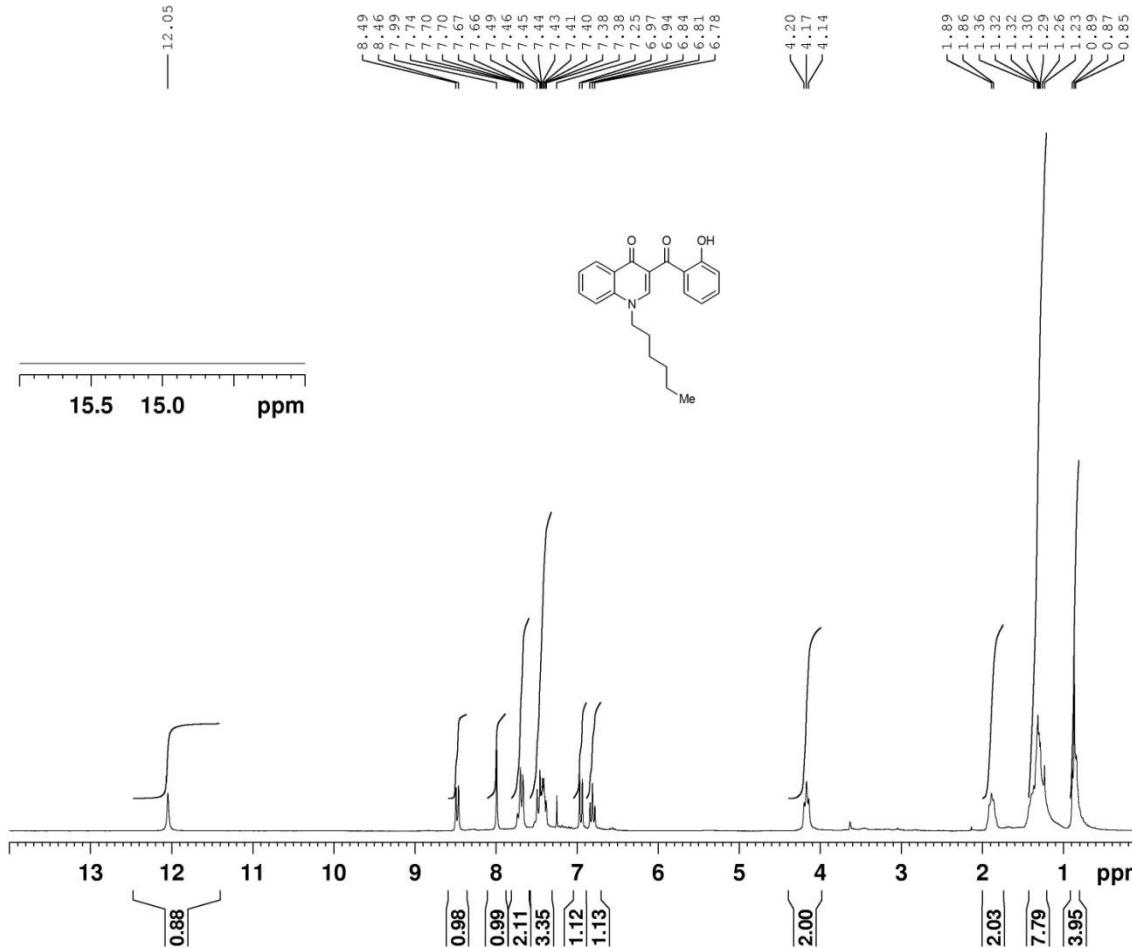


Compound 4o



Compound 4d'

Mkrtchyan SM844 1H CDCl₃



Current Data Parameters
NAME SM844 140716.205
EXPNO 10
PROCNO 1

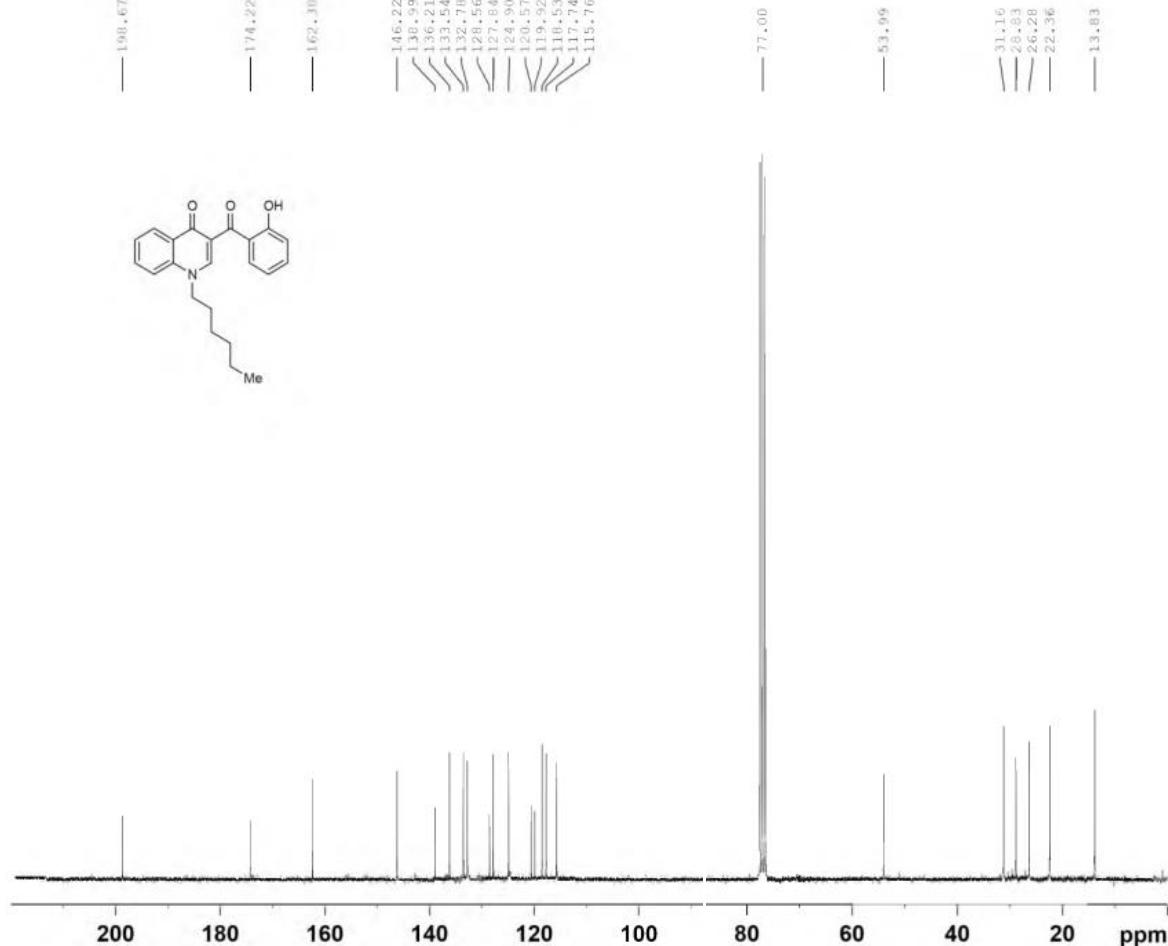
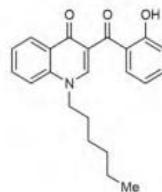
F2 - Acquisition Parameters
Date 20140716
Time 11.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 203
DW 96.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 250.1300029 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 4d'

Mkrtychyan SM844 13C CDCl₃



Current Data Parameters
NAME SM844 140716.205
EXPNO 11
PROCNO 1

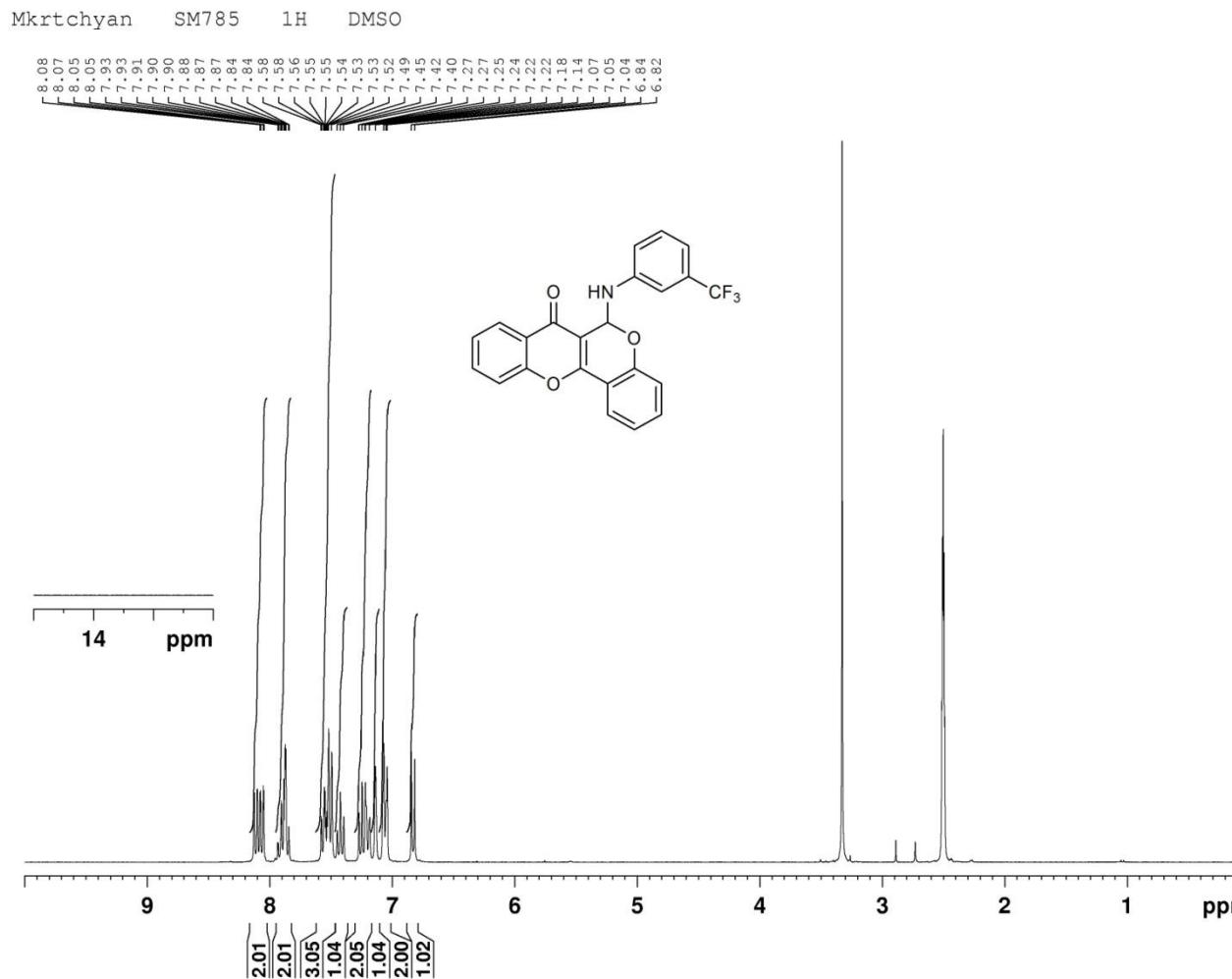
F2 - Acquisition Parameters
Date 20140716
Time 12.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.8999998 sec
TDO 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 62.8952429 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 5a



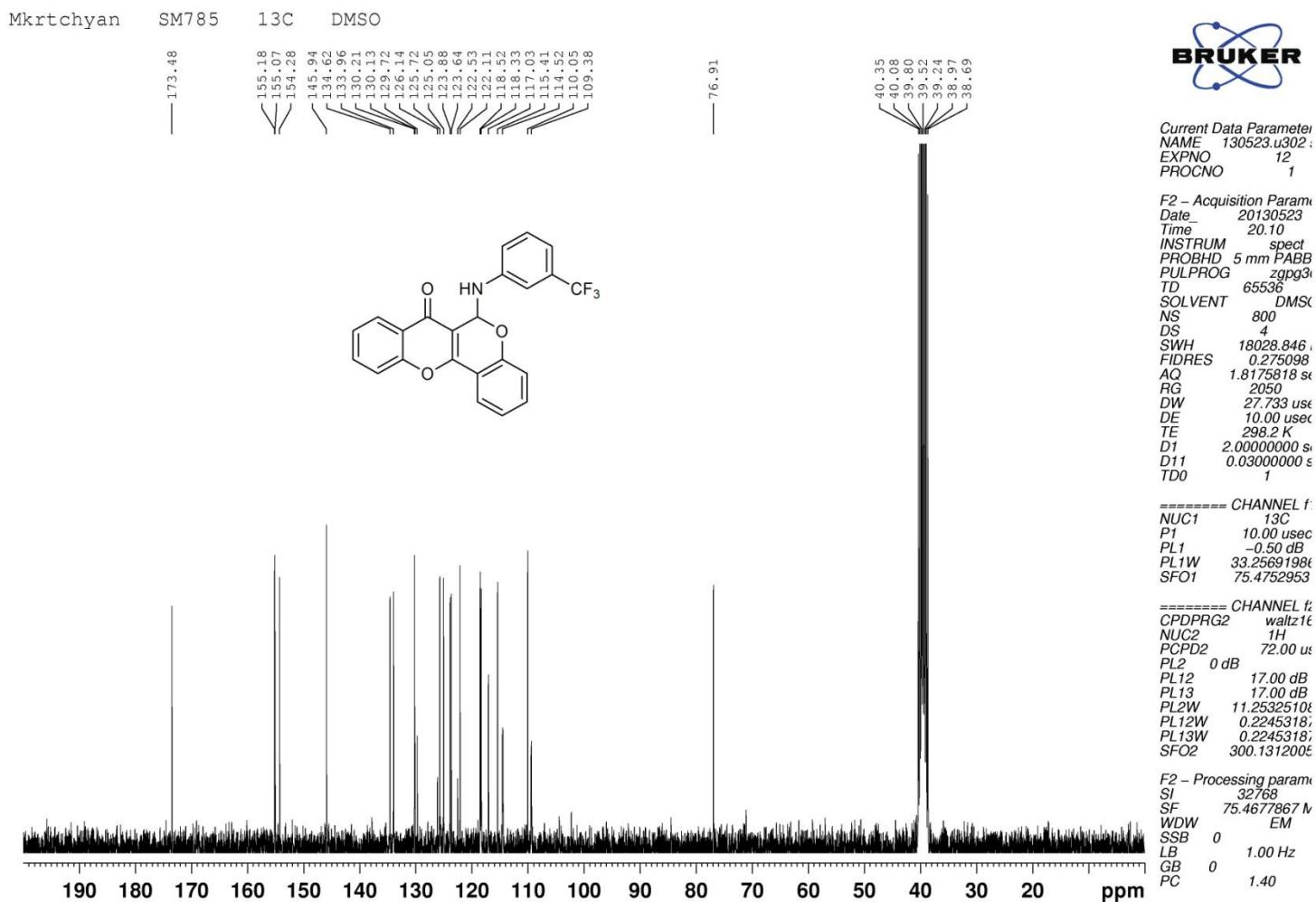
Current Data Parameters
NAME 130523.u302.s
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20130523
Time 9.05
INSTRUM spect
PROBHD 5 mm PABBC
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 t
AQ 5.2953587 sec
RG 228
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TDO 1

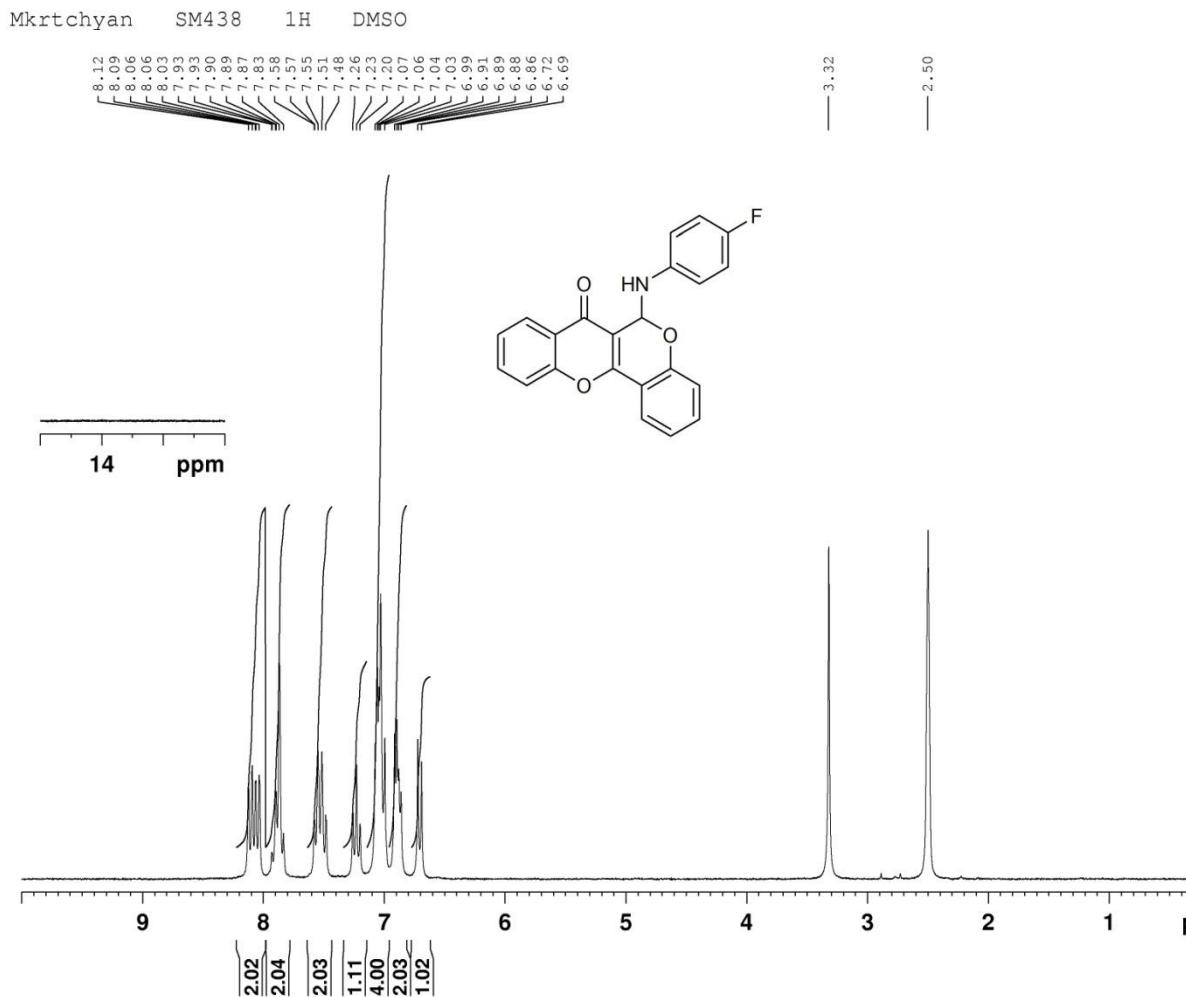
===== CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108
SFO1 300.1318534

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

Compound 5a



Compound 5b



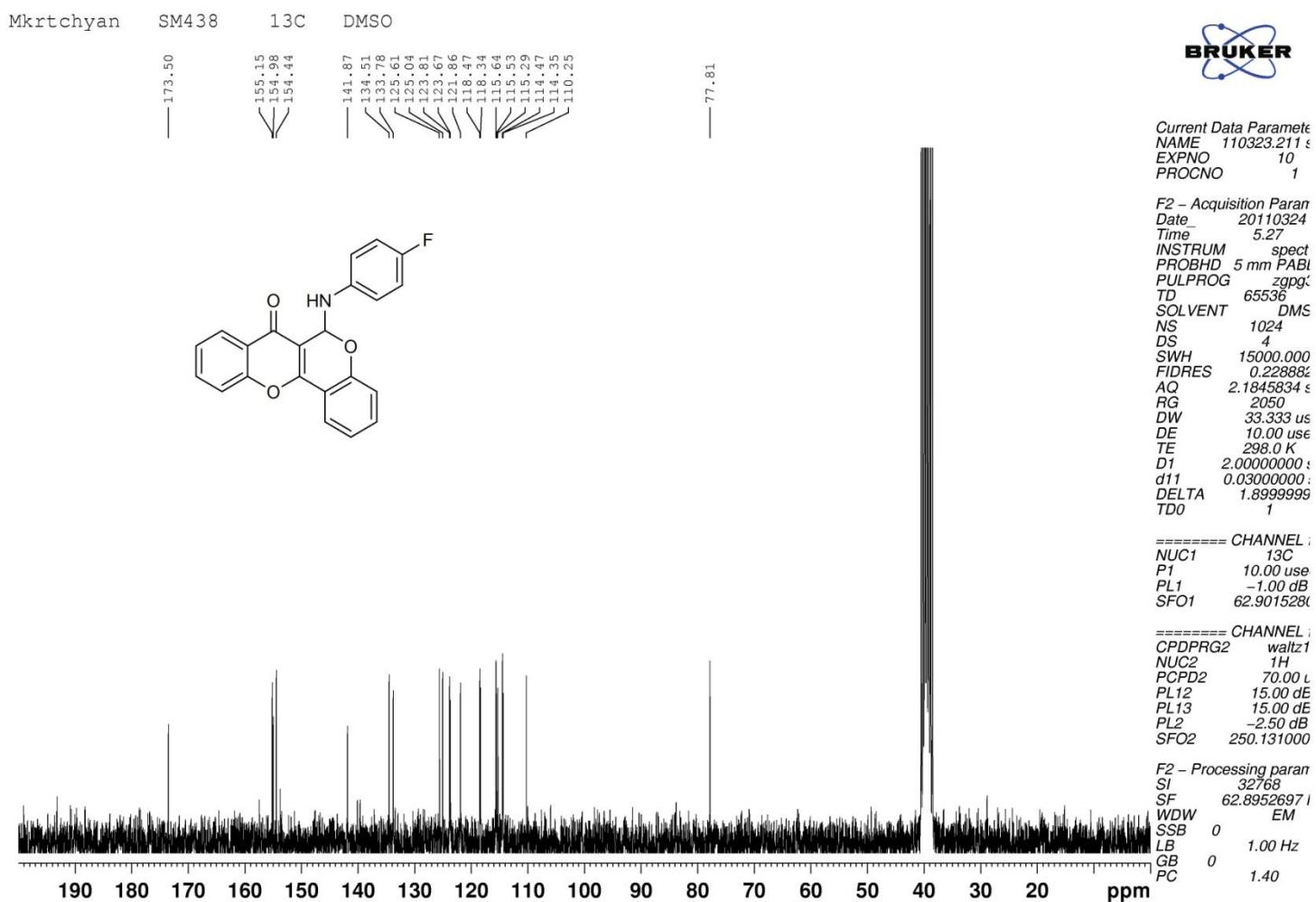
Current Data Parameters
NAME 110322.237 sm.
EXPNO 10
PROCNO 1

F2 – Acquisition Parameters
Date 20110322
Time 15.35
INSTRUM spect
PROBHD 5 mm PABBO
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 1290
DW 96.800 usec
DE 10.00 usec
TE 298.1 K
D1 1.0000000 sec
TD0 1

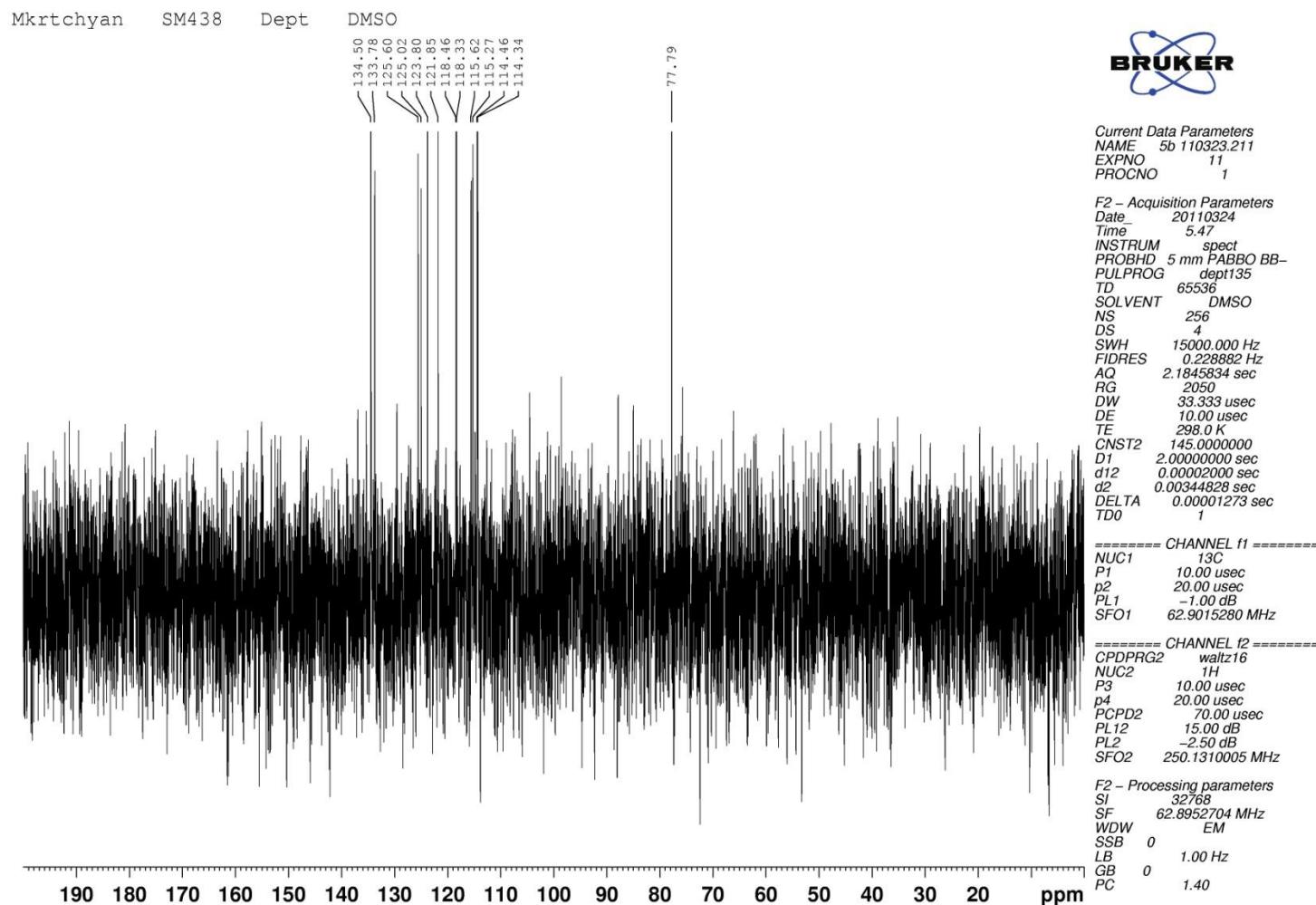
===== CHANNEL f1 =
NUC1 1H
P1 10.00 usec
PL1 -2.50 dB
SFO1 250.1315447 Hz

F2 – Processing parameters
SI 32768
SF 250.1299983 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

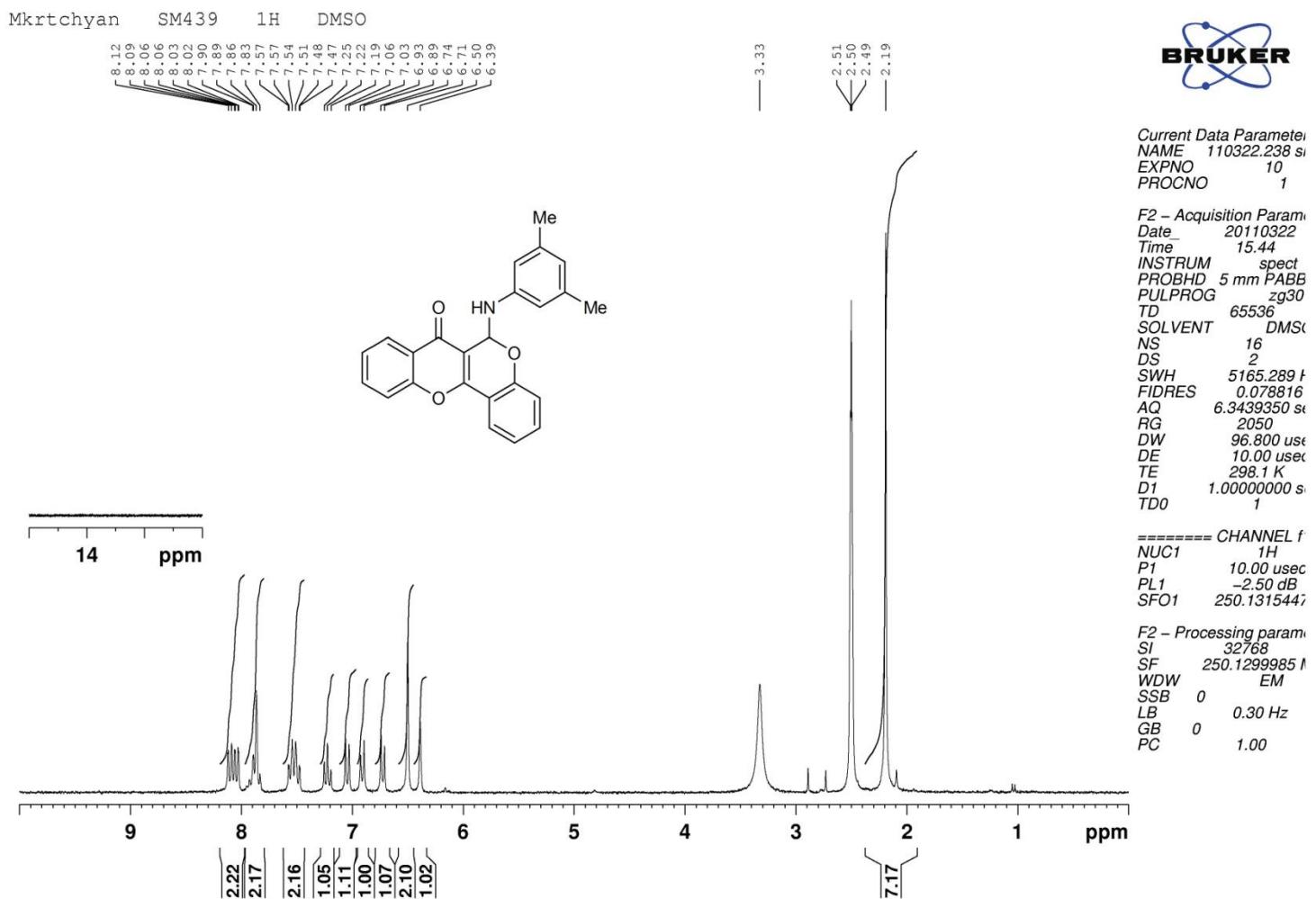
Compound 5b



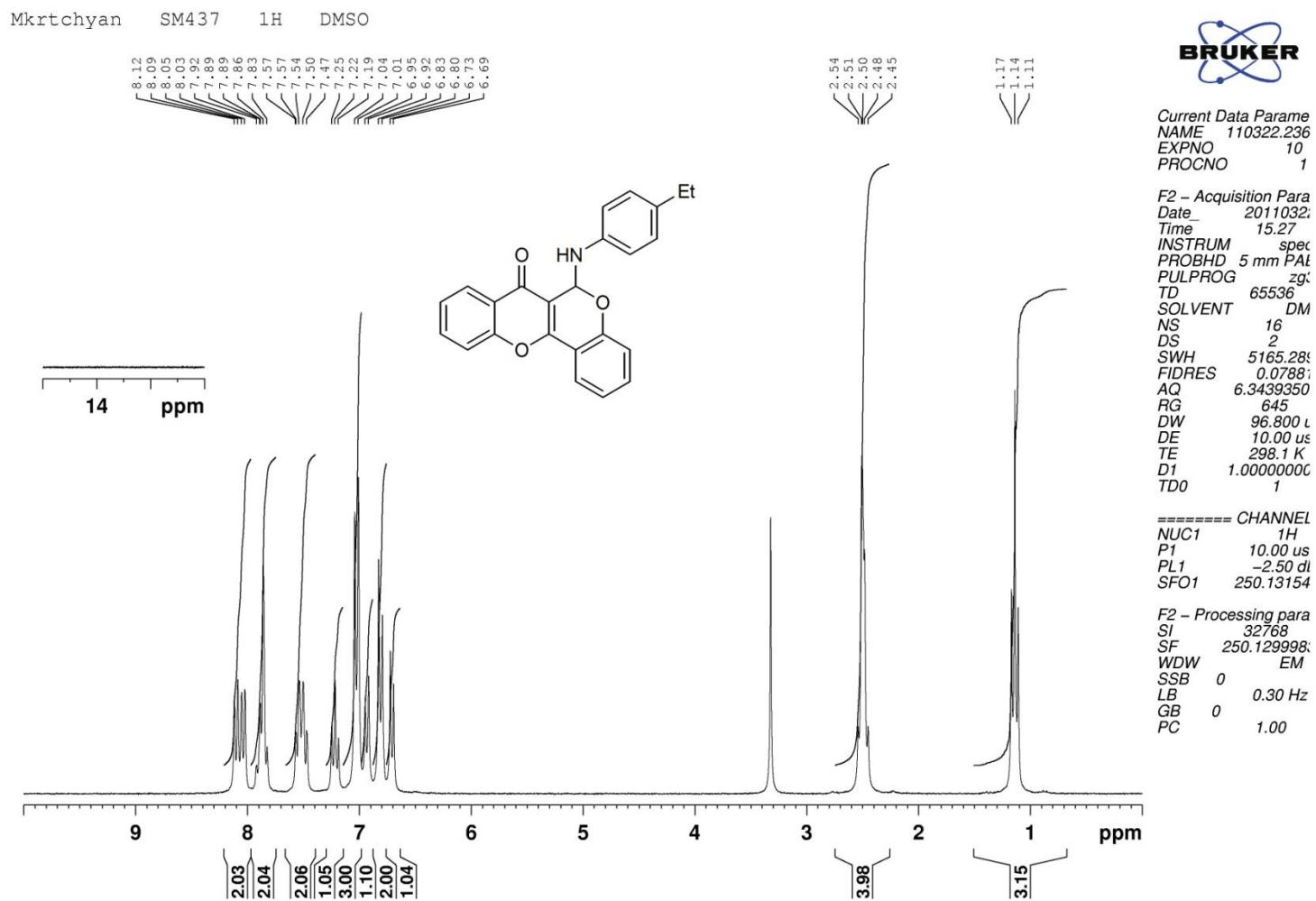
Compound 5b



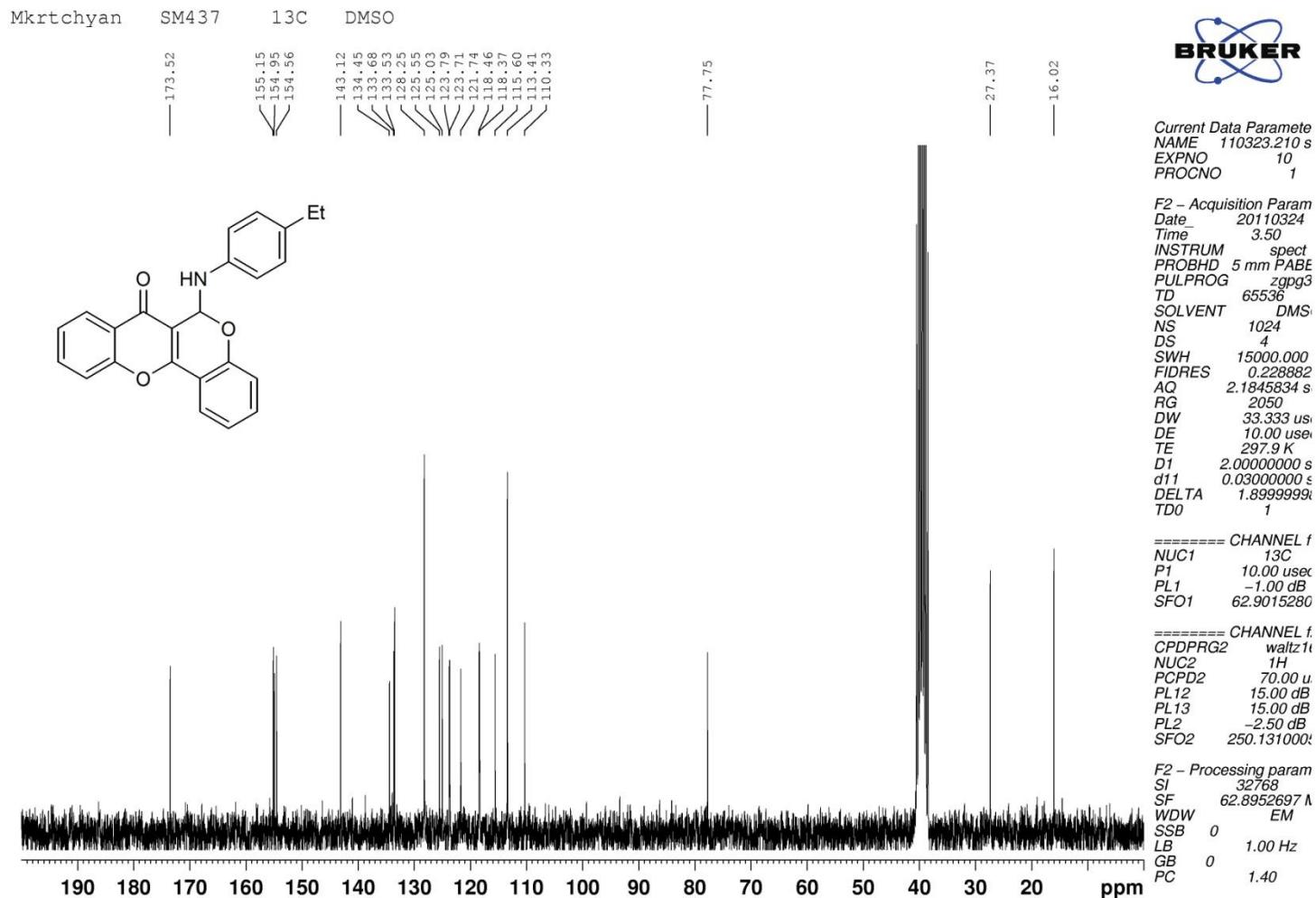
Compound 5c



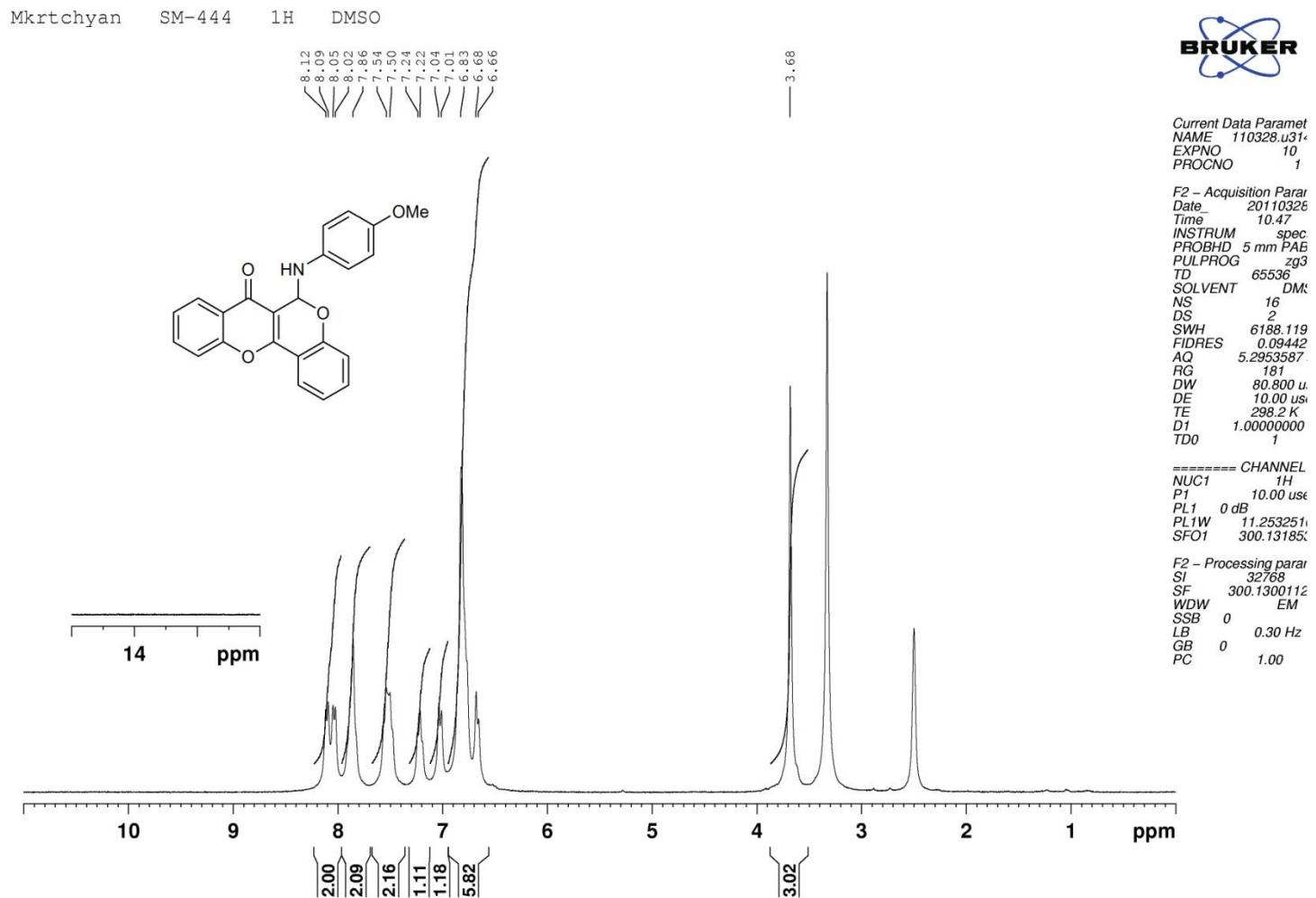
Compound 5d



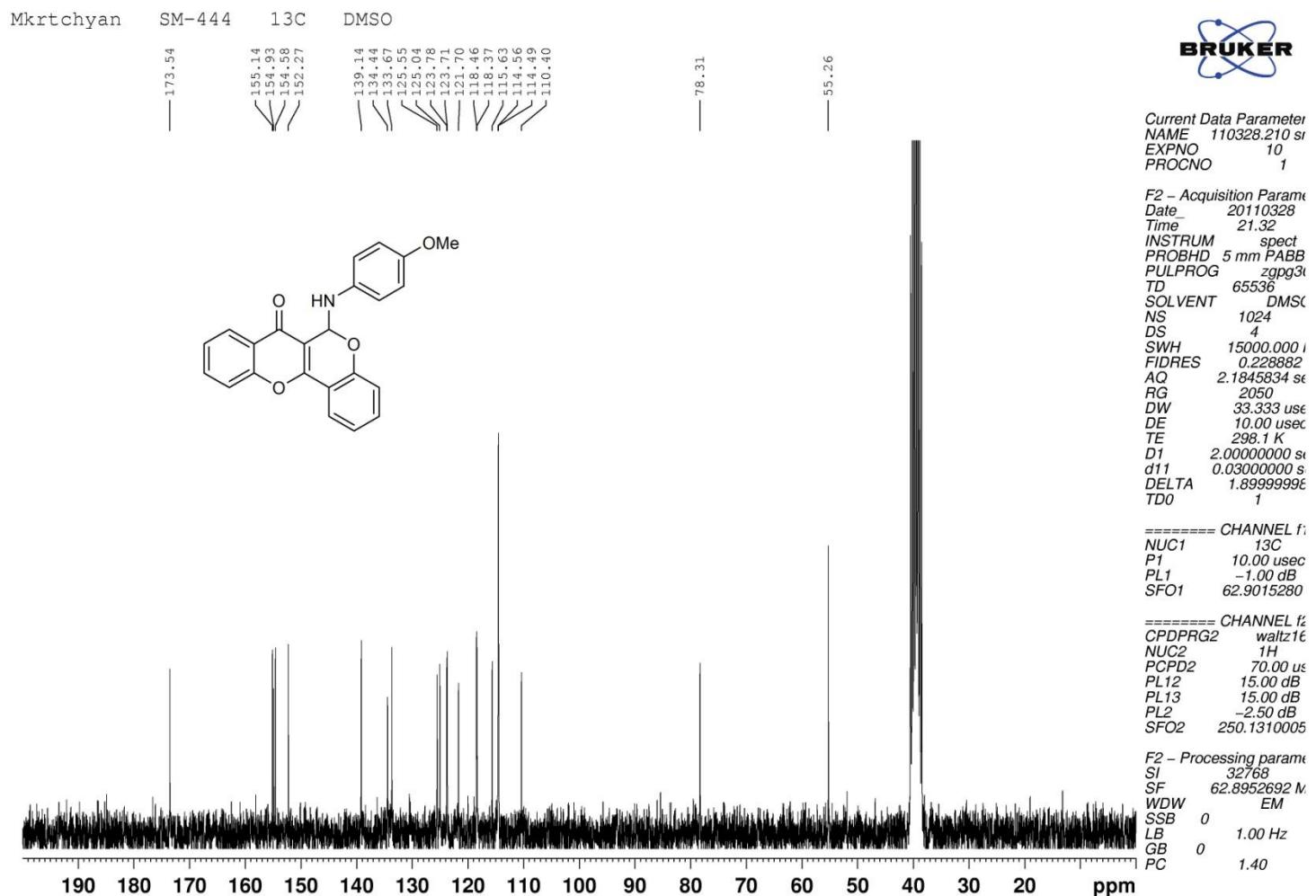
Compound 5d



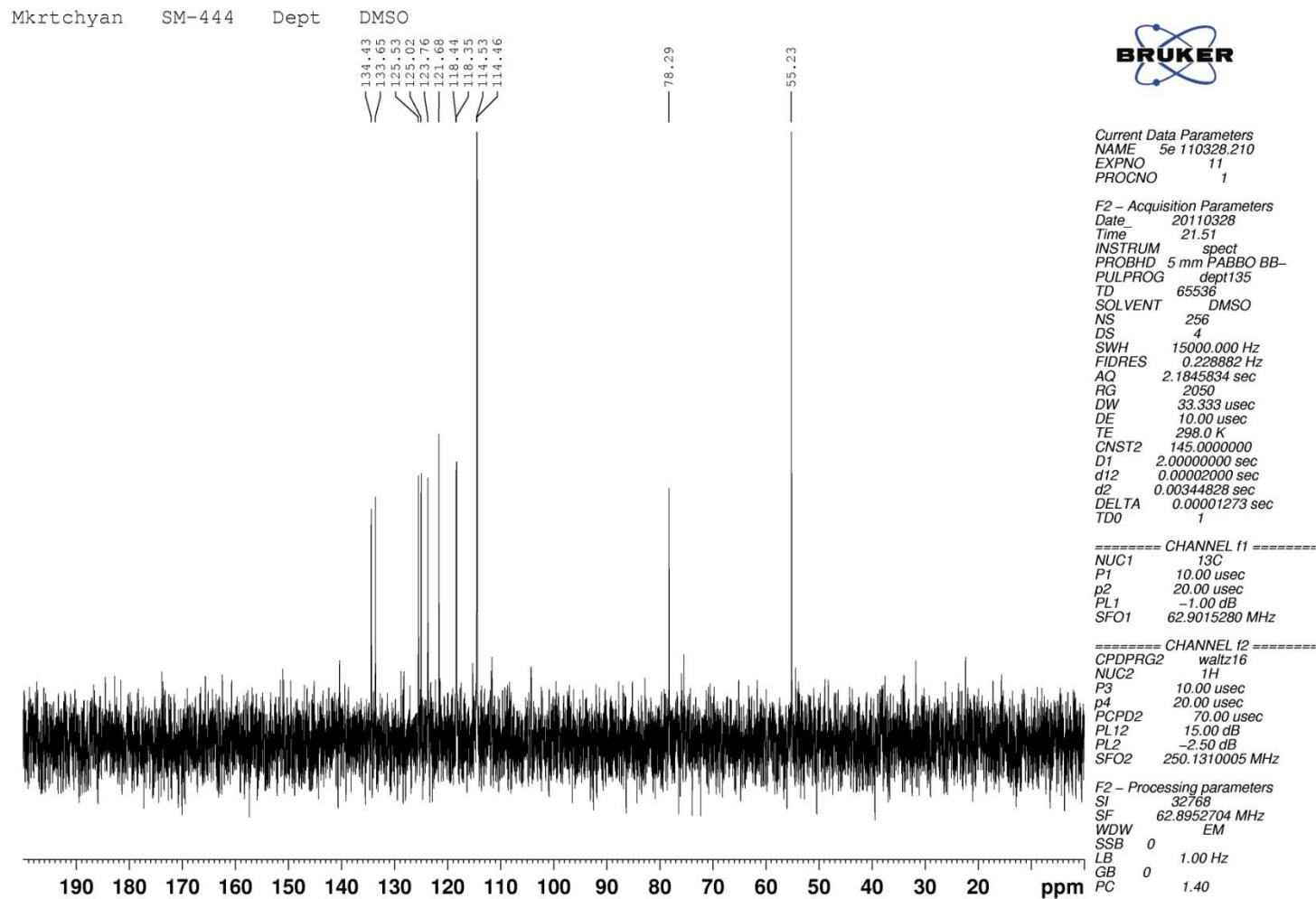
Compound 5e



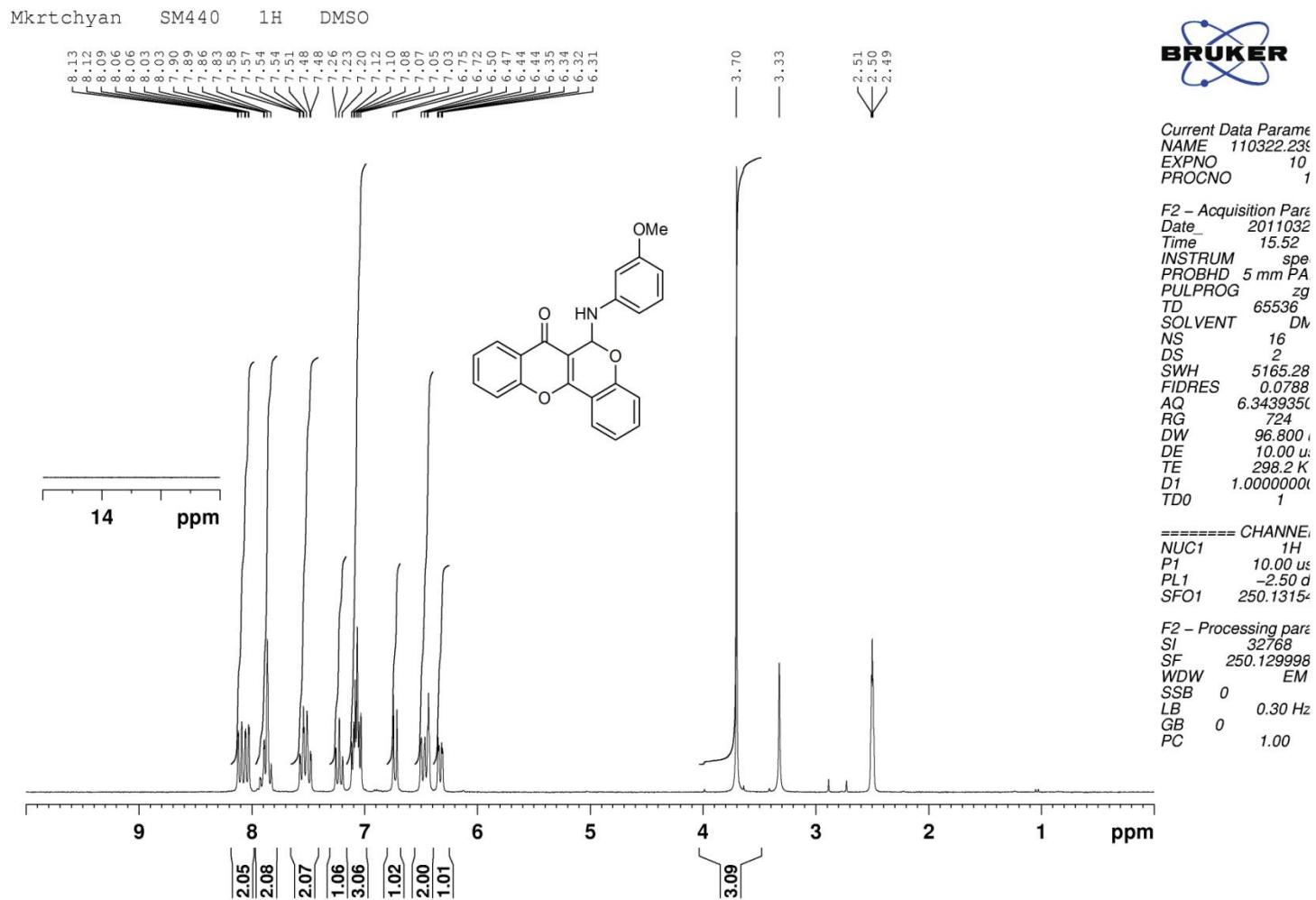
Compound 5e



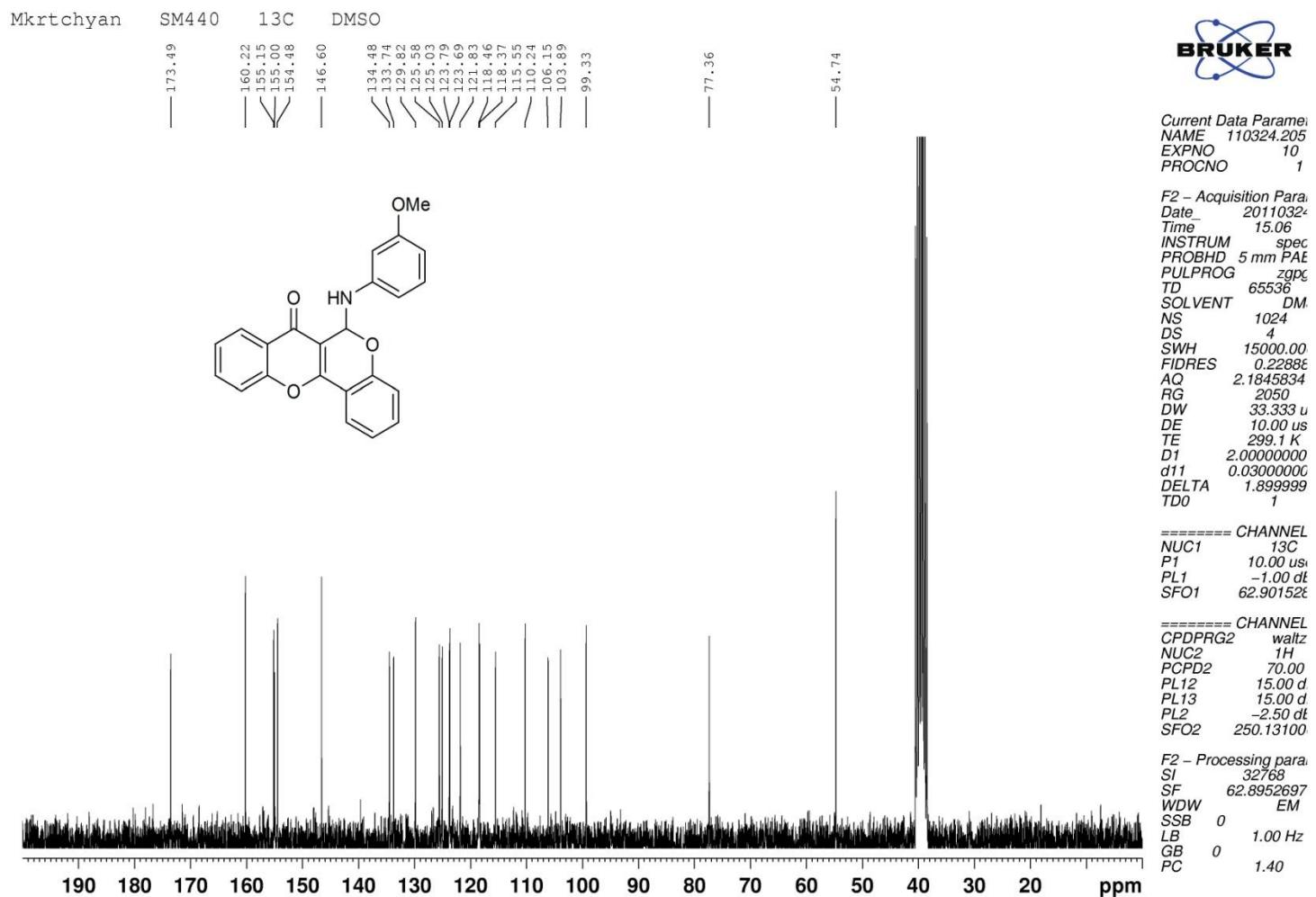
Compound 5e



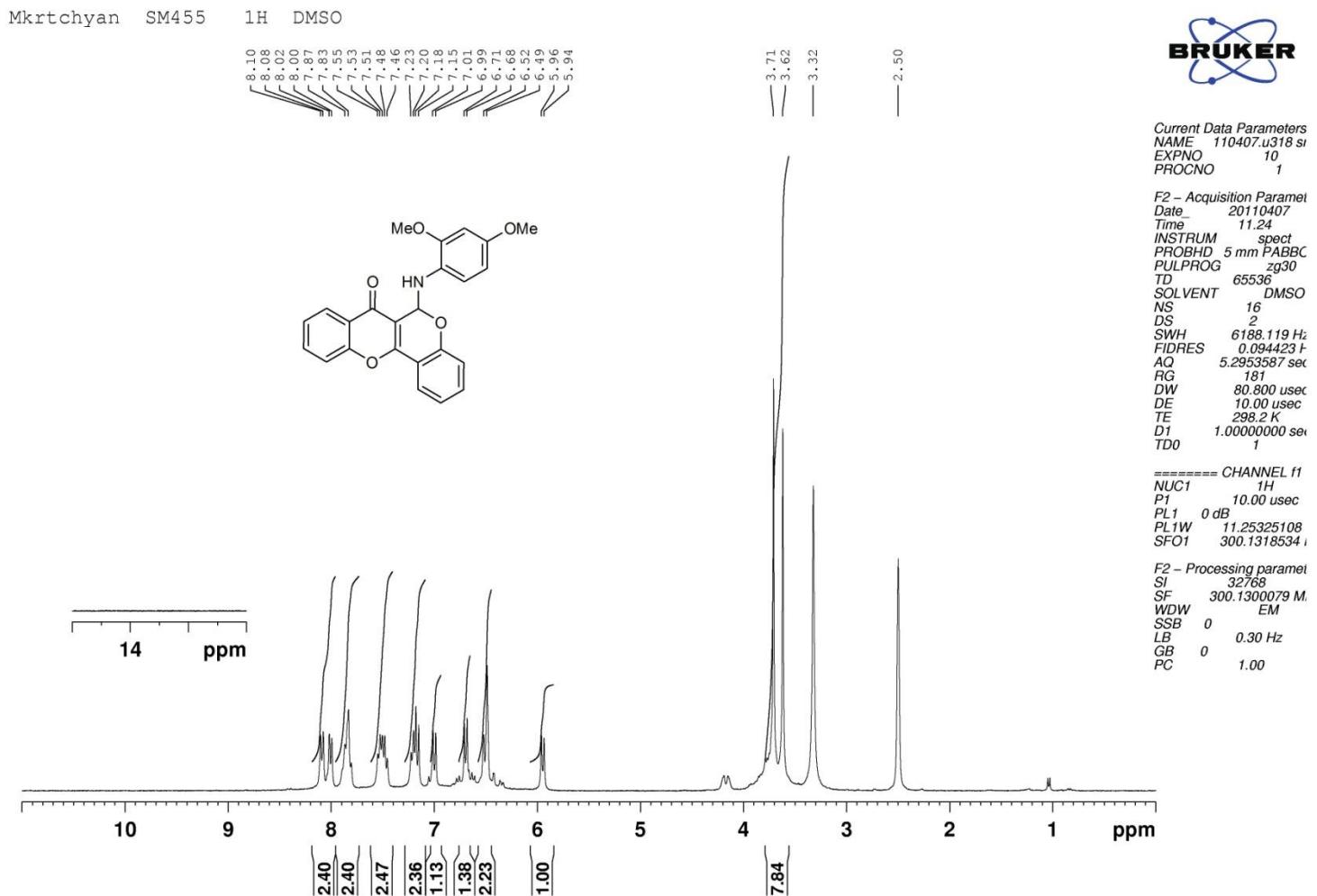
Compound 5f



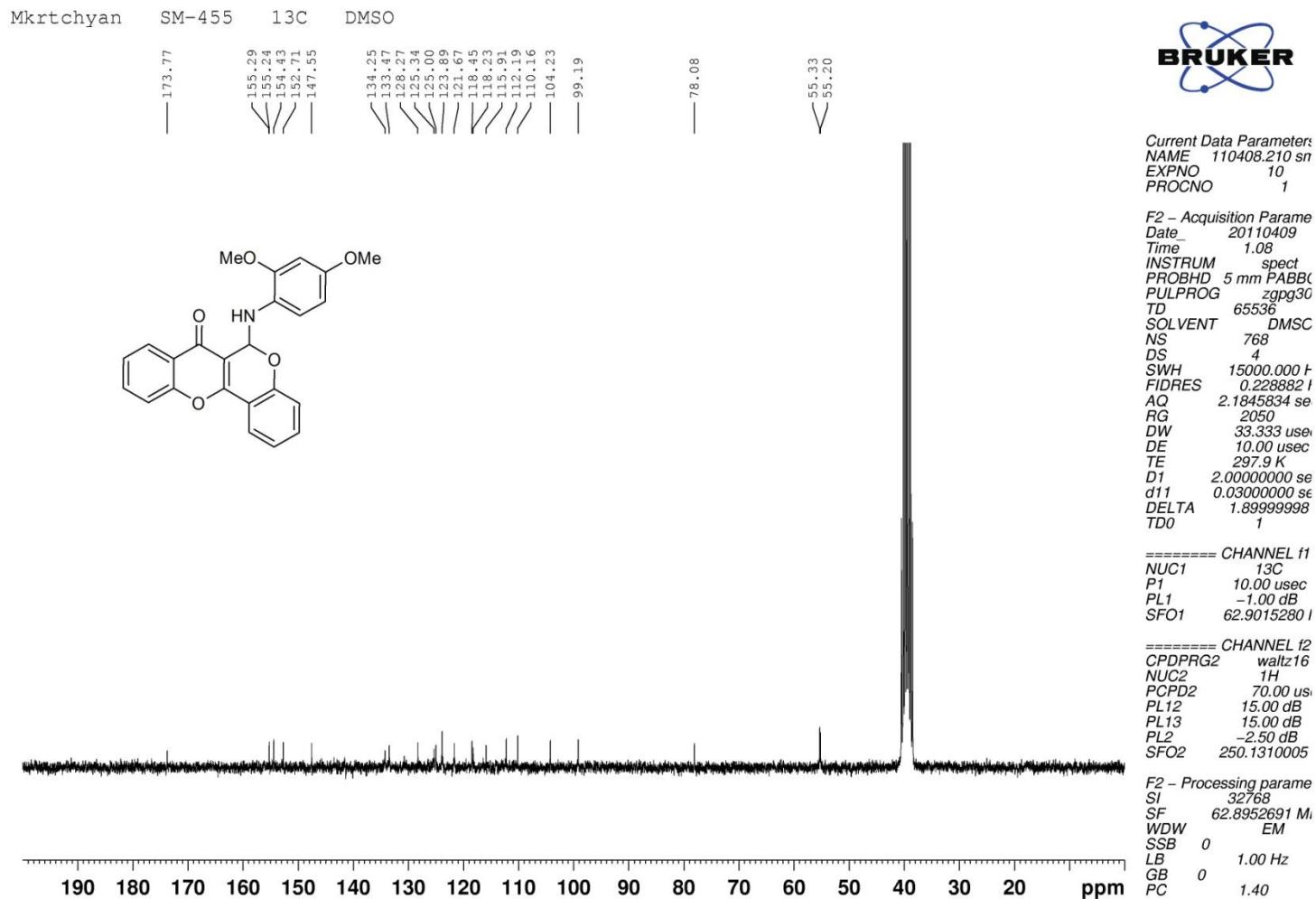
Compound 5f



Compound 5g

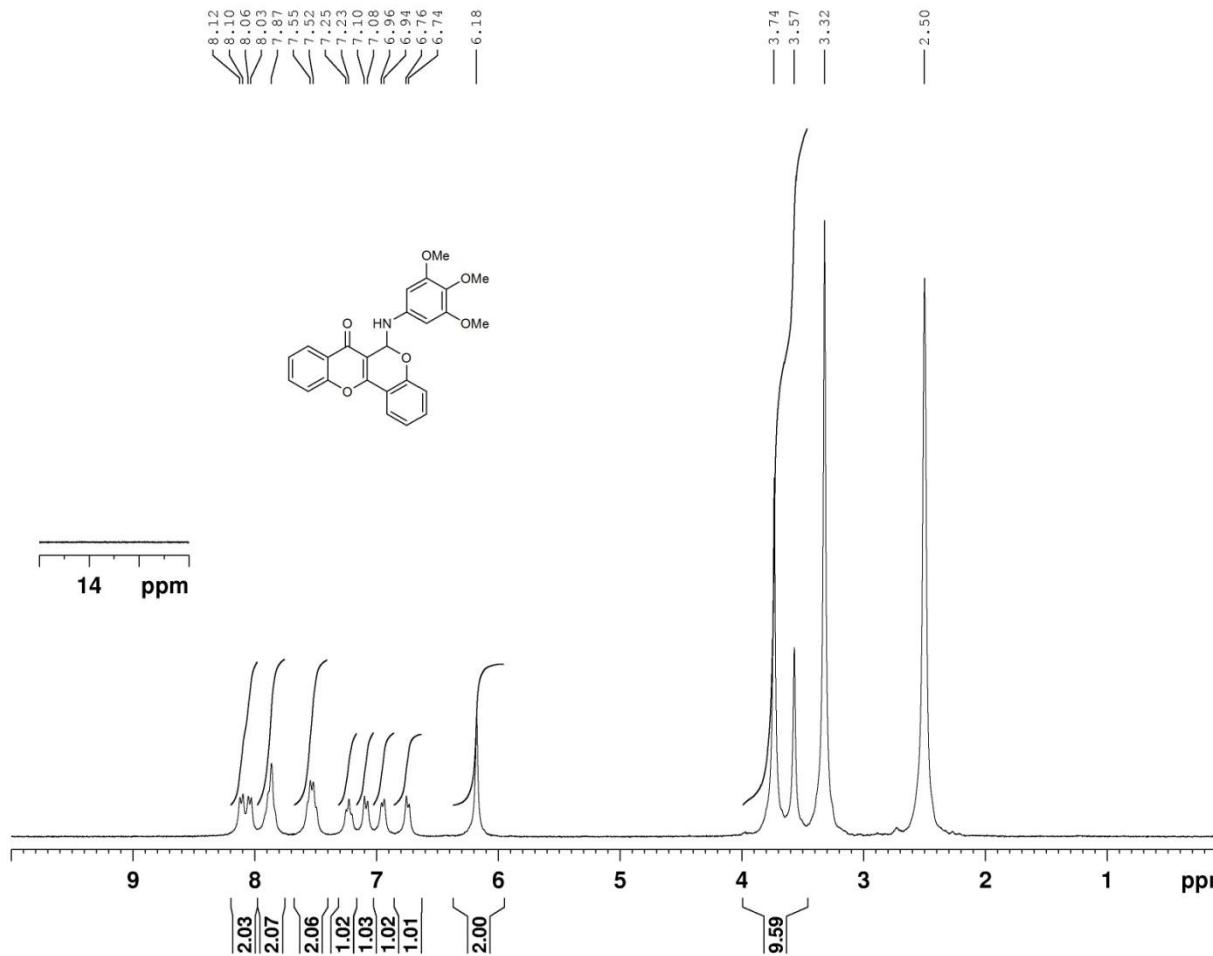


Compound 5g



Compound 5h

Mkrtchyan SM430 1H DMSO



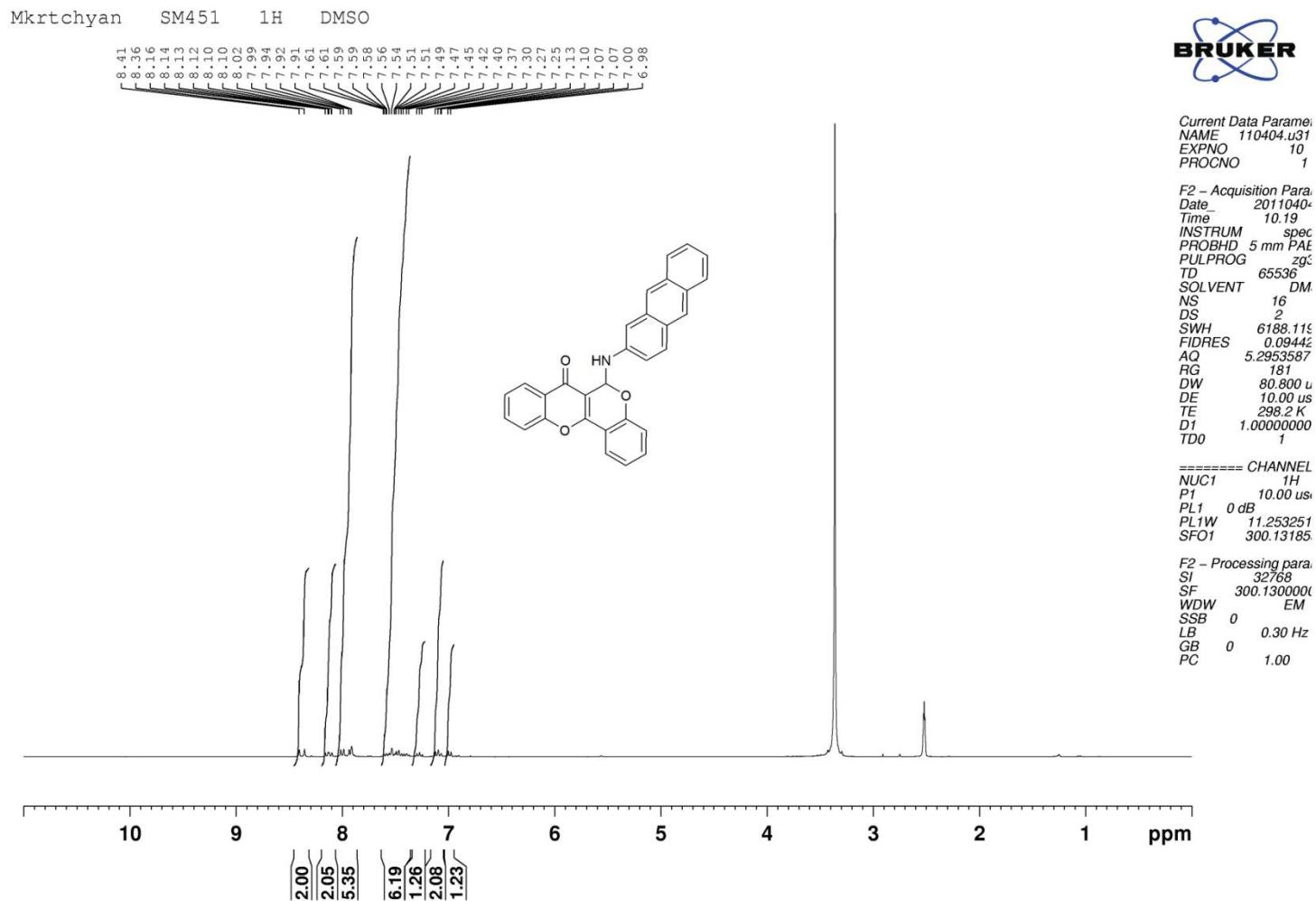
Current Data Parameters
NAME 130902.u312 s, 43
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20130902
Time 11.33
INSTRUM spect
PROBHD 5 mm PABBO BI
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 1.0000000 sec
TD0 1

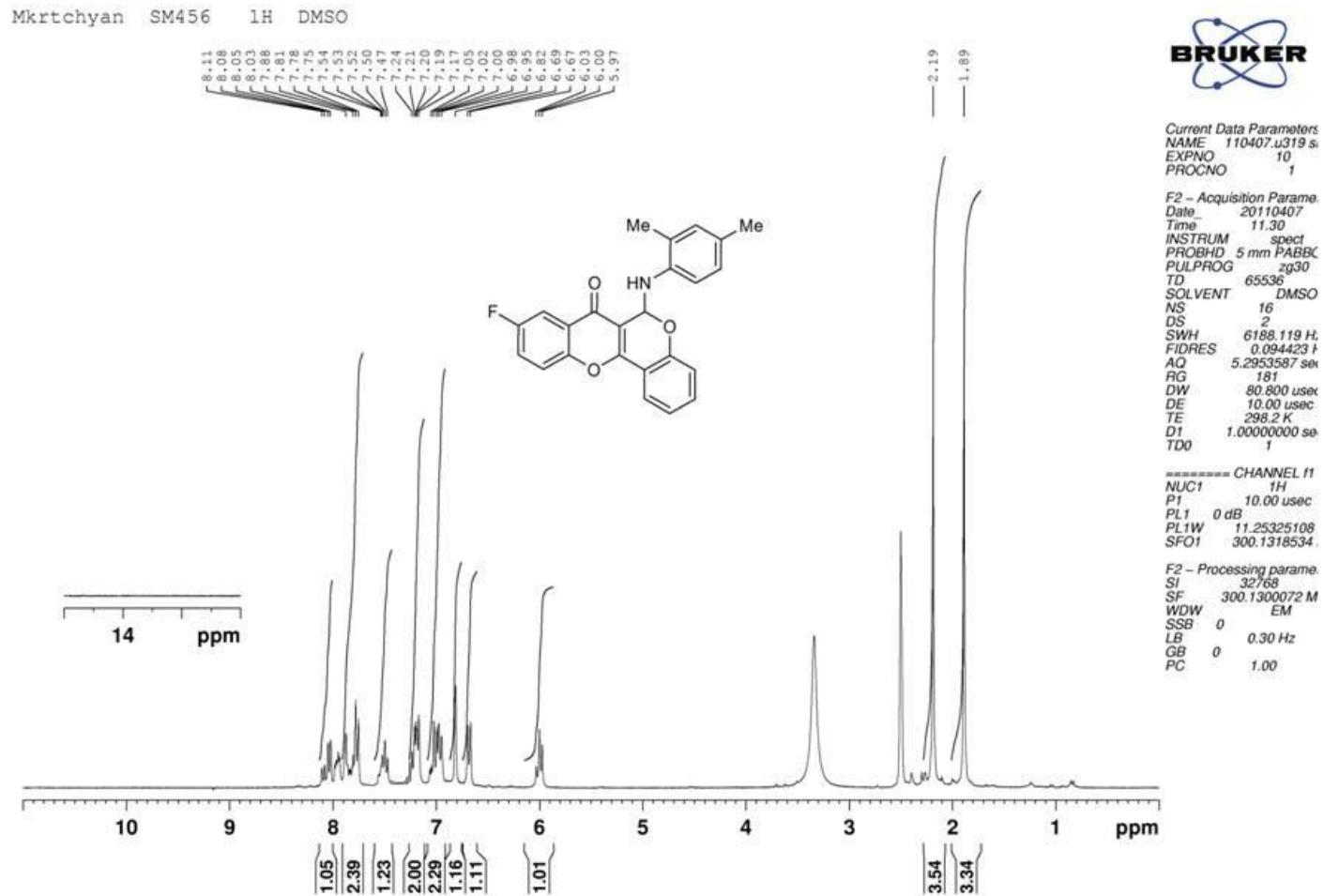
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300354 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

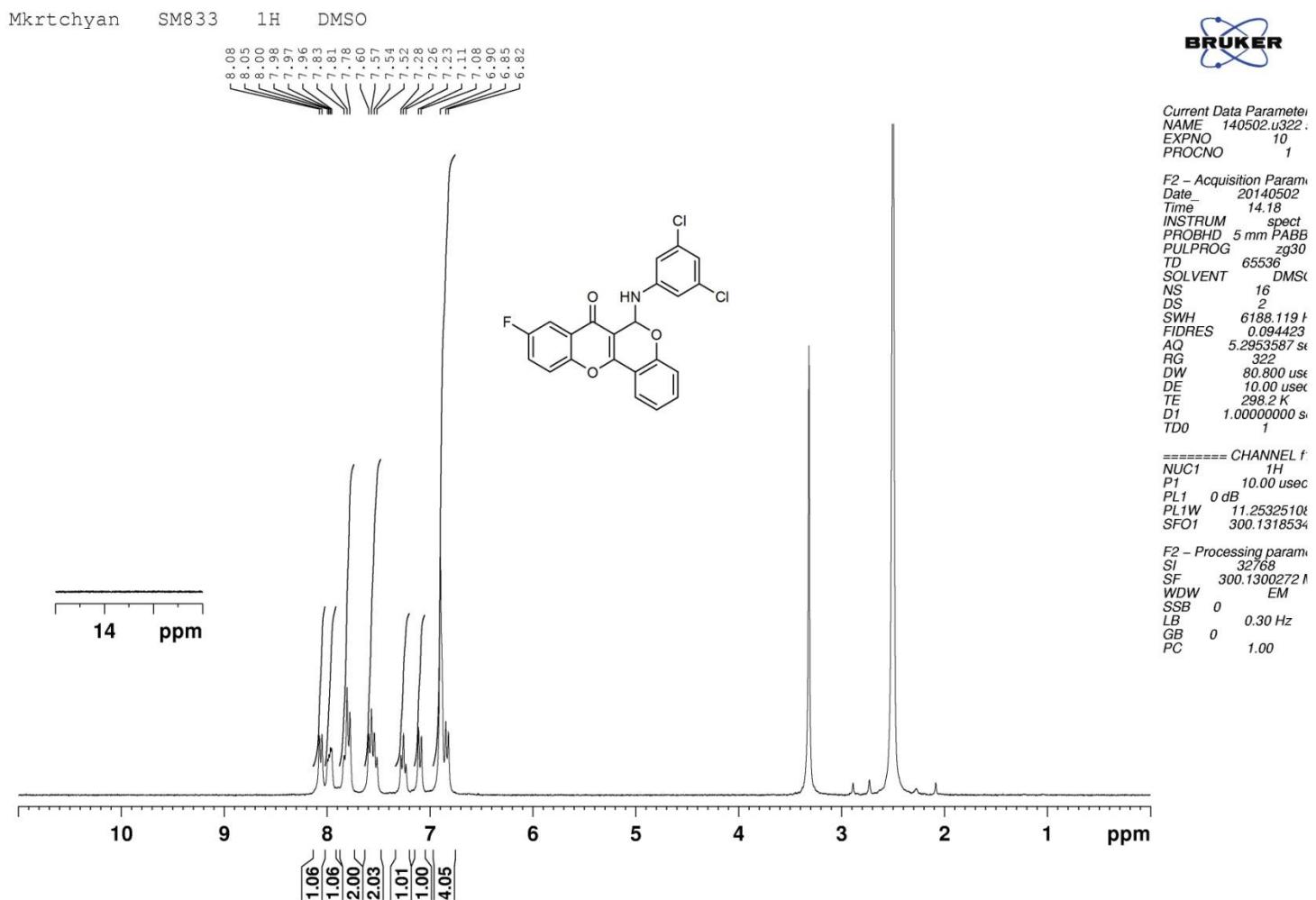
Compound 5i



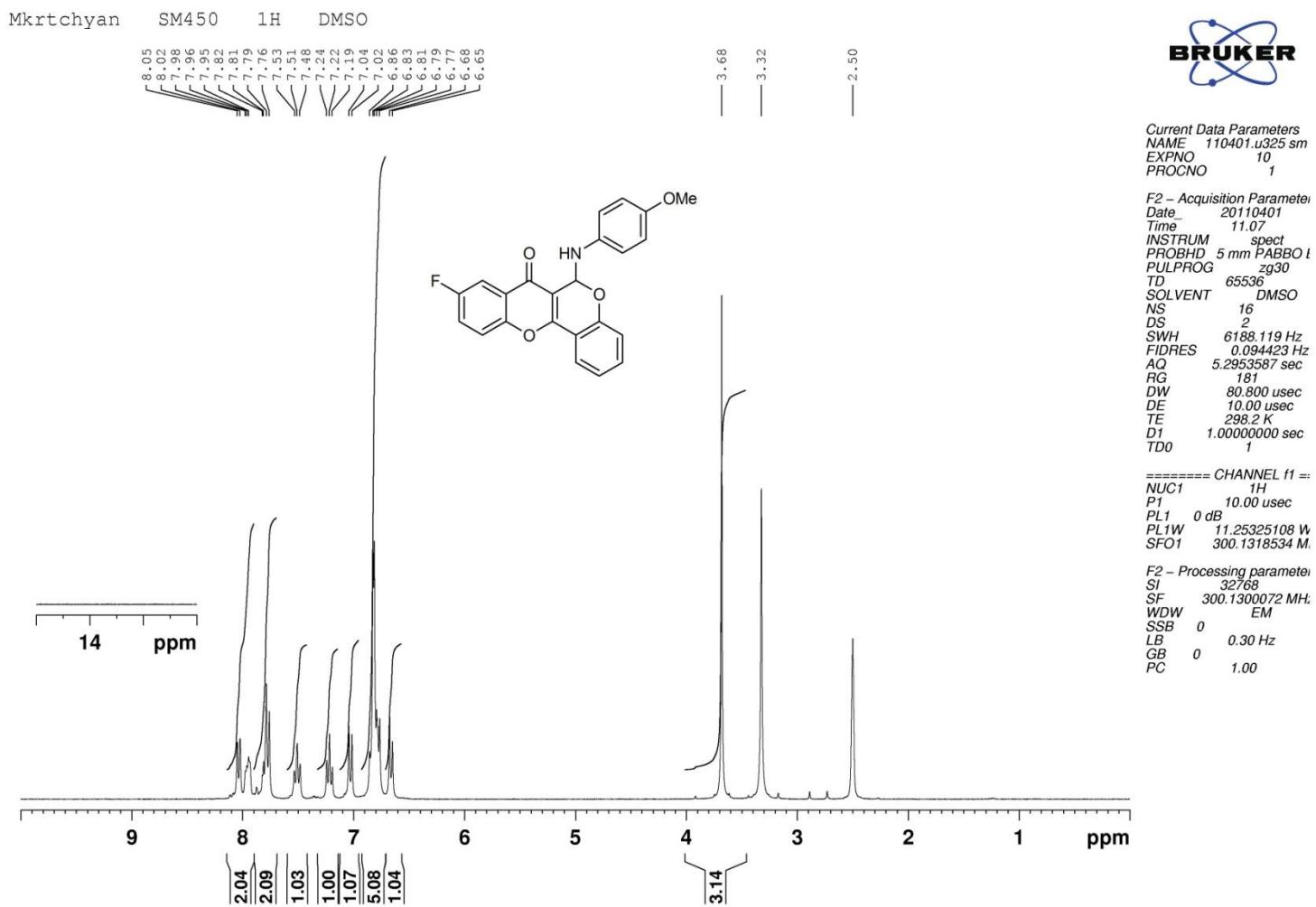
Compound 5j



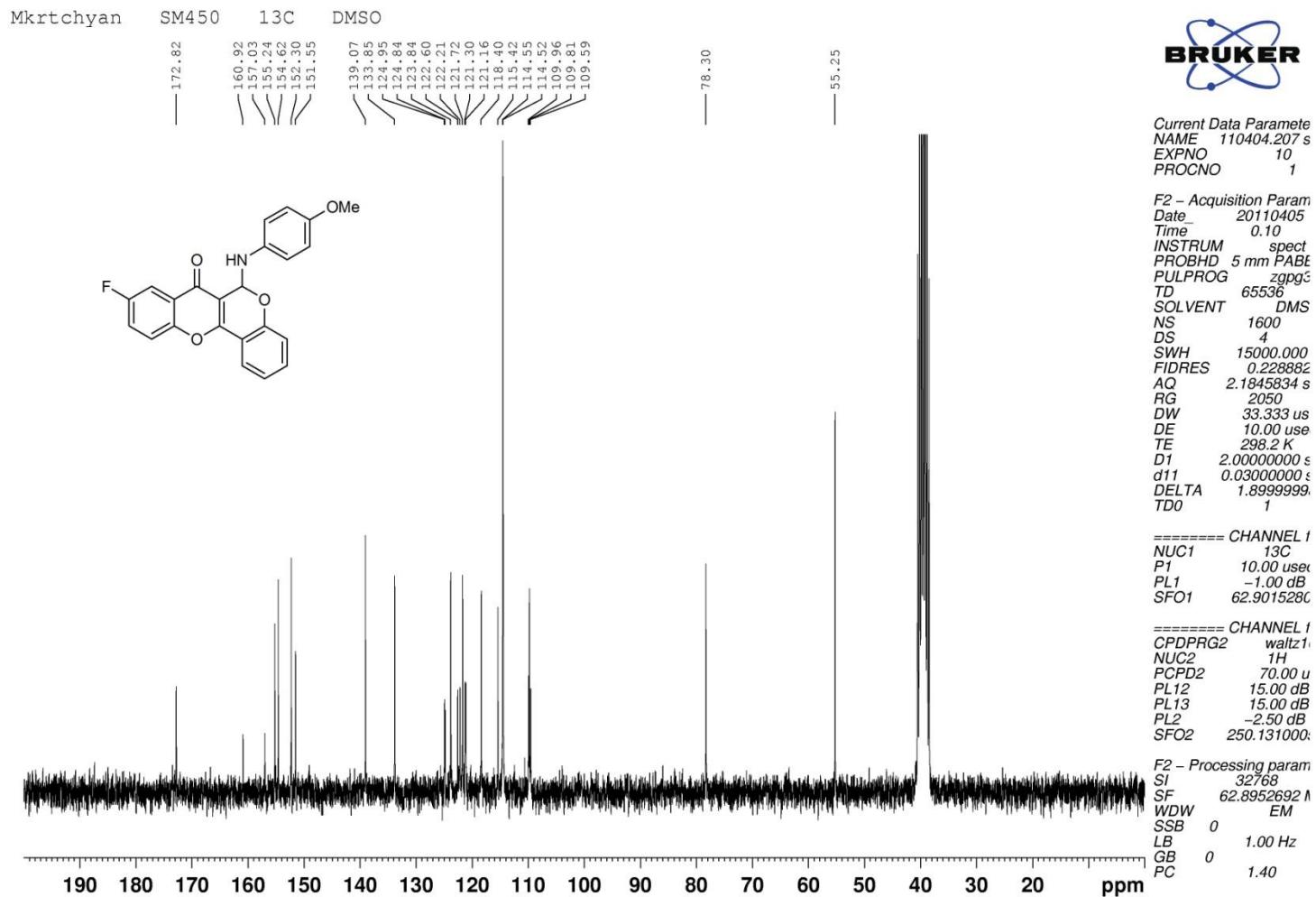
Compound 5k



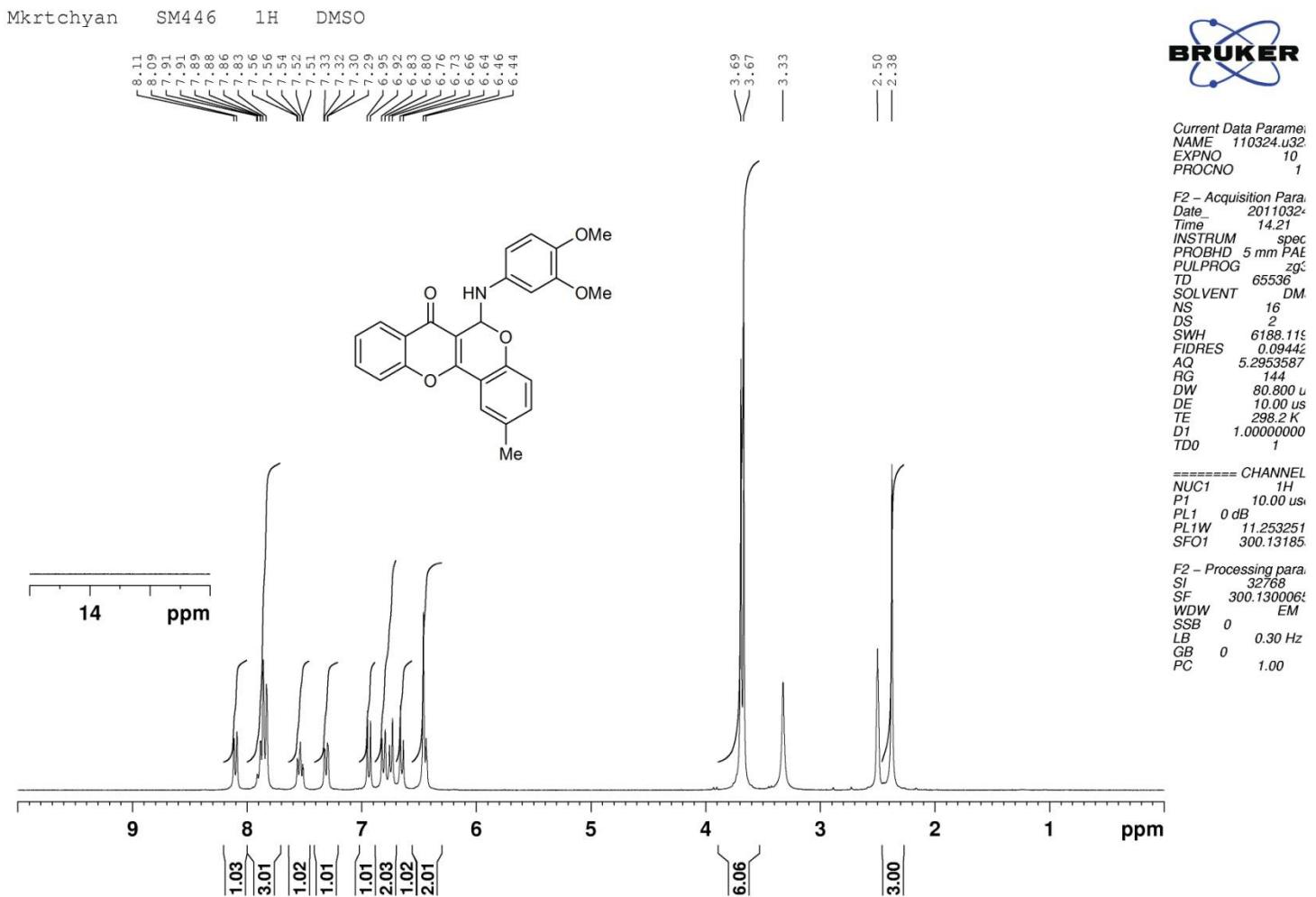
Compound 5l



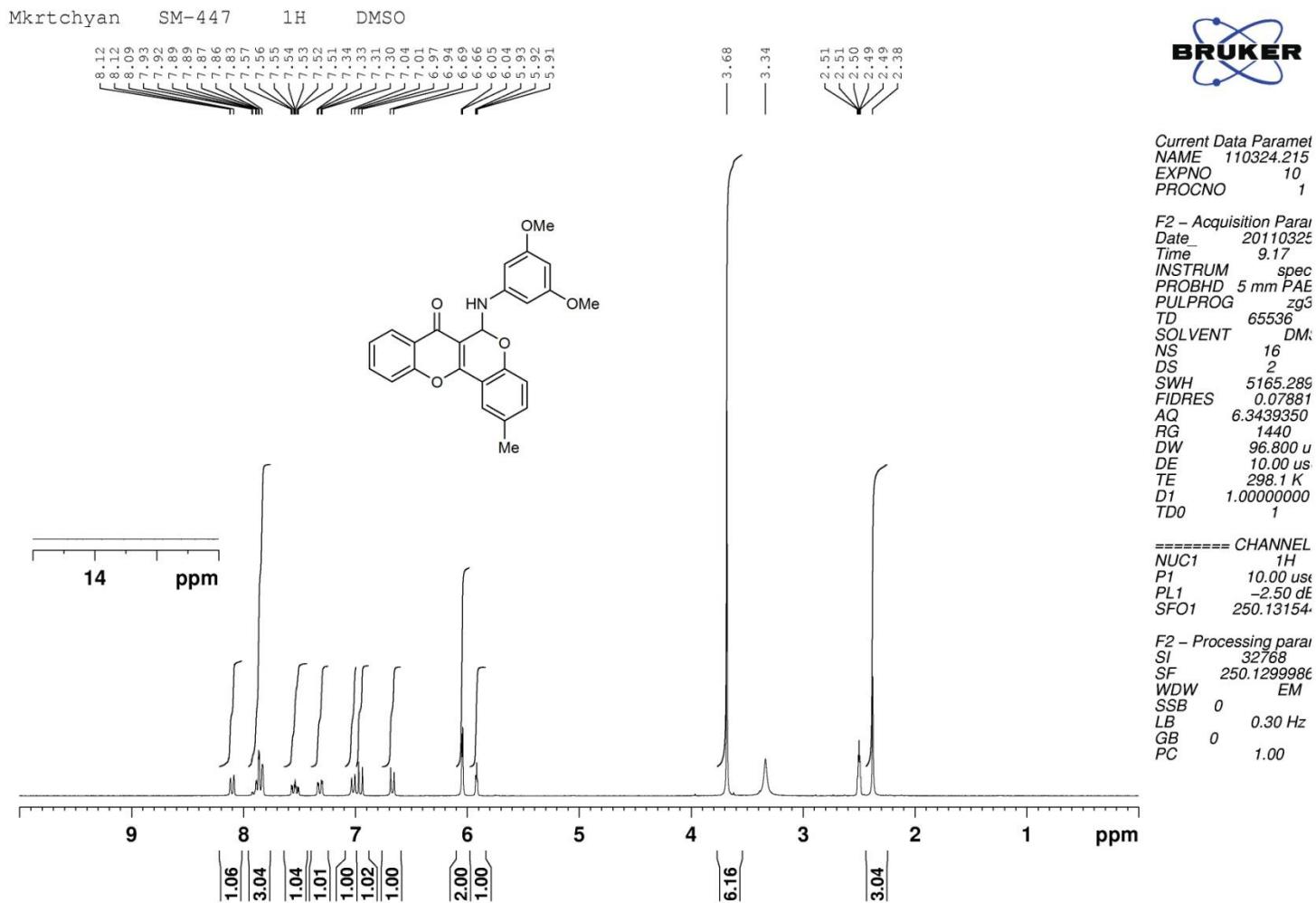
Compound 5l



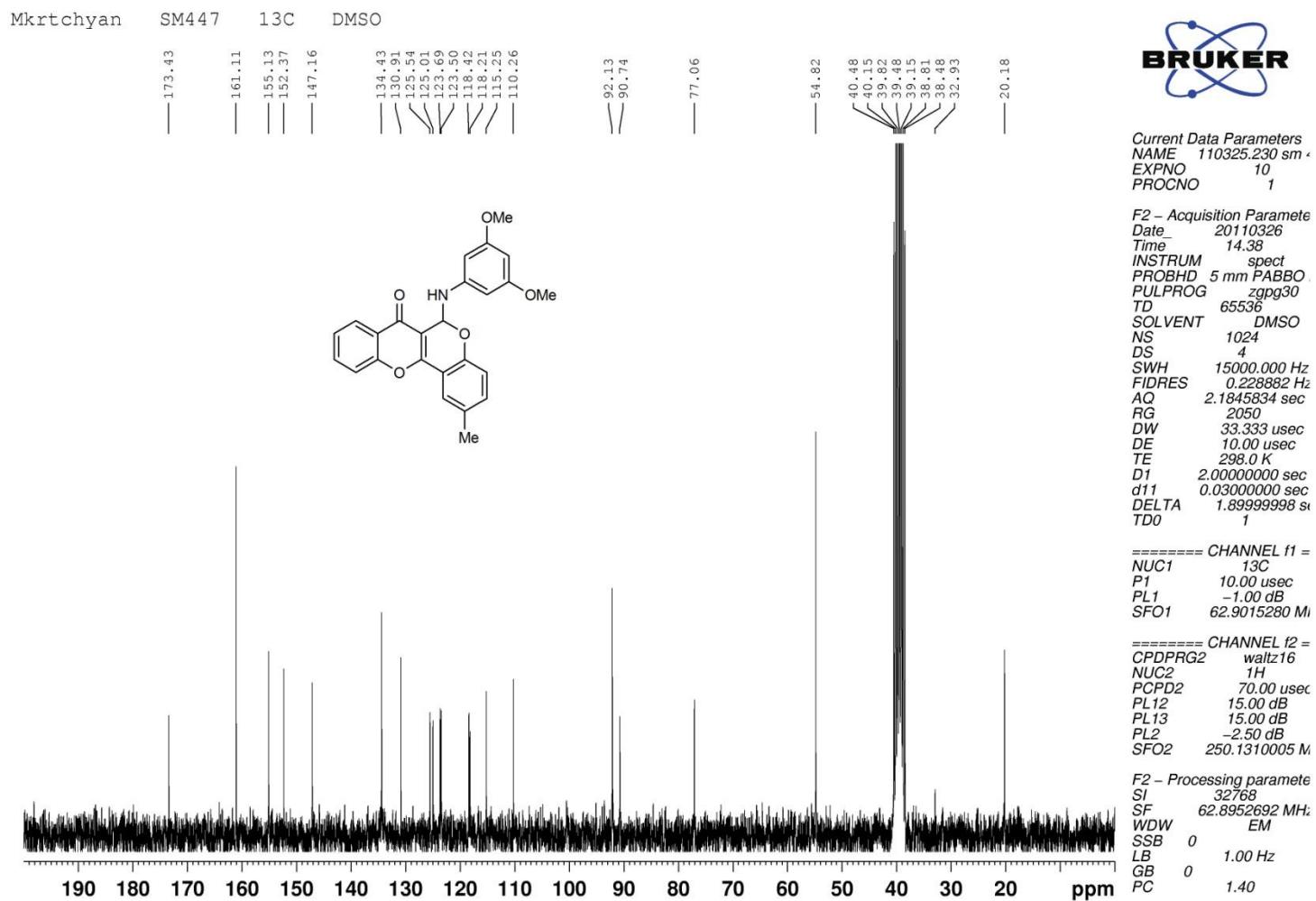
Compound 5m



Compound 5n

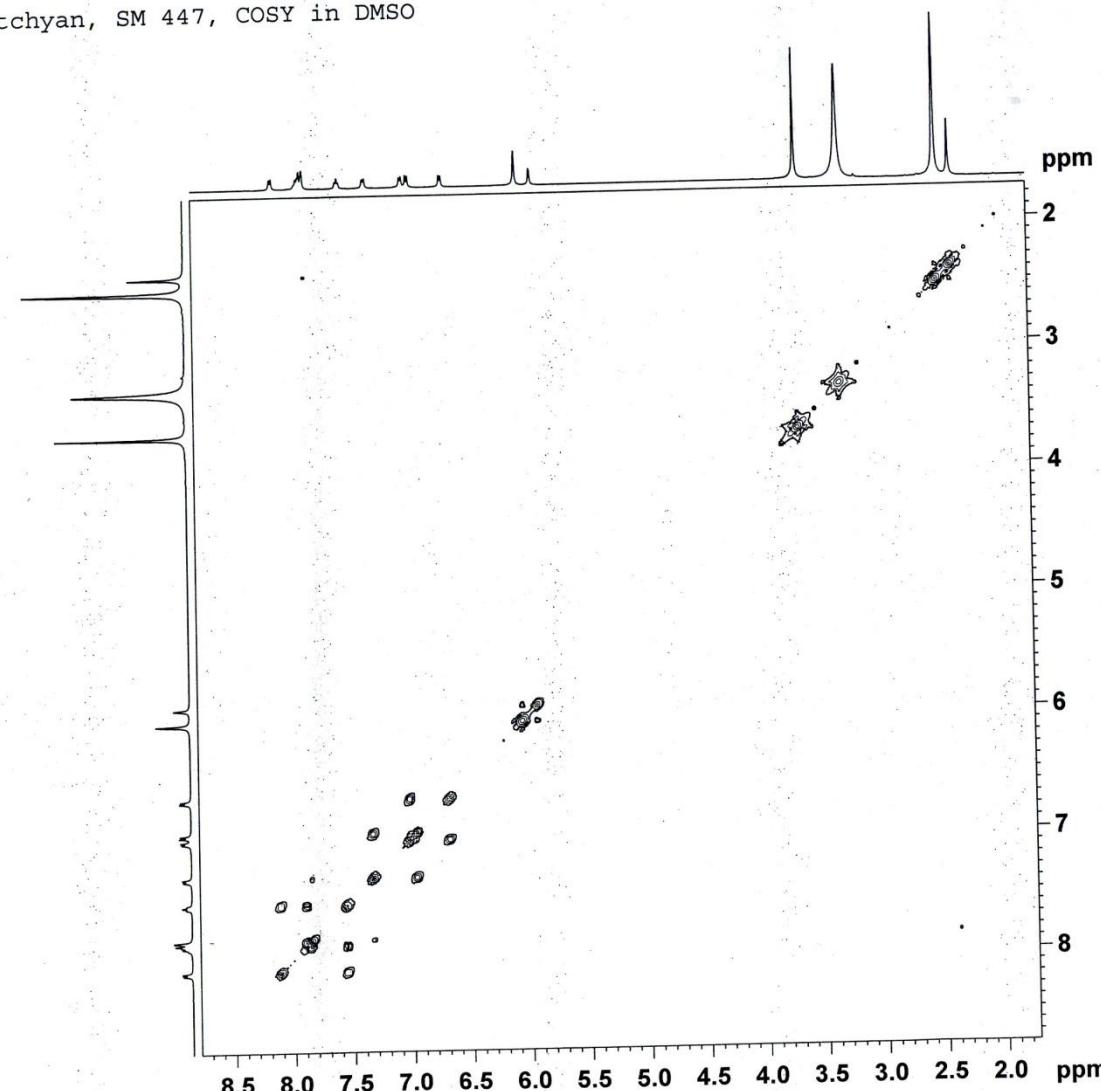


Compound 5n



Compound 5n

Mkrtchyan, SM 447, COSY in DMSO



```

NAME          130903.502
EXPNO         11
PROCNO        1
Date_        20130903
Time       16.32
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG    cosygpqf
TD           2048
SOLVENT      DMSO
NS            2
DS            8
SWH         3531.073 Hz
FIDRES     1.724157 Hz
AQ          0.2901884 sec
RG           161.3
DW           141.600 usec
DE           10.00 usec
TE           300.1 K
DO          0.00000300 sec
D1          1.34967506 sec
D13          0.00000400 sec
D16          0.00020000 sec
IINO         0.00028320 sec

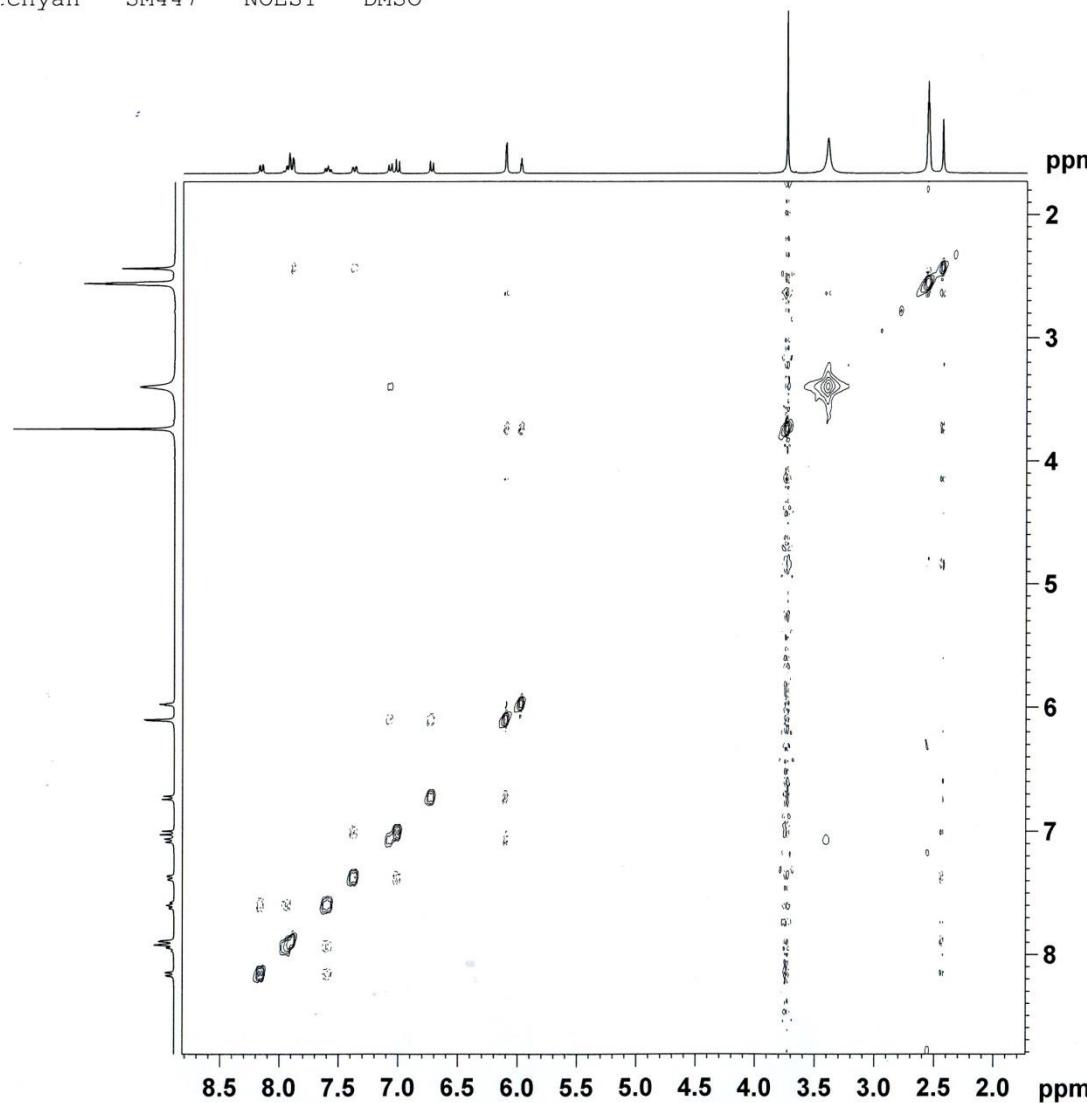
===== CHANNEL f1 =====
NUC1            1H
P0             9.80 usec
P1             9.80 usec
PL1           -3.00 dB
SFO1        500.1326327 MHz

===== GRADIENT CHANNEL =====
GPNAME1        SINE.100
GPZ1           10.00 %
P16          1000.00 usec
ND0              1
TD            128
SFO1        500.1326 MHz
FIDRES     27.586512 Hz
SW           7.060 ppm
FnMODE        QF
SI            1024
SF          500.1300000 MHz
WDW            SINE
SSB             0
LB             0.00 Hz
GB               0
PC            1.40
SI            1024
MC2            QF
SF          500.1300000 MHz
WDW            SINE
SSB             0
LB             0.00 Hz
GB               0

```

Compound 5n

Chyan SM447 NOESY DMSO



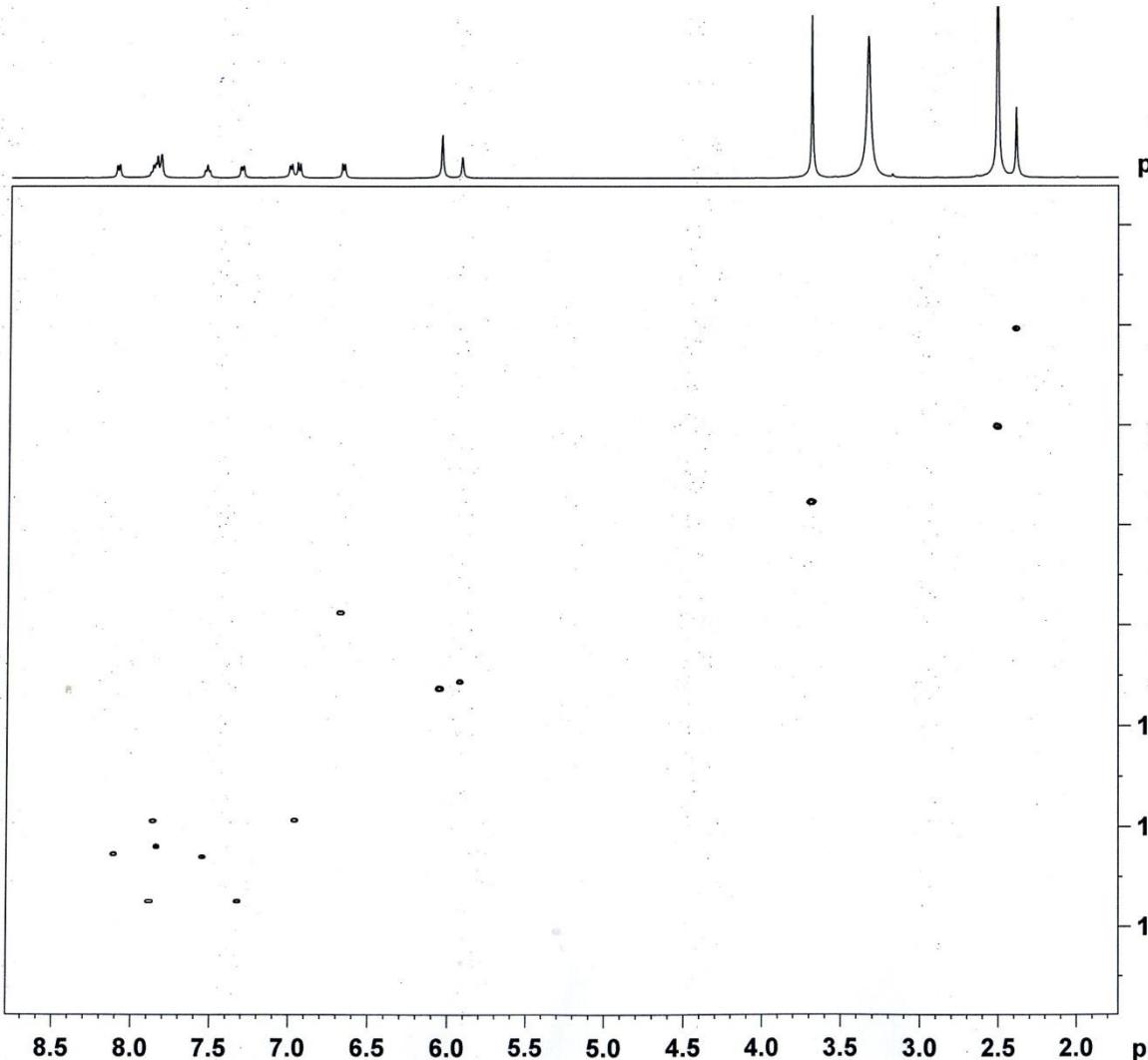
NAME 130830.u340
 EXPNO 14
 PROCN0 1
 Date 20130831
 Time 6.36
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG noesypf
 TD 2048
 SOLVENT DMSO
 NS 16
 DS 4
 SWH 2127.660 Hz
 FIDRES 1.038896 Hz
 AQ 0.4813300 sec
 RG 64
 DW 235.000 usec
 DE 10.00 usec
 TE 298.2 K
 D0 0.00022227 sec
 D1 1.85295296 sec
 D8 1.5000000 sec
 IN0 0.00047000 sec

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

NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 PL1W 11.25325108 W
 SFO1 300.1315826 MHz
 NDO 1
 TD 256
 SFO1 300.1316 MHz
 FIDRES 8.311171 Hz
 SW 7.089 ppm
 FnMODE States-TPPI
 SI 1024
 SF 300.1300000 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.00
 SI 1024
 MC2 States-TPPI
 SF 300.1300000 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

Compound 5n

Mkrtchyan, SM 447, HSQC in DMSO



```

NAME          130903.502
EXPNO         12
PROCNO        1
Date_        20130903
Time_        16.42
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG    hsqcetgps12
TD           1024
SOLVENT      DMSO
NS            4
DS            16
SWH          3531.073 Hz
FIDRES       3.448314 Hz
AQ            0.1451900 sec
RG            18390.4
DW            141.600 usec
DE            1.000 usec
TE            300.0 K
CST2         145.000000 sec
D0           0.0000300 sec
D1           1.43139195 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            0.00 usec
PL1            -3.00 dB
SF01          500.1326327 MHz

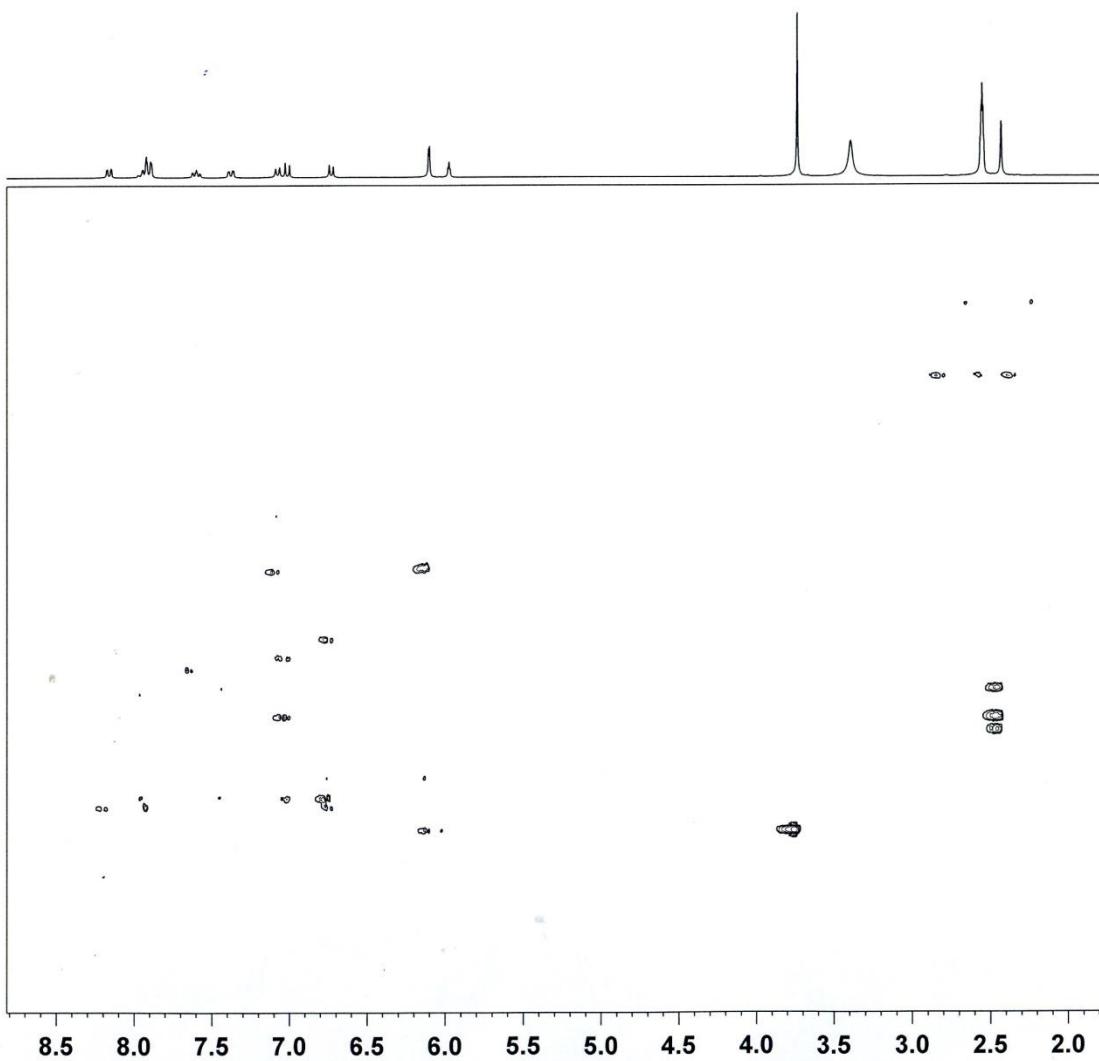
***** CHANNEL f2 *****
CRDPRG2        garp
NUC2           13C
P3             9.00 usec
P4             18.00 usec
PCPD2          72.00 usec
PL2            4.50 dB
PL12           22.00 dB
SF02          125.7672177 MHz

***** GRADIENT CHANNEL *****
GNAM1          SINE,100
GNAM2          SINE,100
GNAM3          SINE,100
GNAM4          SINE,100
GPZ1           80.00 %
GPZ2           20.10 %
GPZ3           11.00 %
GPZ4           -5.00 %
P16            1000.00 usec
P19            600.00 usec
ND00           2
TD            256
SF01          125.7672 MHz
FIDRES        81.380234 Hz
SW            165.650 ppm
FmMODE        Echo-Antiecho
SI             1024
SF            500.1300000 MHz
WDW            QSINE
SSB            2
LB             0.00 Hz
GB             0
PC             1.40
SI             1024
MC2           echo-antiecho
SF            125.7577890 MHz
WDW            QSINE
SSB            2
LB             0.00 Hz
GB             0

```

Compound 5n

Mkrtchyan SM447 HMBC DMSO



```

NAME          130830.u340
EXPNO         13
PROCNO        1
Date_       20130831
Time_        1.52
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG     hmbcgpndqf
TD           4096
SOLVENT      DMSO
NS            64
DS            16
SWH          2127.660 Hz
FIDRES      0.519448 Hz
AQ           0.9626100 sec
RG           2050
DW           235.000 usec
DE           10.00 usec
TE           298.2 K
CNUST13     8.0000000
D0           0.00000300 sec
D1           1.04944003 sec
D6           0.06250000 sec
D16          0.00020000 sec
INO          0.00002985 sec

```

0

```

----- CHANNEL f1 -----
NUC1          1H
P1           10.00 usec
P2           20.00 usec
PL1          0.00 dB
PL1W         11.25325108 W
SF01         300.1315826 MHz

```

20

```

----- CHANNEL f2 -----
NUC2          13C
P3           10.00 usec
PL2          -0.50 dB
PL2W         33.25691986 W
SF02         75.4752833 MHz

```

40

```

----- GRADIENT CHANNEL -----
GPNAME1      SINE.100
GPNAME2      SINE.100
GPNAME3      SINE.100
GPZ1          50.00 %
GPZ2          30.00 %
GPZ3          40.10 %
P16           1000.00 usec
NDO            2
TD             128
SF01          75.47528 MHz
FIDRES      130.958496 Hz
SW            222.095 ppm
FnMODE       QF
SI             1024
SF            300.1300000 MHz
WDW           SINE
SSB            0
LB             0.00 Hz
GB             0
PC             1.40
SI             1024
MC2           QF
SF            75.4677490 MHz
WDW           SINE
SSB            0
LB             0.00 Hz
GB             0

```

60

80

100

120

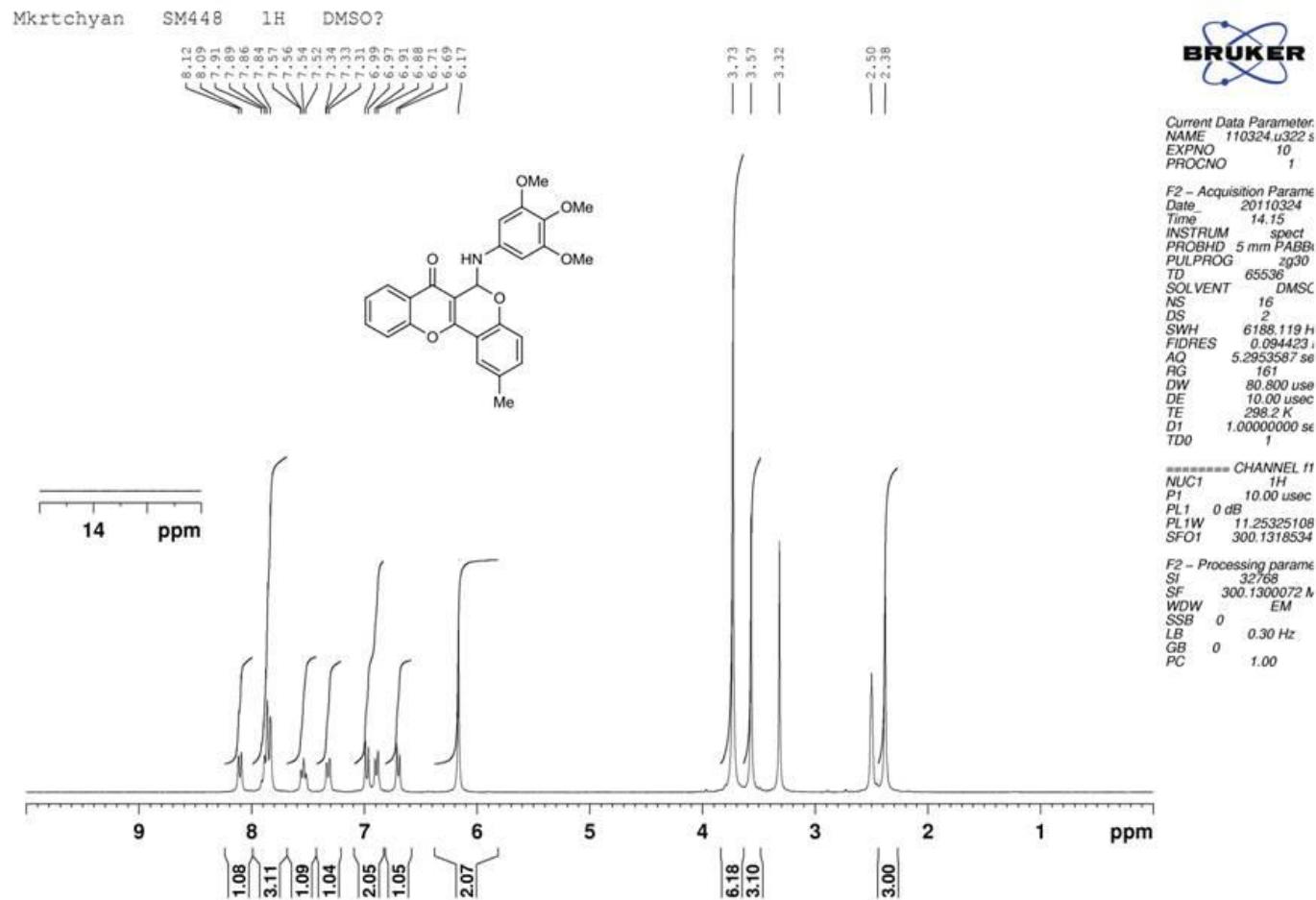
140

160

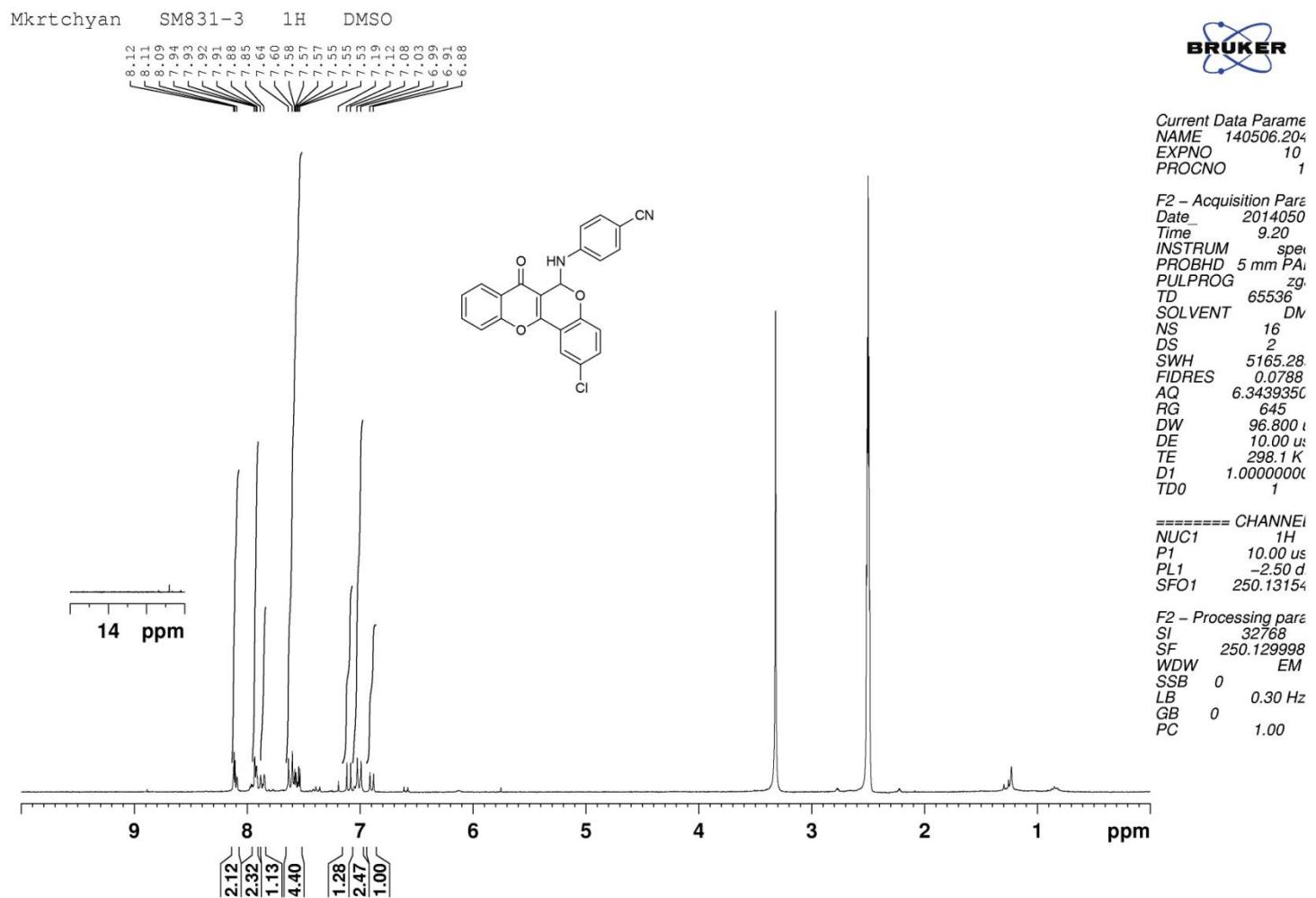
180

200

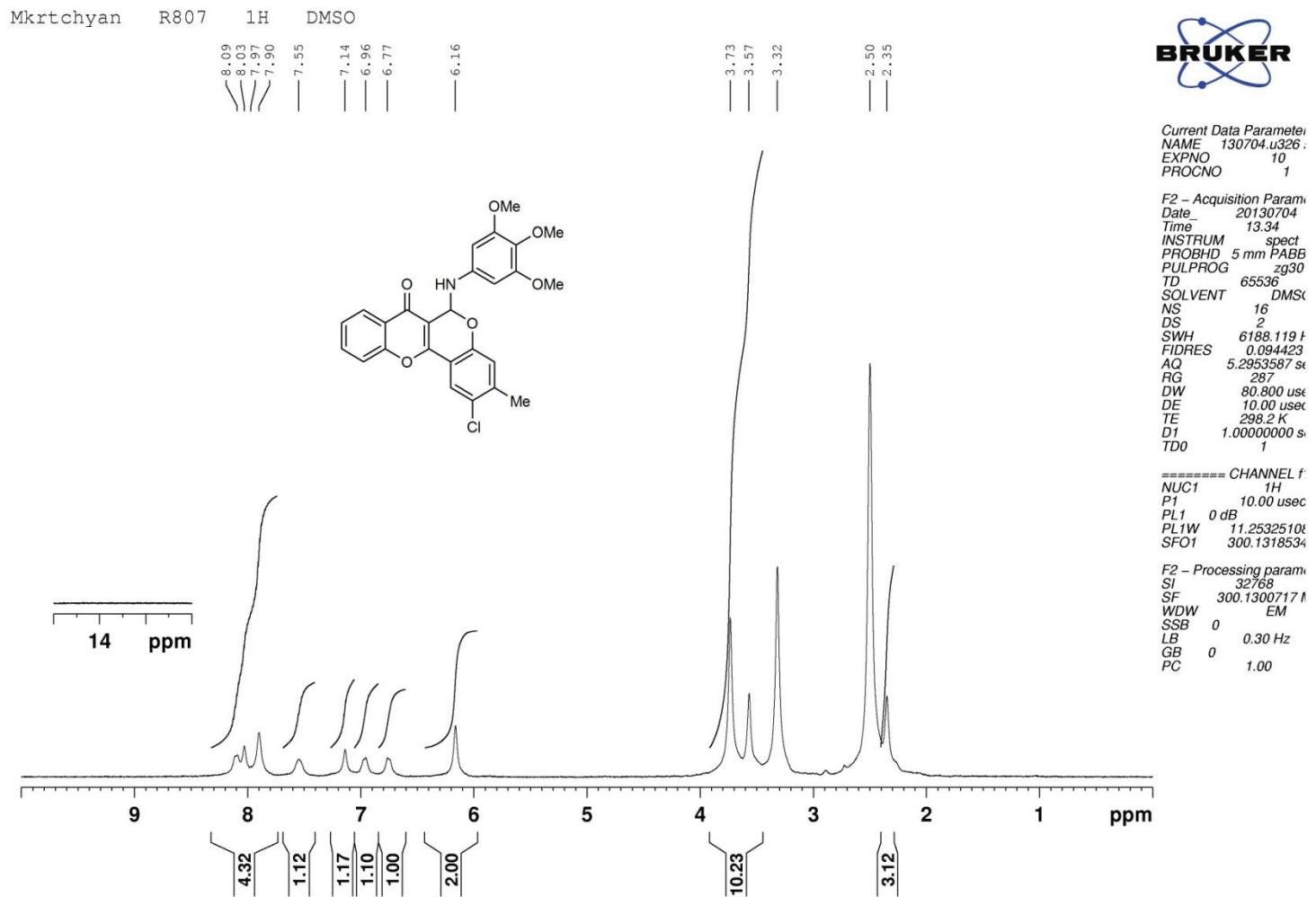
Compound 5o



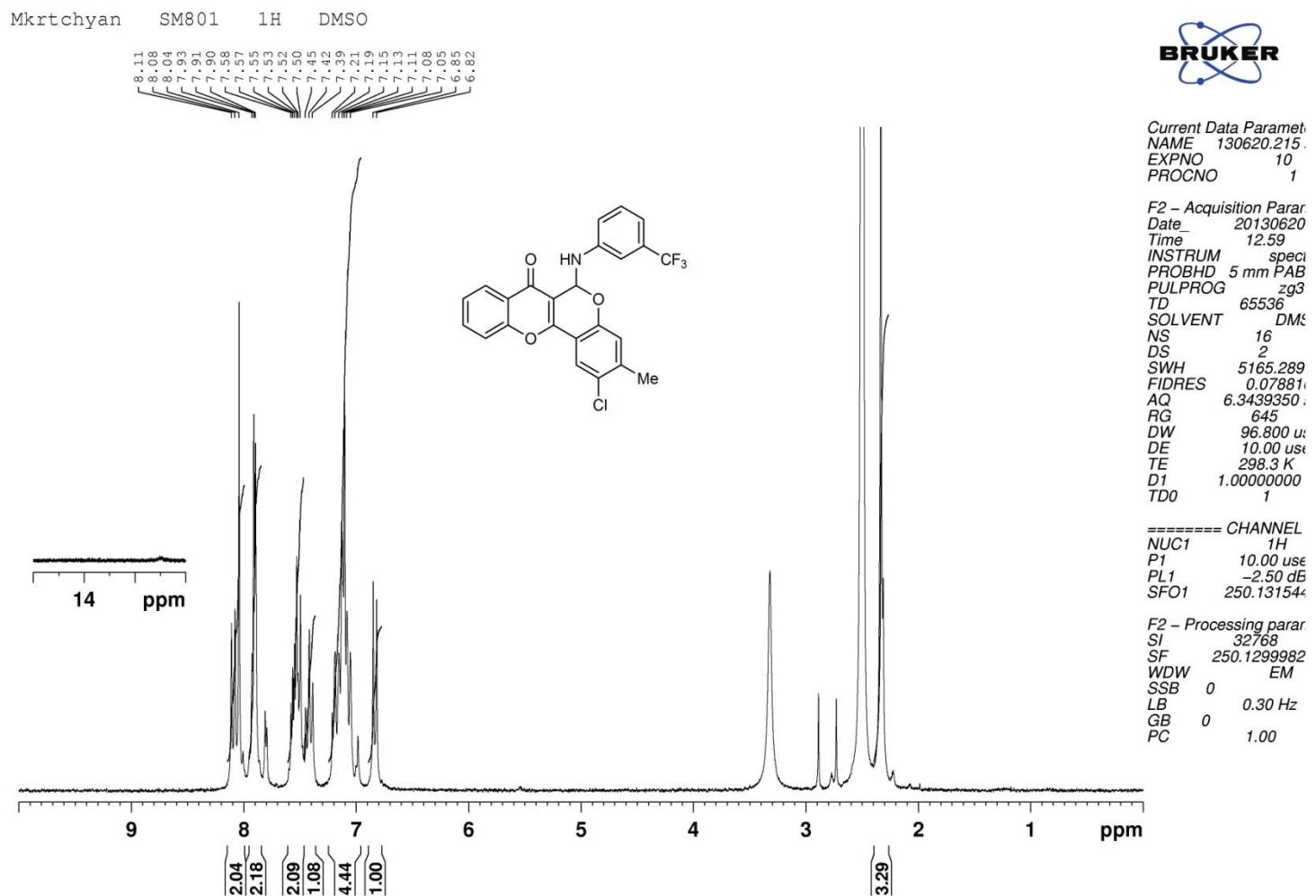
Compound 5p



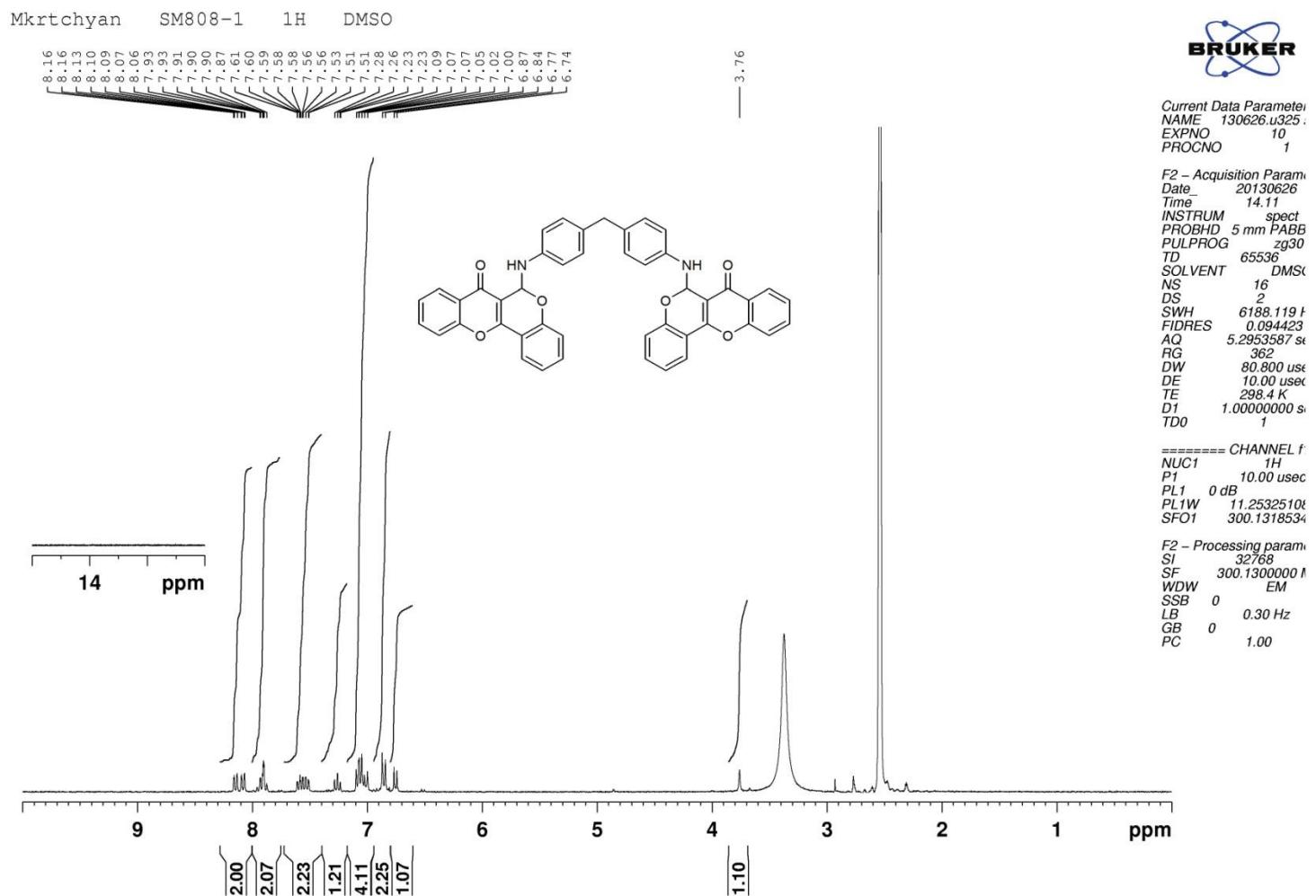
Compound 5q



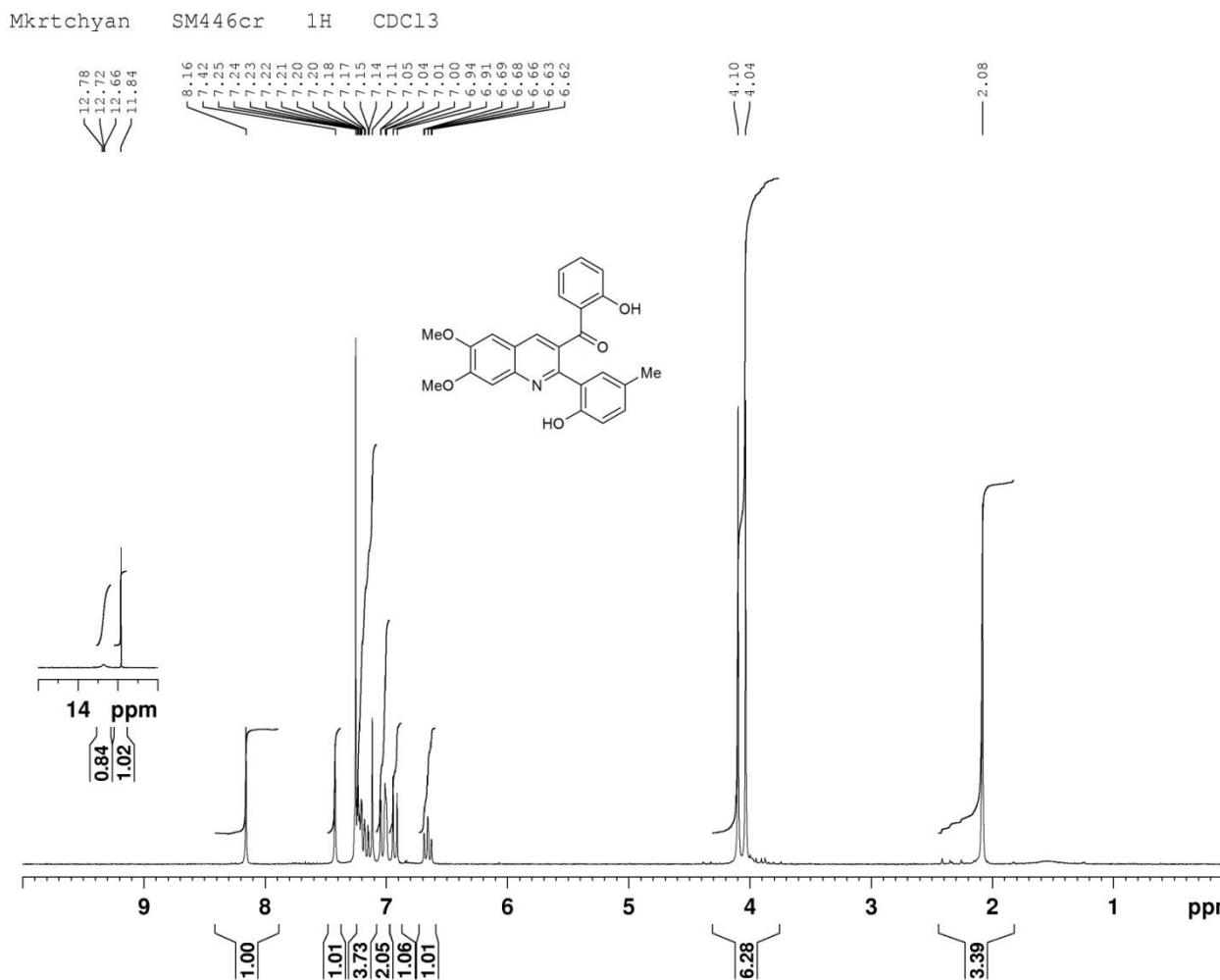
Compound 5r



Compound 5s



Compound 6a



BRUKER

Current Data Parameters
NAME 140430.202 sm.
EXPNO 10
PROCNO 1

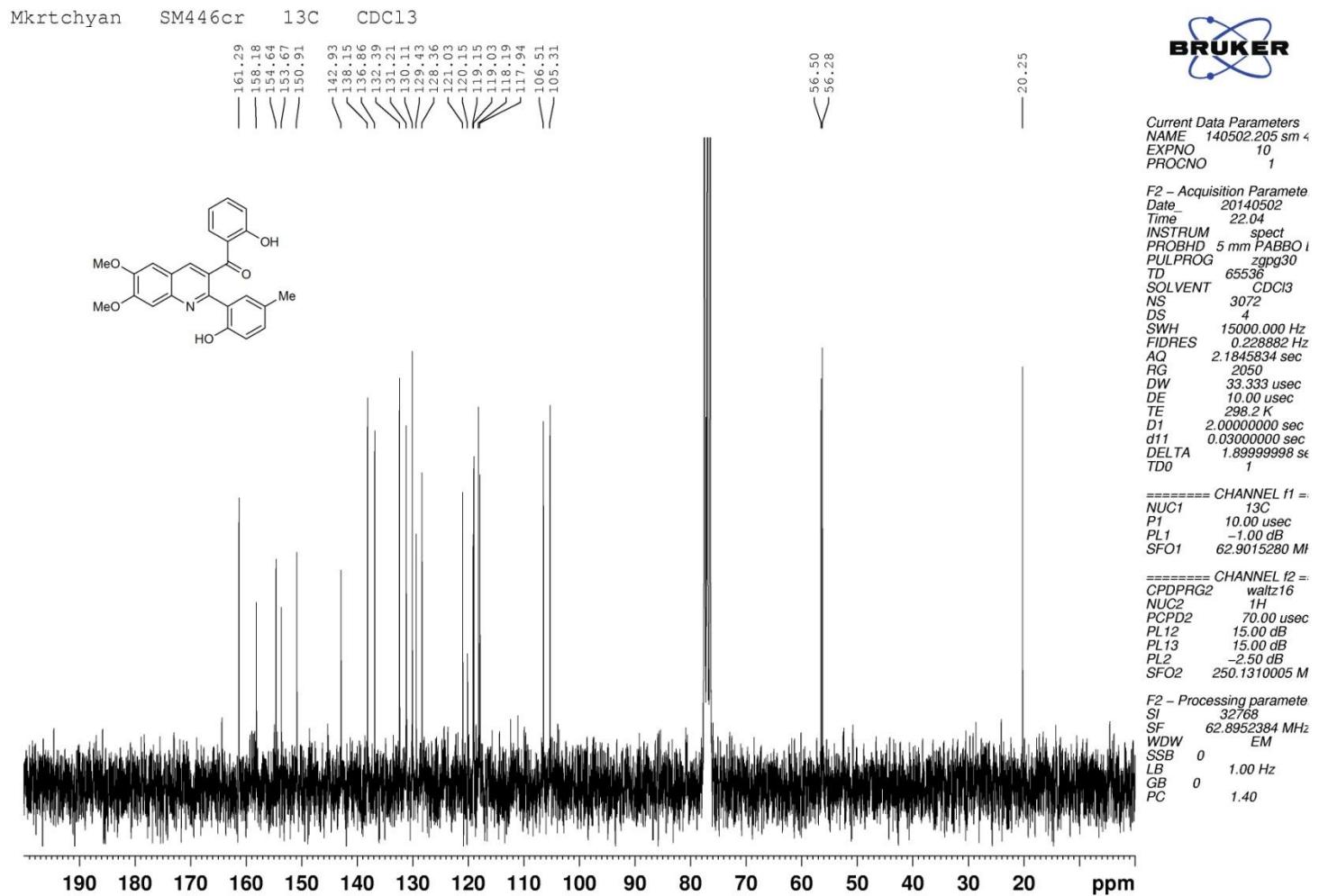
F2 - Acquisition Parameters
 Date _ 20140430
 Time 11.10
 INSTRUM spect
 PROBHD 5 mm PABBO
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 5165.289 Hz
 FIDRES 0.078816 Hz
 AQ 6.3439350 sec
 RG 645
 DW 96.800 usec
 DE 10.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =
NUC1 1H
P1 10.00 usec
PL1 -2.50 dB
SFQ1 250.1315447 N

F2 - Processing parameters

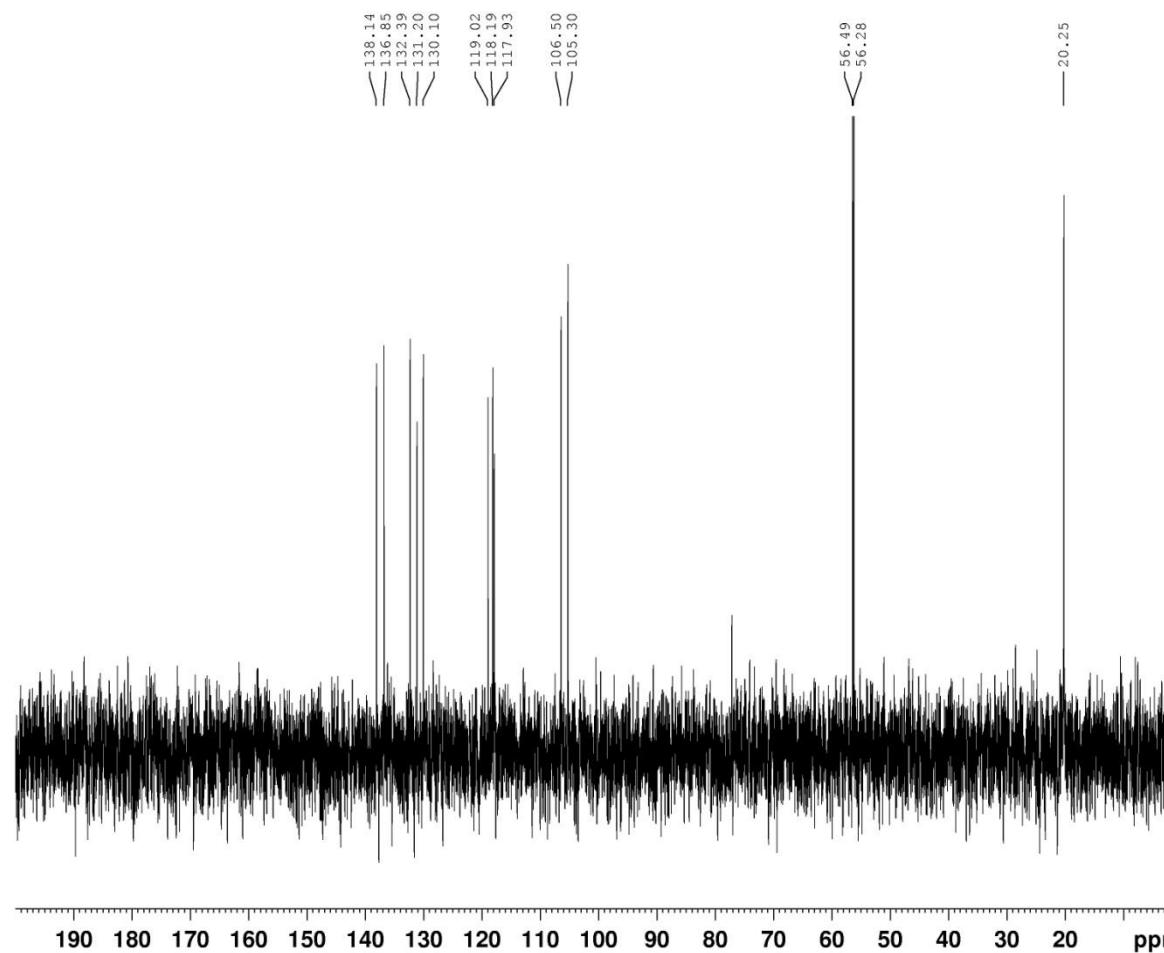
<i>SI</i>	32768
<i>SF</i>	250.1300030 MHz
<i>WDW</i>	EM
<i>SSB</i>	0
<i>LB</i>	0.30 Hz
<i>GB</i>	0
<i>PC</i>	1.00

Compound 6a



Compound 6a

Mkrtchyan SM446cr Dept CDC13



Current Data Parameters
NAME 6a 140502.205
EXPNO 11
PROCNO 1

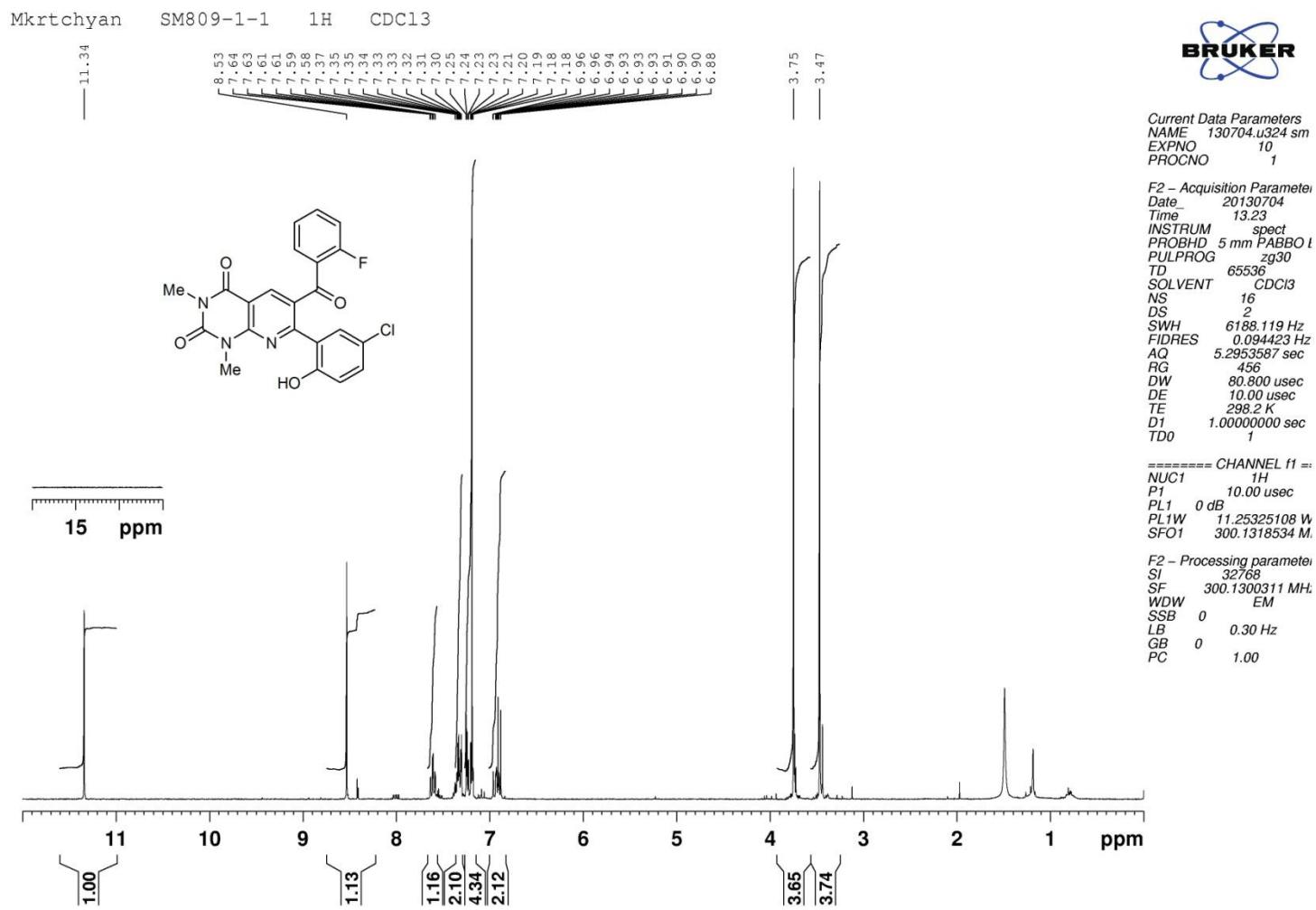
F2 - Acquisition Parameters
Date 20140502
Time 22.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 768
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.1 K
CNST2 145.0000000
D1 2.0000000 sec
d12 0.00002000 sec
d2 0.00344828 sec
DELTA 0.00001273 sec
TD0 1

===== CHANNEL f1 ======
NUC1 ¹³C
P1 10.00 usec
p2 20.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

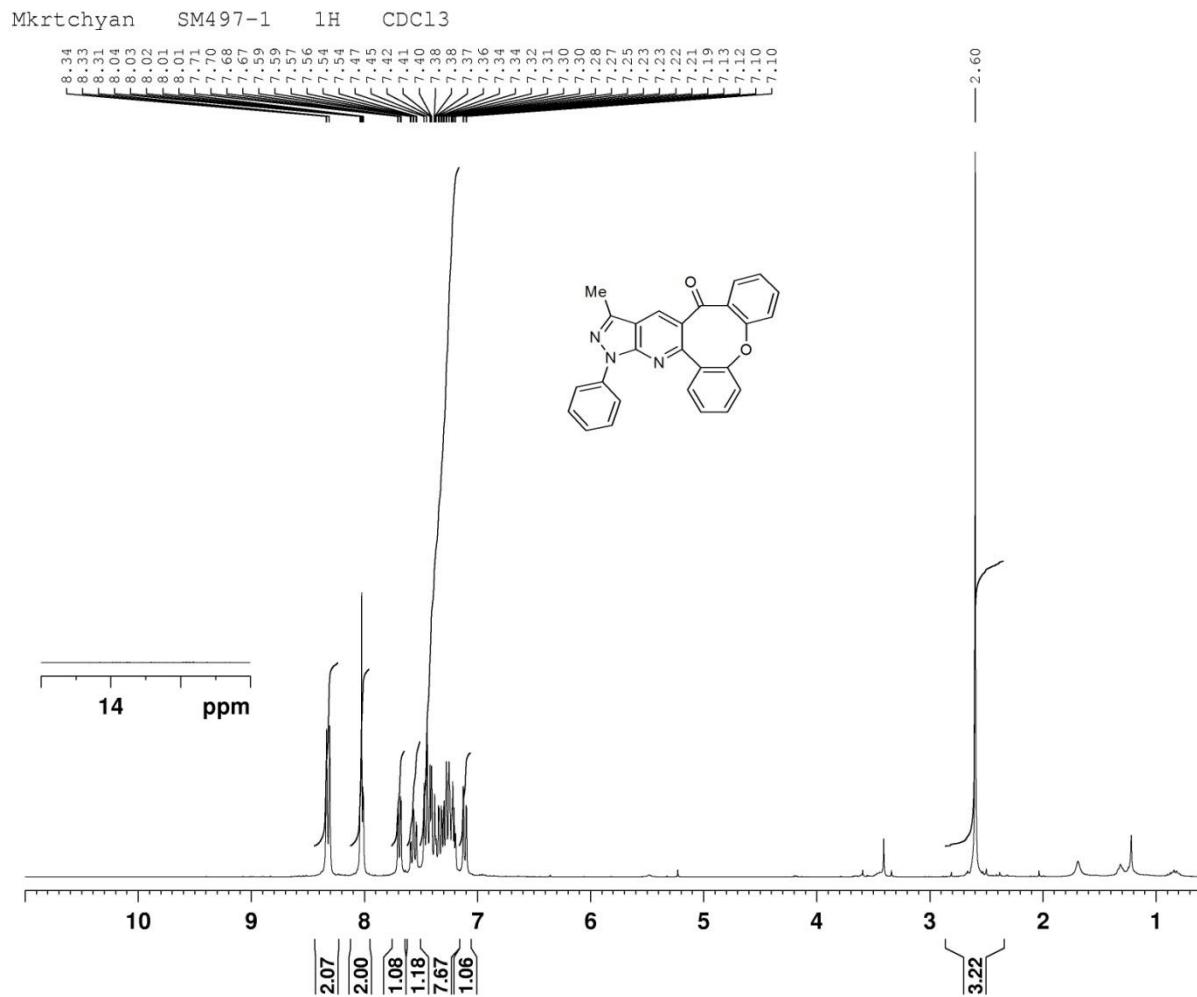
===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
P3 10.00 usec
p4 20.00 usec
PCPD2 70.00 usec
PL12 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 6b



Compound 7a



Current Data Parameters
NAME 110620.u302.s
EXPNO 10
PROCNO 1

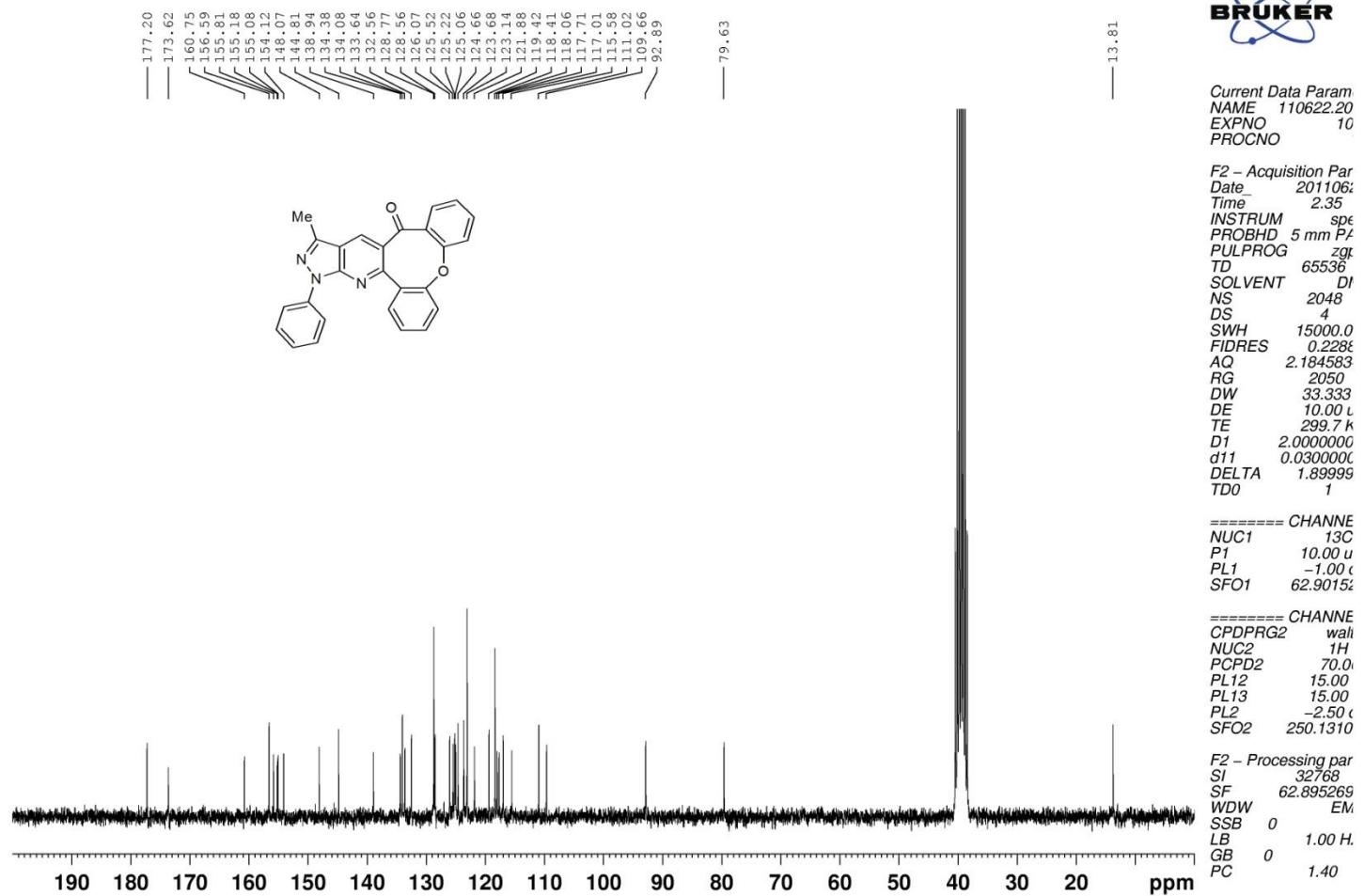
F2 - Acquisition Parameters
Date 20110620
Time 8.12
INSTRUM spect
PROBHD 5 mm PABBC
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 6188.119 H.
FIDRES 0.094423 t
AQ 5.2953587 se
RG 80.6
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 se
TDO 1

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

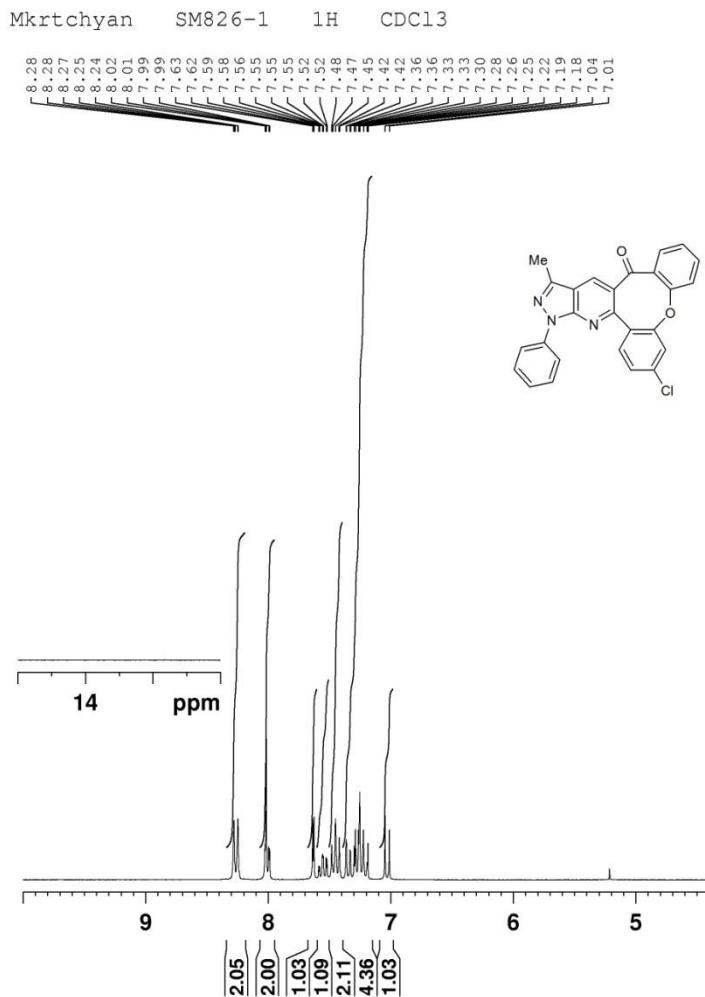
F2 - Processing parameters
SI 32768
SF 300.1300264 M
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 7a

Mkrtchyan, SM 497-2-2, DMSO, ^{13}C



Compound 7b



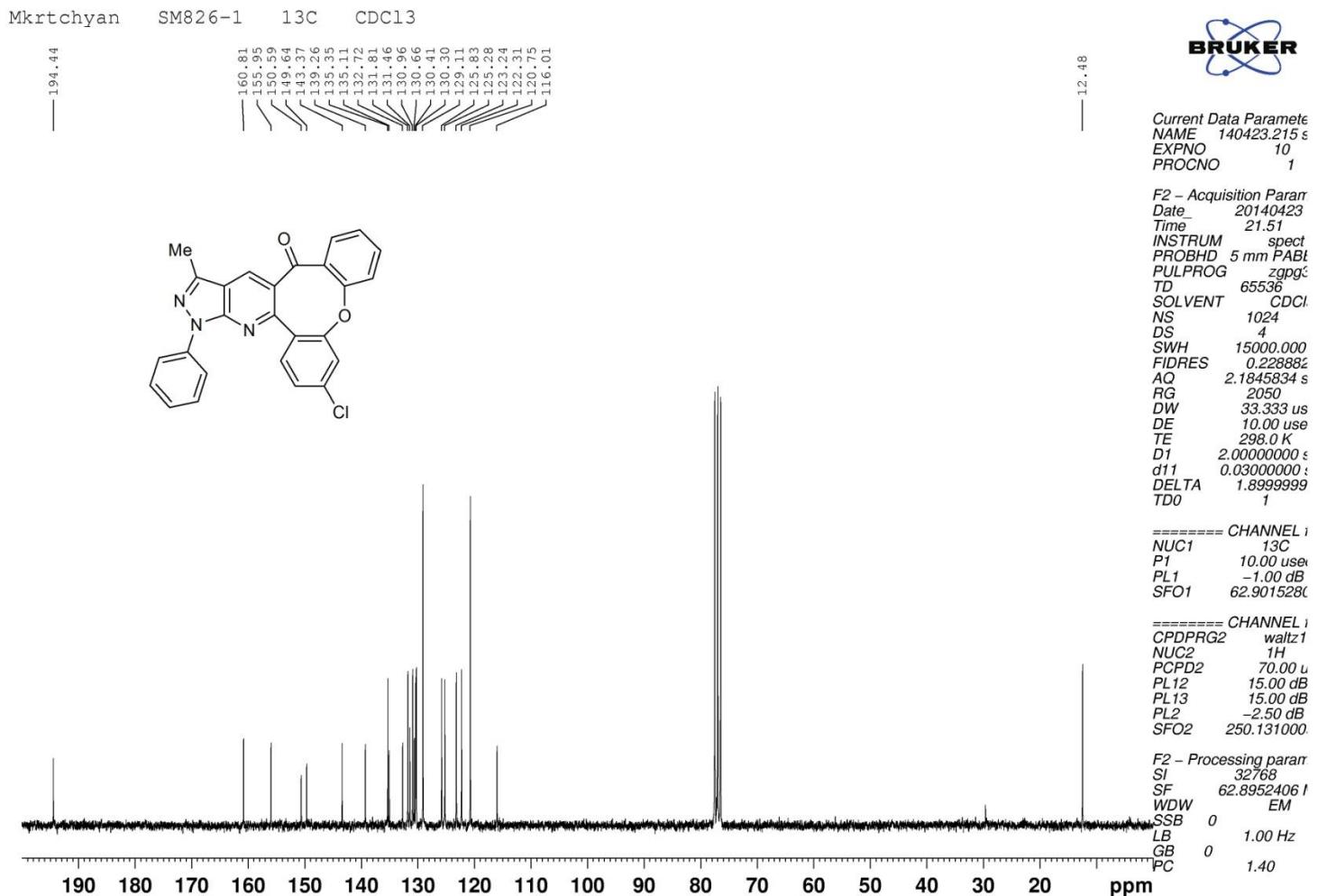
Current Data Parameters
NAME 140425.215.s
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20140426
Time 20.21
INSTRUM spect
PROBHD 5 mm PABBC
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5165.289 H.
FIDRES 0.078816 t
AQ 6.3439350 sec
RG 287
DW 96.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

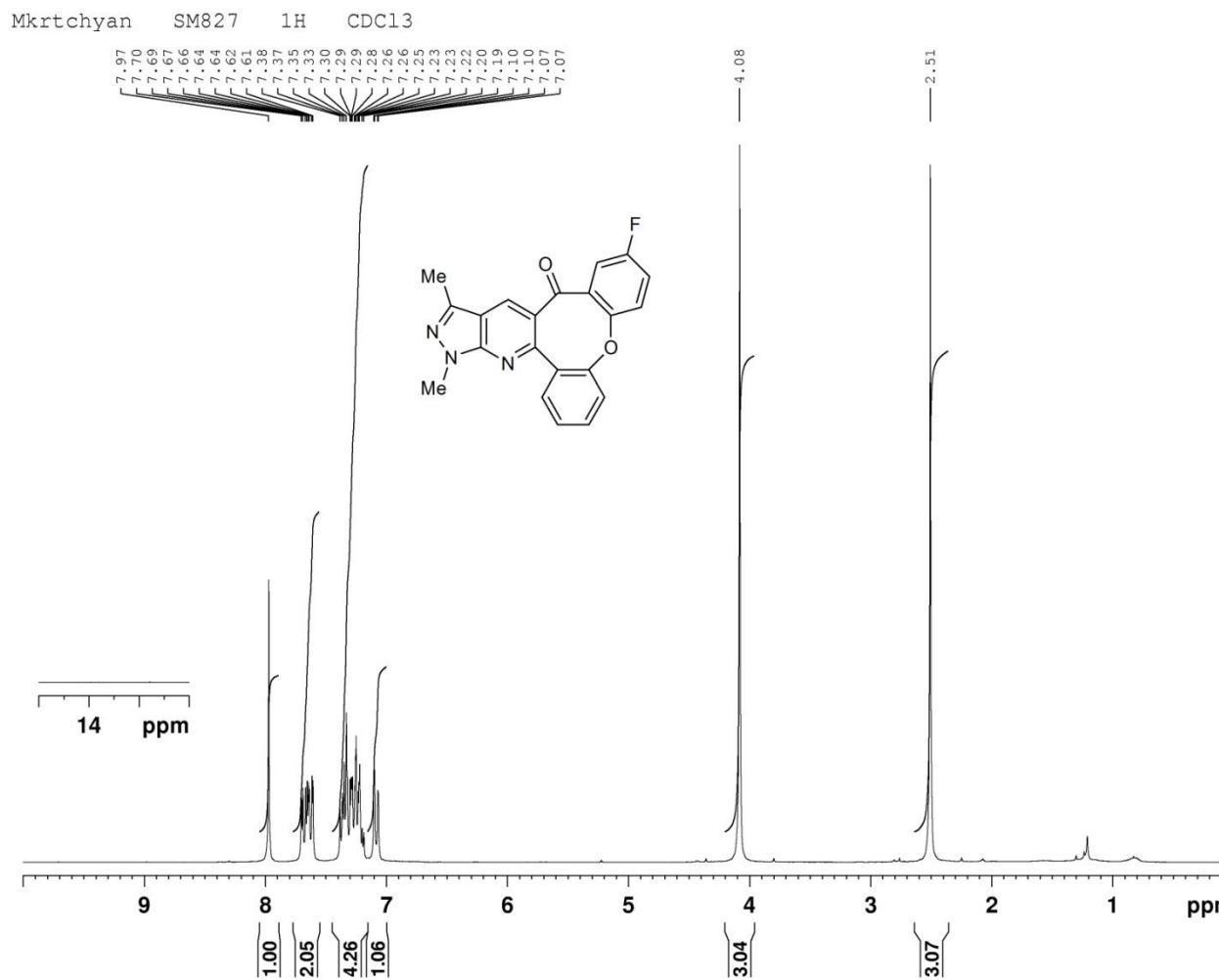
===== CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 -2.50 dB
SFO1 250.1315447

F2 - Processing parameters
SI 32768
SF 250.1300196 M
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Compound 7b



Compound 7c



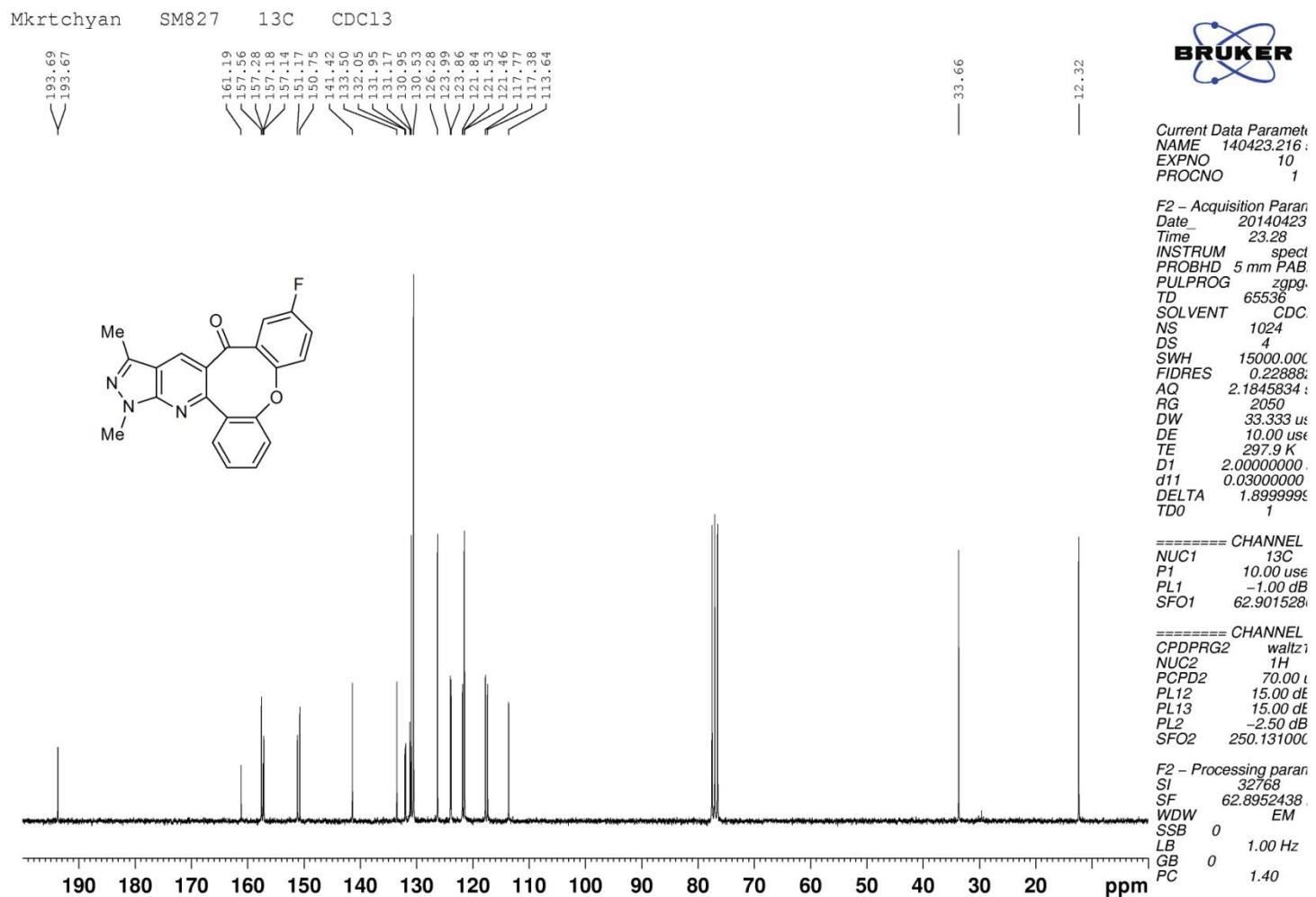
Current Data Parameters
 NAME 140423.207.s.
 EXPNO 10
 PROCNO 1

F2 - Acquisition Param
 Date 20140423
 Time 8.56
 INSTRUM spect
 PROBHD 5 mm PABE
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 5165.289 Hz
 FIDRES 0.078816 s
 AQ 6.3439350 s
 RG 144
 DW 96.800 us
 DE 10.00 us
 TE 298.1 K
 D1 1.00000000 s
 TDO 1

===== CHANNEL f
 NUC1 1H
 P1 10.00 usec
 PL1 -2.50 dB
 SFO1 250.131544;

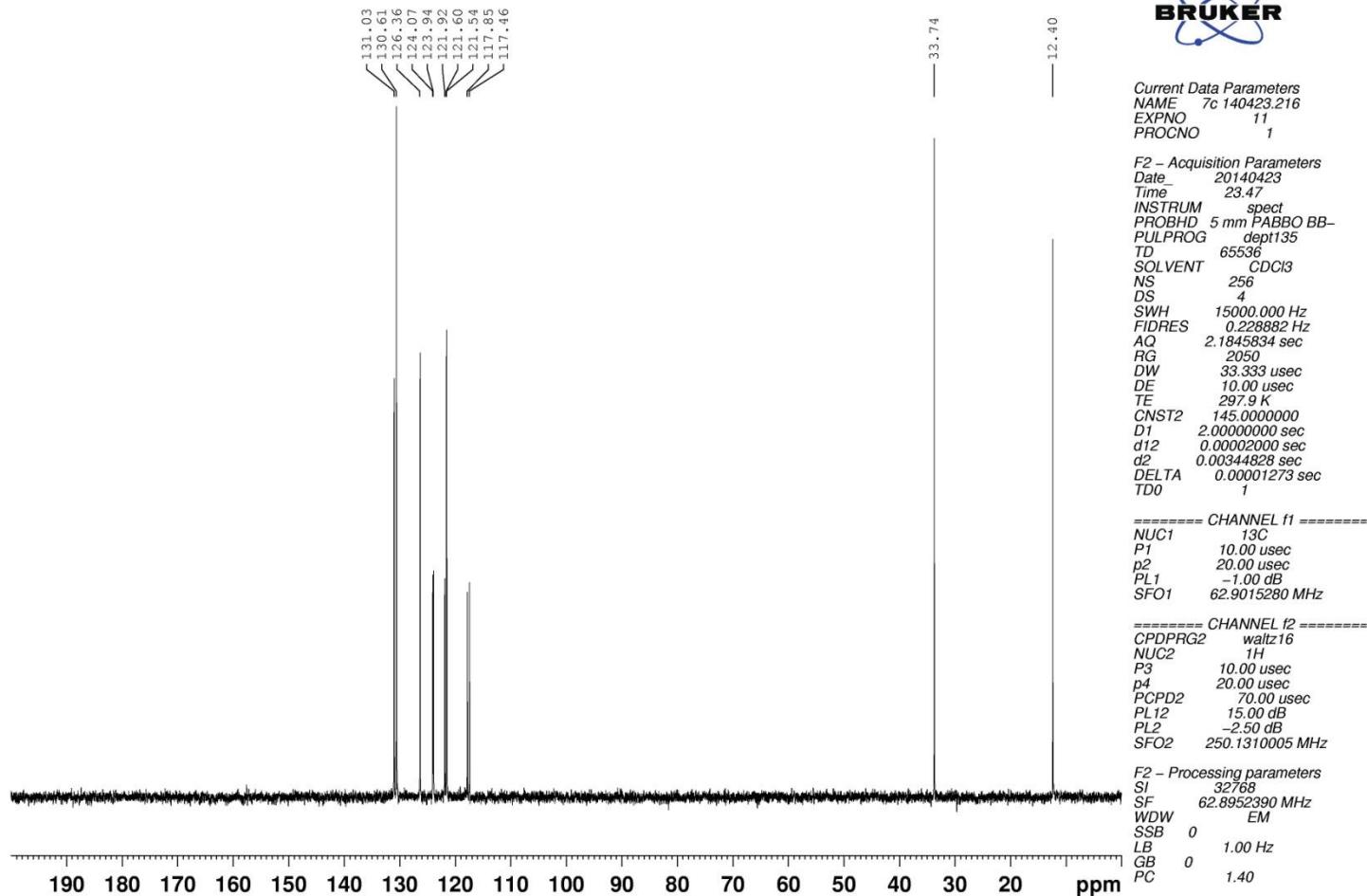
F2 - Processing param
 SI 32768
 SF 250.1300101 Hz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Compound 7c

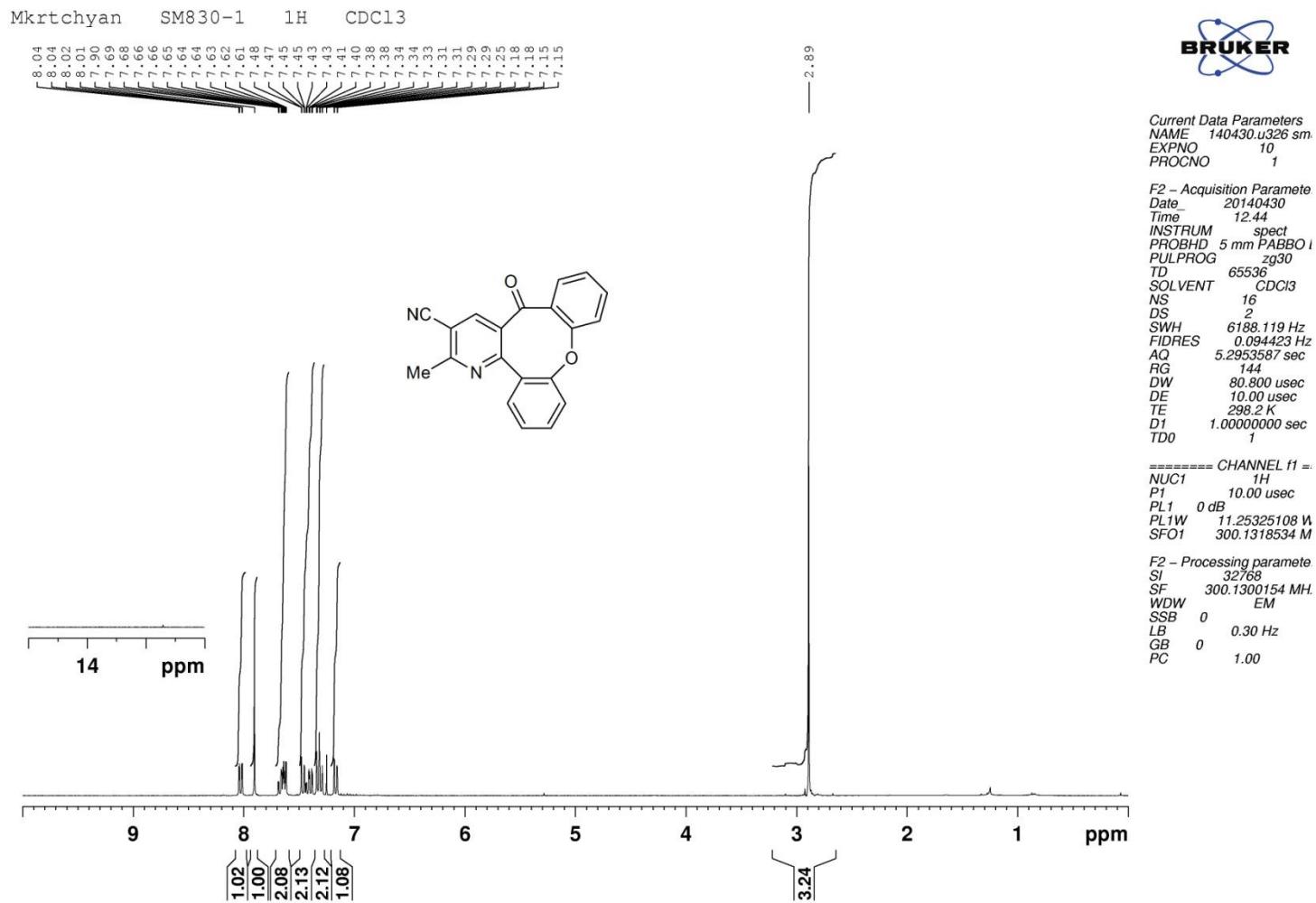


Compound 7c

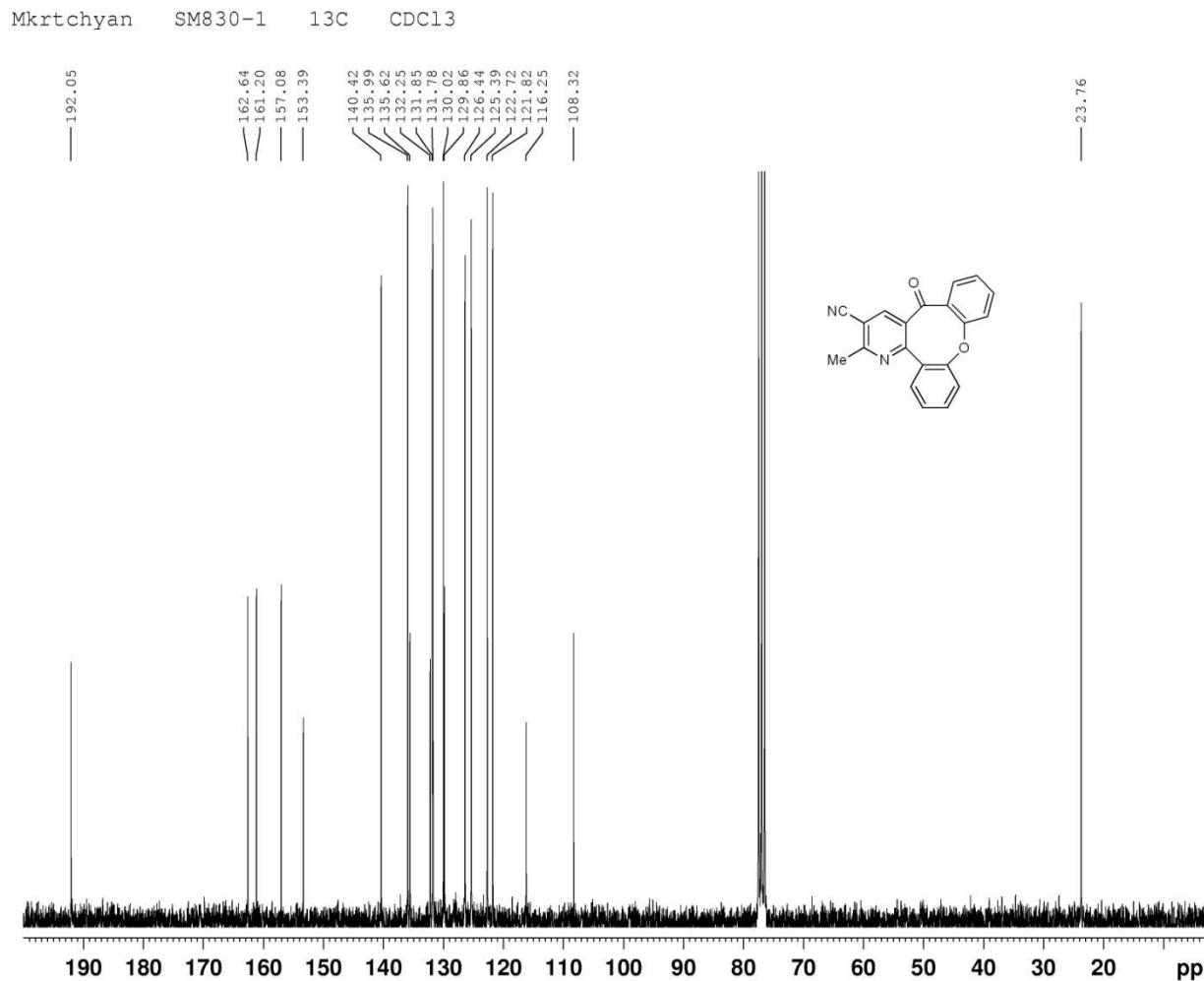
Mkrtchyan SM827 Dept CDC13



Compound 7d



Compound 7d



Current Data Parameters
NAME 140502.209 sm
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20140503
Time 5.10
INSTRUM spect
PROBHD 5 mm PABBC
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 t
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.89999998 :
TD0 1

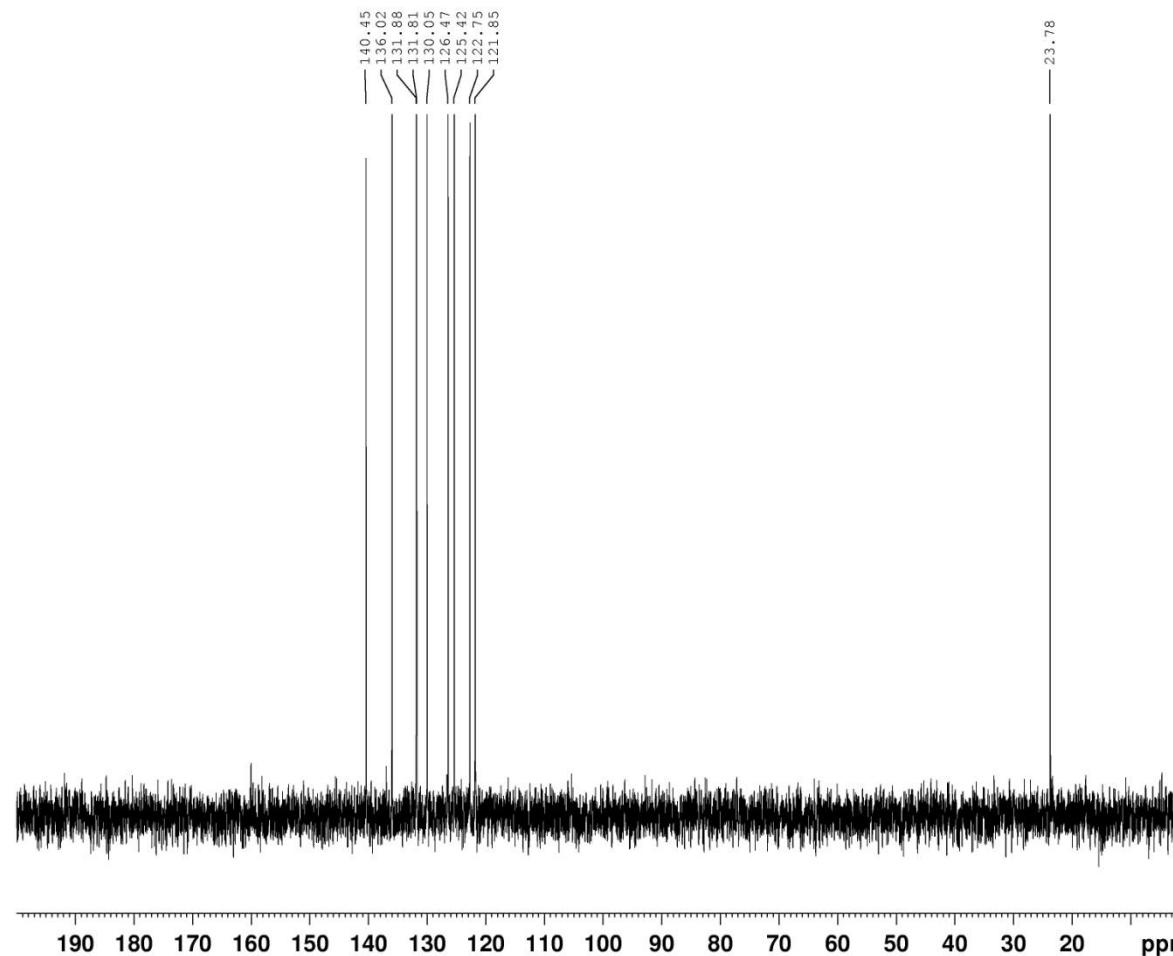
===== CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 Hz

===== CHANNEL f2
CPDPG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 Hz

F2 - Processing parameters
SI 32768
SF 62.8952407 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 7d

Mkrtchyan SM830-1 Dept CDC13



Current Data Parameters
NAME 7d 140502.209
EXPNO 11
PROCNO 1

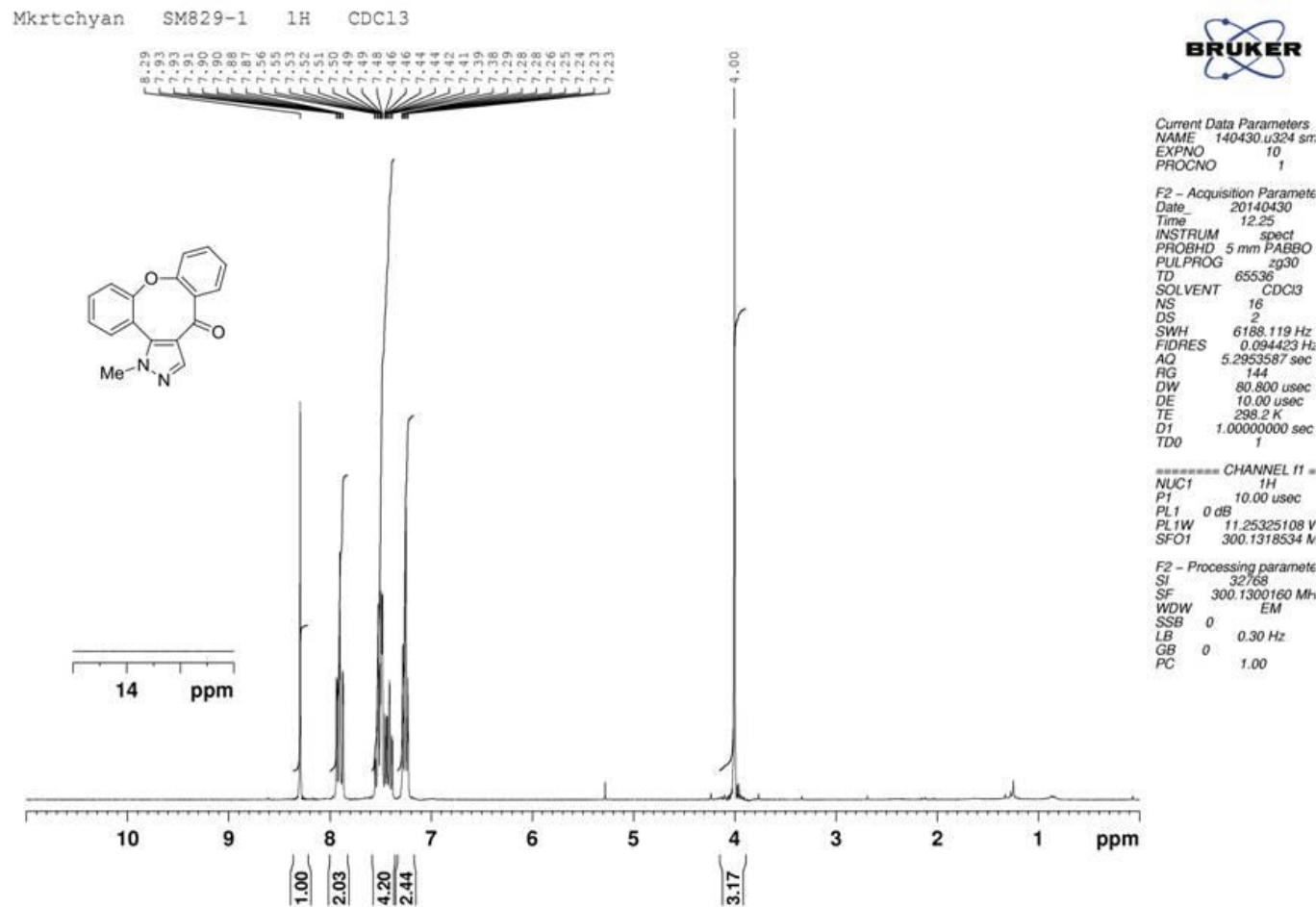
F2 - Acquisition Parameters
Date 20140503
Time 5.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
CNST2 145.0000000
D1 2.0000000 sec
d12 0.00002000 sec
d2 0.00344828 sec
DELTA 0.00001273 sec
TDO 1

===== CHANNEL f1 ======
NUC1 ¹³C
P1 10.00 usec
p2 20.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

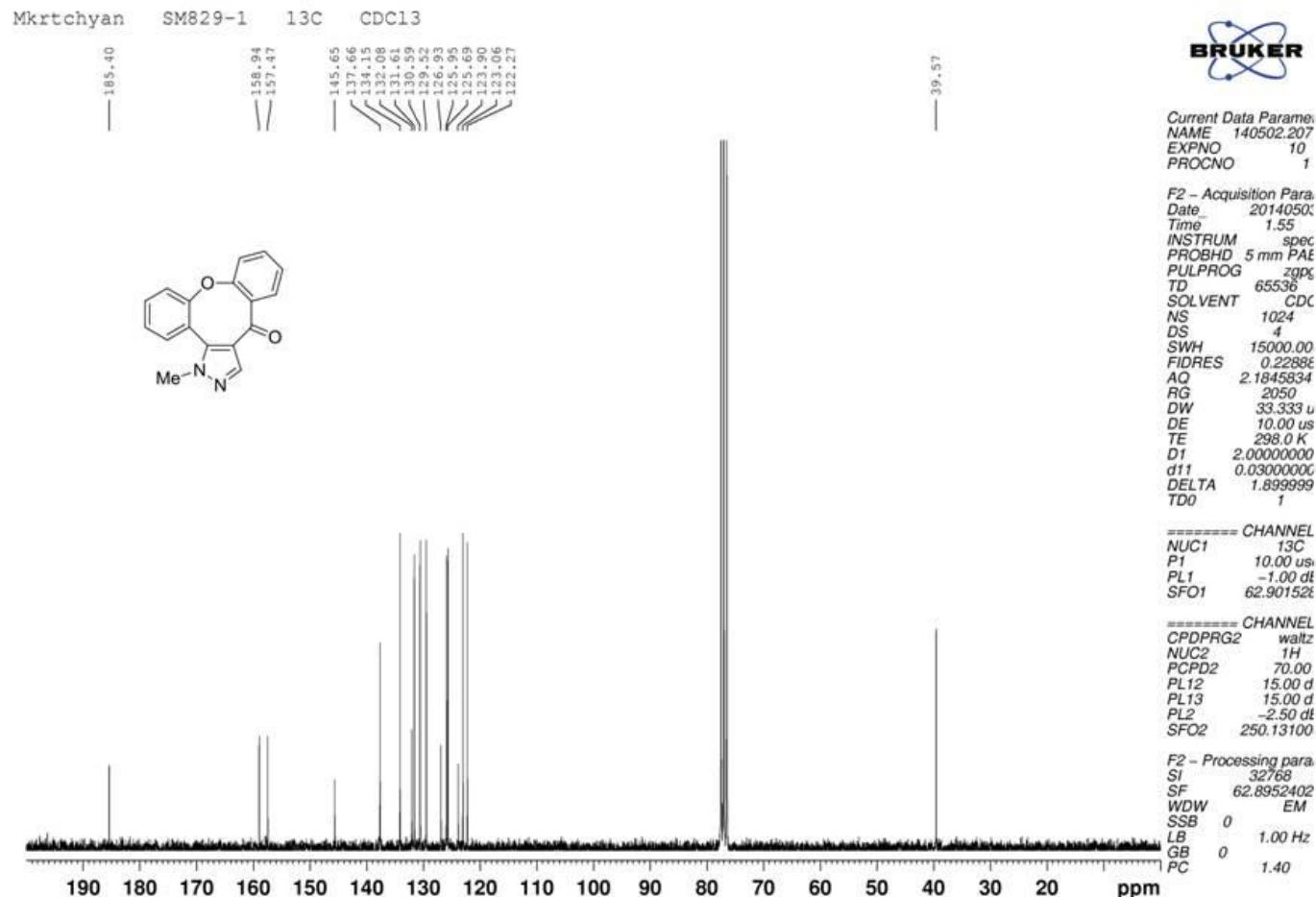
===== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 ¹H
P3 10.00 usec
p4 20.00 usec
PCPD2 70.00 usec
PL12 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 7e

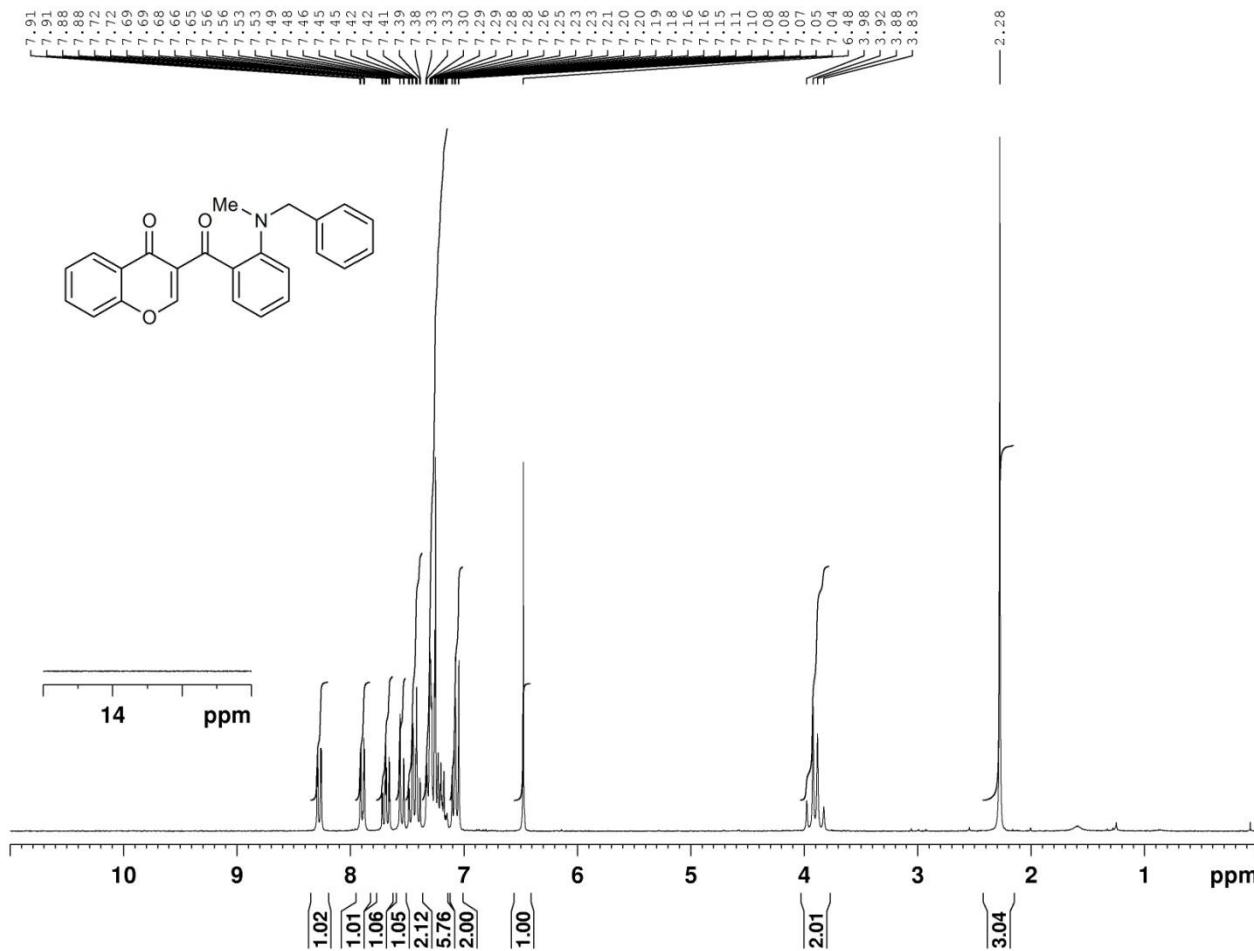
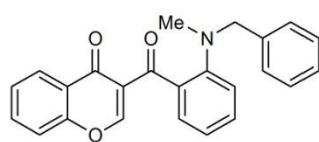


Compound 7e



Compound 8a

Mkrtchyan SM828-1 1H CDC13



BRUKER

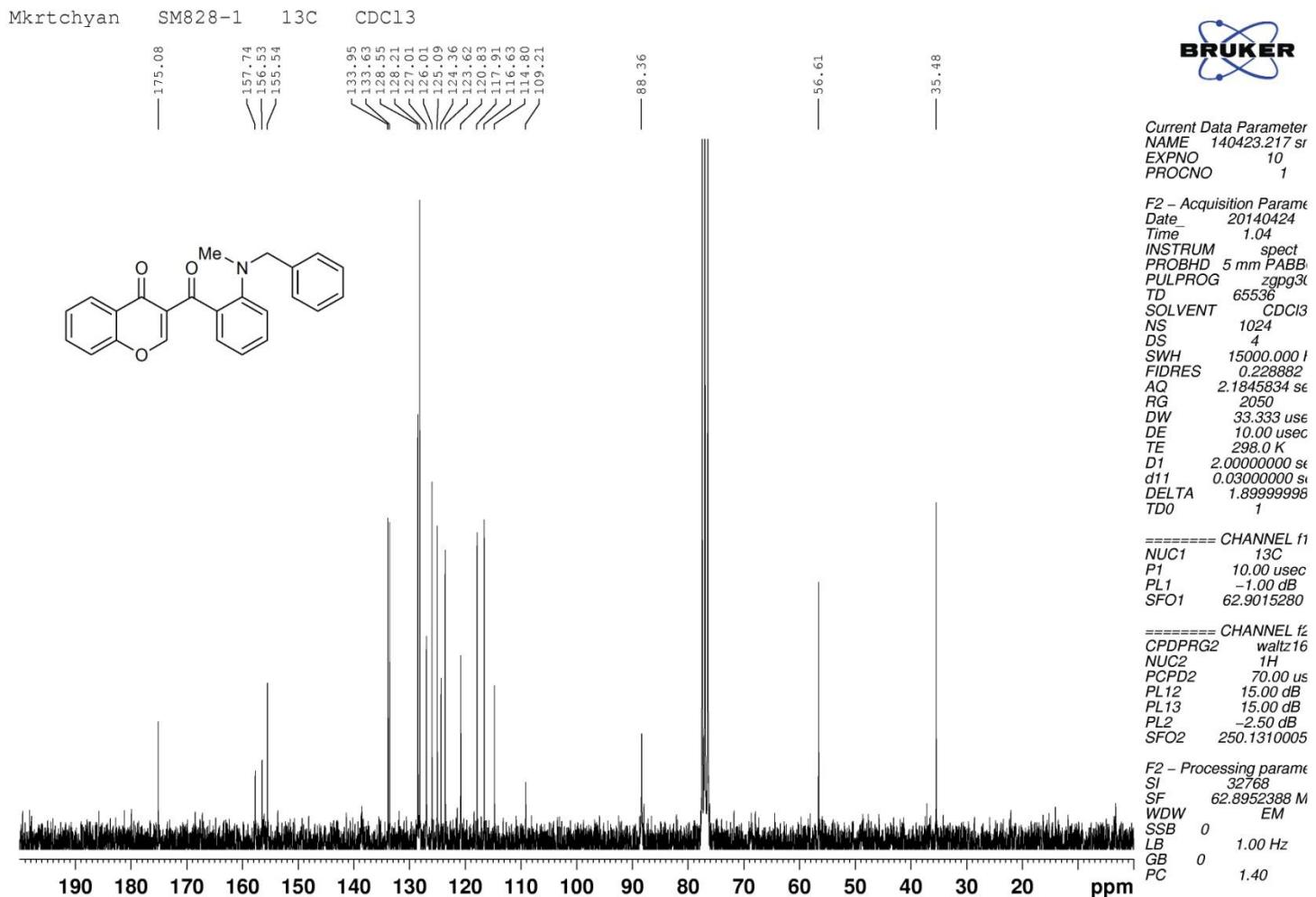
Current Data Paramet
NAME 140423.208
EXPNO 10
PROCNO 1

F2 - Acquisition Para
 Date 20140423
 Time 9.02
 INSTRUM spec
 PROBHDI 5 mm PAB
 PULPROG zg3
 TD 65536
 SOLVENT CDC
 NS 16
 DS 2
 SWH 5165.289
 FIDRES 0.07881
 AQ 6.3439350
 RG 645
 DW 96.800 u.
 DE 10.00 us.
 TE 298.0 K
 D1 1.00000000
 TDO 1

===== CHANNEL
NUC1 1H
P1 10.00 use
PL1 -2.50 dE
SFO1 250.13154

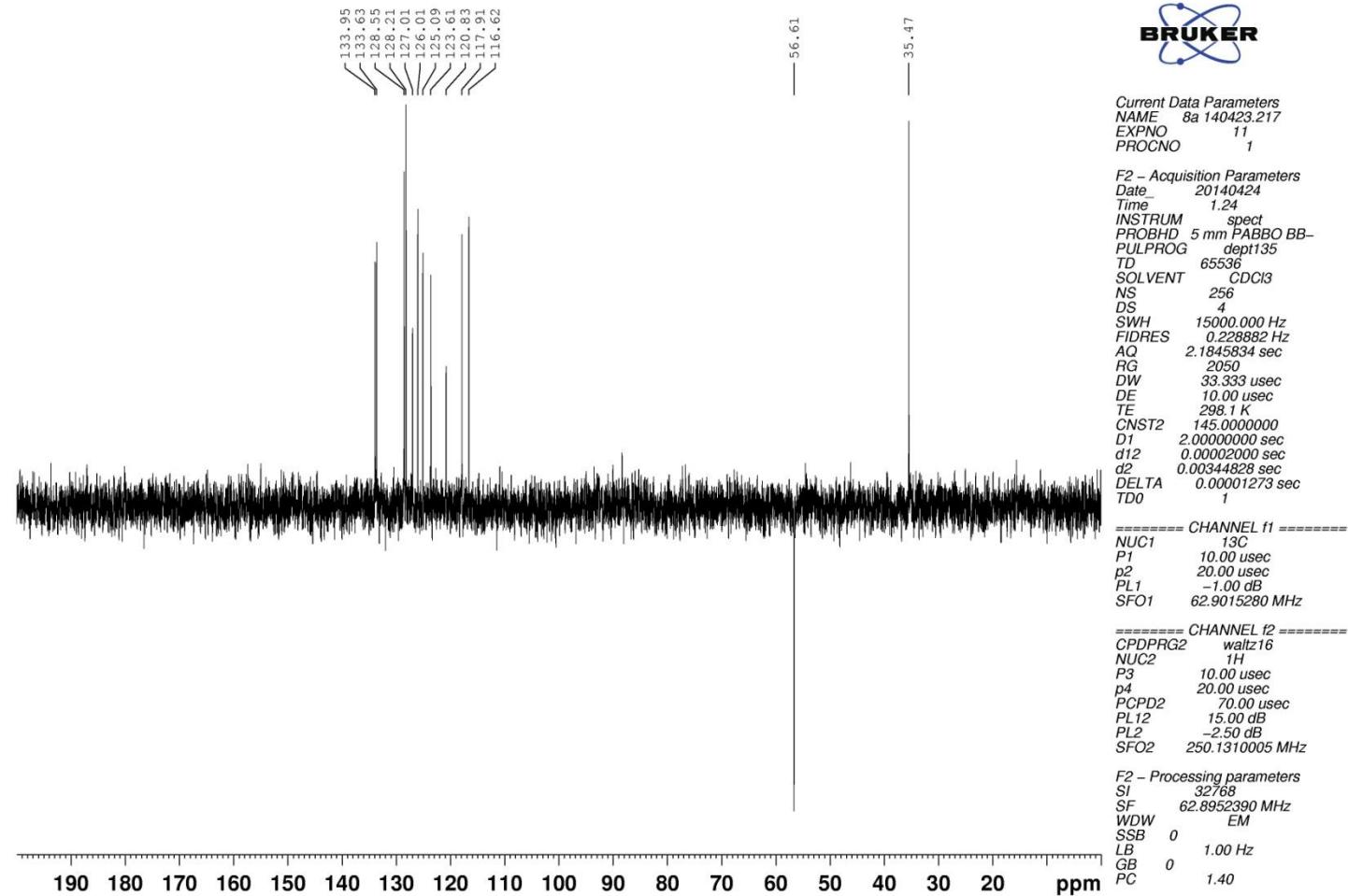
F2 – Processing para
 SI 32768
 SF 250.1300031
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Compound 8a



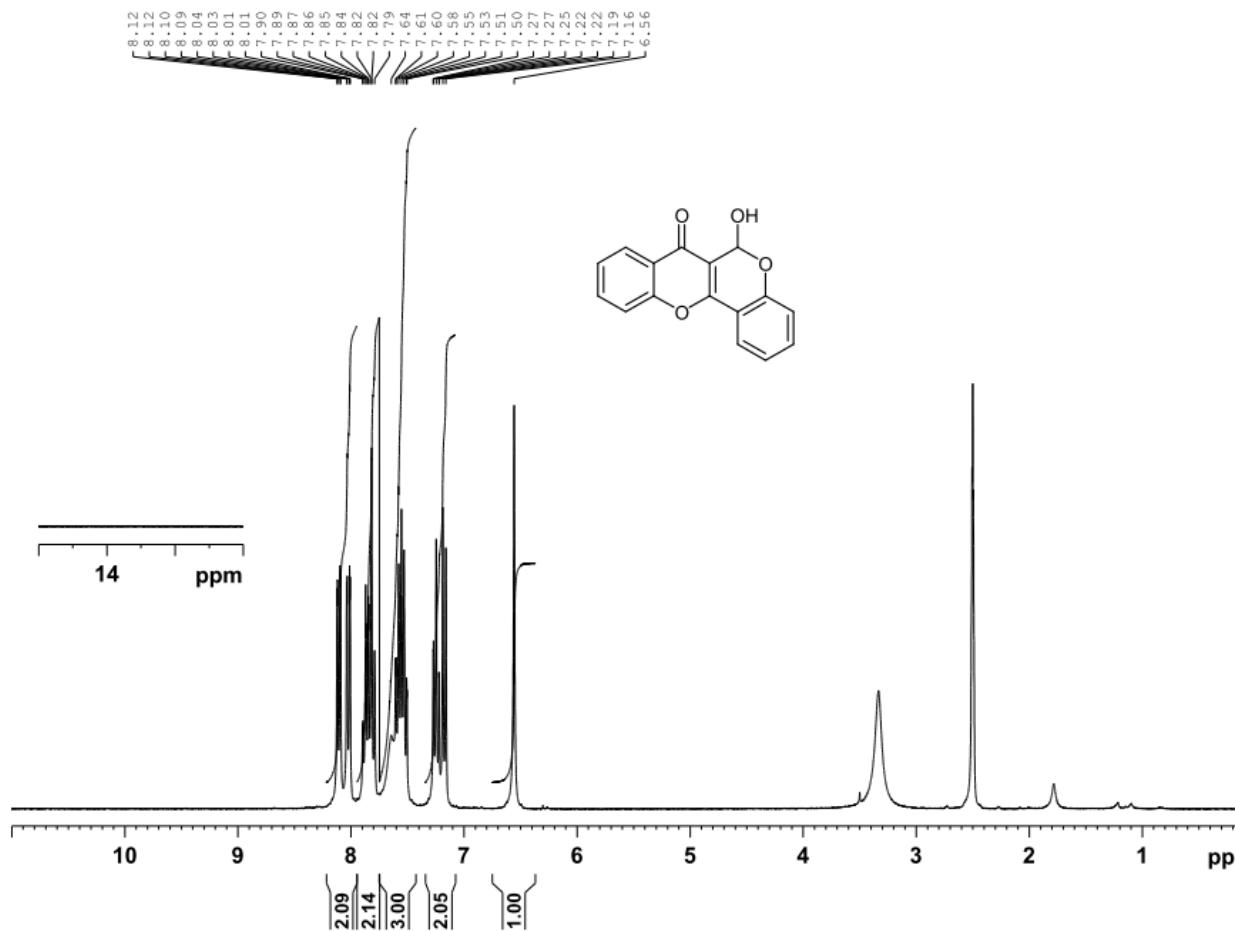
Compound 8a

Mkrtchyan SM828-1 Dept CDC13



Compound 9a

Mkrtchyan, R 407, DMSO, 1H



Current Data Parameters
 NAME 120116.n321 sm 407 r
 EXPNO 10
 PROCNO 1

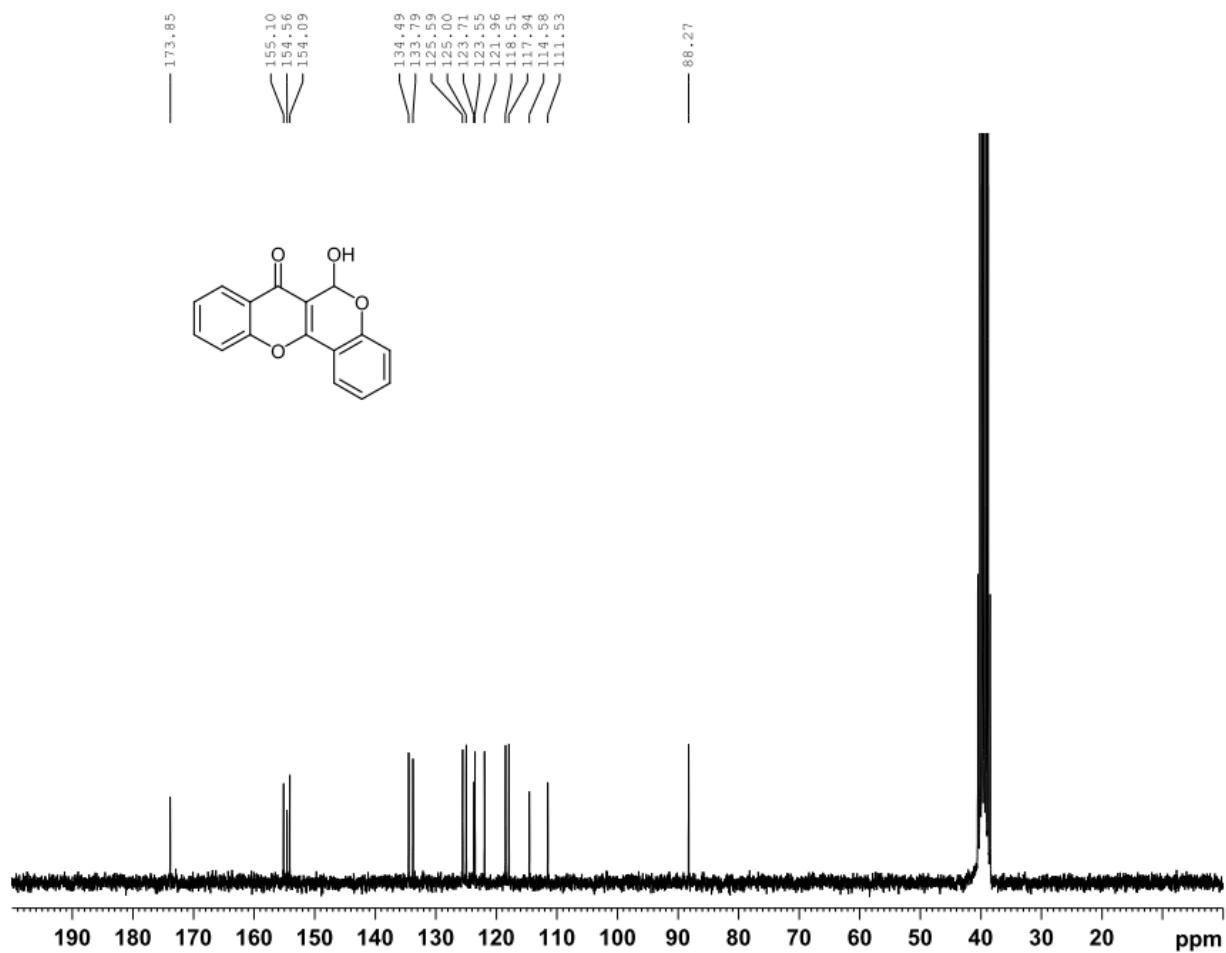
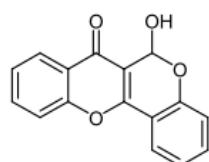
F2 - Acquisition Parameters
 Date 20120116
 Time 12.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2935387 sec
 RG 287
 DW 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 ======
 NUCI 1H
 P1 10.00 usec
 PL1 0.00 dB
 PL1W 11.23325108 W
 SF01 300.1318534 MHz

F2 - Processing parameters
 SP 32768
 SF 300.1300067 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Compound 9a

Mkrtchyan R407 13C DMSO



Current Data Parameters
NAME 120117.208 sm 407 r c
EXPNO 10
PROCNO 1

```

F2 - Acquisition Parameters
Date_ 20120117
Time 22.39
INSTRUM spect
PROBHD 5 mm QNP JH/I3
PULPROG zgpg30
TD 65536
SOLVENT DMSO
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
DI 2.00000000 sec
d1I 0.03000000 sec
DELTA 1.89999998 sec
T0D0 1

```

```
===== CHANNEL f1 =====
NUCI          13C
PI           10.20 usec
PL1          0.00 dB
SFO1        62.901520 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2          walt16
NUC2             1H
PCPD2           70.00 usec
PL12            14.00 dB
PL13            14.00 dB
PL2             -3.00 dB
SEQ2           250,131,0005 MHz
```

F2 - Processing parameters

<i>SI</i>	32768
<i>SF</i>	62.8952678 MHz
<i>WDW</i>	EM
<i>SSB</i>	0
<i>LB</i>	1.00 Hz
<i>GB</i>	0
<i>PC</i>	140