

Supporting Information

2,3-Unsubstituted chromones and their enaminone precursors as versatile reagents for the synthesis of fused pyridines

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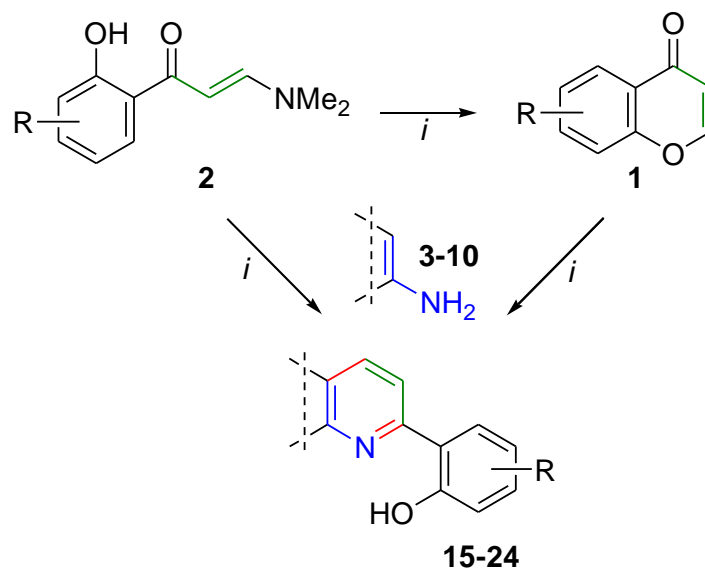
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(A) Experimental Section

All solvents were purified and dried by standard methods. NMR spectra were recorded on a Bruker AV 300 and Bruker AV 400. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. IR spectra were recorded on a Perkin Elmer FT IR 1600 spectrometer (ATR). Mass spectra were obtained on a “Hewlett-Packard” HP GC / MS 5890 / 5972 instrument (EI, 70 eV) by GC inlet or on a MX-1321 instrument (EI, 70 eV) by direct inlet. Column chromatography was performed on silica gel (63–200 mesh, Merck). Silica gel Merck 60F₂₅₄ plates were used for TLC. Satisfactory microanalysis obtained C ± 0.33; H ± 0.45; N ± 0.25. Chemical yields refer to pure isolated substances.

General procedure in DMF/TMSCl: Corresponding chromone **1** or enaminones **2**, **25** (2 mmol) and amine (2.2 mmol) were placed in pressure tube under the flow of dry argon and dissolved in dry DMF (10 mL) containing 1 mL of TMSCl. The mixture was heated at 90–120 °C during 1–4 h (controlled by TLC). Then this solution was evaporated under reduced pressure, treated with water, filtrated, dried on the air, and recrystallized from an appropriate solvent, or was subjected to a column chromatography over silica gel.

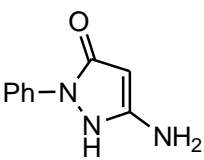
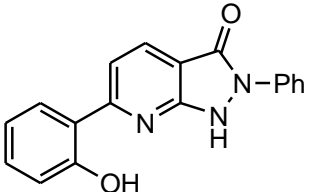
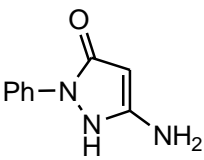
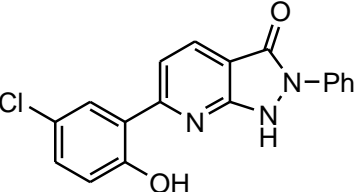
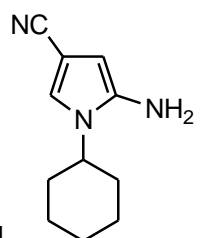
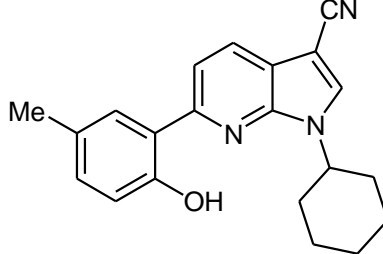
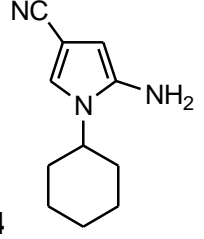
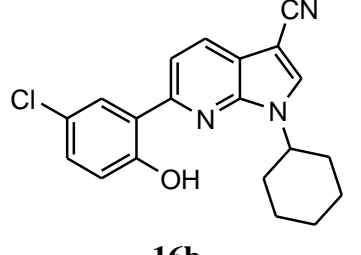
For **21**: Compounds **1c,d** or **2c,d** (1 equiv.) and the corresponding amine **8** (1.1 equiv.) were dissolved in acetic acid (20 mL) and heated under reflux in an inert atmosphere during 2–3 h (controlled by TLC). Then this solution was evaporated under reduced pressure, treated with water, filtrated, dried on the air, and recrystallized from an appropriate solvent.

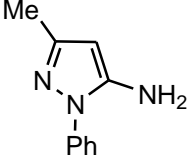
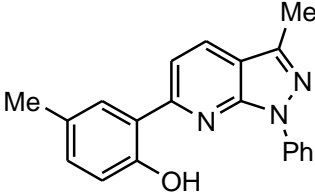
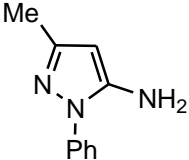
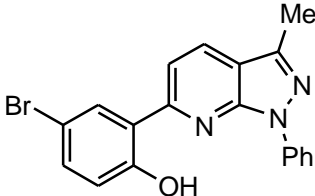
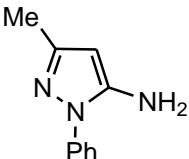
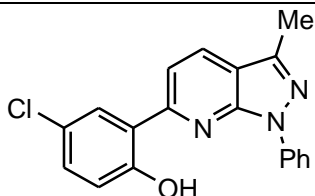
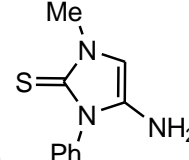
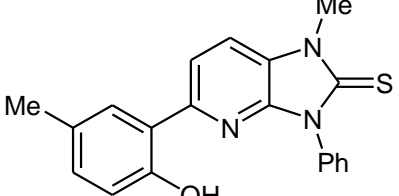


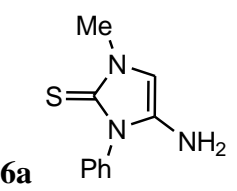
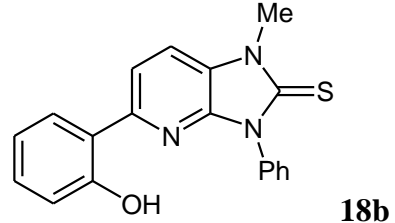
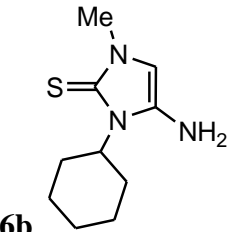
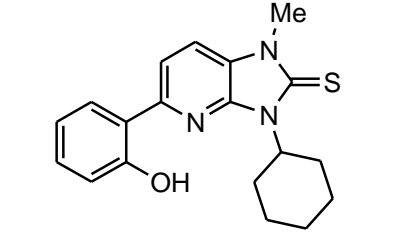
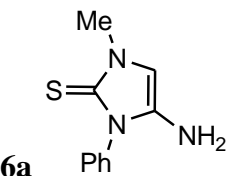
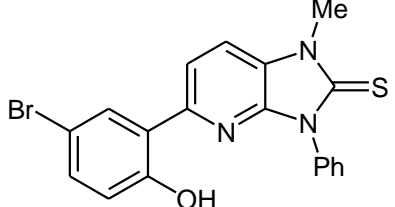
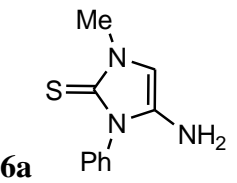
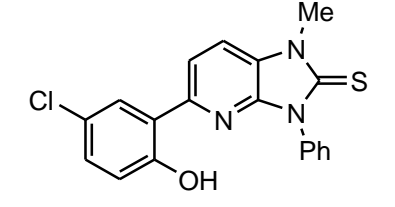
Scheme 1. Reagents and conditions: (i) DMF/TMSCl, under argon, 90–120 °C, 1–4 h.

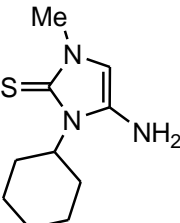
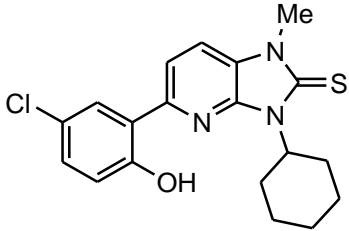
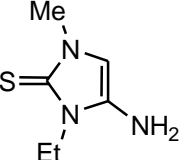
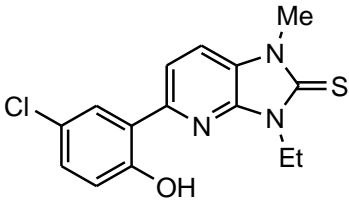
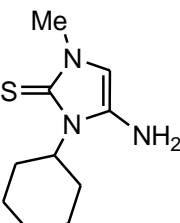
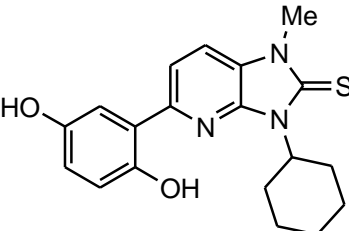
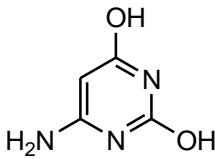
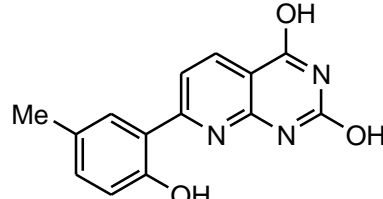
Table 1. Synthesis of fused pyridines **15–24** from chromones **1** and aminoenones **2** (yields are in brackets).

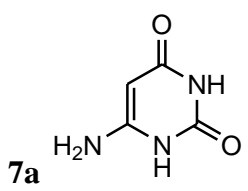
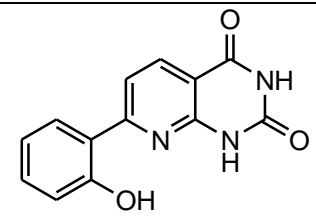
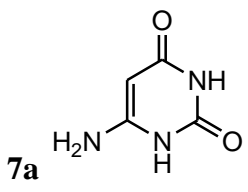
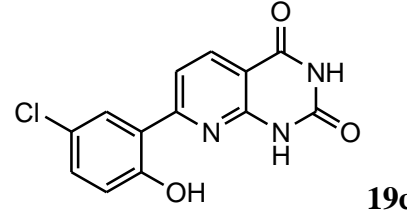
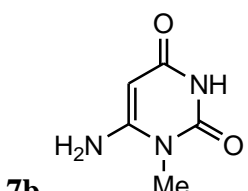
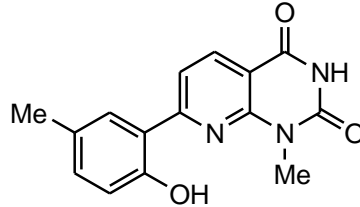
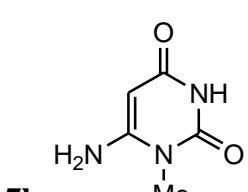
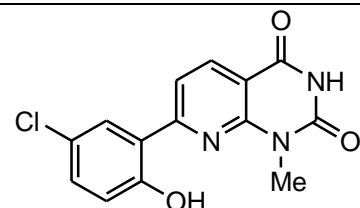
3–10	15–24	Reaction conditions	Yield (%)
 3	 15a	DMF/TMSCl, 100 °C, 1 h	90 (86)

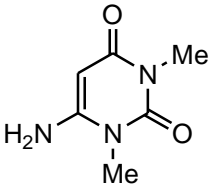
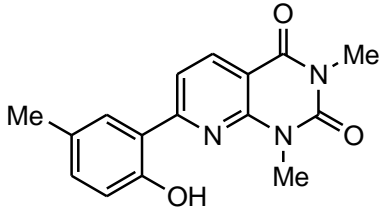
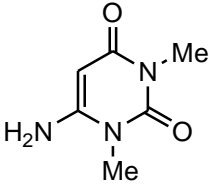
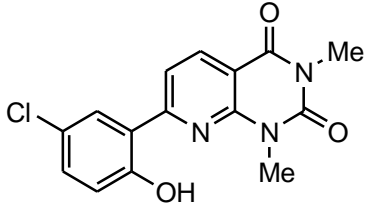
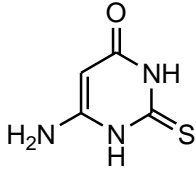
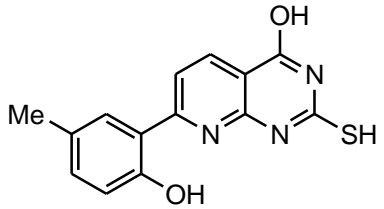
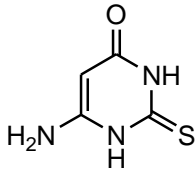
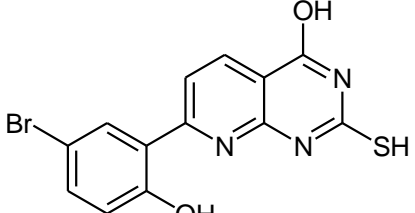
<p>3</p> 	<p>15b</p> 	<p>DMF/TMSCl, 100 °C, 2 h</p>	<p>77 (78)</p>
<p>3</p> 	<p>15c</p> 	<p>DMF/TMSCl, 90 °C, 1 h</p>	<p>92 (90)</p>
<p>4</p> 	<p>16a</p> 	<p>DMF/TMSCl, 90 °C, 1 h</p>	<p>78 (75)</p>
<p>4</p> 	<p>16b</p> 	<p>AcOH, reflux, 1 h</p>	<p>62 (60)</p>

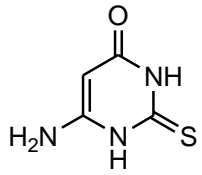
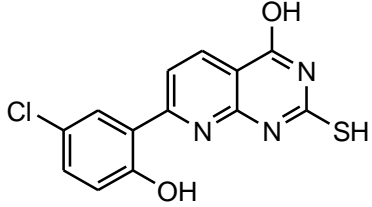
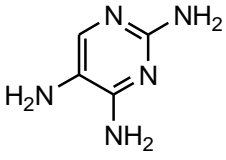
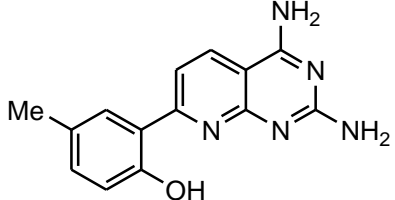
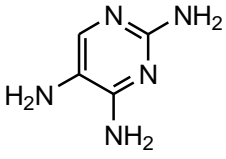
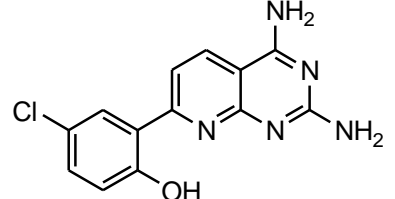
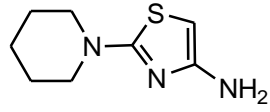
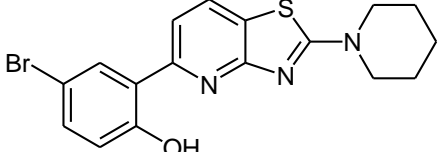
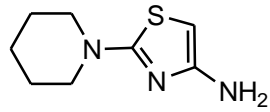
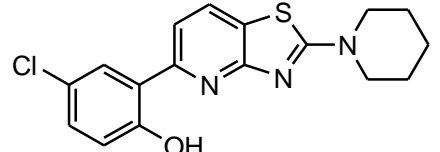
 <p>5</p>	 <p>17a</p>	DMF/TMSCl, 100 °C, 2 h	97 (93)
 <p>5</p>	 <p>17b</p>	DMF/TMSCl, 100 °C, 2 h	92 (92)
 <p>5</p>	 <p>17c</p>	DMF/TMSCl, 90 °C, 1 h	75 (74)
 <p>6a</p>	 <p>18a</p>	DMF/TMSCl, 100 °C, 1 h	90 (86)

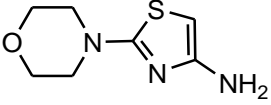
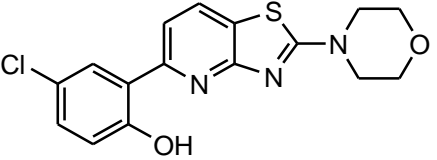
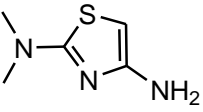
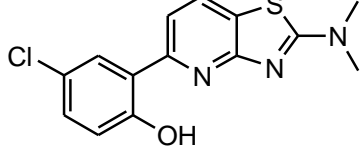
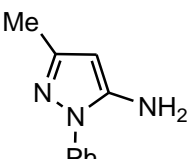
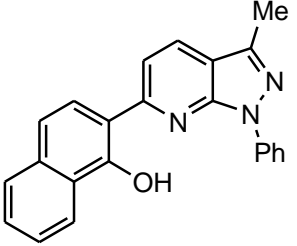
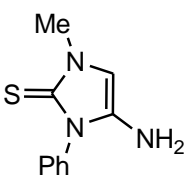
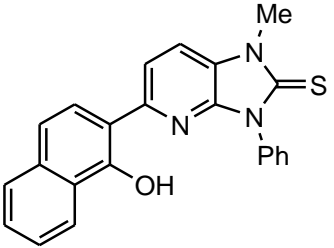
 <p>6a</p>	 <p>18b</p>	DMF/TMSCl, 100 °C, 1 h	90 (89)
 <p>6b</p>	 <p>18c</p>	DMF/TMSCl, 90 °C, 4 h	68
 <p>6a</p>	 <p>18d</p>	DMF/TMSCl, 90 °C, 1 h	76 (74)
 <p>6a</p>	 <p>18e</p>	DMF/TMSCl, 90 °C, 4 h	61 (60)

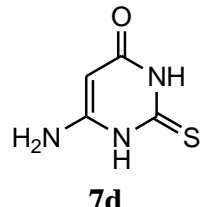
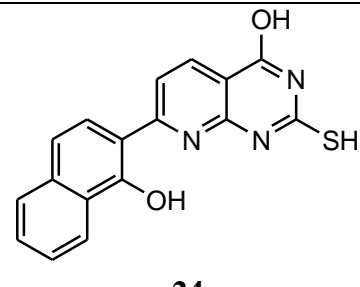
 6b	 18f	DMF/TMSCl, 90 °C, 4 h	59
 6c	 18g	DMF/TMSCl, 90 °C, 4 h	58 (60%)
 6b	 18h	DMF/TMSCl, 100 °C, 4 h	68
 7a	 19a	DMF/TMSCl, 100 °C, 2 h	89 (87)

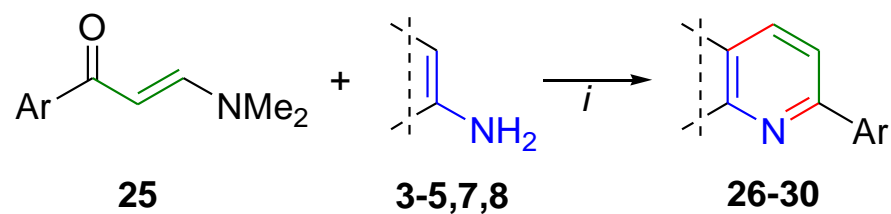
 <p>7a</p>	 <p>19b</p>	DMF/TMSCl, 100 °C, 1 h	88 (87)
 <p>7a</p>	 <p>19c</p>	DMF/TMSCl, 100 °C, 2 h	85 (85)
 <p>7b</p>	 <p>19d</p>	DMF/TMSCl, 100 °C, 2 h	90 (88)
 <p>7b</p>	 <p>19e</p>	DMF/TMSCl, 90 °C, 2 h	65 (66)

 7c	 19f	DMF/TMSCl, 100 °C, 1 h	65 (60)
 7c	 19g	DMF/TMSCl, 90 °C, 1 h	97 (90)
 7d	 19h	DMF/TMSCl, 100 °C, 2 h	89
 7d	 19i	DMF/TMSCl, 100 °C, 2 h	68

<p>7d</p> 	<p>19j</p> 	<p>DMF/TMSCl, 90 °C, 1 h</p>	<p>79</p>
<p>9</p> 	<p>20a</p> 	<p>DMF/TMSCl, 100 °C, 3 h</p>	<p>60</p>
<p>9</p> 	<p>20b</p> 	<p>DMF/TMSCl, 100 °C, 2 h</p>	<p>70</p>
<p>8a</p> 	<p>21a</p> 	<p>AcOH, reflux, 3 h</p>	<p>62 (60)</p>
<p>8a</p> 	<p>21b</p> 	<p>AcOH, reflux, 3 h</p>	<p>55 (50)</p>

 <p>8b</p>	 <p>21c</p>	<p>AcOH, reflux, 2 h</p>	<p>60 (54)</p>
 <p>8c</p>	 <p>21d</p>	<p>AcOH, reflux, 3 h</p>	<p>61 (61)</p>
 <p>5</p>	 <p>22</p>	<p>DMF/TMSCl, 90 °C, 1 h</p>	<p>84 (82)</p>
 <p>6a</p>	 <p>23</p>	<p>DMF/TMSCl, 90 °C, 3 h</p>	<p>72 (77)</p>

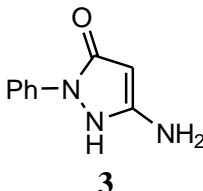
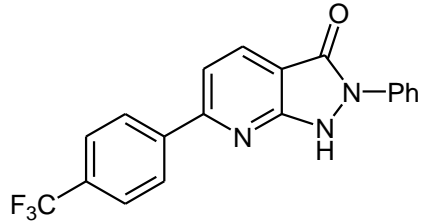
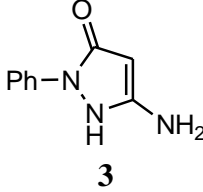
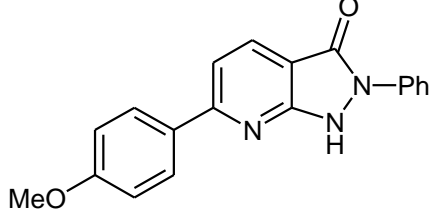
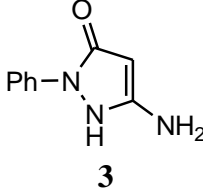
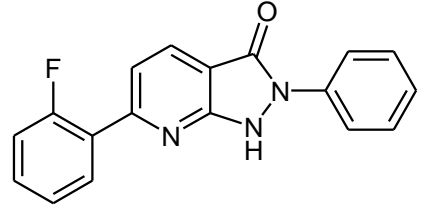
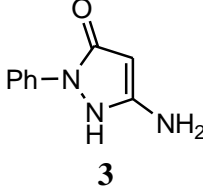
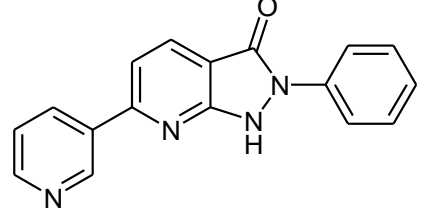
 7d	 24	DMF/TMSCl, 90 °C, 1 h	84
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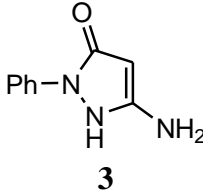
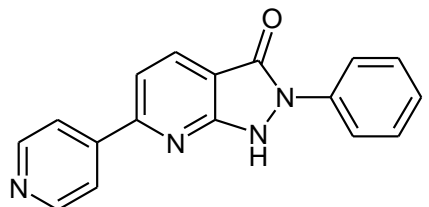
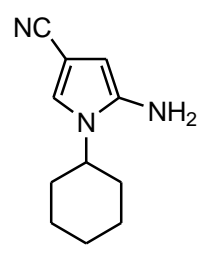
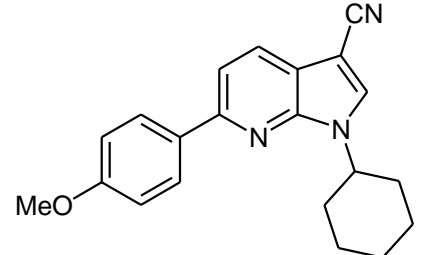
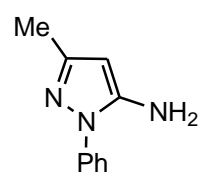
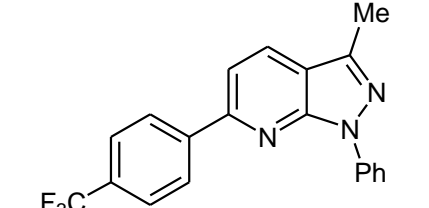
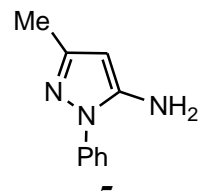
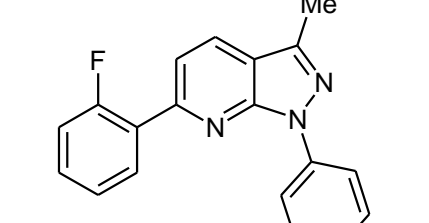


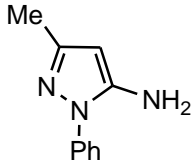
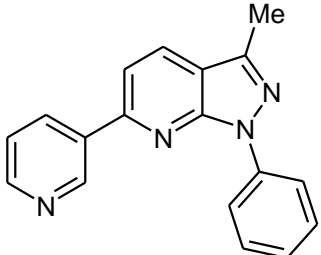
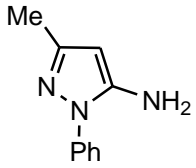
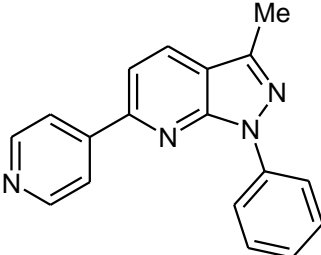
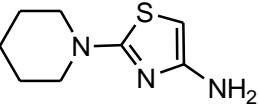
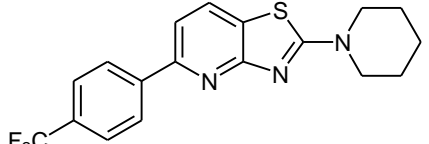
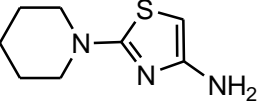
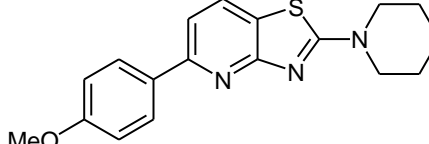
Scheme 2. Reagents and conditions: (i) DMF/TMSCl, under argon, 90–120 °C, 1–2 h.

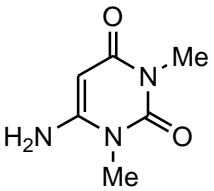
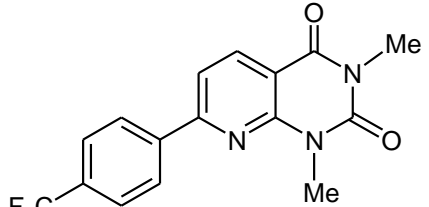
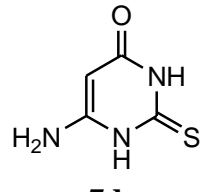
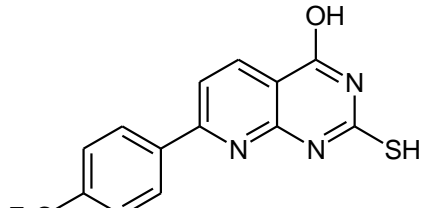
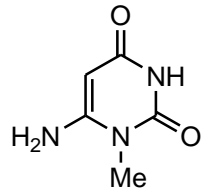
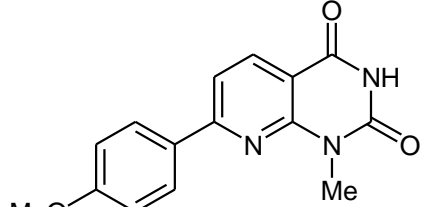
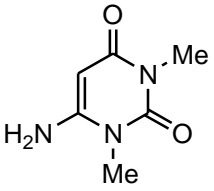
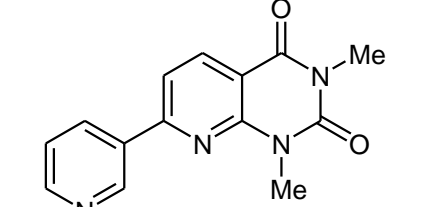
Table 2.

3–5,7,8	26–30	Reaction conditions	Yield (%)
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 3	 26a	DMF/TMSCl, 120 °C, 1 h	70
 3	 26b	DMF/TMSCl, 120 °C, 1 h	72
 3	 26c	DMF/TMSCl, 120 °C, 2 h	78
 3	 26d	DMF/TMSCl, 120 °C, 2 h	70

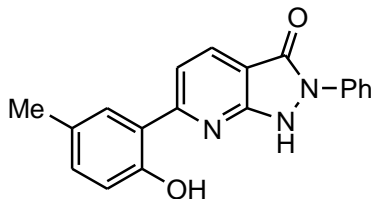
 <p>3</p>	 <p>26e</p>	DMF/TMSCl, 120 °C, 2 h	82
 <p>4</p>	 <p>27</p>	DMF/TMSCl, 120 °C, 1 h	75
 <p>5</p>	 <p>28a</p>	DMF/TMSCl, 100 °C, 1 h	77
 <p>5</p>	 <p>28b</p>	DMF/TMSCl, 120 °C, 2 h	78

 <p>5</p>	 <p>28c</p>	DMF/TMSCl, 120 °C, 2 h	65
 <p>5</p>	 <p>28d</p>	DMF/TMSCl, 120 °C, 2 h	78
 <p>8a</p>	 <p>29a</p>	AcOH, reflux, 2 h	63
 <p>8a</p>	 <p>29b</p>	AcOH, reflux, 2 h	58

 <p>7c</p>	 <p>30a</p>	<p>DMF/TMSCl, 120 °C, 2 h</p>	82
 <p>7d</p>	 <p>30b</p>	<p>DMF/TMSCl, 120 °C, 2 h</p>	85
 <p>7b</p>	 <p>30c</p>	<p>DMF/TMSCl, 120 °C, 2 h</p>	80
 <p>7c</p>	 <p>30d</p>	<p>DMF/TMSCl, 120 °C, 2 h</p>	77

(B) Spectral data

1,2-Dihydro-6-(2-hydroxy-5-methylphenyl)-2-phenylpyrazolo[3,4-*b*]pyridin-3-one (15a)



Brown solid, mp 238–240 °C (*i*-PrOH).

¹H NMR (300 MHz, DMSO-*d*₆): δ = 2.30 (s, 3H, Me), 6.94 (d, 1H, ³*J* = 8.3 Hz), 7.18 (dd, 1H, ³*J* = 8.3 Hz, ⁴*J* = 1.7 Hz), 7.25–7.30 (m, 1H), 7.49–7.55 (m, 2H), 7.85–7.97 (m, 4H), 8.32 (d, 1H, ³*J* = 8.3 Hz), 9.02 (br s, 1H, OH), 11.04 (br s, 1H, NH).

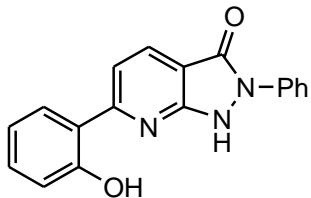
¹³C NMR (62.9 MHz, DMSO-*d*₆): δ = 34.0, 108.5, 114.7, 117.7, 119.3, 119.7, 125.2, 127.9, 128.7, 129.1, 132.9, 134.4, 137.2, 154.9, 156.2, 158.1, 160.0.

MS (EI, 70 eV): *m/z* (%) = 317 (M⁺, 100), 288 (19), 77 (14).

HRMS (EI): calcd for C₁₉H₁₅N₃O₂ (M⁺) 317.11588, found 317.115490.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2967 (w), 2766 (w), 2456 (w), 1665 (w), 1593 (m), 1486 (m), 1447 (m), 1392 (w), 1295 (m), 1231 (m), 1124 (m), 1076 (w), 1026 (w), 884 (w), 809 (m), 746 (s), 684 (s), 603 (m).

1,2-Dihydro-6-(2-hydroxyphenyl)-2-phenylpyrazolo[3,4-*b*]pyridin-3-one (15b)



Orange solid, mp 180–182 °C (heptane:*i*-PrOH/1:5).

¹H NMR (300 MHz, DMSO-*d*₆): δ = 6.95–7.02 (m, 2H), 7.25–7.30 (m, 1H), 7.35–7.41 (m, 1H), 7.50–7.55 (m, 2H), 7.93 (d, 3H, ³*J* = 7.6 Hz), 8.05 (d, 1H, ³*J* = 7.7 Hz), 8.33 (d, 1H, ³*J* = 8.3 Hz), 11.80 (br s, 1H, OH), 12.67 (br s, 1H, NH).

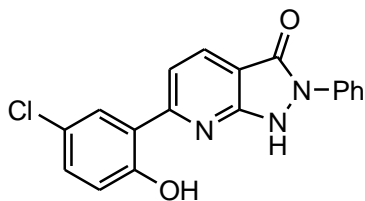
^{13}C NMR (62.9 MHz, $\text{DMSO-}d_6$): $\delta = 108.6, 114.8, 117.8, 119.3, 119.4, 120.0, 125.2, 128.7, 129.1, 132.3, 134.8, 137.1, 155.0, 158.0, 158.4, 160.0$.

MS (EI, 70 eV): m/z (%) = 302 (M^+ , 100), 274 (22), 77 (43).

HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{14}\text{N}_3\text{O}_2$ ($\text{M}+\text{H}$) 303.10023, found 303.100464.

IR (ATR, cm^{-1}): $\tilde{\nu} = 3024$ (w), 1661 (m), 1600 (m), 1484 (m), 1445 (m), 1414 (m), 1295 (w), 1273 (m), 1239 (m), 1187 (w), 1154 (w), 1033 (w), 935 (w), 903 (w), 815 (m), 752 (s), 689 (m), 603 (m).

6-(5-Chloro-2-hydroxyphenyl)-1,2-dihydro-2-phenylpyrazolo[3,4-*b*]pyridin-3-one (15c)



Brown solid, mp 301–303 °C (heptane: *i*-PrOH/1:15).

^1H NMR (250 MHz, $\text{DMSO-}d_6$): $\delta = 7.07$ (d, 1H, $^3J = 8.7$ Hz), 7.27 (t, 1H, $^3J = 7.5$ Hz), 7.39 (dd, 1H, $^3J = 8.7$ Hz, $^3J = 2.7$ Hz), 7.49–7.55 (m, 2H), 7.92–8.06 (m, 4H), 8.31 (d, 1H, $^3J = 8.3$ Hz), 11.92 (br s, 1H, OH), 12.39 (br s, 1H, NH).

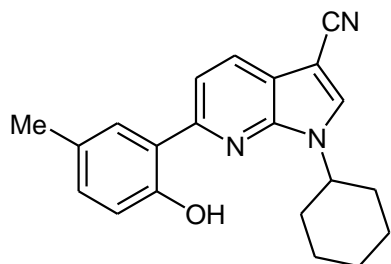
^{13}C NMR (62.9 MHz, $\text{DMSO-}d_6$): $\delta = 109.0, 115.9, 119.4, 119.5, 122.5, 123.0, 125.3, 128.3, 129.1, 131.4, 134.7, 155.3, 155.4, 156.8, 158.0, 178.9$.

MS (EI, 70 eV): m/z (%) = 337 (M^+ , 100), 308 (13).

HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{13}\text{ClN}_3\text{O}_2$ ($\text{M}+\text{H}$) 338.79255, found 338.79257.

IR (ATR, cm^{-1}): $\tilde{\nu} = 3391$ (w), 2991 (w), 2771 (w), 2450 (w), 1661 (m), 1591 (m), 1486 (m), 1447 (m), 1389 (m), 1336 (w), 1292 (m), 1276 (m), 1245 (m), 1207 (w), 1175 (m), 1158 (w), 1126 (w), 1099 (w), 1075 (w), 1023 (w), 944 (w), 868 (w), 828 (m), 810 (m), 757 (s), 719 (s), 686 (m), 598 (m), 577 (m), 539 (m).

1-Cyclohexyl-6-(2-hydroxy-5-methylphenyl)-1*H*-pyrrolo[2,3-*b*]pyridine-3-carbonitrile (16a)



Yellow solid, mp 168–170 °C (heptane: *i*-PrOH/1:10).

^1H NMR (300 MHz, DMSO- d_6): δ = 1.24–1.54 (m, 4H, CH₂), 1.72–2.08 (m, 6H, CH₂), 2.30 (s, 3H, Me), 4.53–4.61 (m, 1H, NCH), 6.86 (d, 1H, 3J = 8.4 Hz), 7.11 (d, 1H, 3J = 7.9 Hz), 7.81 (s, 1H), 8.05 (d, 1H, 3J = 8.4 Hz), 8.25 (d, 1H, 3J = 8.7 Hz), 8.61 (s, 1H), 12.37 (s, 1H, OH).

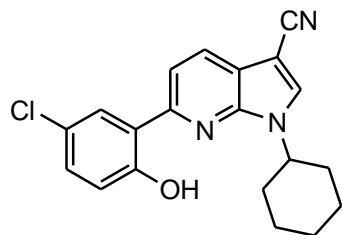
^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 20.2, 24.8, 25.2, 32.1, 55.0, 83.1, 115.2, 115.6, 117.4, 118.2, 120.3, 127.8, 128.2, 129.5, 131.6, 135.6, 143.2, 152.1, 155.4.

MS (GC, 70 eV): m/z (%) = 331 (M^+ , 77), 246 (100), 220 (13).

HRMS (ESI): calcd for C₂₁H₂₁N₃O (M^+) 331.16791, found 331.167627.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3114 (w), 2922 (m), 2857 (m), 2219 (s), 1604 (w), 1579 (m), 1521 (m), 1490 (m), 1443 (s), 1403 (m), 1361 (m), 1282 (s), 1245 (m), 1222 (s), 1209 (s), 1184 (s), 1152 (m), 1028 (m), 955 (w), 894 (w), 862 (w), 819 (s), 791 (s), 764 (m), 732 (m), 673 (m), 648 (s), 615 (m), 553 (m).

6-(5-Chloro-2-hydroxyphenyl)-1-cyclohexyl-1H-pyrrolo[2,3-*b*]pyridine-3-carbonitrile (16b)



Yellow solid, mp 202–210 °C (heptane: *i*-PrOH/1:10).

^1H NMR (300 MHz, DMSO- d_6): δ = 1.23–1.86 (m, 6H, CH₂), 1.97–2.02 (m, 2H, CH₂), 2.16–2.23 (m, 2H, CH₂), 4.52–4.63 (m, 1H, NCH), 6.98 (d, 1H, 3J = 8.9 Hz), 7.25 (dd, 1H, 3J = 8.5 Hz, 3J = 2.5 Hz), 7.79–7.83 (m, 3H), 8.19 (d, 1H, 3J = 8.5 Hz), 13.34 (s, 1H, OH).

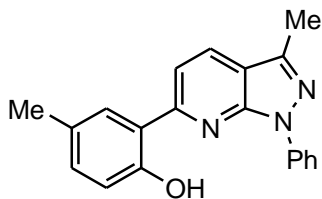
^{13}C NMR (62.9 MHz, CDCl_3): δ = 25.2, 25.5, 33.1, 55.6, 85.3, 114.3, 114.6, 119.3, 120.6, 124.2, 126.5, 130.3, 131.1, 132.8, 143.8, 143.0, 152.0, 157.4.

MS (GC, 70 eV): m/z (%) = 351 (M^+ , 100).

HRMS (EI): calcd for $\text{C}_{20}\text{H}_{18}\text{ClN}_3\text{O}$ (M^+) 351.11329, found 351.113058.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3113 (w), 922 (w), 2219 (w), 1639 (w), 1580 (w), 1539 (w), 1522 (w), 1474 (m), 1446 (m), 1399 (m), 1357 (w), 1278 (m), 1242 (m), 1215 (m), 1185 (m), 1027 (w), 891 (w), 862 (w), 817 (s), 795 (m), 727 (m), 680 (m), 648 (s), 615 (m).

4-Methyl-2-(3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridin-6-yl)phenol (17a)



Yellow solid, mp 139–140 °C (heptane: *i*-PrOH/1:1).

^1H NMR (300 MHz, $\text{DMSO}-d_6$): δ = 2.30 (s, 3H, Me), 2.60 (s, 3H, Me), 6.88 (d, 1H, 3J = 8.8 Hz), 7.14 (dd, 1H, 3J = 8.3 Hz, 3J = 1.9 Hz), 7.38 (t, 1H, 3J = 7.8 Hz), 7.59 (t, 2H, 3J = 7.8 Hz), 7.86 (s, 1H), 7.97–8.04 (m, 3H), 8.42 (d, 1H, 3J = 8.8 Hz), 12.43 (s, 1H, OH).

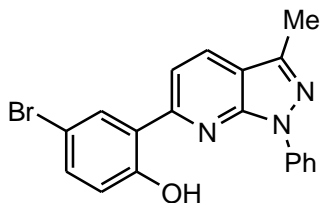
^{13}C NMR (62.9 MHz, $\text{DMSO}-d_6$): δ = 12.1, 20.2, 114.8, 115.1, 117.5, 120.2, 121.2, 126.2, 127.8, 128.7, 129.4, 131.8, 132.3, 138.5, 143.2, 147.7, 155.9, 156.3.

MS (GC, 70 eV): m/z (%) = 315 (M^+ , 100), 286 (20).

HRMS (EI): calcd for $\text{C}_{20}\text{H}_{17}\text{N}_3\text{O}$ (M^+) 315.13661, found 315.136368.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3380 (m), 2984 (m), 2770 (m), 2447 (w), 1580 (m), 1468 (s), 1439 (m), 1403 (m), 1307 (w), 1284 (m), 1245 (m), 1193 (m), 1163 (m), 1130 (m), 1081 (m), 1022 (m), 961 (w), 888 (w), 813 (s), 765 (m), 748 (s), 729 (s), 686 (s), 666 (s), 636 (s).

4-Bromo-2-(3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridin-6-yl)phenol (17b)



Yellow solid, mp 180–181 °C (MeOH: H₂O/3:1).

¹H NMR (300 MHz, DMSO-*d*₆): δ = 2.62 (s, 3H, Me), 6.94 (d, 1H, ³*J* = 8.8 Hz), 7.38 (t, 1H, ³*J* = 7.7 Hz), 7.47 (dd, 1H, ³*J* = 8.8 Hz, ⁴*J* = 2.2 Hz), 7.86 (t, 2H, ³*J* = 7.7 Hz), 8.00–8.09 (m, 3H), 8.18 (s, 1H), 8.44 (d, 1H, ³*J* = 8.8 Hz), 12.44 (s, 1H, OH).

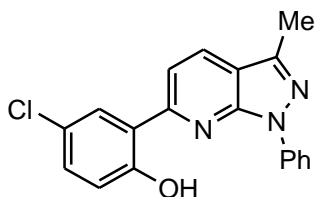
¹³C NMR (62.9 MHz, DMSO-*d*₆): δ = 12.1, 110.5, 115.5, 115.6, 119.7, 121.1, 123.4, 126.2, 129.3, 131.1, 131.9, 133.8, 138.5, 143.2, 147.9, 154.5, 156.9.

MS (GC, 70 eV): *m/z* (%) = 379 (M⁺, 100).

HRMS (ESI): calcd for C₁₉H₁₅BrN₃O (M+1) 380.0393, found 380.03927.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3061 (m), 1593 (s), 1578 (m), 1510 (m), 1474 (m), 1430 (m), 1398 (m), 1362 (m), 1286 (s), 1240 (m), 1206 (s), 1192 (m), 1171 (m), 1092 (m), 1013 (w), 954 (w), 852 (w), 814 (s), 779 (m), 747 (s), 701 (m), 687 (s), 665 (s), 633 (s), 596 (m).

4-Chloro-2-(3-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)phenol (17c)



Yellow solid, mp 186–188 °C (MeOH: H₂O/2:1).

¹H NMR (300 MHz, DMSO-*d*₆): δ = 3.31 (s, 3H, Me), 6.93–7.60 (m, 5H), 8.08 (s, 4H), 8.33–8.64 (m, 1H), 12.42 (s, 1H, OH).

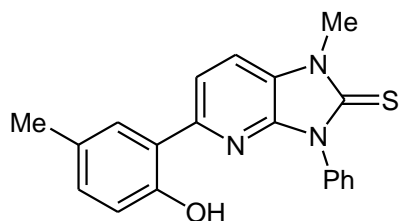
¹³C NMR (62.9 MHz, DMSO-*d*₆): δ = 12.1, 112.2, 115.6, 119.3, 121.1, 123.0, 123.9, 126.2, 128.3, 129.4, 131.0, 132.0, 134.1, 138.5, 143.2, 156.5, 157.3.

MS (GC, 70 eV): *m/z* (%) = 335 (M⁺, 100).

HRMS (EI): calcd for C₁₉H₁₄ClN₃O (M⁺) 335.08199, found 335.081761.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3063 (m), 1641 (w), 1596 (m), 1579 (m), 1513 (m), 1480 (m), 1466 (m), 1434 (m), 1398 (m), 1364 (m), 1331 (w), 1286 (s), 1241 (m), 1207 (m), 1194 (m), 1133 (w), 1104 (m), 1081 (m), 1024 (w), 901 (w), 834 (w), 812 (s), 779 (m), 746 (s), 713 (m), 687 (s), 653 (m), 633 (m).

5-(2-Hydroxy-5-methylphenyl)-1-methyl-3-phenyl-1*H*-imidazo[4,5-*b*]pyridine-2(3*H*)-thione (18a)



Green solid, mp 224–225 °C (heptane: *i*-PrOH/1:3).

^1H NMR (300 MHz, DMSO- d_6): δ = 2.25 (s, 3H, Me), 3.80 (s, 3H, NMe), 6.70 (d, 1H, 3J = 8.2 Hz), 7.01 (dd, 1H, 3J = 8.2 Hz, 4J = 1.5 Hz), 7.48–7.66 (m, 5H, Ph), 7.70 (s, 1H), 7.99–8.05 (m, 2H), 11.76 (s, 1H, OH).

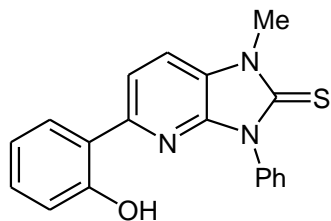
^{13}C NMR (69.2 MHz, DMSO- d_6): δ = 20.2, 31.2, 115.6, 117.4, 118.7, 119.4, 124.8, 127.3, 127.6, 128.1, 129.0, 129.2, 131.2, 134.2, 142.7, 150.0, 154.9, 170.6.

MS (GC, 70 eV): m/z (%) = 347 (M^+ , 100), 332 (15).

HRMS (ESI): calcd for $\text{C}_{20}\text{H}_{18}\text{N}_3\text{OS}$ ($\text{M}+\text{H}$) 348.2558, found 348.2559.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2912 (w), 1496 (w), 1464 (m), 1434 (m), 1381 (m), 1329 (m), 1282 (s), 1249 (s), 1215 (m), 1183 (m), 1135 (m), 1189 (m), 1024 (w), 911 (w), 815 (s), 793 (s), 773 (m), 758 (s), 733 (m), 686 (s), 648 (m).

5-(2-Hydroxyphenyl)-1-methyl-3-phenyl-1H-imidazo[4,5-b]pyridine-2(3H)-thione (18b)



White solid, mp 220–222 °C (heptane: *i*-PrOH/1:3).

^1H NMR (300 MHz, DMSO- d_6): δ = 3.82 (s, 3H, Me), 6.81–6.91 (m, 2H), 7.19–7.25 (m, 1H), 7.54–7.67 (m, 5H, Ph), 7.91 (dd, 1H, 3J = 8.1 Hz, 4J = 1.4 Hz), 8.03–8.10 (m, 2H), 11.90 (s, 1H, OH).

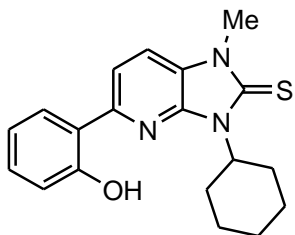
^{13}C NMR (75.5 MHz, DMSO- d_6): δ = 31.2, 116.0, 117.5, 118.7, 119.2, 120.2, 125.0, 127.5, 128.2, 129.0, 129.3, 130.5, 134.2, 142.9, 149.9, 157.0, 170.7.

MS (GC, 70 eV): m/z (%) = 333 (M^+ , 100), 318 (19).

HRMS (EI): calcd for $\text{C}_{19}\text{H}_{15}\text{N}_3\text{OS}$ (M^+) 333.08521, found 333.092105.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3051 (w), 1615 (w), 1593 (w), 1499 (w), 1466 (m), 1427 (m), 1332 (s), 1296 (m), 1281 (m), 1248 (m), 1227 (m), 1203 (m), 1164 (m), 1041 (m), 1090 (m), 1022 (w), 963 (w), 932 (w), 812 (s), 753 (s), 734 (m), 706 (s), 689 (s), 636 (s).

3-Cyclohexyl-5-(2-hydroxyphenyl)-1-methyl-1H-imidazo[4,5-b]pyridine-2(3H)-thione (18c)



Yellow solid, mp 250–251 °C (*i*-PrOH).

^1H NMR (300 MHz, $\text{DMSO-}d_6$): δ = 1.16–1.49 (m, 3H, CH_2), 1.75–1.93 (m, 5H, CH_2), 2.35–2.43 (m, 2H, CH_2), 3.75 (s, 3H, Me), 5.07–5.15 (m, 1H, NCH), 6.93–7.00 (m, 2H), 7.26–7.33 (m, 1H), 7.96–8.08 (m, 3H), 12.02 (s, 1H, OH).

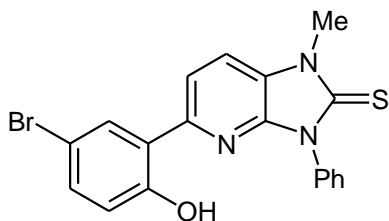
^{13}C NMR (62.9 MHz, $\text{DMSO-}d_6$): δ = 25.0, 25.5, 29.0, 31.4, 56.1, 115.9, 117.4, 118.3, 119.5, 121.3, 124.8, 128.1, 130.4, 142.2, 149.0, 156.8, 169.8.

MS (GC, 70 eV): m/z (%) = 339 (M^+ , 48), 257 (100).

HRMS (EI): calcd for $\text{C}_{19}\text{H}_{21}\text{N}_3\text{OS}$ (M^+) 339.13998, found 339.139863.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2918 (w), 2858 (w), 1614 (w), 1504 (w), 1465 (m), 1428 (m), 1382 (m), 1325 (m), 1282 (m), 1238 (m), 1167 (m), 1139 (m), 1044 (m), 894 (w), 808 (s), 738 (s), 685 (m), 657 (m), 620 (m).

5-(5-Bromo-2-hydroxyphenyl)-1-methyl-3-phenyl-1H-imidazo[4,5-b]pyridine-2(3H)-thione (18d)



Brown solid, mp 248–250 °C (MeOH: H_2O /15:1).

^1H NMR (250 MHz, DMSO- d_6): δ = 3.58 (s, 3H, Me), 6.57 (d, 1H, 3J = 8.9 Hz), 7.11 (dd, 1H, 3J = 8.7 Hz, 4J = 2.2 Hz), 7.29–7.42 (m, 5H, Ph), 7.79–7.80 (m, 2H), 7.83 (s, 1H), 11.64 (s, 1H, OH).

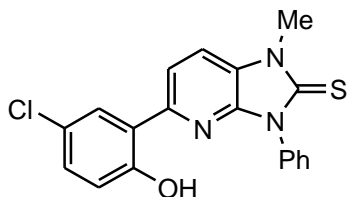
^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 31.2, 110.5, 116.9, 118.5, 119.7, 123.0, 125.5, 128.2, 129.0, 129.2, 129.9, 132.8, 134.2, 141.2, 143.2, 148.1, 156.0, 171.0.

MS (GC, 70 eV): m/z (%) = 412 (M^+ , 100), 166 (12).

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{15}\text{ClN}_3\text{OS}$ ($\text{M}+\text{H}$) 413.11258, found 413.11261

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2913 (w), 1499 (w), 1463 (m), 1431 (w), 1384 (m), 1329 (m), 1280 (s), 1247 (m), 1200 (m), 1148 (m), 1090 (w), 969 (w), 934 (w), 864 (w), 819 (s), 714 (w), 687 (s), 640 (m), 582 (w).

5-(5-Chloro-2-hydroxyphenyl)-1-methyl-3-phenyl-1*H*-imidazo[4,5-*b*]pyridine-2(3*H*)-thione (18e)



Yellow solid, mp 252–254 °C (*i*-PrOH).

^1H NMR (300 MHz, DMSO- d_6): δ = 3.83 (s, 3H, Me), 6.87 (d, 1H, 3J = 8.7 Hz), 7.23 (s, 1H), 7.62 (s, 5H, Ph), 7.92 (s, 1H), 8.05–8.18 (m, 2H), 11.90 (br s, 1H, OH).

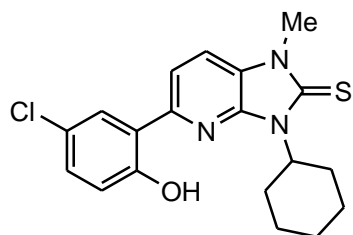
^{13}C NMR due to bed solubility was not possible to measure.

MS (GC, 70 eV): m/z (%) = 367 (M^+ , 100), 352 (11).

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{15}\text{ClN}_3\text{OS}$ ($\text{M}+\text{H}$) 368.06189, found 368.06207.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2915 (w), 1618 (w), 1498 (m), 1462 (s), 1434 (m), 1383 (m), 1330 (s), 1297 (s), 1279 (s), 1247 (m), 1189 (m), 1150 (m), 1086 (m), 1026 (w), 971 (w), 935 (w), 904 (w), 865 (w), 819 (s), 754 (m), 722 (m), 687 (s), 658 (m), 584 (m).

5-(5-Chloro-2-hydroxyphenyl)-3-cyclohexyl-1-methyl-1*H*-imidazo[4,5-*b*]pyridine-2(3*H*)-thione (18f)



Yellow solid, mp 185–187 °C (heptane: *i*-PrOH/1:10).

^1H NMR (300 MHz, DMSO- d_6): δ = 1.16–1.48 (m, 3H, CH₂), 1.61–1.99 (m, 5H, CH₂), 2.36–2.44 (m, 2H, CH₂), 3.75 (s, 3H, Me), 5.05–5.13 (m, 1H, NCH), 7.02 (d, 1H, 3J = 8.5 Hz, CH_{Ar}), 7.30 (dd, 1H, 3J = 8.8 Hz, 4J = 2.5 Hz, CH_{Ar}), 7.95–8.02 (m, 2H, CH_{Ar}), 8.14 (d, 1H, 3J = 8.8 Hz, CH_{Ar}), 11.91 (s, 1H, OH).

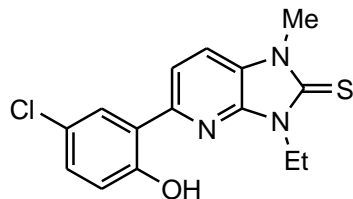
^{13}C NMR (75.5 MHz, DMSO- d_6): δ = 25.0, 25.5, 29.0, 31.4, 56.2, 116.7, 118.0, 119.1, 123.1, 123.4, 125.2, 127.6, 129.7, 142.5, 147.2, 155.4, 170.0.

MS (GC, 70 eV): m/z (%) = 373 (M⁺, 42), 291 (100).

HRMS (ESI): calcd for C₁₉H₂₁ClN₃OS (M+H) 374.10884, found 374.10876.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2934 (w), 2854 (w), 1615 (w), 1468 (m), 1434 (m), 1383 (m), 1338 (m), 1323 (m), 1295 (m), 1279 (s), 1244 (m), 1213 (w), 1170 (m), 1141 (m), 1092 (w), 1047 (w), 933 (w), 864 (w), 825 (m), 806 (s), 718 (m), 655 (m), 625 (w), 582 (m).

5-(5-Chloro-2-hydroxyphenyl)-3-ethyl-1-methyl-1H-imidazo[4,5-*b*]pyridine-2(3H)-thione (18g)



Green solid, mp 204–206 °C (*i*-PrOH).

^1H NMR (300 MHz, DMSO- d_6): δ = 1.33 (t, 3H, 3J = 7.1 Hz, CH₂Me), 3.73 (s, 3H, Me), 4.34 (q, 2H, CH₂), 6.96 (d, 1H, 3J = 8.5 Hz), 7.26 (dd, 1H, 3J = 8.7 Hz, 4J = 2.7 Hz), 7.89–7.93 (m, 2H), 8.05 (d, 1H, 3J = 8.5 Hz), 11.64 (br s, 1H, OH).

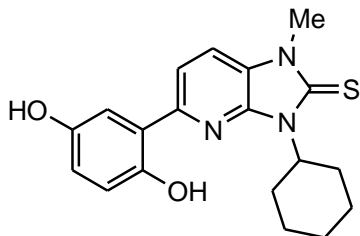
^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 12.7, 30.9, 38.1, 117.2, 117.7, 118.9, 123.0, 123.7, 125.0, 127.7, 129.8, 142.5, 147.8, 155.2, 169.9.

MS (GC, 70 eV): m/z (%) = 319 (M⁺, 100), 291 (50).

HRMS (ESI): calcd for C₁₅H₁₅ClN₃OS (M+H) 320.06189, found 320.06194.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2938 (w), 1469 (m), 1436, 1383 (s), 1341 (m), 1316 (m), 1278 (s), 1244 (m), 1187 (m), 1148 (w), 1122 (s), 1089 (m), 1028 (w), 957 (w), 867 (w), 858 (w), 846 (w), 829 (m), 802 (s), 774 (w), 753 (w), 718 (m), 673 (w), 652 (m), 595 (m), 570 (w), 548 (w).

3-Cyclohexyl-5-(2,5-dihydroxyphenyl)-1-methyl-1*H*-imidazo[4,5-*b*]pyridine-2(3*H*)-thione (18h)



Yellow solid, mp 307–309 °C (*i*-PrOH).

^1H NMR (300 MHz, $\text{DMSO-}d_6$): δ = 1.21–1.53 (m, 3H, CH_2), 1.62–2.11 (m, 5H, CH_2), 2.29–2.40 (m, 2H, CH_2), 3.73 (s, 3H, Me), 5.06–5.14 (m, 1H, NCH), 6.36–6.41 (m, 2H), 7.82 (d, 1H, $^3J = 8.7$ Hz), 7.88–7.95 (m, 2H), 9.77 (s, 1H, OH), 12.44 (s, 1H, OH).

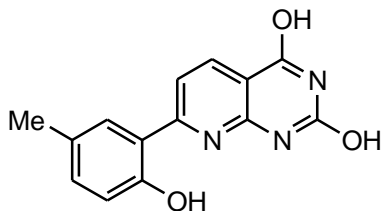
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$): δ = 25.6, 29.0, 31.4, 56.0, 62.0, 103.4, 107.8, 112.2, 114.2, 118.7, 123.9, 128.8, 141.6, 150.0, 158.7, 160.0, 169.2.

MS (GC, 70 eV): m/z (%) = 355 (M^+ , 74), 273 (100), 168 (10).

HRMS (ESI): calcd for $\text{C}_{19}\text{H}_{21}\text{N}_3\text{O}_2\text{S}$ (M^+) 355.13490, found 355.134366.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3305 (w), 3139 (w), 2929 (m), 2862 (w), 1610 (m), 1465 (s), 1437 (s), 1385 (m), 1323 (s), 1298 (s), 1250 (s), 1221 (m), 1169 (s), 1140 (s), 1122 (m), 1046 (m), 976 (m), 946 (m), 840 (w), 791 (s), 721 (m), 652 (m), 611 (m).

7-(2-Hydroxy-5-methylphenyl)pyrido[2,3-*d*]pyrimidine-2,4-diol (19a)



Green solid, mp more than 375 °C (EE: *i*-PrOH/1:2).

^1H NMR (300 MHz, $\text{DMSO-}d_6$): δ = 2.28 (s, 3H, Me), 6.86 (d, 1H, $^3J = 8.2$ Hz), 7.17 (dd, 1H, $^3J = 8.4$ Hz, $^4J = 1.7$ Hz), 7.83 (s, 1H), 7.93 (d, 1H, $^3J = 8.4$ Hz), 8.30 (d, 1H, $^3J = 8.4$ Hz), 8.93, 11.45, 12.00 (all s, 1H, OH).

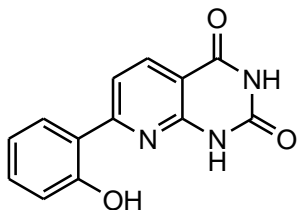
^{13}C NMR (62.9 MHz, $\text{DMSO-}d_6$): δ = 20.1, 107.7, 114.8, 118.1, 118.2, 127.8, 128.2, 133.5, 137.4, 150.4, 150.7, 156.8, 160.9, 161.8.

MS (GC, 70 eV): m/z (%) = 269 (M^+ , 100), 198 (16).

HRMS (EI): calcd for $\text{C}_{14}\text{H}_{11}\text{N}_3\text{O}_3$ (M^+) 269.07949, found 269.079464.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3426 (w), 2981 (w), 2764 (m), 2457 (w), 1709 (m), 1661 (s), 1591 (s), 1472 (m), 1409 (s), 1365 (m), 1266 (m), 1241 (m), 1203 (m), 1115 (w), 1054 (w), 1025 (m), 950 (w), 878 (w), 800 (s), 767 (s), 706 (m), 678 (m), 651 (m), 588 (m).

7-(2-Hydroxyphenyl)pyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (19b)



White solid, mp > 375 °C (EE: *i*-PrOH/1:3).

^1H NMR (300 MHz, $\text{DMSO-}d_6$): δ = 6.92–7.00 (m, 2H), 7.35–7.41 (m, 1H), 7.96 (d, 1H, 3J = 8.4 Hz), 8.04 (dd, 1H, 3J = 8.0 Hz, 4J = 1.4 Hz), 8.33 (d, 1H, 3J = 8.4 Hz), 11.51 (s, 1H, OH), 12.03 (s, 1H, NH), 12.52 (s, 1H, NH).

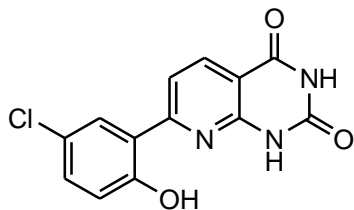
^{13}C NMR (62.9 MHz, $\text{DMSO-}d_6$): δ = 107.9, 114.9, 118.2, 118.7, 119.2, 128.4, 132.7, 137.5, 150.4, 150.7, 158.9, 160.8, 161.8.

MS (GC, 70 eV): m/z (%) = 255 (M^+ , 12), 184 (20).

HRMS (ESI): calcd for $\text{C}_{13}\text{H}_{10}\text{N}_3\text{O}_3$ ($\text{M}+1$) 256.07167, found 256.07177.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3152 (w), 2984 (w), 2765 (m), 1710 (m), 1667 (m), 1592 (m), 1475 (m), 1414 (m), 1384 (m), 1277 (m), 1220 (m), 1151 (m), 1007 (w), 942 (w), 859 (m), 803 (m), 749 (s), 680 (m), 643 (m).

7-(5-Chloro-2-hydroxyphenyl)pyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (19c)



Orange solid, mp > 375 °C (EE: *i*-PrOH/1:3).

^1H NMR (300 MHz, DMSO- d_6): δ = 6.99 (d, 1H, 3J = 8.8 Hz), 7.38 (dd, 1H, 3J = 8.8 Hz, 4J = 2.5 Hz), 8.00–8.07 (m, 2H), 8.31 (d, 1H, 3J = 8.4 Hz), 11.52 (s, 1H, OH), 11.99 (s, 1H, NH), 12.40 (s, 1H, NH).

^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 108.5, 115.7, 120.0, 120.6, 123.0, 127.8, 132.1, 137.6, 150.3, 150.8, 157.4, 159.1, 161.8.

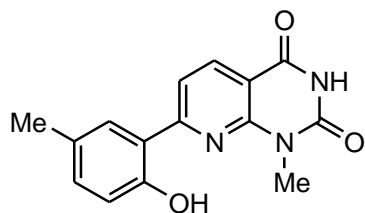
MS (EI, 70 eV): m/z (%) = 289 (M^+ , 100), 218 (27).

HRMS (EI): calcd for $\text{C}_{13}\text{H}_9\text{ClN}_3\text{O}_3$ ($\text{M}+1$) 290.0327, found 290.0331.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3167 (w), 3043 (w), 1716 (m), 1659 (m), 1586 (m), 1467 (m), 1403 (m), 1344 (m), 1265 (m), 1241 (m), 1171 (m), 1100 (w), 1045 (w), 946 (w), 829 (m), 799 (s), 773 (m), 730 (m), 693 (s), 646 (m).

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7-(2-Hydroxy-5-methylphenyl)-1-methylpyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (19d)



White solid, mp 332–333 °C (EE: *i*-PrOH/1:3).

^1H NMR (300 MHz, DMSO- d_6): δ = 2.29 (s, 3H, Me), 3.54 (s, 3H, NMe), 6.91 (d, 1H, 3J = 8.6 Hz), 7.16 (dd, 1H, 3J = 8.2 Hz, 4J = 2.0 Hz), 7.81 (s, 1H), 7.98 (d, 1H, 3J = 8.2 Hz), 8.35 (d, 1H, 3J = 8.2 Hz), 11.46 (br s, 2H, OH).

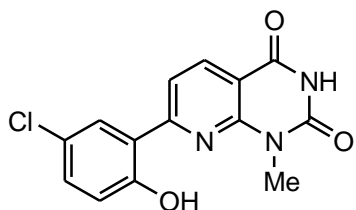
^{13}C NMR due to bed solubility was not possible to measure.

MS (GC, 70 eV): m/z (%) = 283 (M^+ , 100), 254 (33), 185 (20).

HRMS (EI): calcd for $\text{C}_{15}\text{H}_{13}\text{N}_3\text{O}_3$ (M^+) 283.09514, found 283.094282.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3182 (w), 2764 (m), 2457 (w), 1714 (m), 1682 (s), 1595 (s), 1470 (m), 1404 (m), 1365 (m), 1277 (m), 1225 (m), 1159 (w), 1131 (w), 1078 (w), 1027 (w), 831 (m), 804 (m), 774 (m), 734 (m), 690 (m), 669 (m), 611 (w).

7-(5-Chloro-2-hydroxyphenyl)-1-methylpyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (19e)



Yellow solid, mp 148–150 °C (MeOH: H₂O/2:1).

¹H NMR (300 MHz, DMSO-*d*₆): δ = 3.54 (s, 3H, Me), 7.04 (d, 1H, ³*J* = 7.8 Hz), 7.40 (d, 1H, ³*J* = 8.0 Hz), 8.07–8.11 (m, 2H), 8.39 (d, 1H, ³*J* = 7.3 Hz), 11.76 (s, 2H, OH, NH).

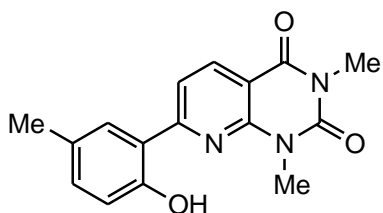
¹³C NMR due to bed solubility was not possible to measure.

MS (EI, 70 eV): *m/z* (%) = 303 (M⁺, 100), 274 (23), 205 (27), 168 (20), 99 (11), 78 (36).

HRMS (EI): calcd for C₁₄H₁₀ClN₃O₃ (M⁺) 303.04052, found 303.040878.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3047 (w), 1727 (w), 1709 (m), 1689 (m), 1594 (s), 1484 (m), 1469 (m), 1406 (s), 1365 (m), 1285 (s), 1239 (w), 1219 (w), 1202 (w), 1162 (w), 1130 (w), 1102 (w), 1074 (w), 1025 (w), 979 (w), 838 (m), 806 (m), 734 (w), 719 (s), 697 (m), 686 (m), 651 (w).

7-(2-Hydroxy-5-methylphenyl)-1,3-dimethylpyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (19f)



White solid, mp 304–306 °C (*i*-PrOH).

¹H NMR (300 MHz, CDCl₃-*d*₆): δ = 2.35 (s, 3H, Me), 3.50 (s, 3H, NMe), 3.75 (s, 3H, NMe), 6.95 (d, 1H, ³*J* = 8.4 Hz), 7.22 (dd, 1H, ³*J* = 8.4 Hz, ⁴*J* = 1.4 Hz), 7.65 (s, 1H), 8.53 (d, 1H, ³*J* = 8.4 Hz), 12.94 (br s, 2H, OH).

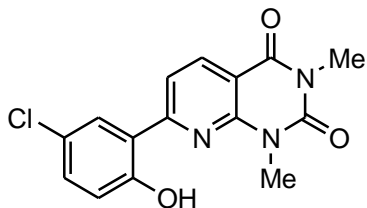
¹³C NMR (62.9 MHz, CDCl₃): δ = 20.7, 28.6, 29.8, 105.8, 108.3, 114.2, 118.6, 127.5, 128.8, 134.5, 138.7, 143.1, 149.4, 151.3, 155.0, 162.1.

MS (GC, 70 eV): *m/z* (%) = 297 (M⁺, 100), 268 (25), 185 (14).

HRMS (EI): calcd for C₁₆H₁₅N₃O₃ (M⁺) 297.11079, found 297.110626.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2930 (w), 1712 (w), 1652 (s), 1599 (s), 1478 (m), 1424 (s), 1395 (m), 1358 (s), 1298 (m), 1280 (s), 1233 (m), 1221 (s), 1130 (m), 1103 (m), 1063 (w), 1018 (m), 831 (m), 798 (s), 776 (m), 747 (s), 734 (m), 712 (s), 665 (m), 646 (m), 543 (m).

7-(5-Chloro-2-hydroxyphenyl)-1,3-dimethylpyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (19g)



Yellow solid, mp 252–253 °C (heptane: *i*-PrOH/1:5).

¹H NMR (300 MHz, DMSO-*d*₆): δ = 3.32 (s, 3H, NMe), 3.62 (s, 3H, NMe), 7.11 (d, 1H, ³*J* = 8.7 Hz), 6.39 (dd, 1H, ³*J* = 9.0 Hz, ⁴*J* = 3.0 Hz), 8.05 (d, 1H, ³*J* = 2.7 Hz), 8.12 (d, 1H, ³*J* = 8.3 Hz), 8.43 (d, 1H, ³*J* = 8.3 Hz), 11.70 (s, 1H, OH).

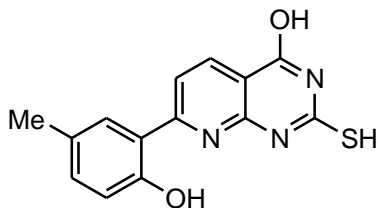
¹³C NMR (75.5 MHz, DMSO-*d*₆): δ = 28.1, 29.2, 108.8, 117.9, 119.2, 123.1, 123.4, 128.8, 131.5, 137.7, 149.8, 151.0, 156.3, 158.0, 160.4.

MS (GC, 70 eV): *m/z* (%) = 317 (M⁺, 100), 288 (21), 205 (19).

HRMS (EI): calcd for C₁₅H₁₂ClN₃O₃ (M⁺) 317.05617, found 317.05629.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3362 (w), 2962 (w), 2767 (m), 2452 (w), 1708 (m), 1658 (s), 1598 (s), 1468 (s), 1424 (s), 1354 (m), 1284 (m), 1238 (m), 1211 (m), 1122 (w), 1096 (m), 1052 (w), 1022 (m), 865 (w), 847 (m), 804 (s), 747 (m), 711 (m), 691 (m), 651 (m), 641 (m).

7-(2-Hydroxy-5-methylphenyl)-2-mercaptopyrido[2,3-*d*]pyrimidin-4-ol (19h)



Green solid, mp 371–373 °C (heptane: *i*-PrOH/1:5).

¹H NMR (300 MHz, DMSO-*d*₆): δ = 2.29 (s, 3H, Me), 6.87 (d, 1H, ³*J* = 8.4 Hz), 7.20 (dd, 1H, ³*J* = 8.4 Hz, ⁴*J* = 1.7 Hz), 7.87 (s, 1H), 8.04 (d, 1H, ³*J* = 8.7 Hz), 8.33 (d, 1H, ³*J* = 8.7 Hz), 12.08 (s, 1H, OH), 12.65 (s, 1H, OH), 13.47 (s, 1H, SH).

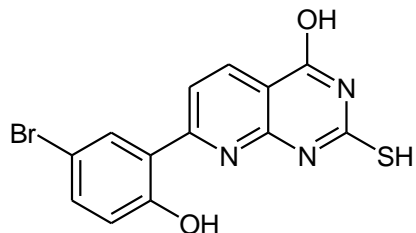
¹³C NMR (62.9 MHz, DMSO-*d*₆): δ = 20.1, 109.8, 116.3, 118.0, 118.3, 127.9, 128.3, 133.8, 137.2, 149.8, 156.9, 159.2, 161.2, 175.9.

MS (GC, 70 eV): *m/z* (%) = 285 (M⁺, 100), 168 (26), 99 (14).

HRMS (EI): calcd for C₁₄H₁₁N₃O₂S (M⁺) 285.05665, found 285.056686.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3134 (w), 3018 (w), 2768 (w), 1683 (m), 1609 (s), 1589 (s), 1567 (s), 1545 (s), 1481 (s), 1417 (m), 1282 (m), 1239 (s), 1200 (s), 1161 (s), 1133 (s), 1052 (w), 988 (w), 836 (m), 812 (s), 777 (s), 692 (m), 660 (m), 610 (w), 578 (s), 543 (s).

7-(5-Bromo-2-hydroxyphenyl)-4-mercaptopyrido[2,3-*d*]pyrimidin-2-ol (19i)



Brown solid, mp > 375 °C (heptane: *i*-PrOH/1:5).

^1H NMR (300 MHz, $\text{DMSO-}d_6$): δ = 7.00 (d, 1H, 3J = 8.8 Hz), 7.52 (dd, 1H, 3J = 8.8 Hz, 4J = 2.5 Hz), 8.14 (d, 1H, 3J = 8.6 Hz), 8.23 (s, 1H), 8.34 (d, 1H, 3J = 8.6 Hz), 12.20 (s, 1H, OH), 12.67 (s, 1H, OH), 13.44 (s, 1H, SH).

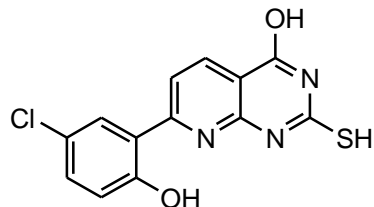
^{13}C NMR (62.9 MHz, $\text{DMSO-}d_6$): δ = 110.4, 110.5, 117.5, 120.5, 121.2, 130.9, 135.1, 137.3, 150.0, 157.8, 159.2, 159.4, 175.9.

MS (GC, 70 eV): m/z (%) = 348 (M^+ , 100), 207 (16).

HRMS (EI): calcd for $\text{C}_{13}\text{H}_8\text{BrN}_3\text{O}_2\text{S}$ (M^+) 348.95151, found 348.950828.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3184 (w), 2932 (w), 2758 (m), 2456 (w), 1665 (s), 1621 (m), 1586 (s), 1548 (m), 1470 (s), 1413 (m), 1356 (s), 1272 (s), 1236 (s), 1205 (s), 1175 (s), 1087 (w), 1026 (w), 939 (w), 838 (m), 814 (m), 787 (s), 723 (m), 664 (m).

7-(5-Chloro-2-hydroxyphenyl)-2-mercaptopyrido[2,3-*d*]pyrimidin-4-ol (19j)



Yellow solid, mp > 375 °C (MeOH: H_2O /2:1).

^1H NMR (250 MHz, $\text{DMSO-}d_6$): δ = 7.01 (d, 1H, 3J = 8.4 Hz), 7.41 (td, 1H, 3J = 8.8 Hz, 4J = 2.5 Hz), 8.11–8.15 (m, 2H), 8.35 (d, 1H, 3J = 8.4 Hz), 12.24 (s, 1H, OH), 12.69 (s, 1H, OH), 13.47 (s, 1H, SH).

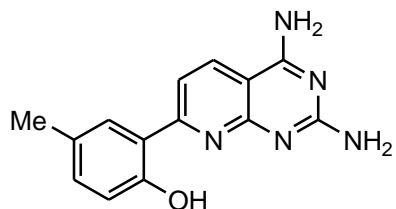
^{13}C NMR (62.9 MHz, $\text{DMSO-}d_6$): δ = 110.5, 117.1, 120.2, 120.3, 123.1, 127.8, 132.4, 137.4, 149.9, 157.6, 159.2, 159.5, 176.0.

MS (GC, 70 eV): m/z (%) = 305 (M^+ , 100), 277 (12), 218 (12), 168 (28), 99 (16).

HRMS (EI): calcd for $C_{13}H_8ClN_3O_2S$ (M^+) 305.00203, found 305.001007.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3186 (w), 1665 (m), 1606 (m), 1587 (s), 1558 (m), 1470 (m), 1414 (m), 1356 (m), 1271 (m), 1236 (m), 1192 (m), 1136 (m), 1098 (w), 1051 (w), 941 (w), 838 (m), 815 (m), 785 (s), 735 (m), 699 (w), 667 (m), 575 (m), 540 (m).

2-(2,4-Diaminopyrido[2,3-*d*]pyrimidin-7-yl)-4-methylphenol (20a)



Yellow solid, mp 352–354 °C (EE: *i*-PrOH/2:1).

1H NMR (250 MHz, $DMSO-d_6$): δ = 2.28 (s, 3H, Me), 6.90 (d, 1H, $^3J = 8.2$ Hz), 7.19 (d, 1H, $^3J = 8.0$ Hz), 7.88 (br s, 2H, NH_2), 8.17 (d, 1H, $^3J = 8.5$ Hz), 8.50 (br s, 1H, NH_2), 8.87 (d, 1H, $^3J = 8.5$ Hz), 9.04 (br s, 1H, NH_2), 11.94 (br s, 1H, NH_2), 13.20 (s, 1H, OH).

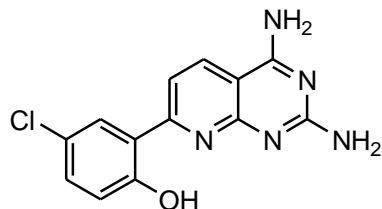
^{13}C NMR (62.9 MHz, $DMSO-d_6$): δ = 20.1, 103.1, 117.5, 117.8, 118.9, 128.0, 128.9, 133.8, 135.5, 148.7, 156.0, 156.6, 161.6, 162.7.

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

HRMS (EI): calcd for $C_{14}H_{13}N_5O$ (M^+) 267.11146, found 267.111500.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3412 (w), 3131 (w), 2861 (w), 1645 (m), 1608 (m), 1524 (w), 1480 (m), 1460 (m), 1370 (m), 1344 (m), 1291 (m), 1242 (m), 1214 (m), 1184 (m), 1147 (m), 1043 (m), 1004 (m), 874 (w), 835 (m), 800 (s), 770 (m), 742 (s), 701 (s), 674 (s), 646 (s).

2-(2,4-Diaminopyrido[2,3-*d*]pyrimidin-7-yl)-4-chlorophenol (20b)



Yellow solid, mp > 375 °C (EE: *i*-PrOH/1:3).

^1H NMR (250 MHz, DMSO- d_6): δ = 7.08 (d, 1H, 3J = 8.9 Hz), 7.40 (td, 1H, 3J = 8.9 Hz, 4J = 2.5 Hz), 7.81 (br s, 1H, NH₂), 8.08 (d, 1H, 3J = 2.5 Hz), 8.23 (d, 1H, 3J = 8.9 Hz), 8.52 (br s, 1H, NH₂), 8.88 (d, 1H, 3J = 8.5 Hz), 9.07 (br s, 1H, NH₂), 9.41 (br s, 1H, NH₂), 12.04 (s, 1H, OH).

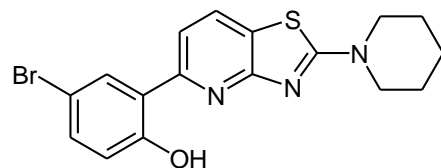
^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 103.4, 118.5, 119.7, 121.6, 123.1, 128.4, 132.1, 135.6, 148.9, 156.1, 157.0, 159.7, 162.7.

MS (GC, 70 eV): m/z (%) = 287 (M⁺, 100), 122 (16), 105 (36), 77 (16).

HRMS (ESI): calcd for C₁₃H₁₁ClN₅O (M+1) 288.06466, found 288.06522.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3307 (w), 3140 (w), 2586 (w), 1682 (w), 1645 (s), 1605 (s), 1525 (w), 1453 (s), 1400 (w), 1285 (m), 1235 (m), 1192 (m), 1145 (w), 1041 (w), 981 (w), 802 (s), 738 (m), 695 (m).

4-Bromo-2-(2-(piperidin-1-yl)thiazolo[4,5-*b*]pyridin-5-yl)phenol (21a)



Brown solid, mp 194–196 °C (EE: *i*-PrOH/1:2).

^1H NMR (300 MHz, DMSO- d_6): δ = 1.66 (s, 6H, CH₂), 3.67 (s, 4H, CH₂), 6.87–6.90 (m, 1H), 7.42 (s, 1H), 7.89 (s, 1H), 8.16 (s, 1H), 8.33–8.35 (s, 1H), 14.15 (s, 1H, OH).

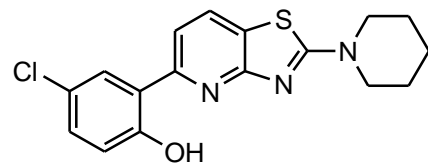
^{13}C NMR due to bed solubility was not possible to measure.

MS (EI, 70 eV): m/z (%) = 389 (M⁺, 100).

HRMS (ESI): calcd for C₁₇H₁₇BrN₃OS (M+H) 390.02702, found 390.02783.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2925 (w), 1573 (m), 1523 (s), 1485 (m), 1423 (m), 1365 (m), 1328 (m), 1281 (s), 1272 (s), 1249 (s), 1213 (s), 1172 (m), 1123 (m), 1086 (m), 1009 (m), 956 (w), 909 (m), 872 (m), 857 (m), 823 (s), 811 (s), 747 (m), 696 (w), 655 (m), 622 (m).

4-Chloro-2-(2-(piperidin-1-yl)thiazolo[4,5-*b*]pyridin-5-yl)phenol (21b)



Brown solid, mp 178–180 °C (EE: *i*-PrOH/1:2).

^1H NMR (300 MHz, CDCl_3): δ = 1.72 (s, 6H, CH_2), 3.66 (s, 4H, CH_2), 6.97 (d, 1H, 3J = 8.5 Hz), 7.18 (dd, 1H, 3J = 8.7 Hz, 4J = 1.8 Hz), 7.42 (d, 1H, 3J = 8.2 Hz), 7.69 (d, 1H, 3J = 2.2 Hz), 7.91 (d, 1H, 3J = 8.2 Hz), 13.77 (s, 1H, OH).

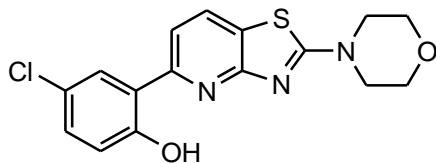
^{13}C NMR (62.9 MHz, CDCl_3): δ = 24.0, 25.3, 49.6, 111.3, 119.9, 120.4, 123.3, 123.4, 125.9, 130.3, 130.5, 153.0, 158.0, 161.4, 170.6.

MS (EI, 70 eV): m/z (%) = 345 (M^+ , 100), 316 (21), 289 (16), 227 (15), 207 (11), 172 (11), 155 (16).

HRMS (ESI): calcd for $\text{C}_{17}\text{H}_{17}\text{ClN}_3\text{OS}$ ($\text{M}+\text{H}$) 346.07754, found 346.07691.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2925 (w), 1573 (w), 1519 (m), 1487 (m), 1423 (m), 1360 (m), 1326 (m), 1269 (s), 1244 (s), 1214 (s), 1122 (m), 1042 (w), 1009 (w), 957 (w), 901 (m), 857 (m), 824 (s), 811 (s), 747 (m), 730 (m), 698 (w), 666 (s), 623 (m).

4-Chloro-2-(2-morpholinothiazolo[4,5-*b*]pyridin-5-yl)phenol (21c)



Red-brown solid, mp 257–259 °C (EE: *i*-PrOH/1:2).

^1H NMR (300 MHz, $\text{DMSO}-d_6$): δ = 3.74 (s, 8H, CH_2), 6.96 (s, 1H), 7.30 (s, 1H), 7.95–8.07 (m, 2H), 8.40 (s, 1H), 14.05 (s, 1H, OH).

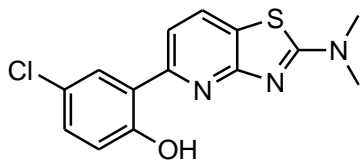
^{13}C NMR (62.9 MHz, CDCl_3): δ = 47.9, 65.4, 112.8, 119.6, 120.9, 122.6, 123.4, 126.5, 130.3, 131.9, 152.3, 157.5, 160.8, 171.2.

MS (EI, 70 eV): m/z (%) = 347 (M^+ , 62), 269 (100), 206 (12).

HRMS (EI): calcd for $\text{C}_{16}\text{H}_{14}\text{ClN}_3\text{O}_2\text{S}$ (M^+) 347.04898, found 347.048741.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2966 (w), 1575 (w), 1529 (s), 1478 (m), 1426 (m), 1371 (m), 1330 (m), 1280 (s), 1230 (s), 1217 (m), 1189 (m), 1115 (s), 1030 (m), 965 (w), 896 (m), 872 (m), 825 (s), 730 (m), 666 (s), 621 (m).

4-Chloro-2-(2-(dimethylamino)thiazolo[4,5-*b*]pyridin-5-yl)phenol (21d)



Brown solid, mp 255–256 °C (EE: *i*-PrOH/1:3).

^1H NMR (250 MHz, $\text{DMSO}-d_6$): δ = 3.23 (s, 6H, Me), 6.94 (d, 1H, 3J = 8.1 Hz), 7.30 (d, 1H, 3J = 7.0 Hz), 7.89 (d, 1H, 3J = 7.6 Hz), 8.06 (s, 1H), 8.36 (d, 1H, 3J = 7.6 Hz), 14.21 (s, 1H, OH).

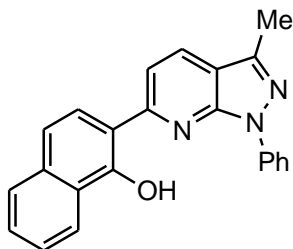
^{13}C NMR (62.9 MHz, CDCl_3): $\delta = 26.1, 112.1, 119.6, 120.9, 122.5, 124.0, 126.4, 130.3, 131.6, 134.0, 152.1, 157.6, 161.2$.

MS (EI, 70 eV): m/z (%) = 305 (M^+ , 100), 290 (12), 276 (12).

HRMS (ESI): calcd for $\text{C}_{14}\text{H}_{13}\text{ClN}_3\text{OS}$ ($\text{M}+\text{H}$) 306.04624, found 306.04684.

IR (ATR, cm^{-1}): $\tilde{\nu} = 2890$ (w), 1598 (w), 1579 (w), 1538 (m), 1488 (w), 1404 (w), 1348 (m), 1278 (m), 1218 (m), 1173 (m), 1140 (m), 1100 (w), 1083 (m), 961 (w), 914 (m), 877 (m), 817 (s), 747 (m), 731 (m), 709 (m), 660 (s).

2-(3-Methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)naphthalen-1-ol (22)



White solid, mp 186–187 °C (from EE: *i*-PrOH/1:2).

^1H NMR (300 MHz, $\text{DMSO-}d_6$): $\delta = 2.65$ (s, 3H, Me), 7.46–7.71 (m, 6H), 7.88–7.97 (m, 3H), 8.20–8.25 (m, 2H), 8.33 (d, 1H, $^3J = 8.0$ Hz), 8.57 (d, 1H, $^3J = 8.5$ Hz), 14.88 (s, 1H, OH).

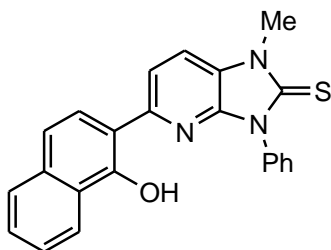
^{13}C NMR (62.9 MHz, $\text{DMSO-}d_6$): $\delta = 12.1, 112.0, 113.8, 115.2, 118.6, 121.9, 123.0, 124.3, 125.3, 125.6, 126.8, 127.3, 128.1, 129.6, 132.9, 134.9, 138.2, 143.5, 146.8, 156.2, 156.7$.

MS (GC, 70 eV): m/z (%) = 351 (M^+ , 100).

HRMS (ESI): calcd for $\text{C}_{23}\text{H}_{18}\text{N}_3\text{O}$ ($\text{M}+\text{H}$) 352.1444, found 352.14452.

IR (ATR, cm^{-1}): $\tilde{\nu} = 3400$ (w), 2980 (m), 2763 (s), 2456 (w), 1582 (s), 1508 (m), 1480 (m), 1431 (m), 1389 (s), 1349 (m), 1304 (m), 1231 (m), 1176 (m), 1148 (w), 1119 (w), 1057 (m), 1023 (m), 948 (w), 850 (m), 804 (m), 790 (s), 772 (s), 753 (s), 722 (m), 691 (s), 648 (s), 608 (m), 570 (m).

5-(1-Hydroxynaphthalen-2-yl)-1-methyl-3-phenyl-1*H*-imidazo[4,5-*b*]pyridine-2(3*H*)-thione (23)



Green solid, mp 305–306 °C (*i*-PrOH).

^1H NMR (300 MHz, DMSO- d_6): δ = 3.85 (s, 3H, Me), 7.42–7.54 (m, 3H), 7.64–7.73 (m, 5H, Ph), 7.82 (d, 1H), 8.09–8.24 (m, 4H), 13.61 (br s, 1H, OH).

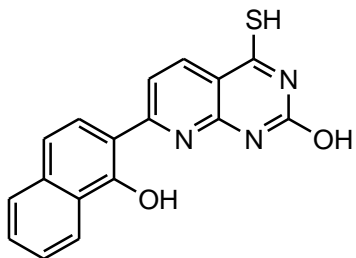
^{13}C NMR due to bed solubility was not possible to measure.

MS (GC, 70 eV): m/z (%) = 383 (M^+ , 100), 207 (13).

HRMS (EI): calcd for $\text{C}_{23}\text{H}_{17}\text{N}_3\text{OS}$ (M^+) 383.10868, found 383.107368.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3049 (w), 1614 (w), 1569 (w), 1499 (w), 1462 (s), 1438 (m), 1402 (m), 1337 (s), 1295 (s), 1223 (m), 1203 (m), 1139 (m), 1063 (w), 1027 (w), 977 (w), 853 (w), 795 (s), 769 (m), 723 (m), 704 (m), 622 (m).

7-(1-Hydroxynaphthalen-2-yl)-4-mercaptopyrido[2,3-*d*]pyrimidin-2-ol (24)



Brown solid, mp 278–280 °C (EE: *i*-PrOH/1:1).

^1H NMR (300 MHz, DMSO- d_6): δ = 7.41 (d, 1H, 3J = 8.8 Hz), 7.51–7.62 (m, 2H), 7.83 (d, 1H, 3J = 7.5 Hz), 8.03–8.06 (m, 2H), 8.30–8.35 (m, 2H), 12.65 (s, 1H, OH), 13.56 (s, 1H, OH), 13.99 (s, 1H, SH).

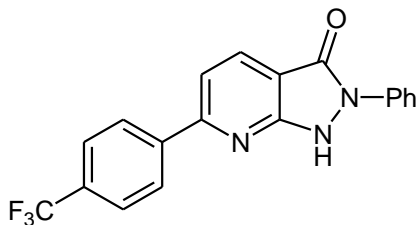
^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 109.4, 110.8, 115.8, 118.6, 123.3, 123.8, 125.4, 125.8, 127.3, 128.6, 135.4, 137.3, 149.5, 157.2, 159.1, 161.2, 175.9.

MS (GC, 70 eV): m/z (%) = 321 (M^+ , 100), 234 (12), 78 (12).

HRMS (EI): calcd for $C_{17}H_{11}N_3O_2S$ (M^+) 321.05665, found 321.056049.

IR (ATR, cm^{-1}): $\tilde{\nu} = 3284$ (w), 1702 (w), 1672 (m), 1611 (m), 1581 (m), 1554 (m), 1512 (m), 1472 (m), 1396 (s), 1344 (m), 1273 (m), 1242 (m), 1207 (m), 1178 (s), 1148 (m), 1126 (s), 1108 (m), 949 (w), 868 (s), 808 (m), 786 (s), 764 (s), 723 (m), 650 (m).

6-(3-(Trifluoromethyl)phenyl)-1,2-dihydro-2-phenylpyrazolo[3,4-*b*]pyridin-3-one (26a)



Yellow solid, mp 161–162 °C (EE: *i*-PrOH/1:3).

1H NMR (300 MHz, DMSO- d_6): $\delta = 7.20$ – 7.31 (m, 1H), 7.45–7.55 (m, 2H), 7.90–7.95 (m, 5H), 8.34–8.40 (m, 3H), 8.32–8.44 (m, 5H), 11.80 (br s, 1H, NH).

^{19}F NMR (282 MHz, DMSO- d_6): $\delta = -61.2$.

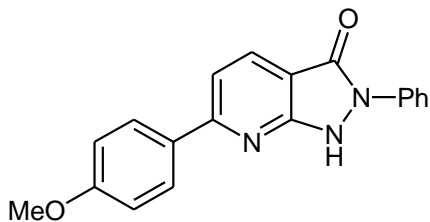
^{13}C NMR due to bed solubility it was not possible to measure.

MS (GC, 70 eV): m/z (%) = 355 (M^+ , 100), 286 (37).

HRMS (EI): calcd for $C_{20}H_{14}F_3N_3$ (M^+) 355.09221, found 355.09222.

IR (ATR, cm^{-1}): $\tilde{\nu} = 3382$ (w), 3013 (m), 2773 (m), 2448 (w), 1651 (m), 1620 (m), 1594 (m), 1501 (m), 1467 (w), 1441 (m), 1403 (m), 1325 (m), 1301 (m), 1158 (m), 1120 (s), 1067 (s), 1017 (s), 935 (w), 857 (m), 825 (s), 792 (s), 746 (s), 711 (s), 682 (s).

1,2-Dihydro-6-(4-methoxyphenyl)-2-phenylpyrazolo[3,4-*b*]pyridin-3-one (26b)



Orange solid, mp 173–174 °C (EE: *i*-PrOH/1:2).

^1H NMR (300 MHz, $\text{DMSO-}d_6$): δ = 3.88 (s, 3H, OMe), 7.11 (d, 2H, 3J = 8.9 Hz), 7.24–7.29 (m, 1H), 7.49–7.55 (m, 2H), 7.75 (d, 1H, 3J = 8.3 Hz), 7.93–7.96 (m, 2H), 8.16 (d, 2H, 3J = 8.9 Hz), 8.23 (d, 1H, 3J = 8.1 Hz), 10.31 (br s, 1H, NH).

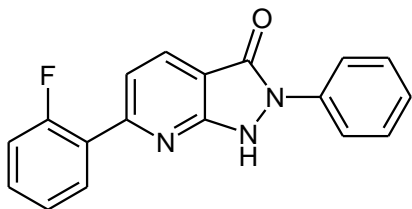
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$): δ = 55.4, 108.5, 113.9, 114.4, 118.8, 119.3, 125.0, 128.9, 129.0, 129.9, 134.2, 135.7, 137.4, 157.4, 158.7, 159.6, 161.1.

MS (EI, 70 eV): m/z (%) = 317 (M^+ , 100), 288 (20).

HRMS (EI): calcd for $\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}_2$ (M^+) 317.11588, found 317.115965.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2936 (w), 2761 (m), 2456 (m), 1899 (w), 1630 (w), 1594 (m), 1576 (m), 1529 (w), 1479 (m), 1439 (m), 1381 (w), 1356 (m), 1319 (m), 1299 (m), 1257 (s), 1221 (m), 1182 (m), 1149 (m), 1064 (m), 1025 (m), 943 (w), 889 (w), 836 (w), 809 (m), 783 (m), 769 (m), 754 (m), 721 (w), 693 (m), 670 (w).

6-(2-Fluorophenyl)-1,2-dihydro-2-phenylpyrazolo[3,4-*b*]pyridin-3-one (26c)



Brown solid, mp 241–243 °C (heptane: *i*-PrOH/1:2).

^1H NMR (300 MHz, $\text{DMSO-}d_6$): δ = 7.25–7.30 (m, 1H), 7.36–7.42 (m, 2H), 7.49–7.60 (m, 4H), 7.92–8.00 (m, 3H), 8.32 (d, 1H, 3J = 8.3 Hz), 11.65 (br s, 1H, NH).

^{19}F NMR (282 MHz, $\text{DMSO-}d_6$): δ = –115.9.

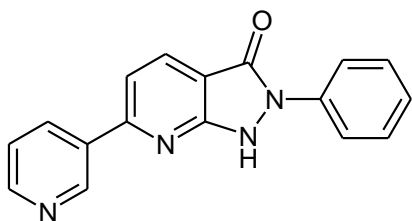
^{13}C NMR due to bed solubility it was not possible to measure.

MS (GC, 70 eV): m/z (%) = 305 (M^+ , 100), 276 (41), 207 (15), 77 (17).

HRMS (ESI): calcd for $\text{C}_{18}\text{H}_{13}\text{FN}_3\text{O}$ ($\text{M}+\text{H}$) 306.10372, found 306.10335.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3043 (w), 1643 (m), 1593 (m), 1497 (m), 1441 (m), 1415 (m), 1335 (w), 1302 (m), 1280 (m), 1203 (m), 1128 (w), 1085 (w), 1026 (w), 937 (w), 893 (w), 789 (w), 760 (s), 740 (s), 712 (w), 661 (s), 590 (s).

1,2-Dihydro-2-phenyl-6-(pyridin-3-yl)pyrazolo[3,4-*b*]pyridin-3-one (26d)



Yellow solid, mp 268–270 °C (MeOH).

^1H NMR (300 MHz, $\text{DMSO-}d_6$): δ = 7.25–7.31 (m, 1H), 7.50–7.55 (m, 2H), 7.91–7.94 (m, 2H), 8.01–8.10 (m, 2H), 8.42 (d, 1H, 3J = 8.1 Hz), 8.96 (d, 1H, 3J = 5.2 Hz), 9.09 (d, 1H, 3J = 8.7 Hz), 9.53 (s, 1H), 11.90 (br s, 1H, NH).

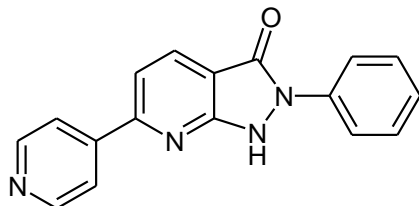
^{13}C NMR (62.9 MHz, $\text{CF}_3\text{COOD/DMSO-}d_6$): δ = 127.3, 131.5, 133.2, 133.3, 137.1, 140.9, 141.0, 144.2, 145.4, 149.1, 157.0, 157.8, 160.5, 164.5, 165.9.

MS (GC, 70 eV): m/z (%) = 288 (M^+ , 100), 259 (50), 77 (28).

HRMS (EI): calcd for $\text{C}_{17}\text{H}_{12}\text{N}_4\text{O}$ ($\text{M}+\text{H}$) 288.10056, found 288.100698.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3052 (w), 2442 (m), 2062 (w), 1651 (s), 1607 (m), 1538 (m), 1495 (m), 1445 (m), 1422 (m), 1345 (m), 1304 (s), 1280 (m), 1236 (m), 1173 (w), 1134 (w), 1108 (w), 1034 (w), 1016 (w), 941 (w), 814 (m), 789 (m), 770 (s), 724 (m), 680 (s), 623 (m), 602 (m).

1,2-Dihydro-2-phenyl-6-(pyridin-4-yl)pyrazolo[3,4-*b*]pyridin-3-one (26e)



Yellow solid, mp 272–274 °C (MeOH).

^1H NMR (300 MHz, $\text{CF}_3\text{COOD/DMSO-}d_6$): δ = 7.20–7.25 (m, 3H), 7.38–7.41 (m, 2H), 7.69 (d, 1H, 3J = 8.2 Hz), 8.37–8.42 (m, 3H), 8.60–8.62 (m, 2H).

^{13}C NMR (75.5 MHz, $\text{CF}_3\text{COOD/DMSO-}d_6$): δ = 114.2, 121.5, 127.8, 129.6, 133.6, 1339, 137.1, 141.4, 145.8, 157.0, 158.4, 158.5, 160.6.

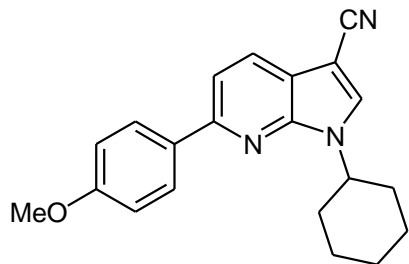
MS (EI, 70 eV): m/z (%) = 288 (M^+ , 100), 259 (39).

HRMS (ESI): calcd for $\text{C}_{17}\text{H}_{13}\text{N}_4\text{O}$ ($\text{M}+\text{H}$) 289.10839, found 289.10874.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3059 (w), 2397 (m), 2068 (w), 1652(m), 1630 (m), 1591 (m), 1510 (w),

1496 (m), 1442 (m), 1417 (m), 1343 (w), 1300 (m), 1279 (m), 1188 (w), 1128 (w), 1083 (w), 1001 (w), 942 (w), 841 (w), 814 (m), 786 (m), 767 (s), 718 (m), 689 (m), 634 (m), 601 (m).

1-Cyclohexyl-6-(4-methoxyphenyl)-1H-pyrrolo[2,3-b]pyridine-3-carbonitrile (27)



Yellow solid, mp 150–152 °C (EE: *i*-PrOH/1:3).

¹H NMR (300 MHz, DMSO-*d*₆): δ = 1.20–1.57 (m, 3H, CH₂), 1.72–1.93 (m, 5H, CH₂), 2.01–2.04 (m, 2H, CH₂), 3.83 (s, 3H, OMe), 4.76–4.84 (m, 1H, NCH), 7.07 (d, 2H, ³*J* = 8.9 Hz), 7.84 (d, 1H, ³*J* = 8.5 Hz), 8.10–8.14 (m, 3H), 8.58 (s, 1H).

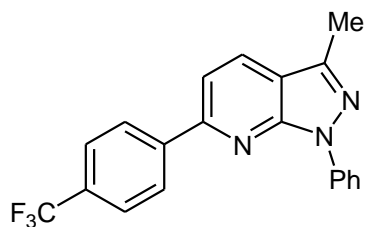
¹³C NMR (62.9 MHz, DMSO-*d*₆): δ = 24.9, 25.2, 32.4, 54.0, 55.2, 82.5, 114.2, 114.6, 115.6, 117.8, 128.0, 128.4, 131.0, 135.3, 145.6, 151.5, 160.1.

MS (GC, 70 eV): *m/z* (%) = 331 (M⁺, 46), 249 (100), 234 (11), 206 (13).

HRMS (EI): calcd for C₂₁H₂₁N₃O (M⁺) 331.4112, found 331.41121.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2922 (m), 2851 (m), 2221 (m), 1698 (w), 1600 (m), 1581 (m), 1513 (m), 1467 (m), 1427 (m), 1396 (m), 1304 (w), 1279 (m), 1251 (s), 1222 (m), 1179 (s), 1106 (m), 1027 (m), 891 (w), 838 (m), 798 (s), 779 (s), 641 (m), 611 (s).

6-(3-(Trifluoromethyl)phenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridine (28a)



Yellow solid, mp 151–152 °C (column chromatography, EE: heptane/2:1).

^1H NMR (300 MHz, DMSO- d_6): δ = 2.62 (s, 3H, Me), 7.29–7.34 (m, 1H), 7.54–7.59 (m, 2H), 7.89 (d, 2H, 3J = 8.5 Hz), 7.97 (d, 1H, 3J = 8.5 Hz), 8.32–8.44 (m, 5H).

^{19}F NMR (282 MHz, DMSO- d_6): δ = -61.0

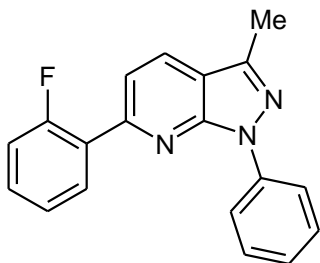
^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 12.3, 115.1, 116.3, 119.9, 122.4 (q, 1J = 281 Hz, CF_3), 125.4, 125.8, 128.1, 129.2, 129.6, 130.6 (q, 2J = 24 Hz, CCF_3), 131.9, 142.3, 143.0, 150.2, 150.9, 154.2, 165.5.

MS (GC, 70 eV): m/z (%) = 353 (M^+ , 100), 338 (17).

HRMS (EI): calcd for $\text{C}_{20}\text{H}_{14}\text{F}_3\text{N}_3$ ($\text{M}+1$) 354.12126, found 354.12094.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3081 (m), 1615 (w), 1592 (m), 1504 (s), 1394 (m), 1315 (s), 1283 (m), 1164 (s), 1124 (s), 1081 (m), 1068 (s), 1013 (m), 956 (w), 908 (w), 856 (w), 838 (w), 815 (s), 749 (s), 690 (s), 665 (s), 593 (m).

6-(2-Fluorophenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridine (28b)



Yellow solid, mp 110 °C (column chromatography, EE: heptane/1:1).

^1H NMR (300 MHz, DMSO- d_6): δ = 2.62 (s, 3H, Me), 7.26–7.31 (m, 1H), 7.35–7.42 (m, 2H), 7.51–7.58 (m, 3H), 7.70 (dd, 1H, 3J = 8.4 Hz, 4J = 2.2 Hz), 8.01 (dt, 1H, 3J = 8.4 Hz, 3J = 2.0 Hz), 8.30–8.33 (m, 2H), 8.41 (d, 1H, 3J = 7.8 Hz).

^{19}F NMR (282 MHz, DMSO- d_6): δ = -116.6.

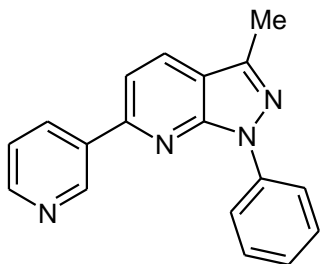
^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 12.2, 113.2 (d, 1J = 240 Hz), 115.6, 116.4 (d, 2J = 22.7 Hz), 118.0 (d, 3J = 8.0 Hz), 119.8, 125.0 (d, 4J = 3.5 Hz), 125.3, 126.9 (d, 3J = 11.4 Hz), 129.1, 131.0, 131.3, 142.9, 150.1, 152.4 (d, 4J = 2.8 Hz), 158.0, 162.0.

MS (GC, 70 eV): m/z (%) = 303 (M^+ , 100), 288 (21).

HRMS (EI): calcd for $\text{C}_{19}\text{H}_{14}\text{FN}_3$ (M^+) 303.11663, found 303.116564.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2924 (w), 1596 (m), 1504 (m), 1493 (m), 1461 (m), 1392 (s), 1309 (m), 1286 (m), 1205 (m), 1161 (m), 1107 (m), 1088 (m), 1030 (m), 957 (w), 901 (w), 820 (m), 797 (m), 742 (s), 682 (s), 658 (s), 631 (m), 598 (m).

3-Methyl-1-phenyl-6-(pyridin-3-yl)-1H-pyrazolo[3,4-b]pyridine (28c)



Yellow solid, mp 196–198 °C (*i*-PrOH).

¹H NMR (300 MHz, DMSO-*d*₆): δ = 2.63 (s, 3H, Me), 7.30–7.35 (m, 1H), 7.54–7.59 (m, 2H), 8.07–8.13 (m, 2H), 8.28–8.31 (m, 2H), 8.52 (d, 1H, ³*J* = 8.3 Hz), 8.94 (dd, 1H, ³*J* = 5.4 Hz, ⁴*J* = 1.0 Hz), 9.16 (dt, 1H, ³*J* = 8.3 Hz, ⁴*J* = 1.8 Hz), 9.59 (s, 1H).

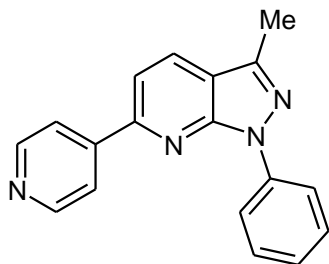
¹³C NMR (62.9 MHz, DMSO-*d*₆): δ = 12.2, 115.1, 116.8, 120.0, 125.5, 126.7, 129.2, 132.2, 136.4, 138.9, 141.5, 142.2, 143.1, 143.8, 149.9, 150.6.

MS (GC, 70 eV): *m/z* (%) = 286 (M⁺, 100), 271 (16).

HRMS (ESI): calcd for C₁₈H₁₅N₄ (M+H) 287.12912, found 287.12936.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3343 (w), 2451 (m), 2072 (w), 1591 (m), 1556 (m), 1486 (m), 1395 (m), 1360 (m), 1283 (w), 1199 (m), 1161 (m), 1113 (w), 1085 (w), 1013 (w), 910 (w), 833 (w), 803 (m), 775 (m), 754 (s), 708 (m), 681 (m), 669 (s), 630 (s).

3-Methyl-1-phenyl-6-(pyridin-4-yl)-1H-pyrazolo[3,4-b]pyridine (28d)



Yellow solid, mp 123–125 °C (*i*-PrOH).

¹H NMR (300 MHz, CF₃COOD/DMSO-*d*₆): δ = 1.42 (s, 3H, Me), 6.10–6.22 (m, 3H), 6.49–6.51 (m, 2H), 6.75 (d, 1H, ³*J* = 8.1 Hz), 7.18 (d, 1H, ³*J* = 8.1 Hz), 7.36–7.38 (m, 2H), 7.59 (m, 1H).

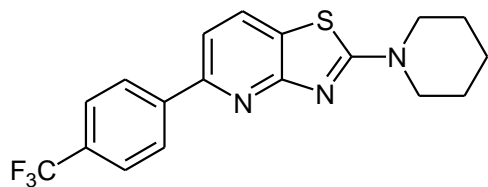
¹³C NMR (62.9 MHz, DMSO-*d*₆): δ = 13.3, 119.8, 120.9, 127.1, 128.6, 132.4, 133.0, 137.5, 138.7, 145.1, 148.0, 152.8, 156.8, 158.9.

MS (GC, 70 eV): m/z (%) = 286 (M^+ , 100), 271 (18).

HRMS (ESI): calcd for $C_{18}H_{15}N_4$ ($M+H$) 287.2256, found 287.2255.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2317 (w), 2064 (w), 1630 (m), 1588 (m), 1498 (m), 1445 (m), 1324 (w), 1247 (m), 1164 (m), 1097 (m), 1082 (m), 997 (m), 833 (m), 803 (s), 763 (s), 692 (m), 661 (m), 594 (m).

5-(3-(Trifluoromethyl)phenyl)-2-(piperidin-1-yl)thiazolo[4,5-*b*]pyridine (29a)



Yellow solid, mp 187–188 °C (EE: heptane/5:1).

1H NMR (300 MHz, $DMSO-d_6$): δ = 1.66 (s, 6H, CH_2), 3.65 (s, 4H, CH_2), 7.71 (d, 1H, 3J = 8.2 Hz), 7.83 (d, 2H, 3J = 8.2 Hz), 8.26-8.33 (m, 3H).

^{19}F NMR (282 MHz, $DMSO-d_6$): δ = -60.9.

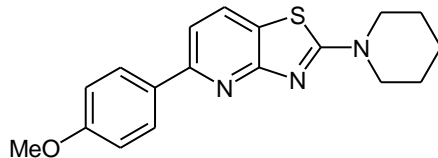
^{13}C NMR (62.9 MHz, $DMSO-d_6$): δ = 23.6, 24.9, 48.9, 109.0, 110.3, 113.3, 120.3 (q, 3J = 230 Hz, CF_3), 124.6, 125.5, 127.1, 128.7 (q, 3J = 31 Hz, CCF_3), 130.4, 142.8, 151.4, 164.4, 169.7.

MS (GC, 70 eV): m/z (%) = 363 (M^+ , 100), 334 (55), 230 (18), 307 (47), 295 (24).

HRMS (EI): calcd for $C_{18}H_{16}F_3N_3S$ (M^+) 363.4115, found 363.4116.

IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2944 (w), 1614 (w), 1582 (w), 1559 (w), 1531 (m), 1444 (w), 1396 (w), 1322 (m), 1263 (m), 1217 (w), 1153 (m), 1105 (s), 1063 (m), 1008 (m), 909 (w), 882 (w), 837 (m), 812 (s), 769 (m), 738 (m), 703 (w).

5-(4-Methoxyphenyl)-2-(piperidin-1-yl)thiazolo[4,5-*b*]pyridine (29b)



Brown solid, mp 173–175 °C (EE: heptane/5:1).

^1H NMR (300 MHz, DMSO- d_6): δ = 1.66 (s, 6H, CH₂), 3.64 (s, 4H, CH₂), 3.81 (s, 3H, OMe), 7.01–7.04 (m, 2H), 7.54 (d, 1H, 3J = 8.1 Hz), 8.02–8.05 (m, 2H), 8.16 (d, 1H, 3J = 8.1 Hz).

^{13}C NMR (62.9 MHz, CDCl₃): δ = 23.6, 24.9, 48.9, 55.2, 112.0, 114.0, 122.3, 127.7, 130.1, 131.4, 145.6, 153.0, 159.9, 164.1, 169.5, 190.8.

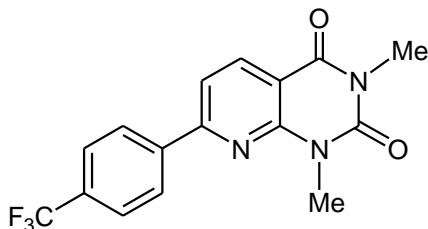
MS (GC, 70 eV): m/z (%) = 325 (M⁺, 100), 296 (28), 289 (16), 282 (15), 269 (31), 242 (19).

HRMS (EI): calcd for C₁₈H₁₉N₃OS (M⁺) 325.12433, found 325.124003.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2934 (w), 1597 (m), 1537 (m), 1507 (m), 1446 (m), 1393 (m), 1359 (m), 1337 (m), 1284 (m), 1245 (s), 1208 (m), 1176 (m), 1136 (m), 1028 (m), 1005 (m), 956 (m), 881 (m), 840 (m), 822 (m), 803 (s), 767 (m), 729 (m), 700 (m), 665 (m), 613 (m).

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7-(3-(Trifluoromethyl)phenyl)-1,3-dimethylpyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (30a)



Yellow solid, mp 173–175 °C (EE: *i*-PrOH/1:1).

^1H NMR (300 MHz, DMSO- d_6): δ = 3.32 (s, 3H, Me), 3.66 (s, 3H, Me), 7.85 (d, 2H, 3J = 8.3 Hz), 7.93 (d, 1H, 3J = 8.3 Hz), 8.36 (d, 2H, 3J = 8.0 Hz), 8.43 (d, 1H, 3J = 8.5 Hz).

^{19}F NMR (282 MHz, DMSO- d_6): δ = -61.4.

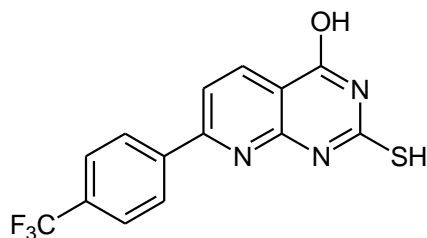
^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 28.1, 29.1, 109.8, 115.7, 116.0, 117.2 (q, 1J = 289 Hz, CF₃), 121.9, 125.9, 126.2, 128.1, 129.6, 138.4, 140.8, 150.7 (q, 2J = 34 Hz, CCF₃), 157.8, 160.5.

MS (GC, 70 eV): m/z (%) = 335 (M⁺, 100), 307 (43), 223 (53).

HRMS (ESI): calcd for C₁₆H₁₃F₃N₃O₂ (M+1) 336.09544, found 336.09613.

IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3362 (m), 2964 (m), 2766 (m), 2457 (w), 1709 (m), 1657 (s), 1595 (s), 1574 (m), 1470 (m), 1424 (m), 1314 (s), 1289 (m), 1170 (m), 1154 (m), 1112 (s), 1072 (s), 1001 (m), 889 (w), 835 (m), 791 (s), 744 (m), 705 (w), 664 (w), 589 (w).

6-(3-(Trifluoromethyl)phenyl)-4-mercaptopyrido[3,2-*d*]pyrimidin-2-ol (30b)



Green solid, mp 172–174 °C (EE: *i*-PrOH/3:1).

^1H NMR (300 MHz, DMSO- d_6): δ = 7.92–7.98 (m, 2H), 8.03 (d, 1H, 3J = 8.0 Hz), 8.37–8.41 (m, 3H), 12.64 (s, 1H, OH), 13.22 (s, 1H, SH).

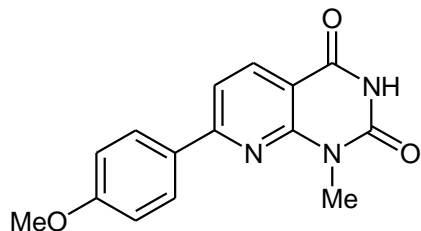
^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 111.5, 117.4, 124.1 (q, 3J = 272 Hz, CF $_3$), 125.8, 125.9, 128.1, 130.5 (q, 3J = 32 Hz, CCF $_3$), 137.7, 140.5, 151.5, 159.0, 159.4, 162.3, 176.1.

MS (GC, 70 eV): m/z (%) = 323 (M $^+$, 100), 280 (18), 265 (13), 236 (12).

HRMS (ESI): calcd for C $_{14}$ H $_9$ FN $_3$ OS (M+1) 324.04129, found 324.04038.

IR (ATR, cm $^{-1}$): $\tilde{\nu}$ = 2938 (w), 2762 (s), 2457 (w), 1682 (m), 1611 (s), 1574 (m), 1476 (m), 1412 (m), 1322 (s), 1276 (m), 1238 (m), 1159 (s), 1110 (s), 1070 (s), 1027 (m), 887 (w), 831 (s), 791 (s), 762 (m), 654 (w).

7-(4-Methoxyphenyl)-1-methylpyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (30c)



Yellow solid, mp 236–238 °C (EE: *i*-PrOH/1:3).

^1H NMR (300 MHz, DMSO- d_6): δ = 3.58 (s, 3H, Me), 3.86 (s, 3H, OMe), 7.09 (d, 2H, 3J = 9.0 Hz), 7.80 (d, 1H, 3J = 8.0 Hz), 8.18 (d, 2H, 3J = 9.0 Hz), 8.29 (d, 1H, 3J = 8.0 Hz), 11.64 (s, 1H, NH).

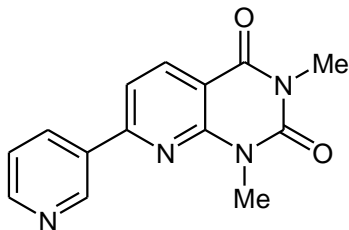
^{13}C NMR (62.9 MHz, DMSO- d_6): δ = 28.0, 55.3, 108.8, 113.9, 114.3, 128.9, 129.4, 137.4, 150.8, 151.7, 159.5, 161.1, 161.4.

MS (EI, 70 eV): m/z (%) = 283 (M $^+$, 100), 254 (34), 185 (26), 170 (13).

HRMS (EI): calcd for C $_{15}$ H $_{13}$ N $_3$ O $_3$ (M $^+$) 283.2865, found 283.2866.

IR (ATR, cm^{-1}): $\tilde{\nu} = 3167$ (w), 3036 (w), 2835 (w), 1692 (s), 1585 (s), 1521 (m), 1454 (m), 1404 (s), 1338 (m), 1299 (m), 1251 (s), 1205 (m), 1177 (m), 1080 (m), 1020 (m), 974 (w), 860 (m), 833 (m), 790 (s), 749 (m), 694 (m), 636 (s).

1,3-Dimethyl-7-(pyridin-3-yl)pyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (30d)



Yellow solid, mp 216 °C (*i*-PrOH).

^1H NMR (300 MHz, $\text{DMSO-}d_6$): $\delta = 3.32$ (s, 3H, Me), 3.68 (s, 3H, Me), 7.95–7.99 (m, 1H), 8.11 (d, 1H, $^3J = 8.1$ Hz), 8.51 (d, 1H, $^3J = 8.1$ Hz), 8.91 (dd, 1H, $^3J = 5.3$ Hz, $^4J = 1.4$ Hz), 9.03 (d, 1H, $^3J = 8.3$ Hz, $^4J = 1.8$ Hz), 9.56 (d, 1H, $^3J = 1.8$ Hz).

^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$): $\delta = 28.1, 29.2, 110.3, 115.8, 125.8, 134.2, 138.6, 139.3, 144.6, 146.9, 150.6, 151.0, 155.6, 160.5$.

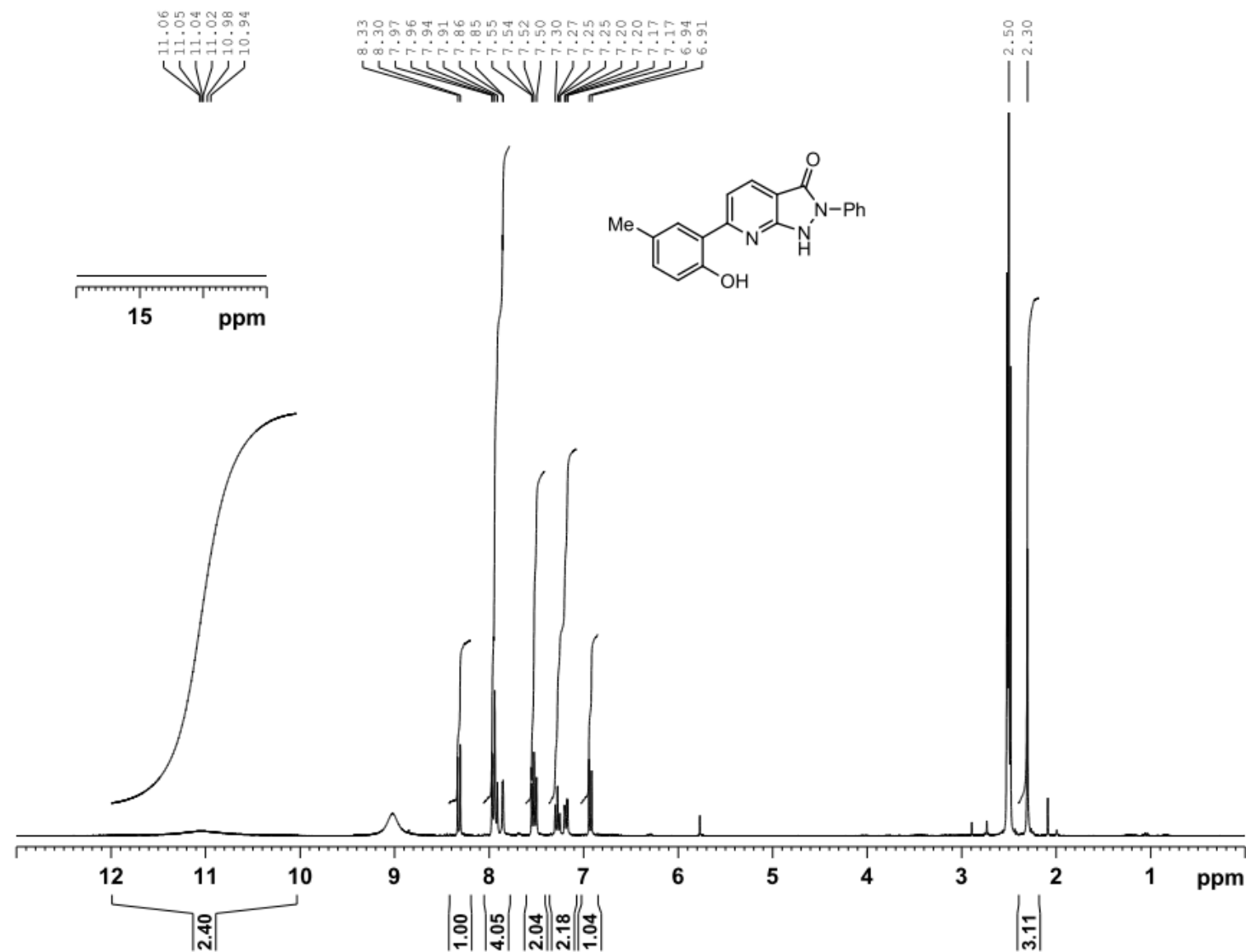
MS (EI, 70 eV): m/z (%) = 268 (M^+ , 100).

HRMS (EI): calcd for $\text{C}_{14}\text{H}_{12}\text{N}_4\text{O}_2$ (M^+) 268.1022, found 268.10233.

IR (ATR, cm^{-1}): $\tilde{\nu} = 3043$ (w), 2351 (w), 2109 (w), 1996 (w), 1705 (m), 1651 (s), 1594 (s), 1553 (m), 1478 (m), 1423 (s), 1373 (m), 1346 (s), 1291 (s), 1226 (m), 1101 (m), 1062 (m), 937 (w), 869 (w), 829 (m), 791 (s), 748 (s), 685 (s), 622 (s).

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

Gevorgyan AG132 (1) 1H DMSO



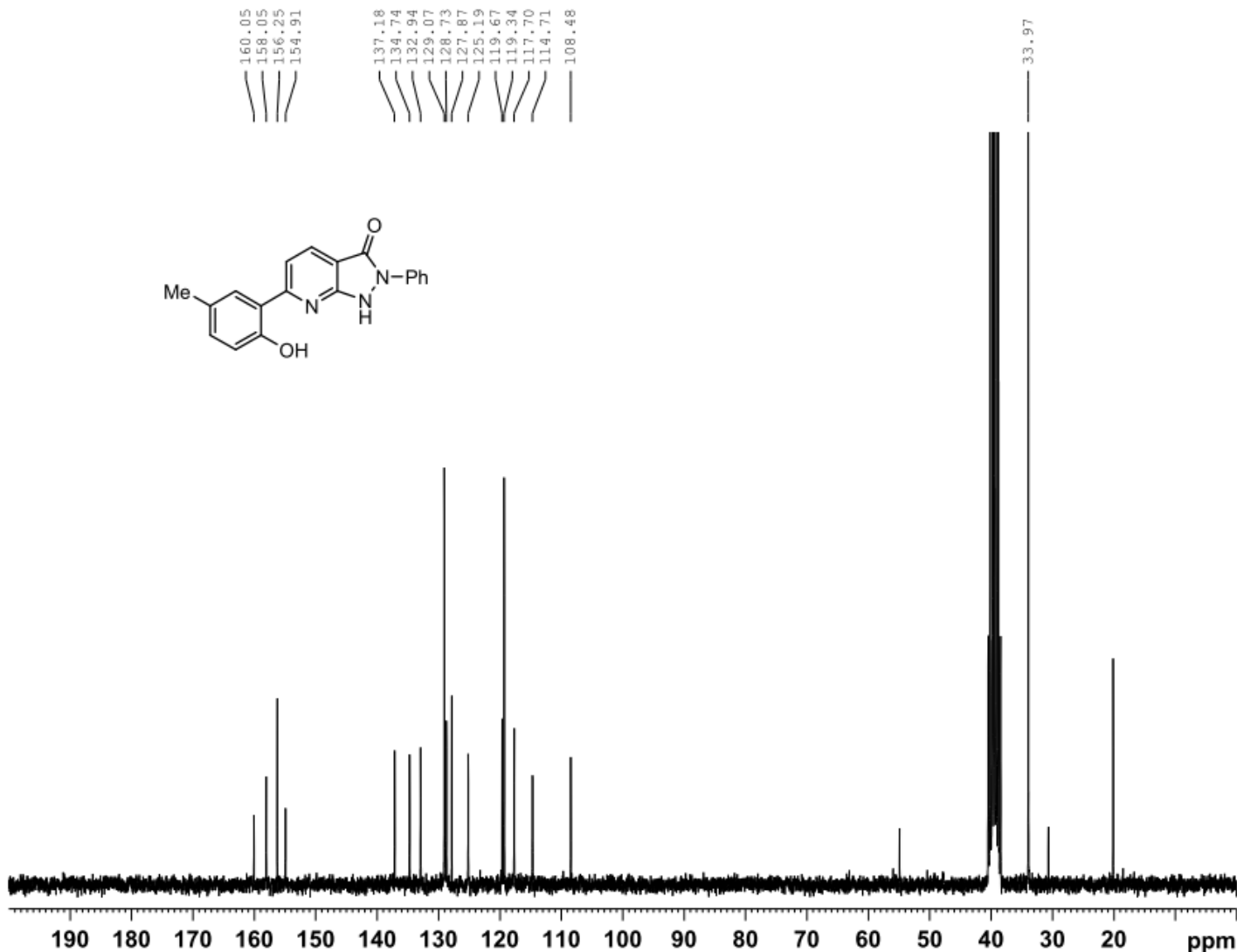
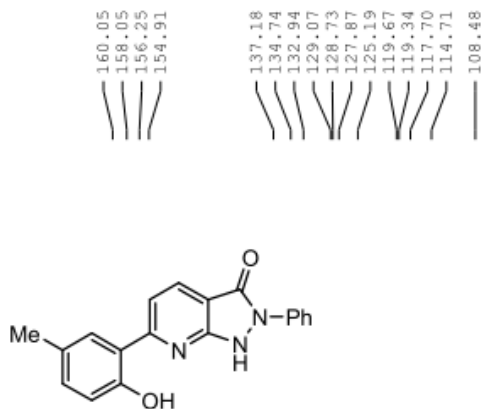
Current Data Parameters
NAME 110105.u308 ag 132-1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110105
Time 8.56
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 5.2953567 sec
RG 101
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300022 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG132 (1) 13C DMSO



Current Data Parameters
NAME 110106.202 ag 132 C
EXPNO 10
PROCNO 1

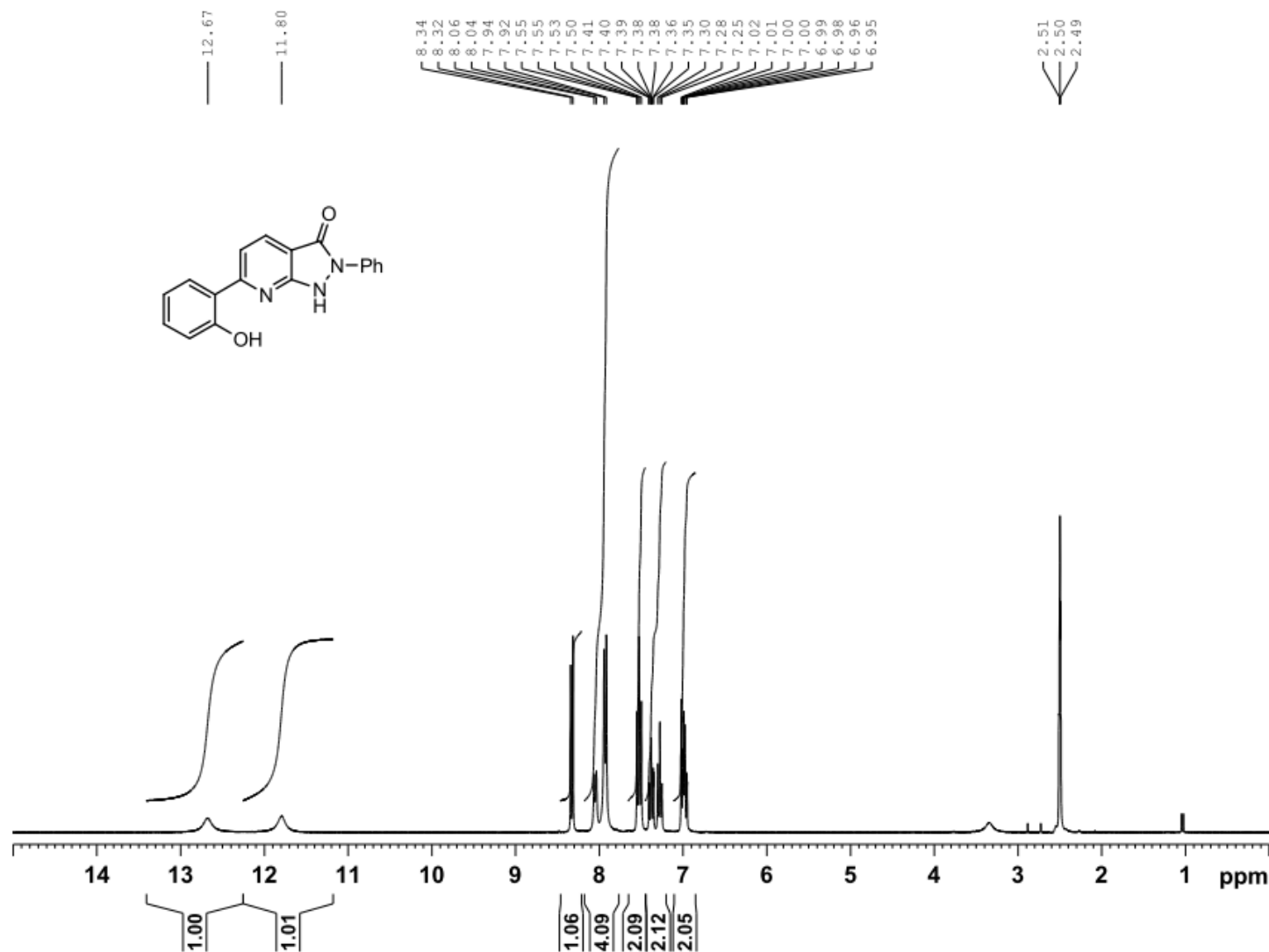
F2 - Acquisition Parameters
Date_ 20110106
Time 13.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.8 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952678 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG145 1H DMSO



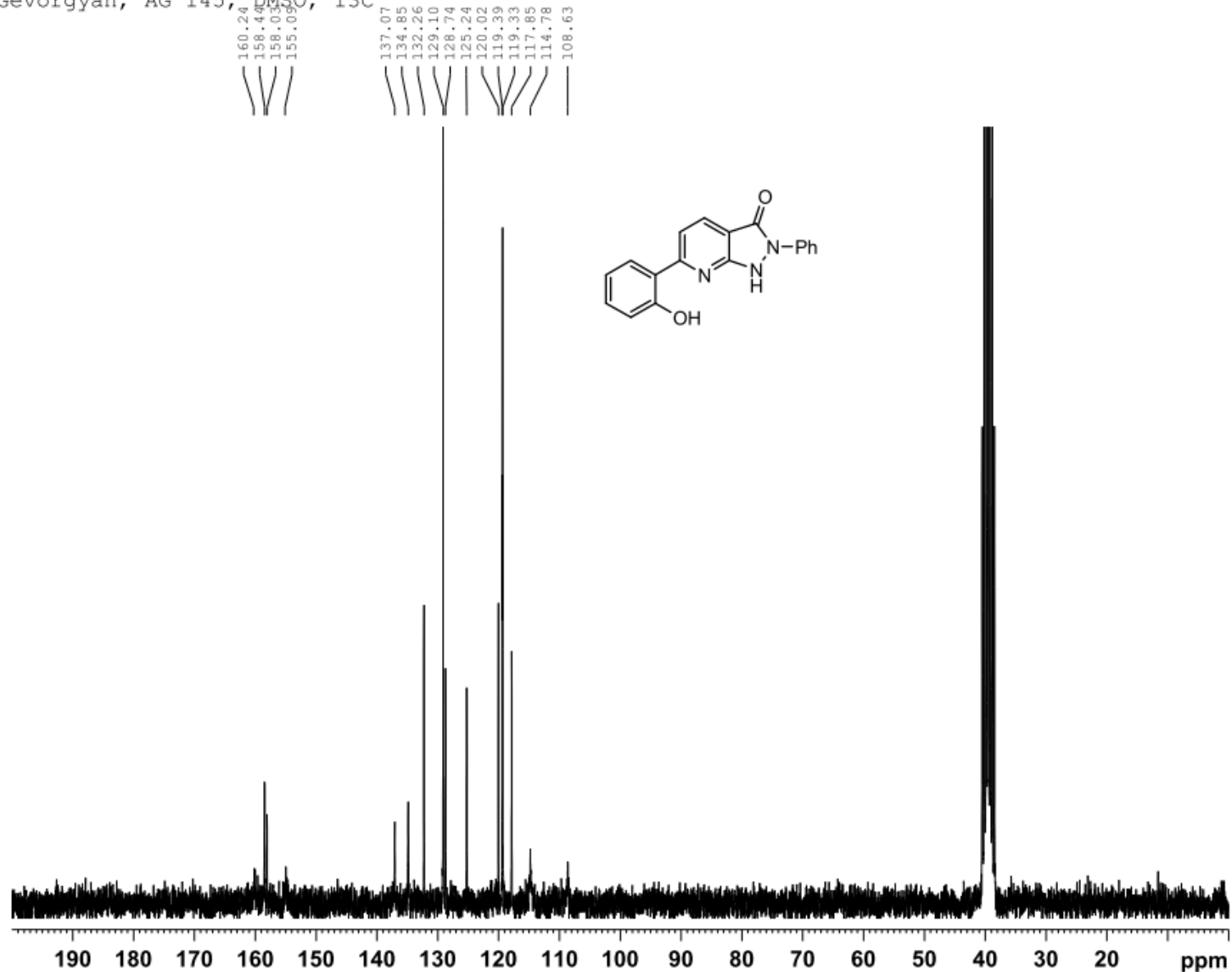
Current Data Parameters
 NAME 110111.u305 ag 145
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110111
 Time 8.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 144
 DW 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

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

F2 - Processing parameters
 SI 32768
 SF 300.1300062 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Gevorgyan, AG 145, DMSO, 13C



Current Data Parameters
NAME 110114.205 ag 145 C
EXPNO 10
PROCNO 1

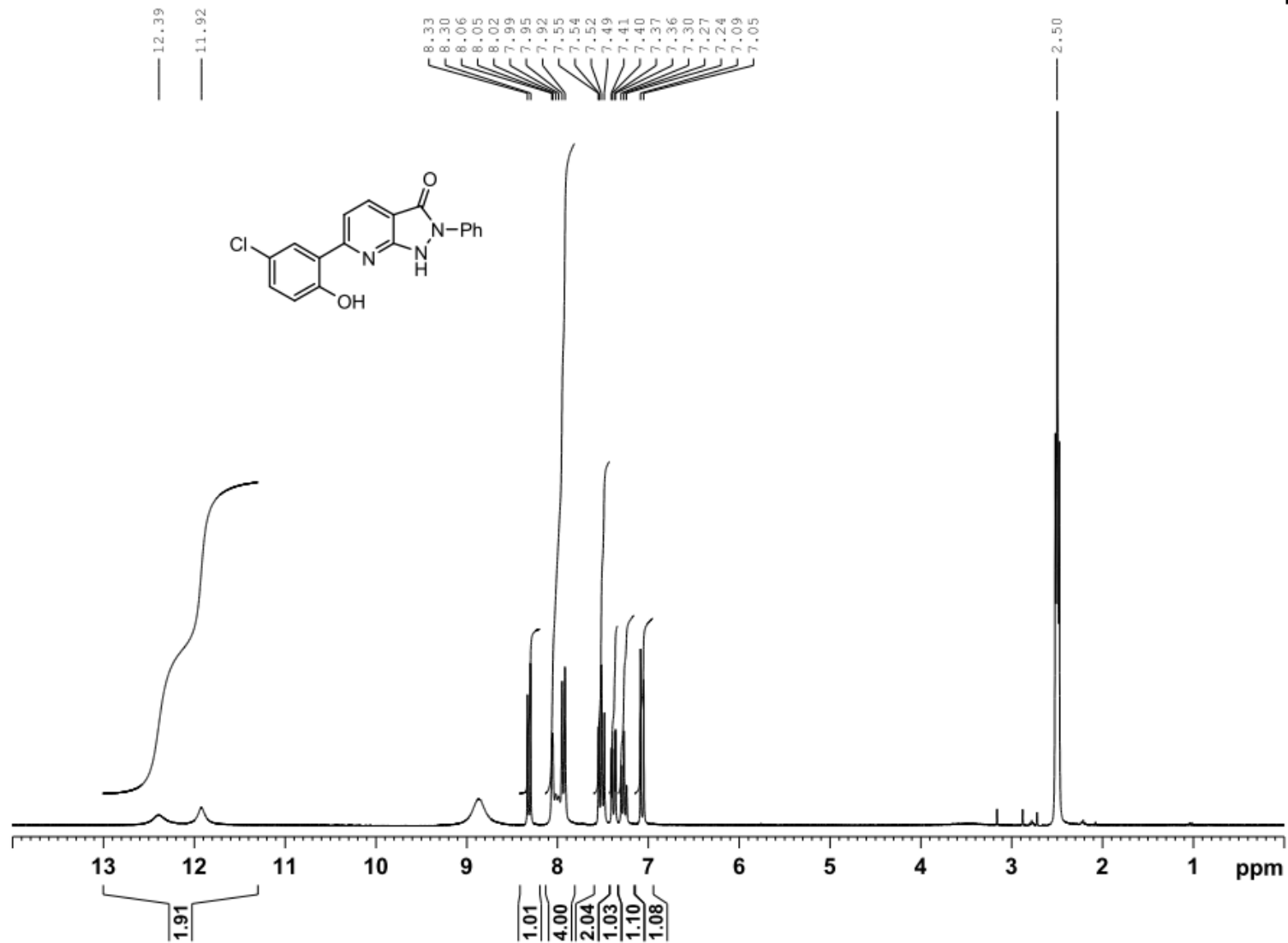
F2 - Acquisition Parameters
Date_ 20110115
Time 3.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.8999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952692 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG124 (1) 1H DMSO



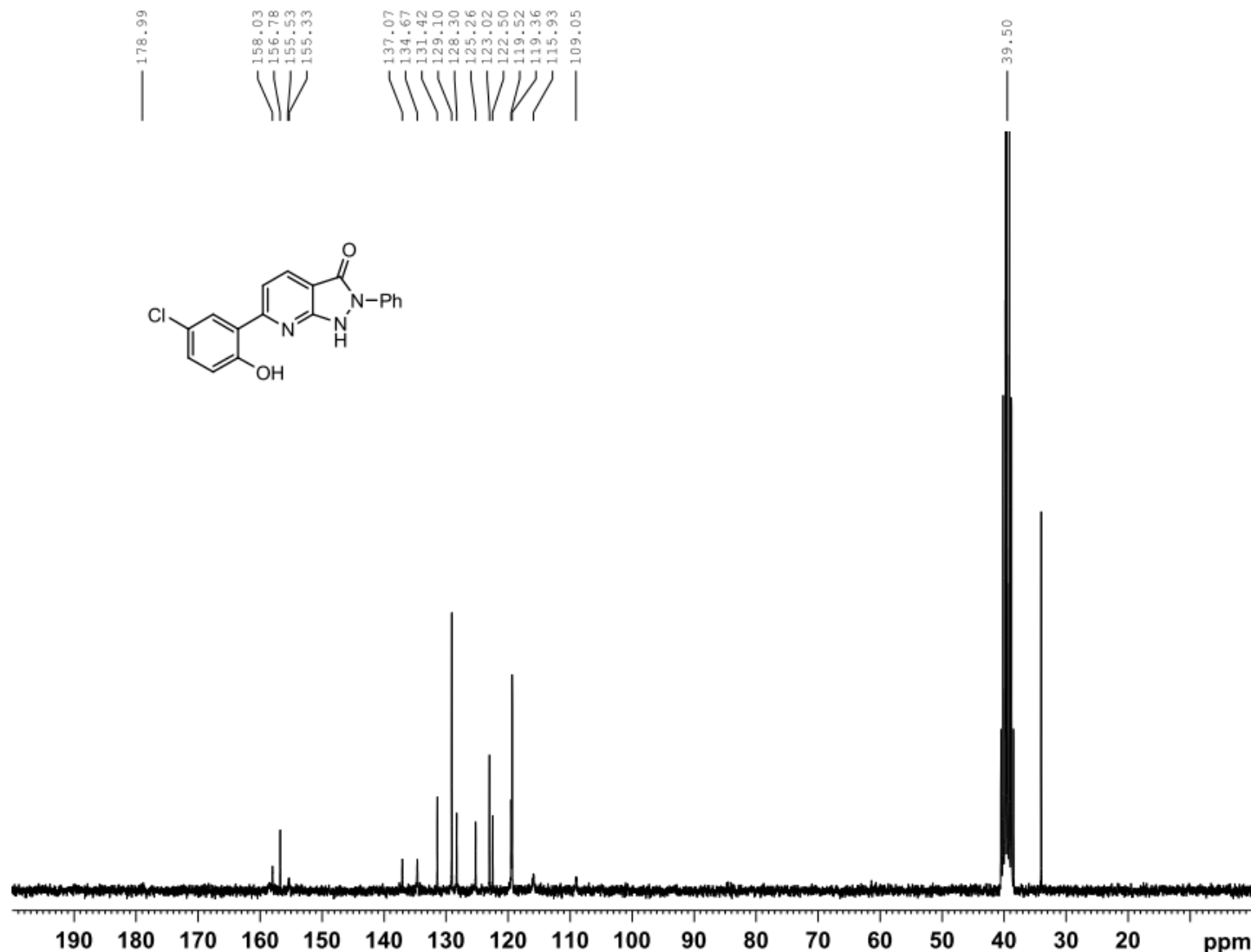
Current Data Parameters
NAME 101220.202 ag 124
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101220
Time 10.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 456
DW 96.800 usec
DE 10.00 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 250.1299982 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG124 (1) 13C DMSO



Current Data Parameters
NAME 101220.202 ag 124
EXPNO 11
PROCNO 1

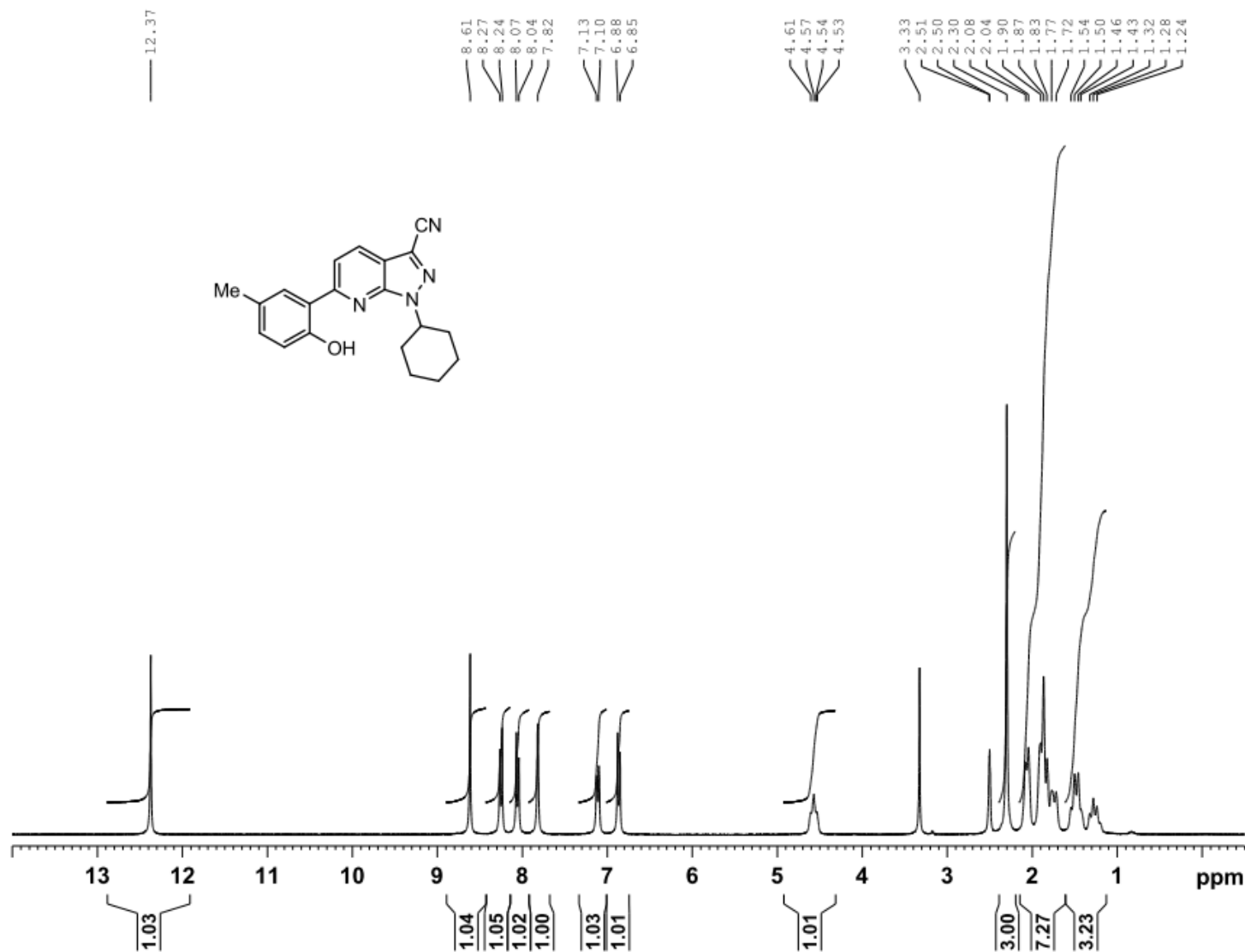
F2 - Acquisition Parameters
Date_ 20101220
Time 18.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 295.9 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952678 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG198 1H DMSO



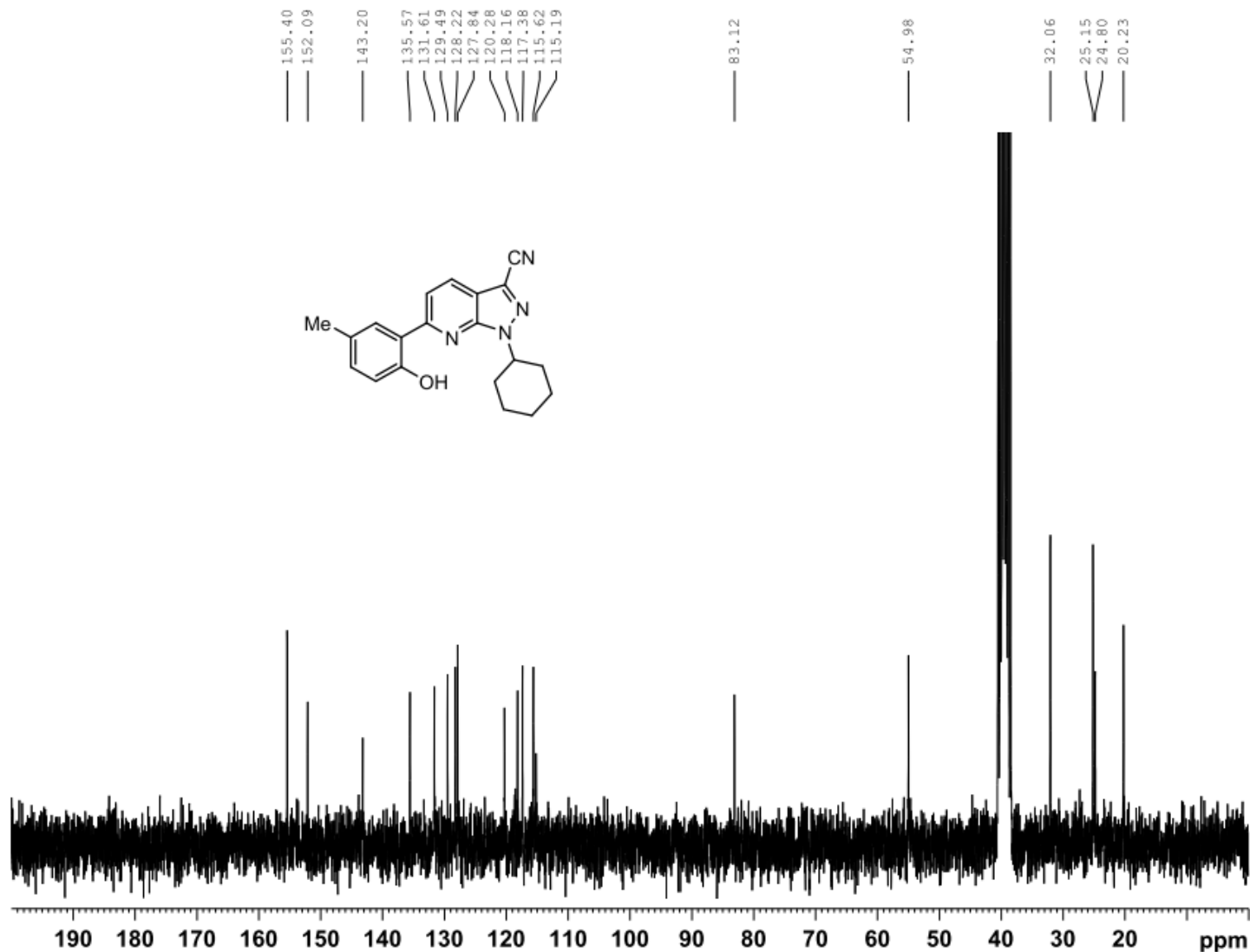
Current Data Parameters
 NAME 110310.u320 ag 198
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110310
 Time 10.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 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 300.1300067 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Gevorgyan AG198 13C DMSO



Current Data Parameters
NAME 110311.219 ag 198 C
EXPNO 10
PROCNO 1

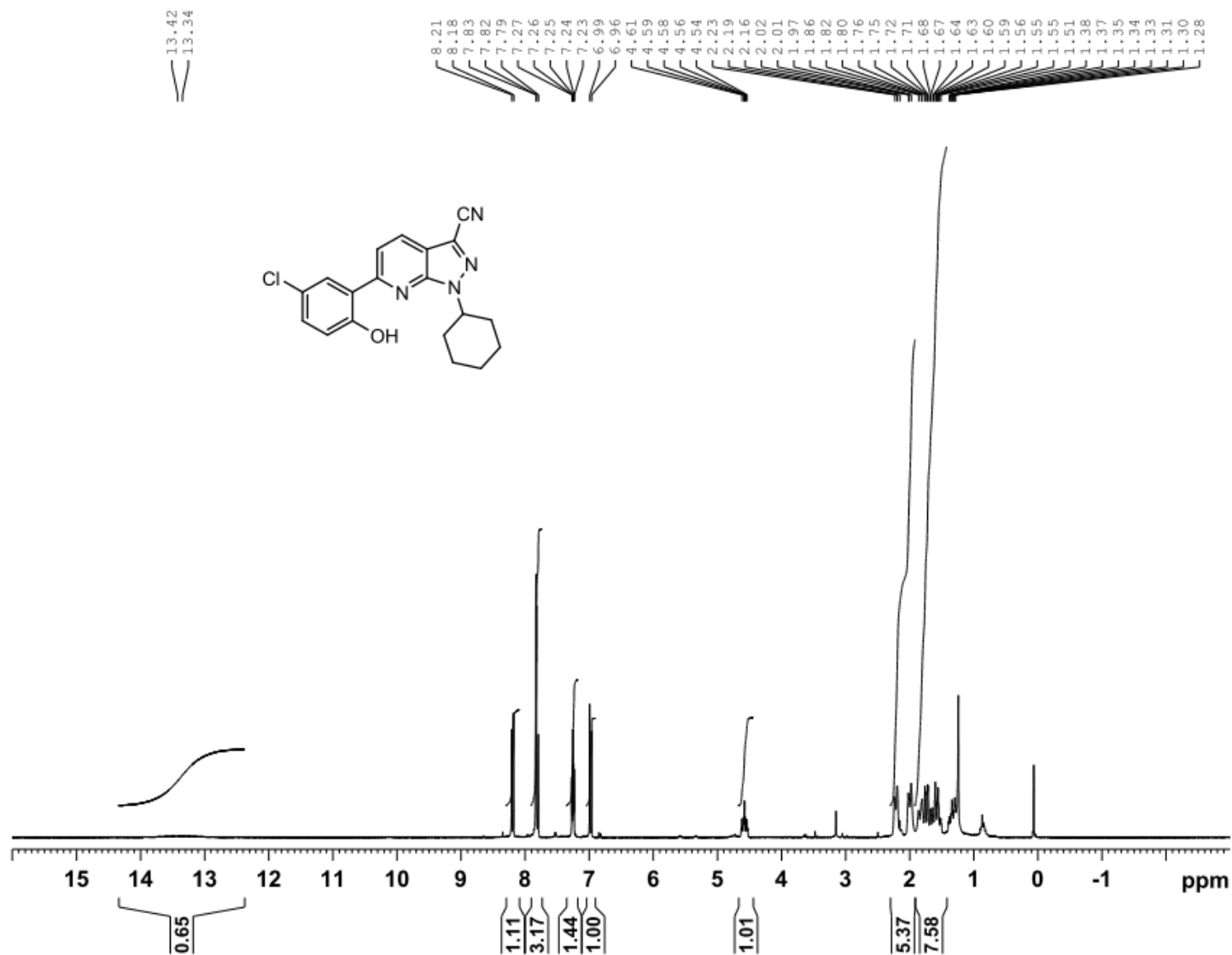
F2 - Acquisition Parameters
Date_ 20110312
Time 14.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952692 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG152 1H CDC13



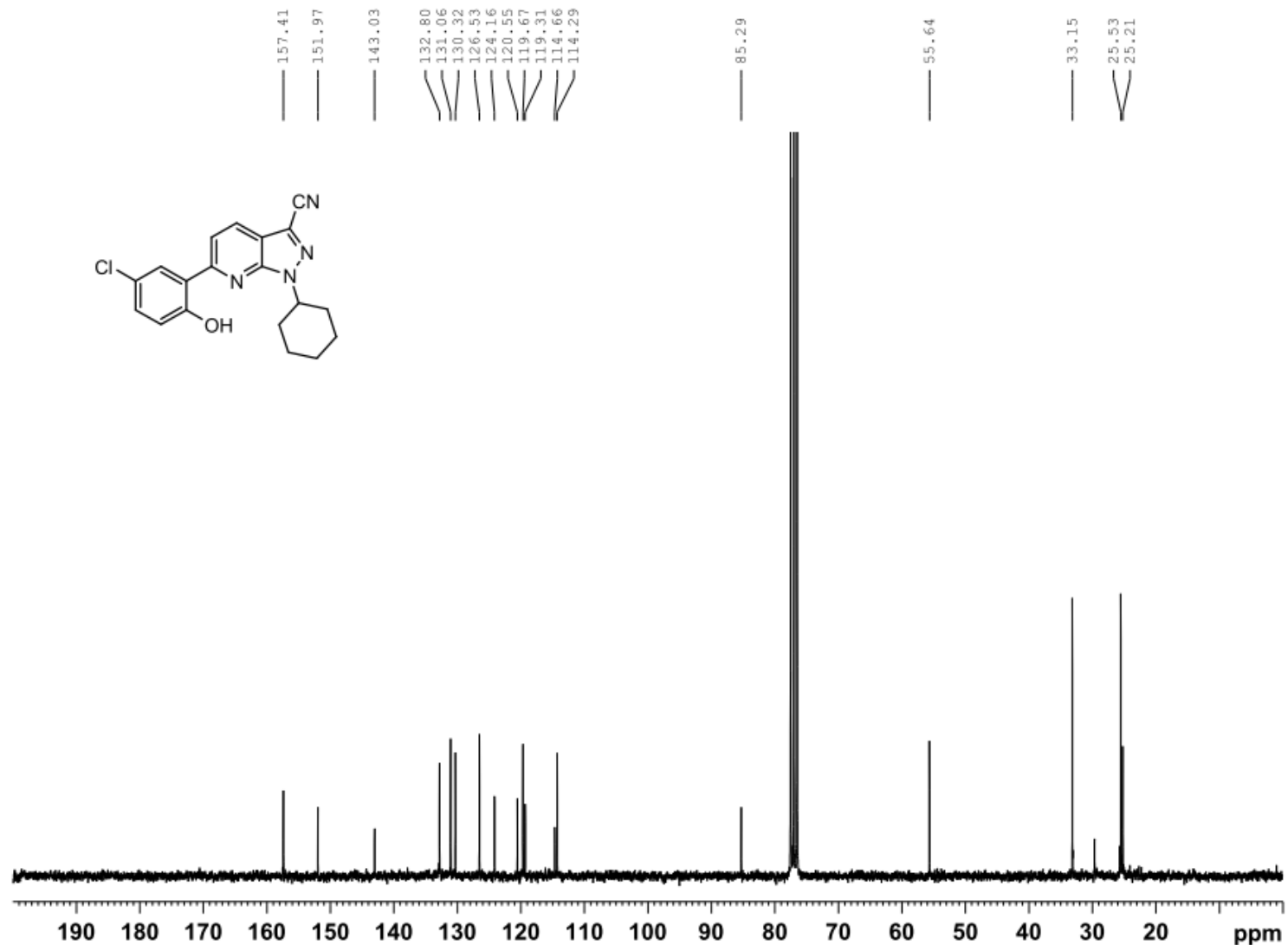
Current Data Parameters
NAME 110124.u304 ag 152
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110124
Time 8.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 101
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG152 (1) 13C CDC13



Current Data Parameters
NAME 110203.216 ag 152 C
EXPNO 10
PROCNO 1

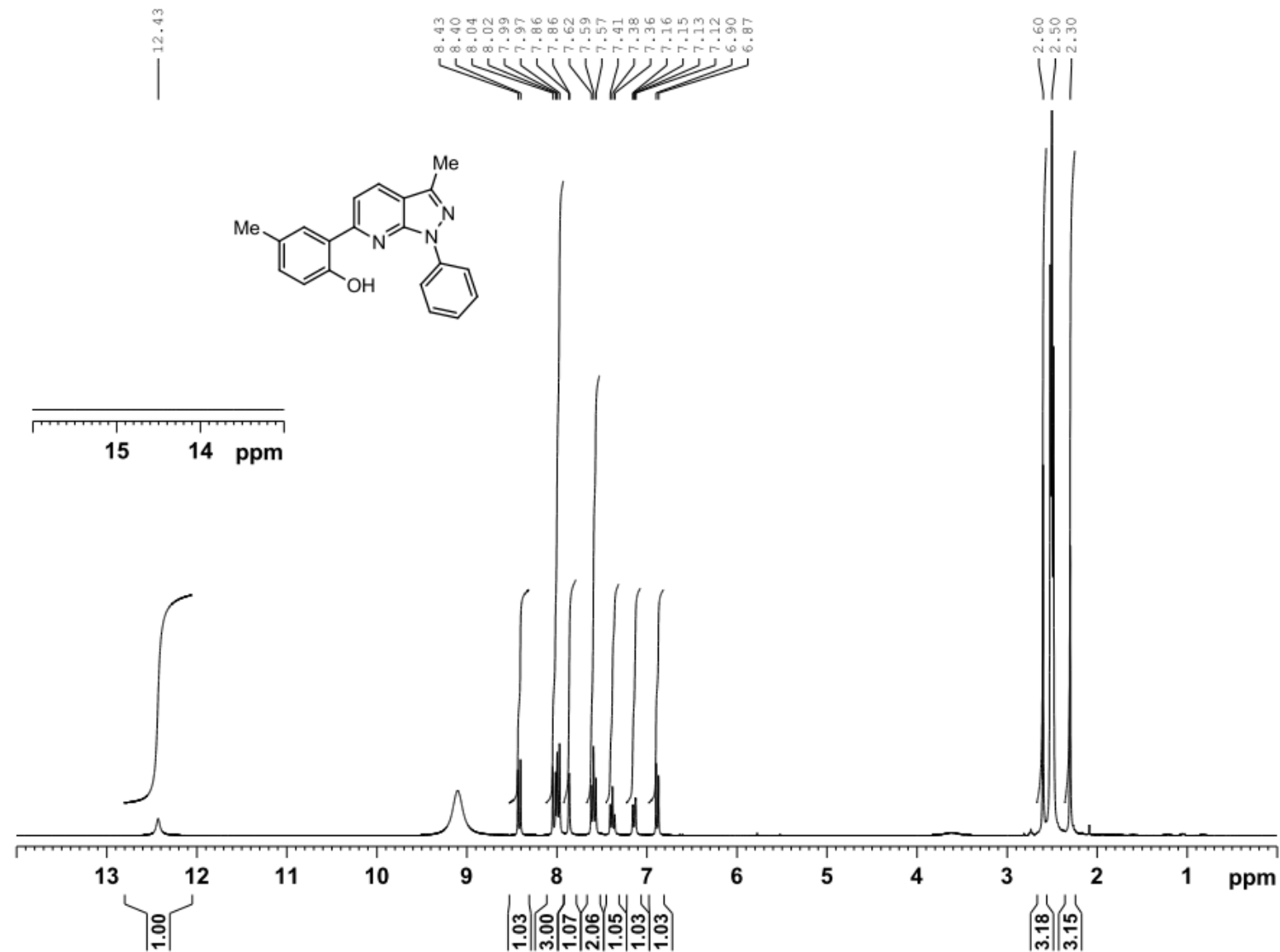
F2 - Acquisition Parameters
Date_ 20110204
Time 8.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1600
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

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

Gevorgyan AG140 1H DMSO



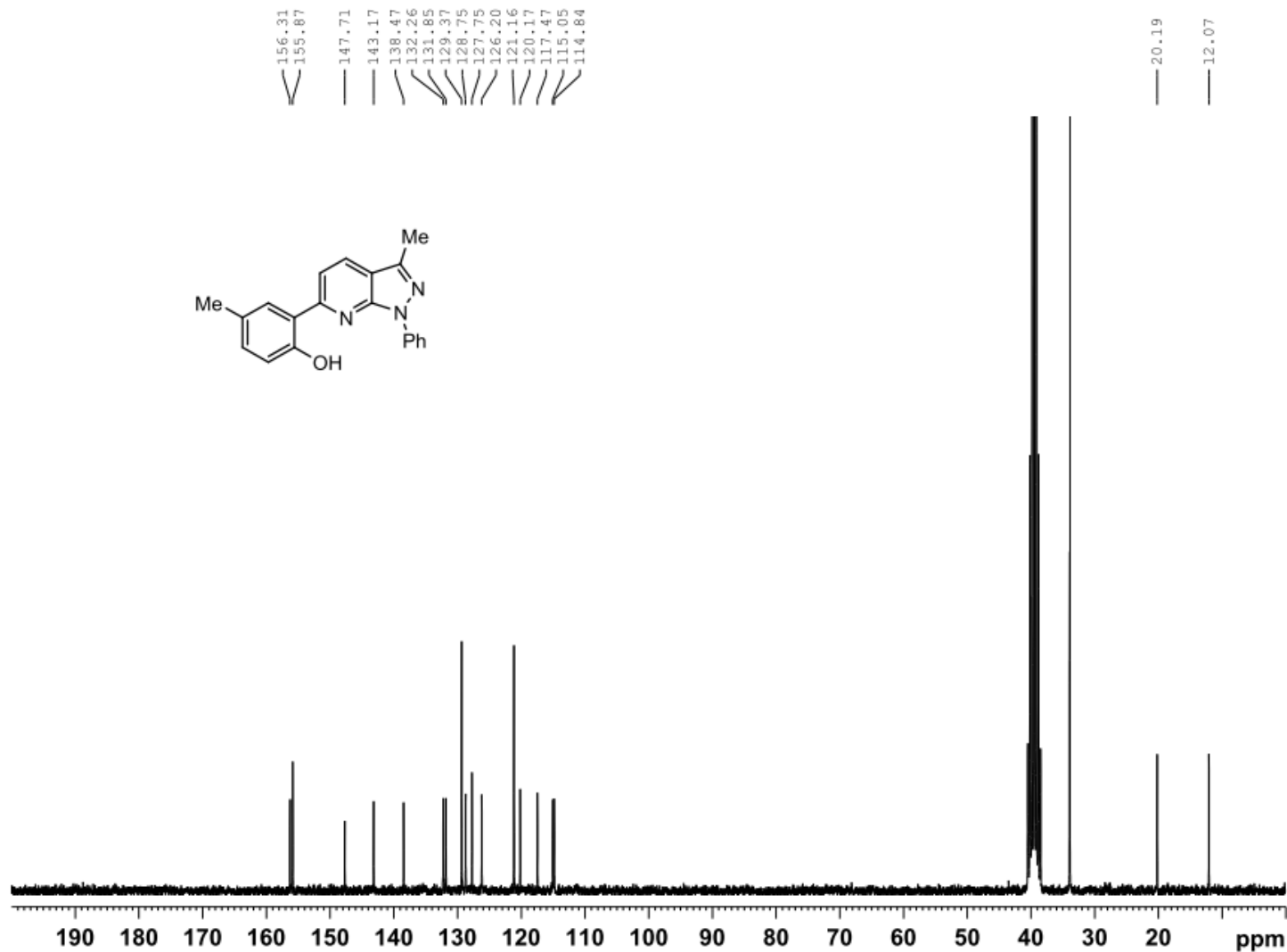
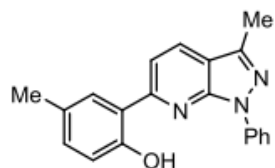
Current Data Parameters
NAME 110110.u303 ag 140
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110110
Time 8.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 71.8
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300026 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG140 13C DMSO

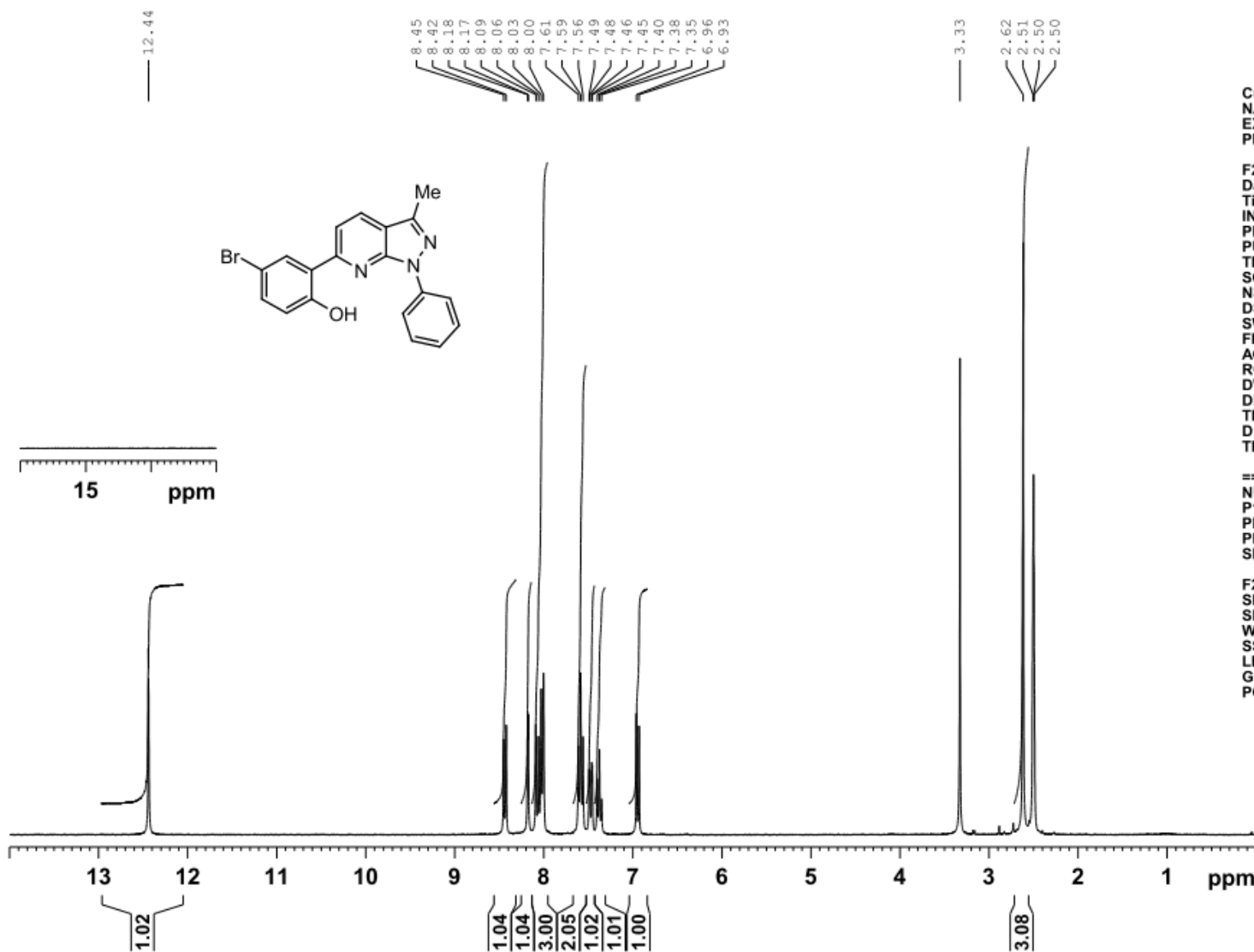


NAME 110111.203 ag 140 C
EXPNO 10
PROCNO 1
Date_ 20110111
Time 15.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952692 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG157 1H DMSO



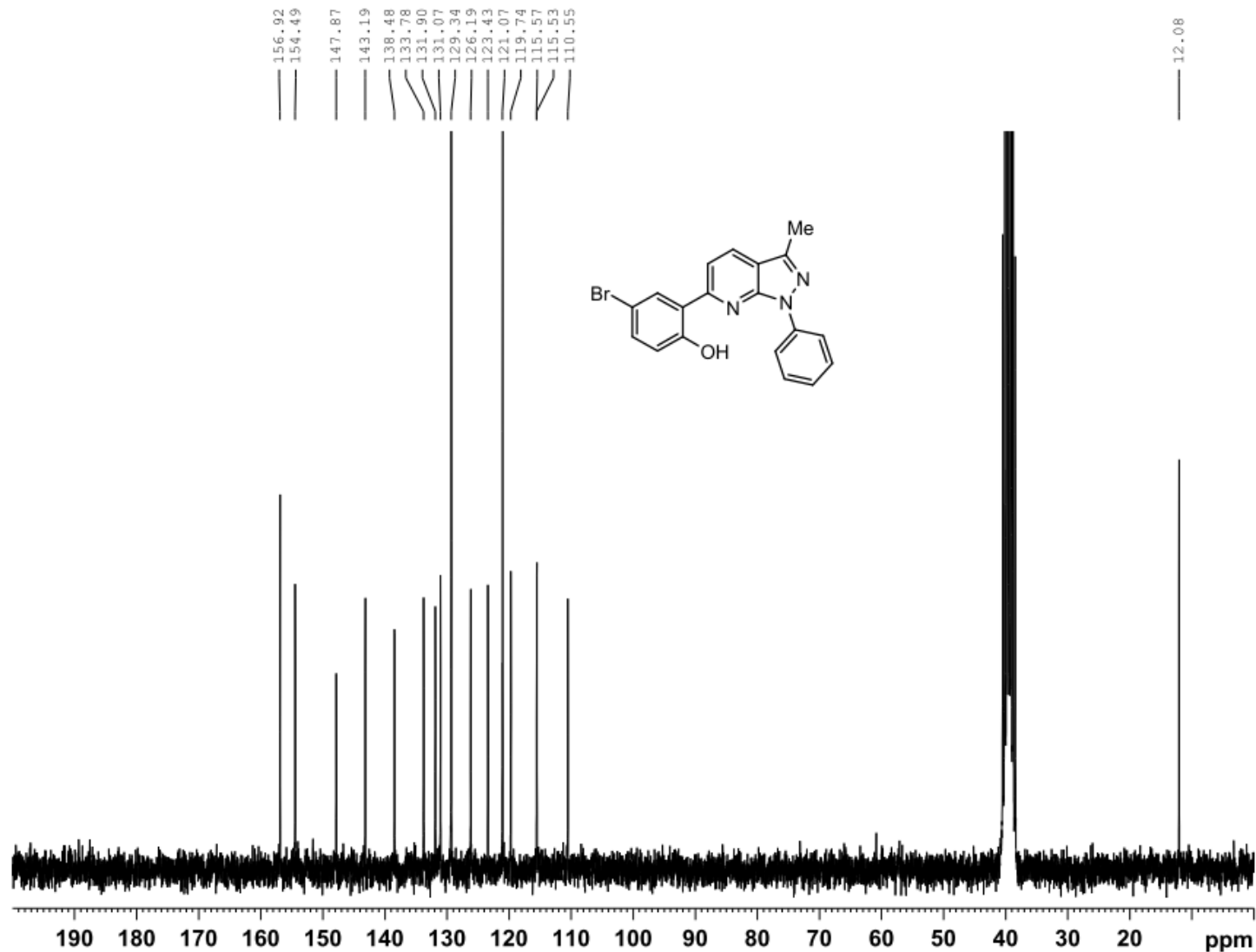
Current Data Parameters
NAME 110120.u308 ag 157
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110120
Time 9.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 161
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 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 300.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG157 13C DMSO



Current Data Parameters
NAME 110121.226 ag 157 C
EXPNO 10
PROCNO 1

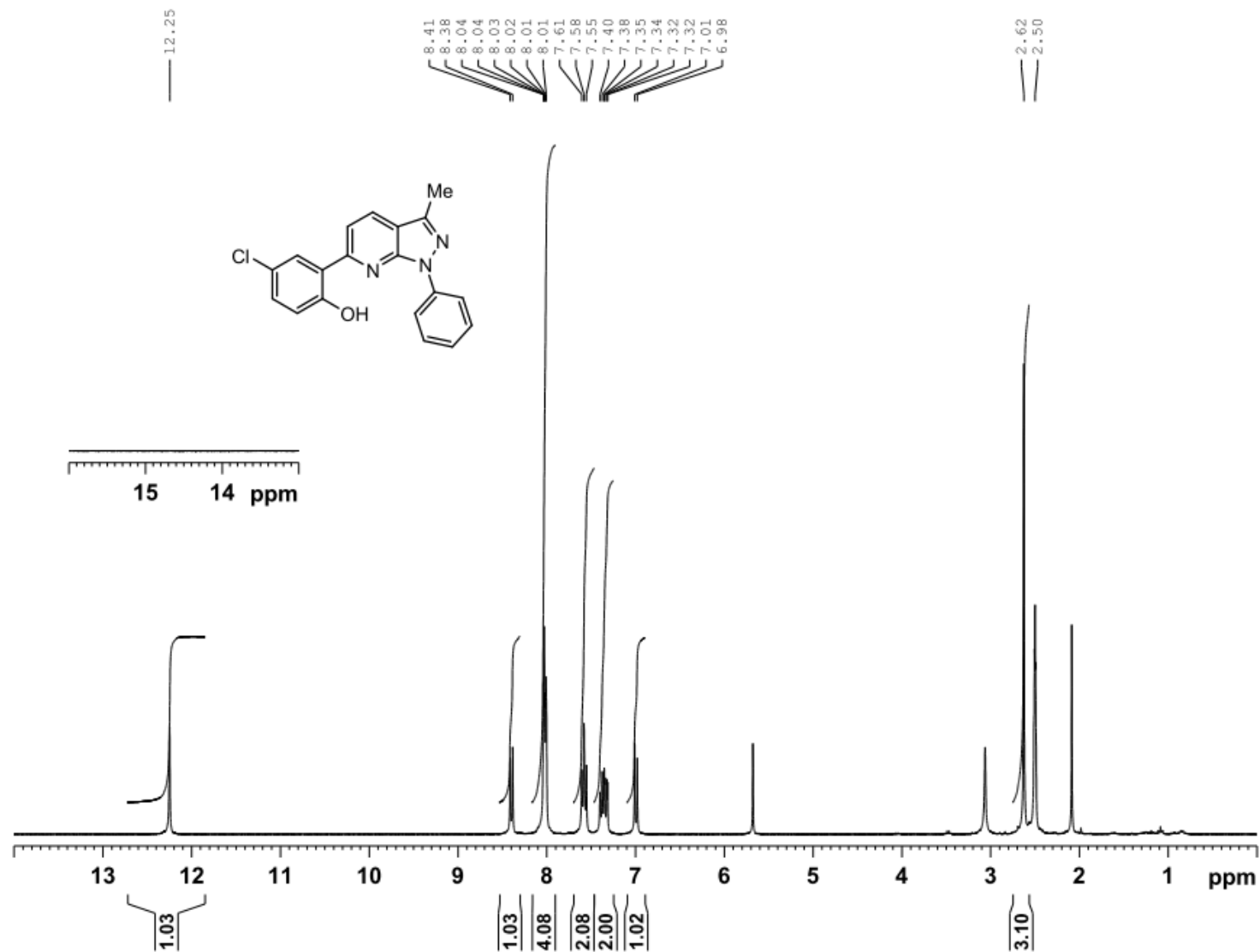
F2 - Acquisition Parameters
Date_ 20110123
Time 16.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1600
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI -32768
SF 62.8952697 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG 134 (3) 1H DMSO 80 grd_C



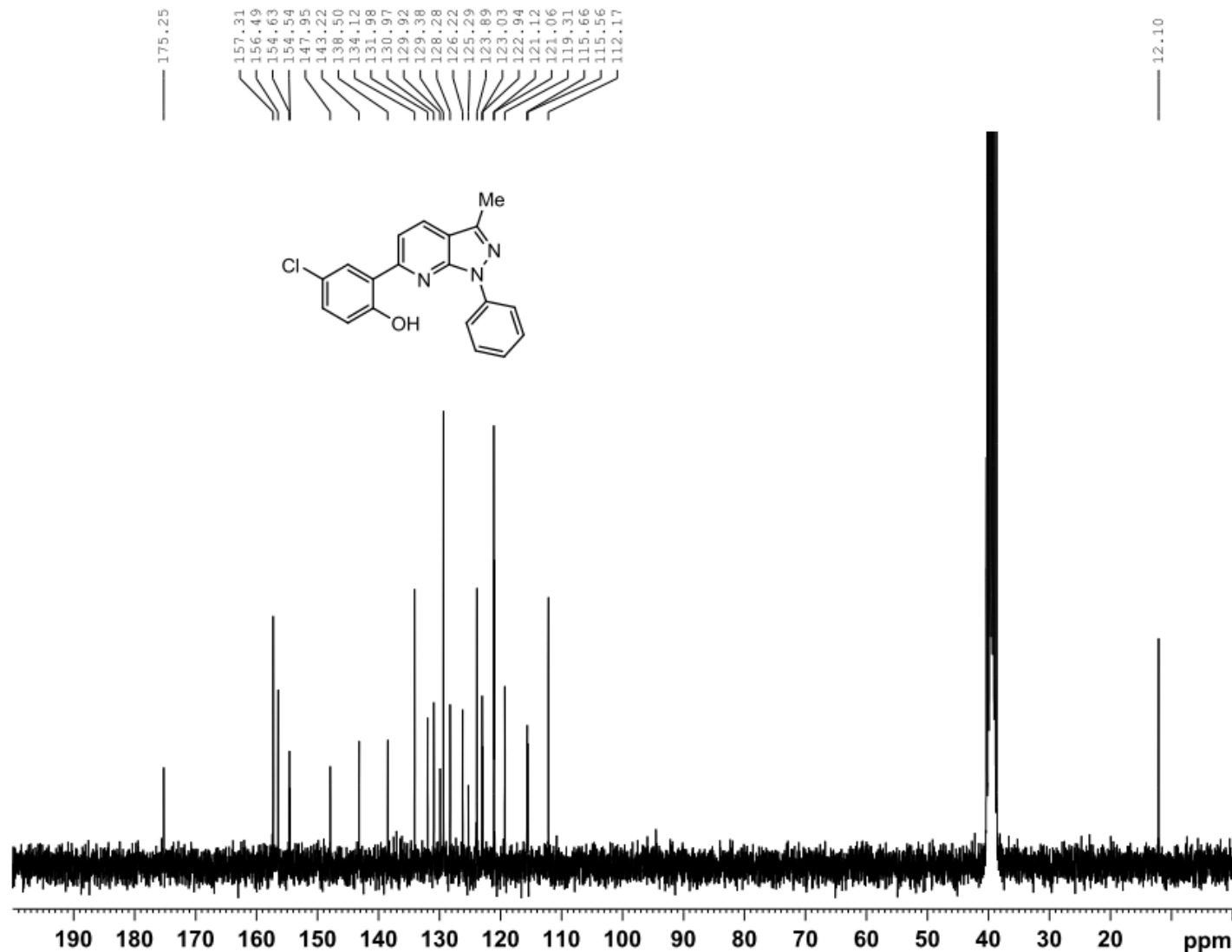
Current Data Parameters
NAME 110310.u342 ag 134
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110310
Time 15.32
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 353.5 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300009 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG134 13C DMSO



Current Data Parameters
NAME 110104.u325 ag 134 C
EXPNO 10
PROCNO 1

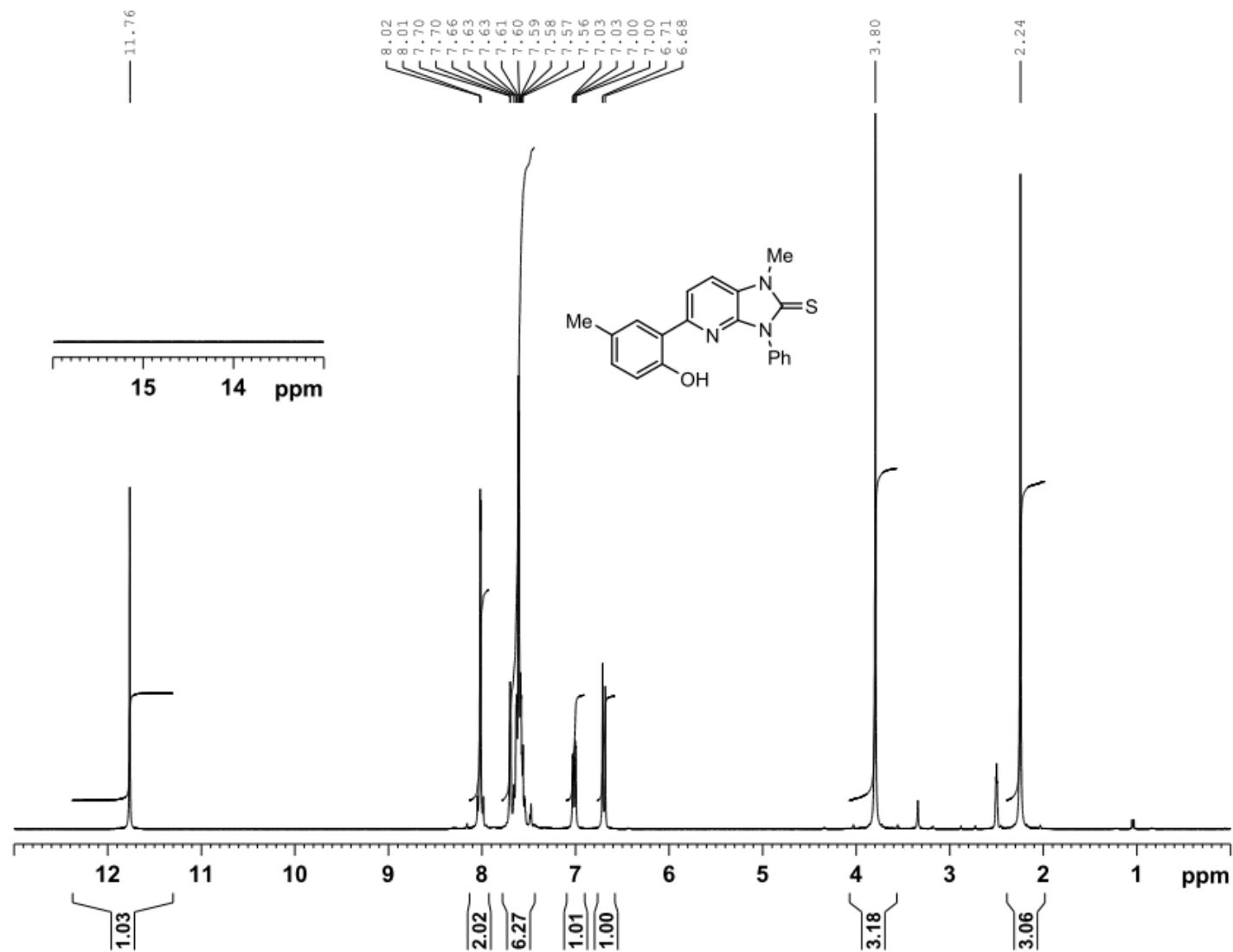
F2 - Acquisition Parameters
Date_ 20110105
Time 5.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1400
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== 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 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677881 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mkrtchyan SM422 1H DMSO



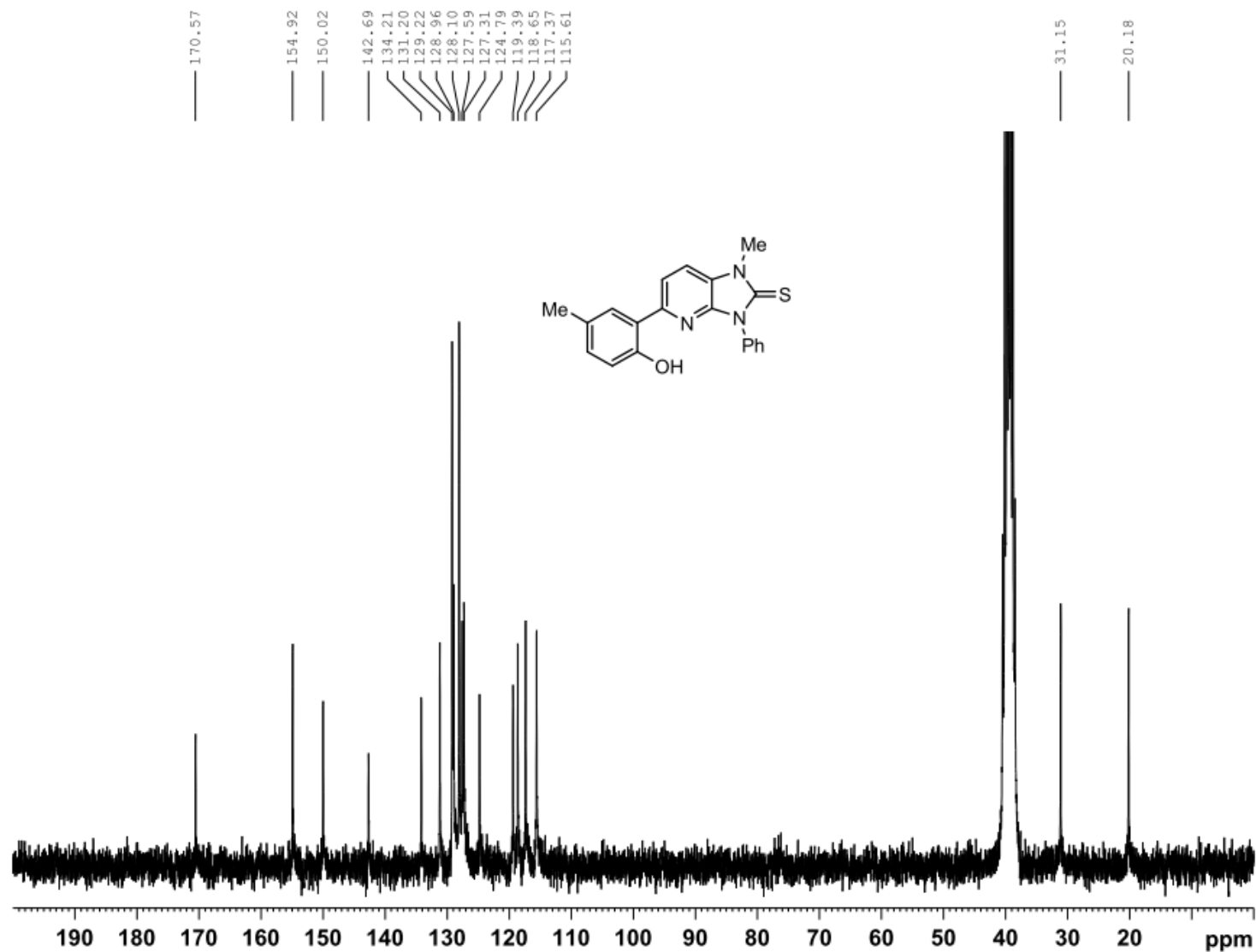
Current Data Parameters
NAME 110303.u308 sm 422
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110303
Time 9.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 90.5
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Mkrtchyan SM422 13C DMSO



Current Data Parameters
NAME 110304.225 sm 422
EXPNO 10
PROCNO 1

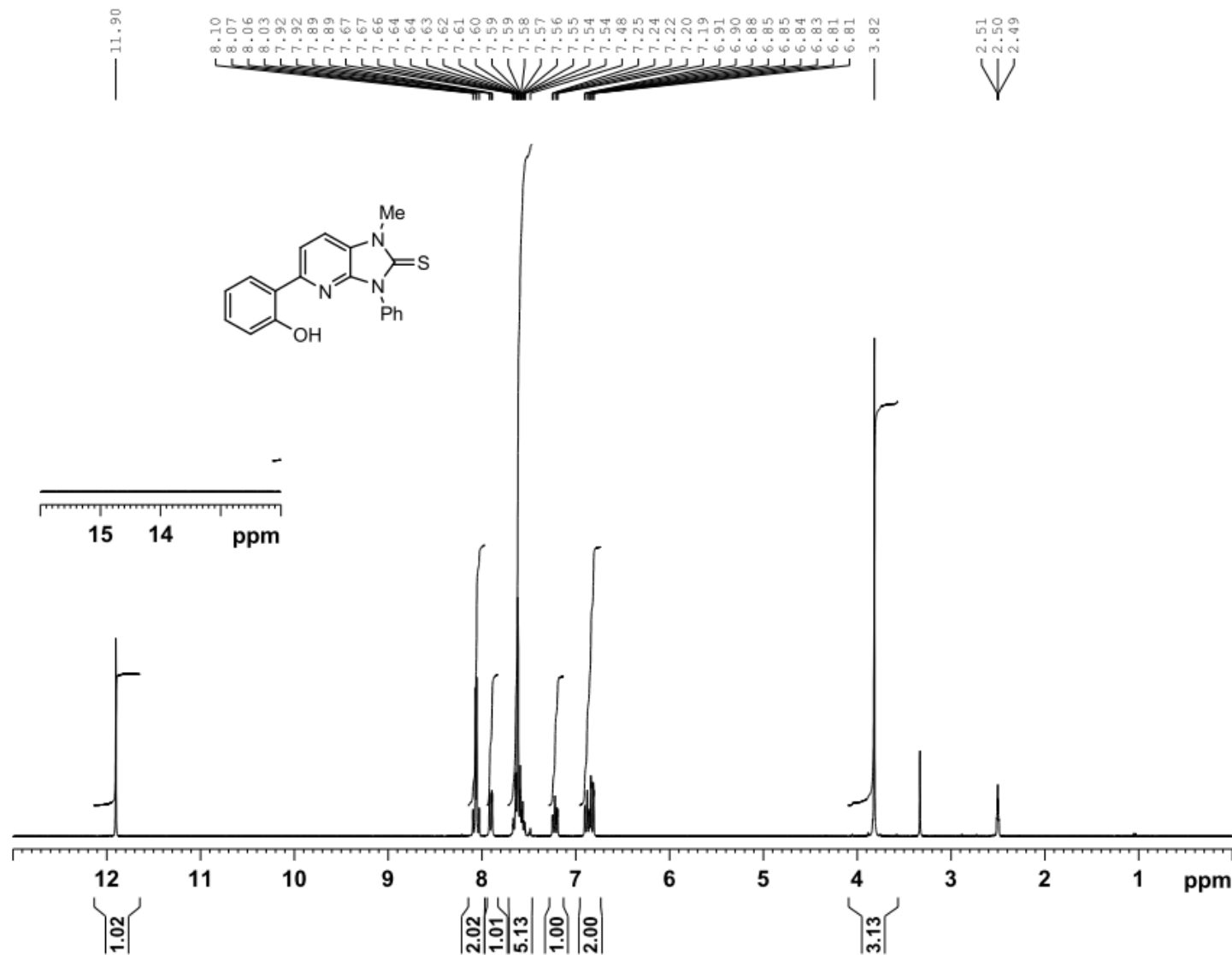
F2 - Acquisition Parameters
Date_ 20110306
Time 10.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952701 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mkrtchyan SM414 1H DMSO



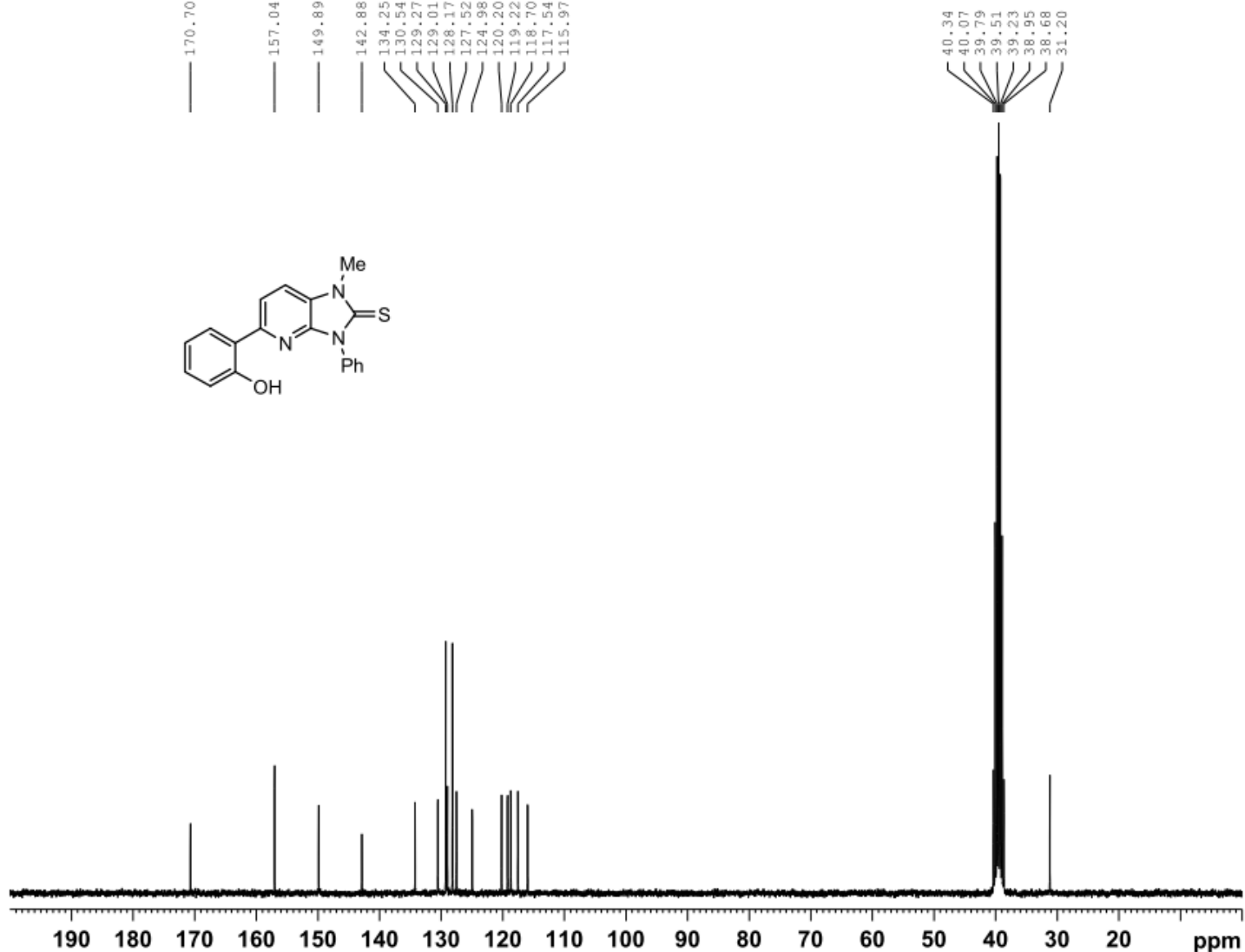
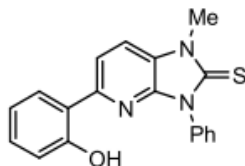
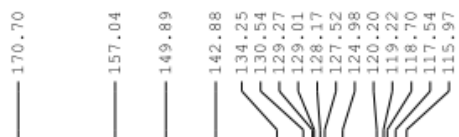
Current Data Parameters
NAME 110228.u310 sm 414
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110228
Time 11.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 144
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Mkrtchyan SM414 13C DMSO



Current Data Parameters
NAME 110301.u337 sm 414 C
EXPNO 10
PROCNO 1

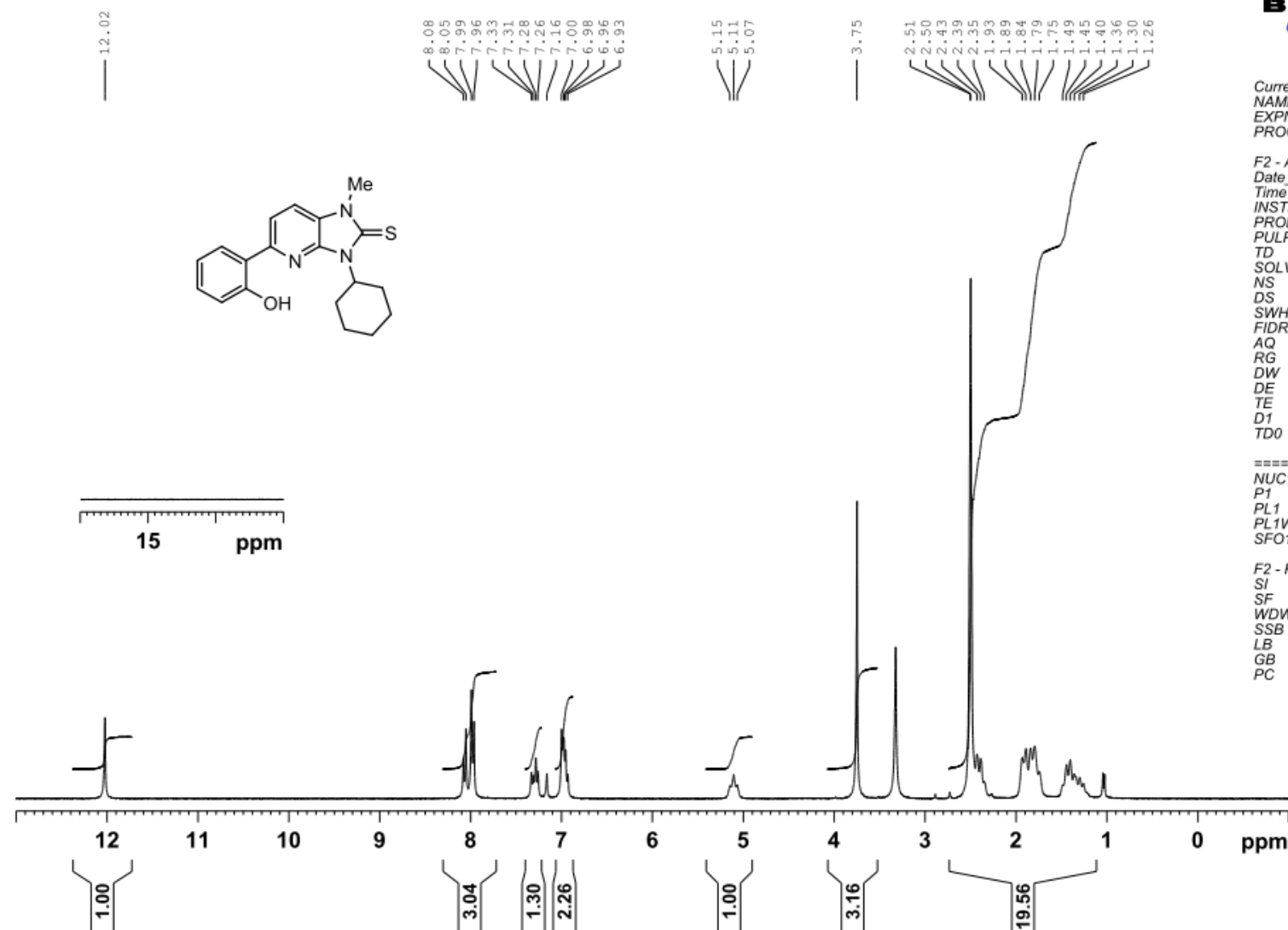
F2 - Acquisition Parameters
Date_ 20110302
Time 7.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 800
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

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

Mkrtchyan SM390 1H DMSO



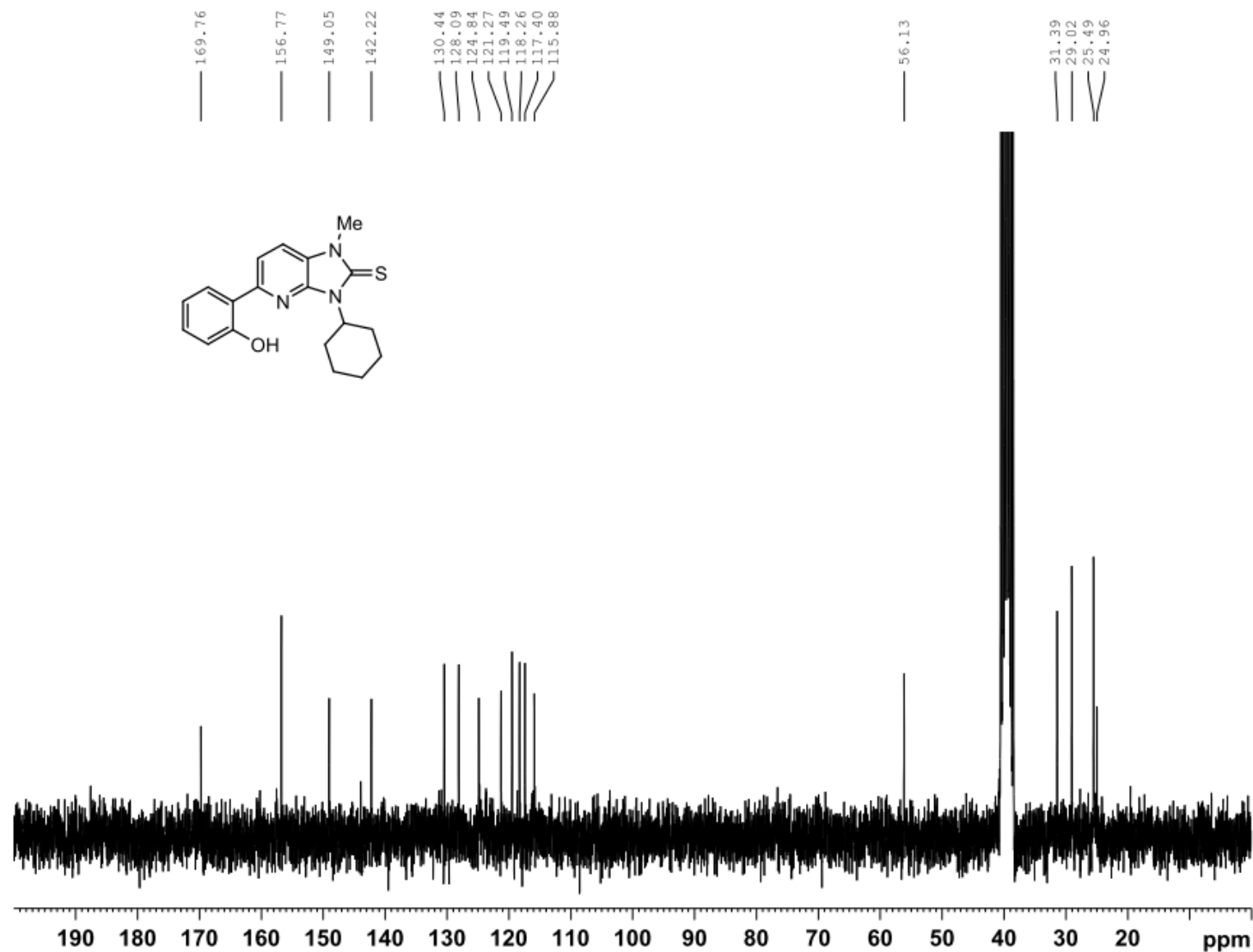
Current Data Parameters
NAME 110111.u302 sm 390
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110111
Time 9.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 144
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 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 300.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Mkrtchyan SM-390 13C DMSO



Current Data Parameters
NAME 110120.215 sm 390 C
EXPNO 10
PROCNO 1

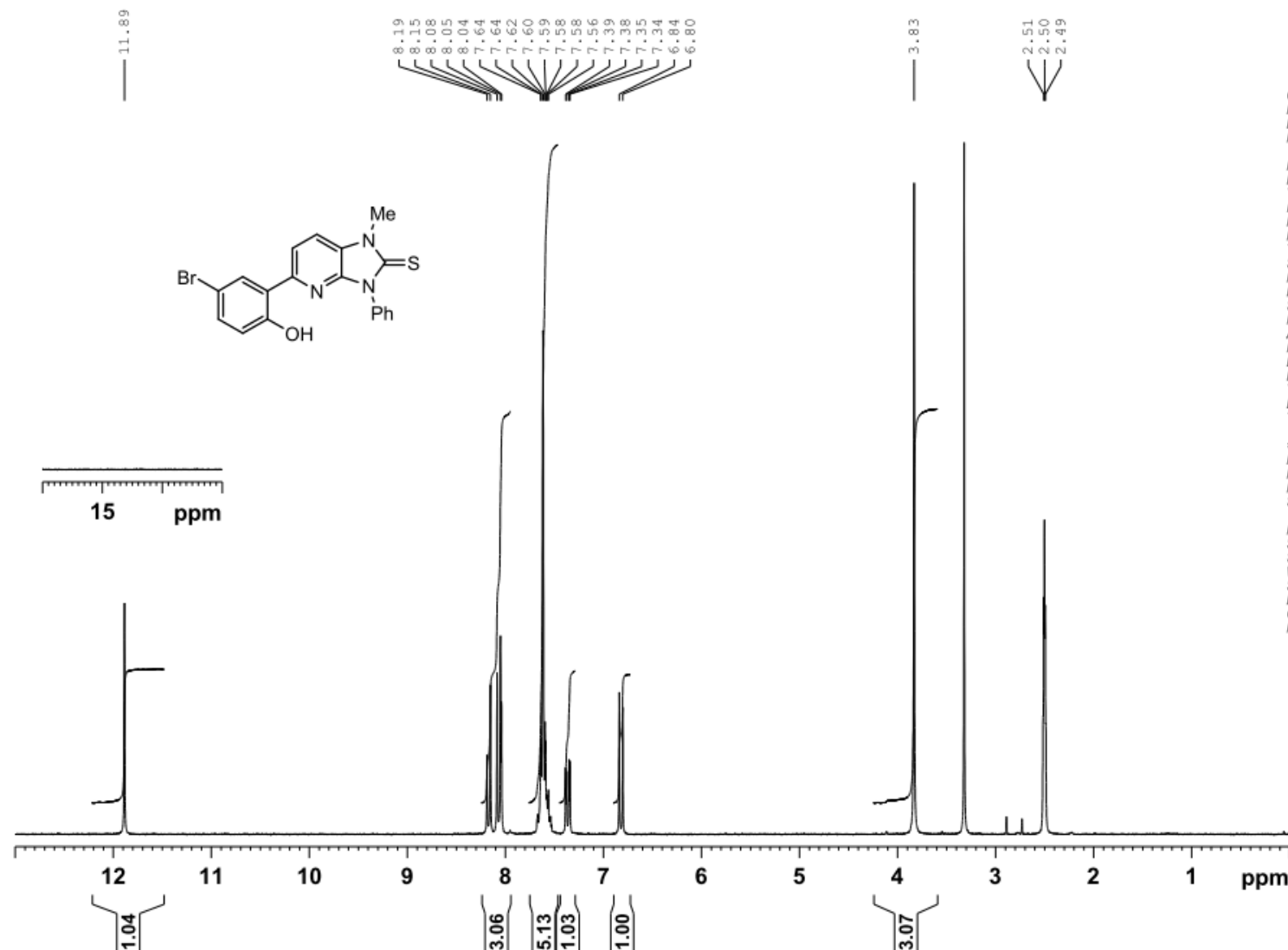
F2 - Acquisition Parameters
Date_ 20110121
Time 7.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1400
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952687 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mkrtchyan SM431 1H DMSO



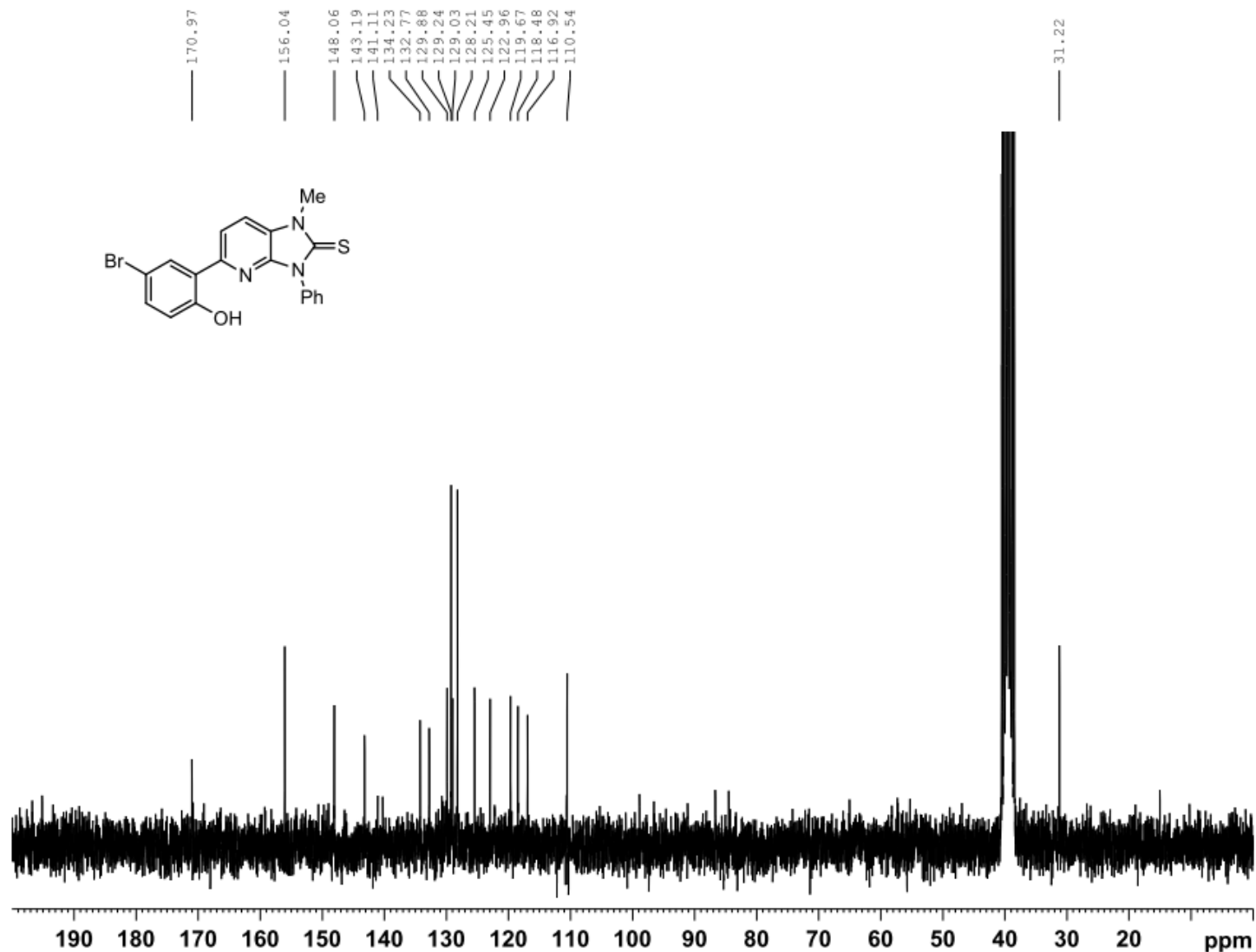
Current Data Parameters
 NAME 110309.216 sm 431
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110309
 Time 12.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 5165.289 Hz
 FIDRES 0.078816 Hz
 AQ 6.3439350 sec
 RG 1440
 DW 96.800 usec
 DE 10.00 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

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

F2 - Processing parameters
 SI 32768
 SF 250.1299985 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Mkrtchyan SM431 13C DMSO



Current Data Parameters
NAME 110310.209 sm 431 C
EXPNO 10
PROCNO 1

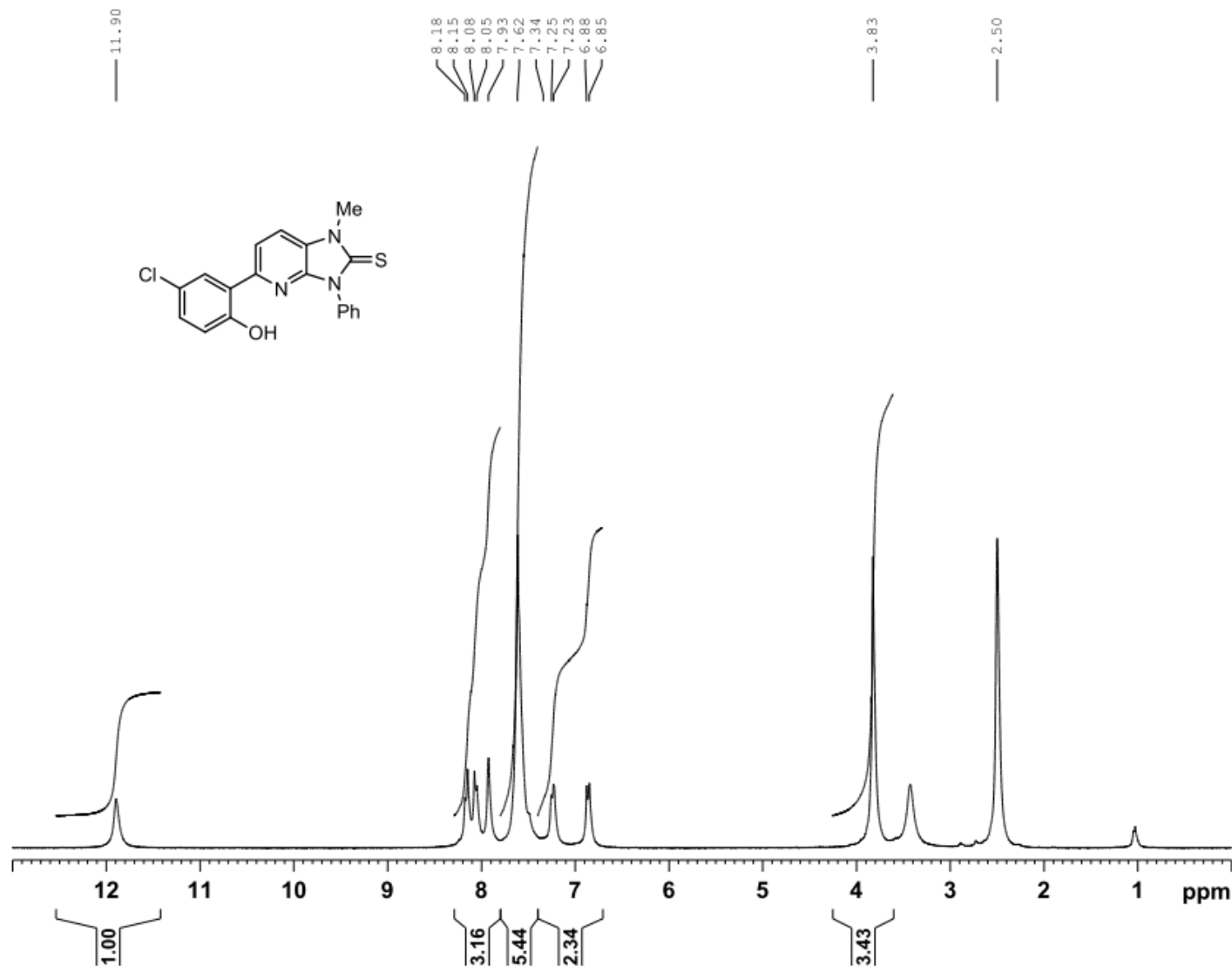
F2 - Acquisition Parameters
Date_ 20110311
Time 1.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952697 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Hakobyan SM 379 1H DMSO



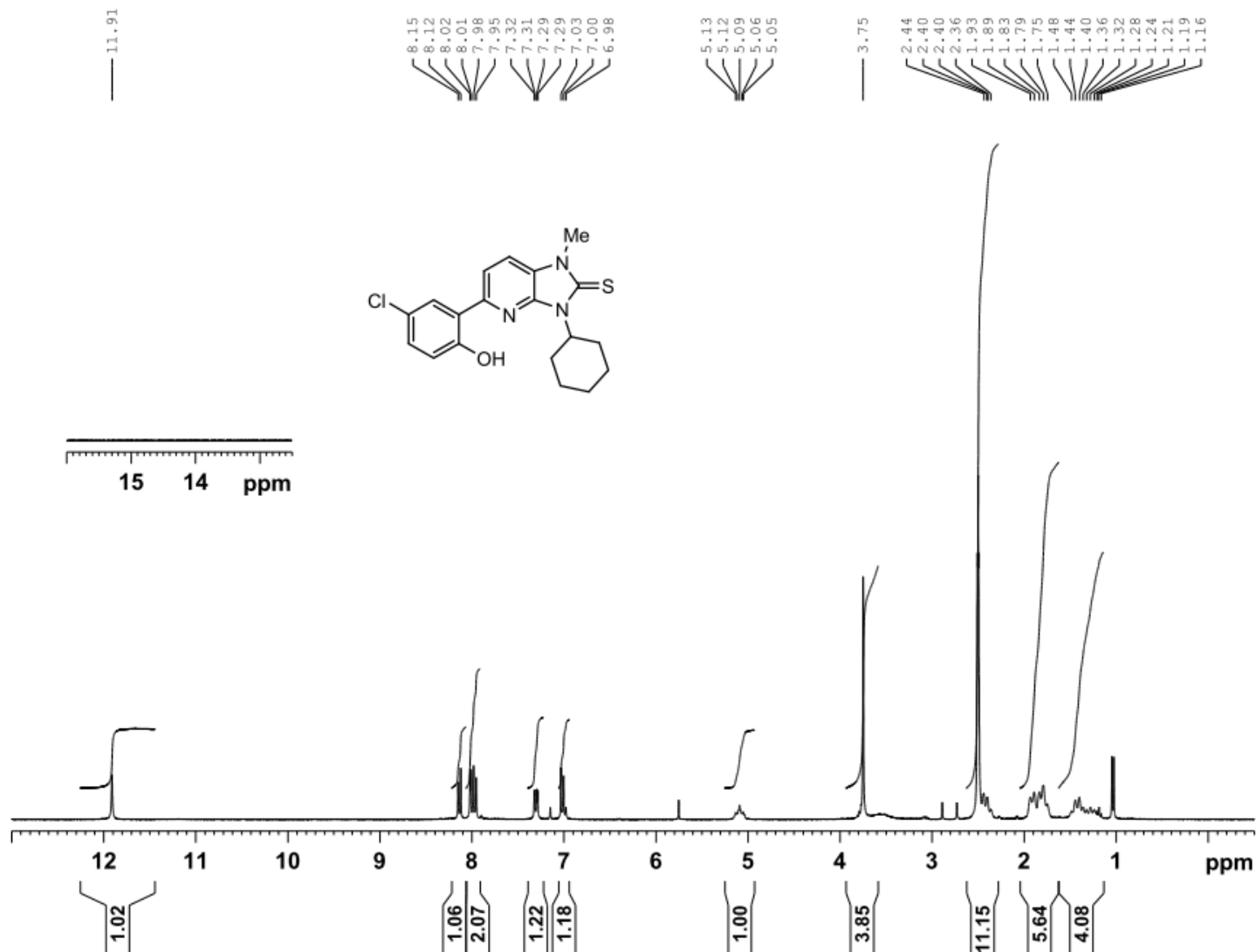
Current Data Parameters
NAME 101209.u315 sm 379
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101209
Time 14.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 114
DW 80.800 usec
DE 10.00 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300201 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Mkrtchyan SM387 1H DMSO



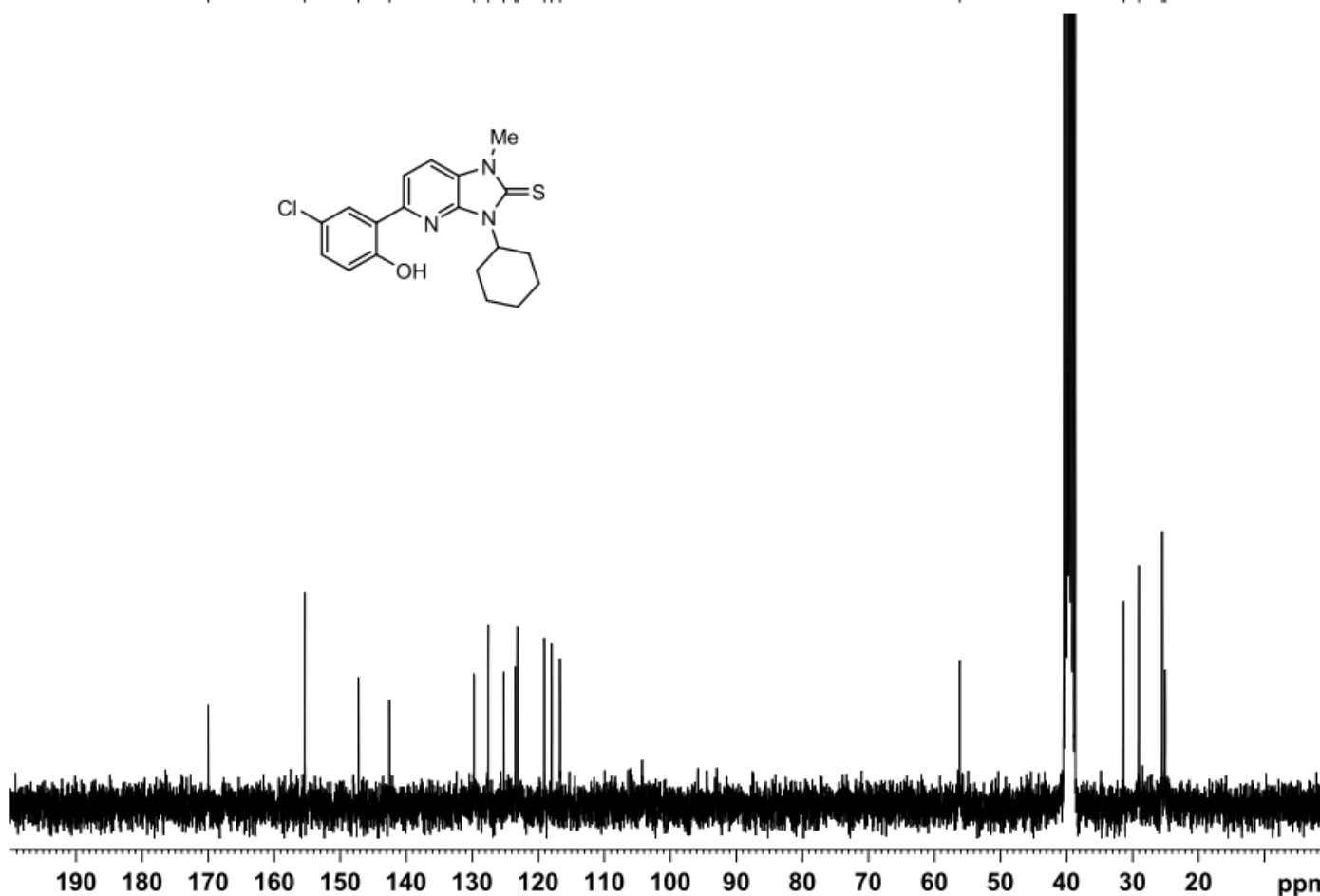
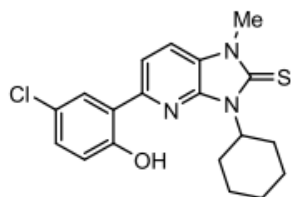
Current Data Parameters
 NAME 101220.u318 sm 387
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101220
 Time 12.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 228
 DW 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

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

F2 - Processing parameters
 SI 32768
 SF 300.1300064 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Mkrtchyan SM387 13C DMSO



Current Data Parameters
 NAME 101220.u318 sm 387
 EXPNO 11
 PROCNO 1

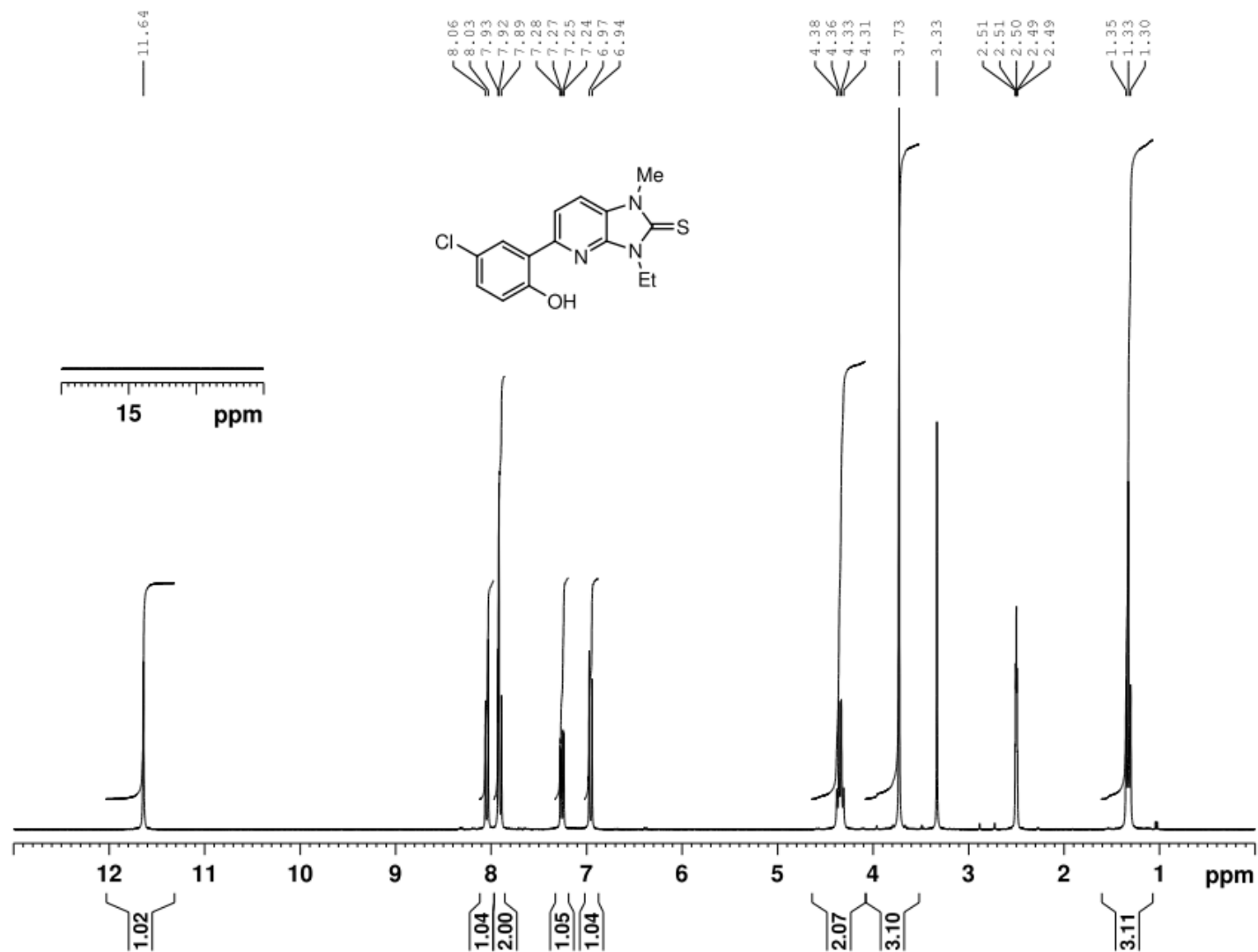
F2 - Acquisition Parameters
 Date_ 20101221
 Time 1.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DW 27.733 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

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

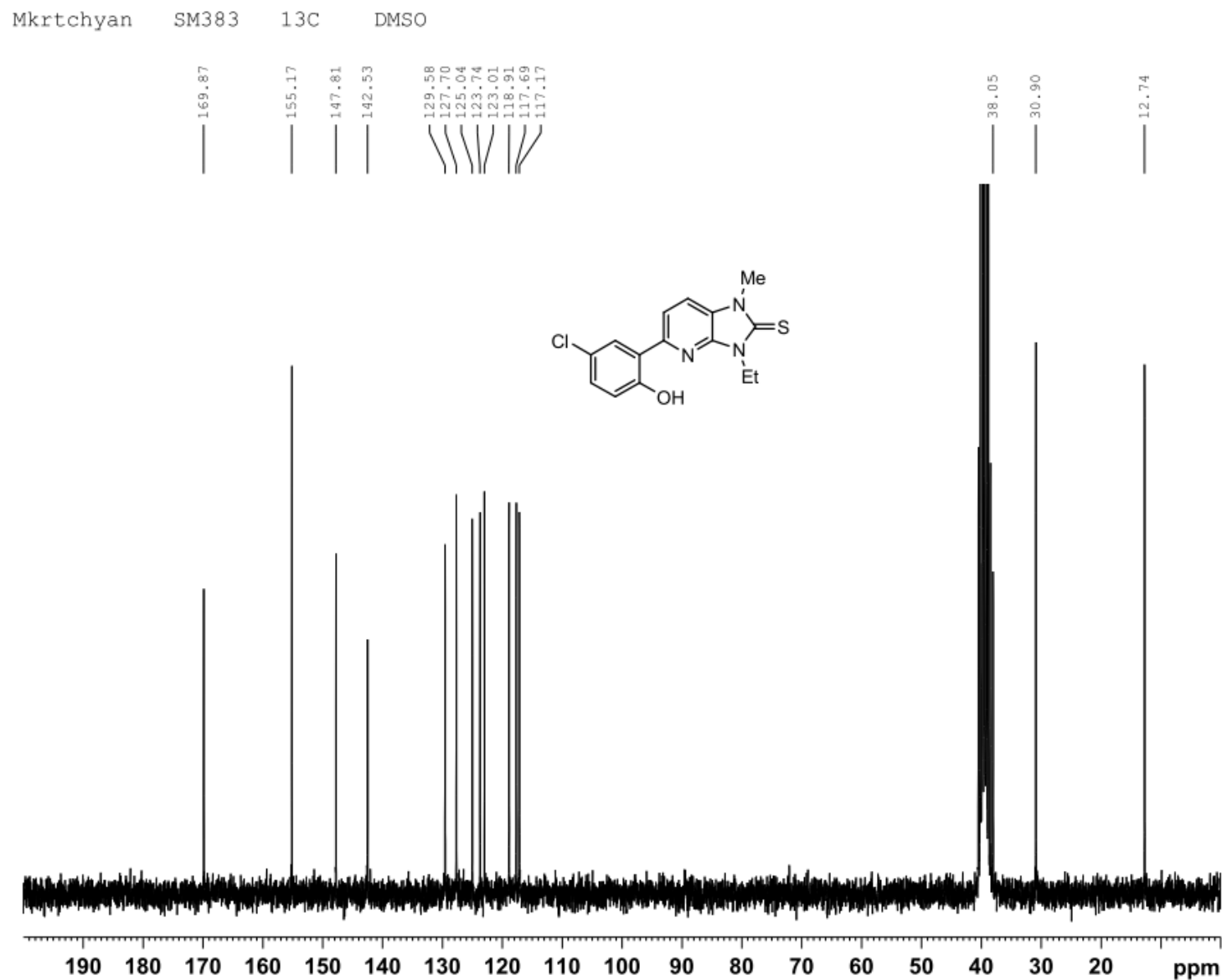
F2 - Processing parameters
 SI 32768
 SF 75.4677876 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Mkrtchyan SM383 1H DMSO



NAME 101214.u317
EXPNO 10
PROCNO 1
Date_ 20101214
Time 10.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
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
SI 32768
SF 300.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 101214.211 sm 383 C
EXPNO 10
PROCNO 1

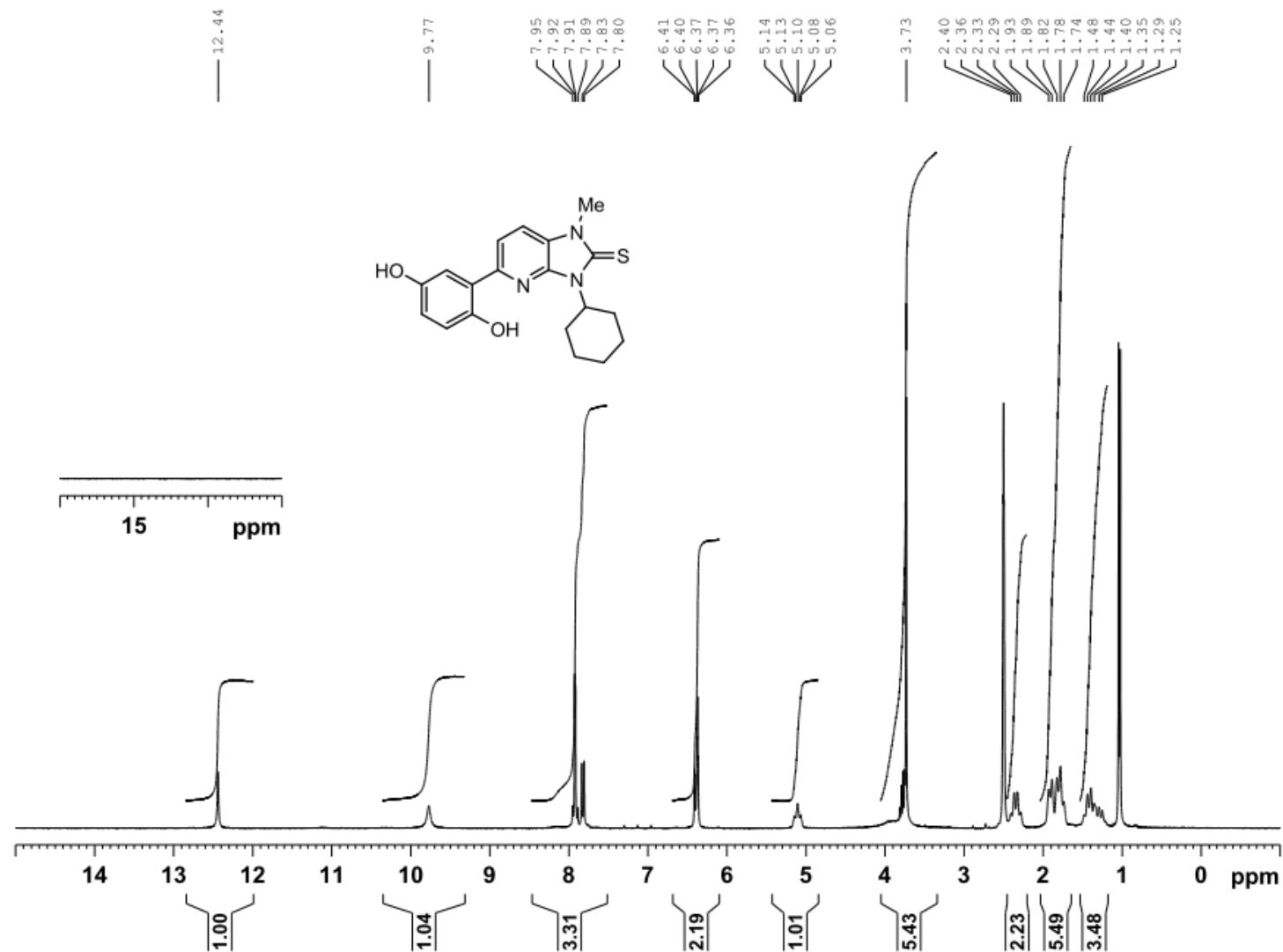
F2 - Acquisition Parameters
Date_ 20101215
Time 1.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 1290
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952697 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mkrtchyan SM389 1H DMSO



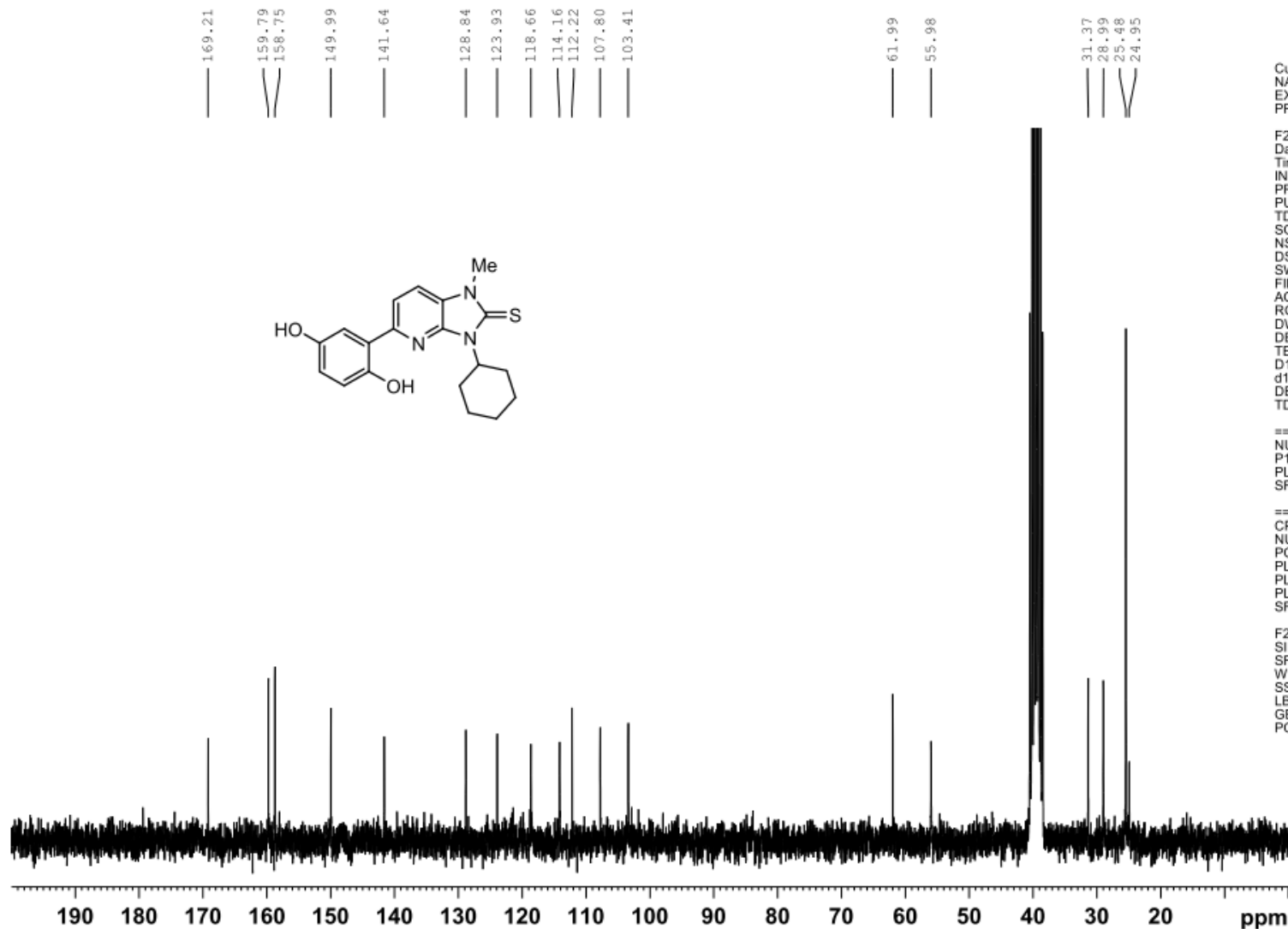
Current Data Parameters
 NAME 101220.u320 sm 389
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101220
 Time 13.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 181
 DW 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

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

F2 - Processing parameters
 SI 32768
 SF 300.1300063 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Mkrtchyan SM389 13C DMSO



Current Data Parameters
NAME 101221.211 sm 389 C
EXPNO 10
PROCNO 1

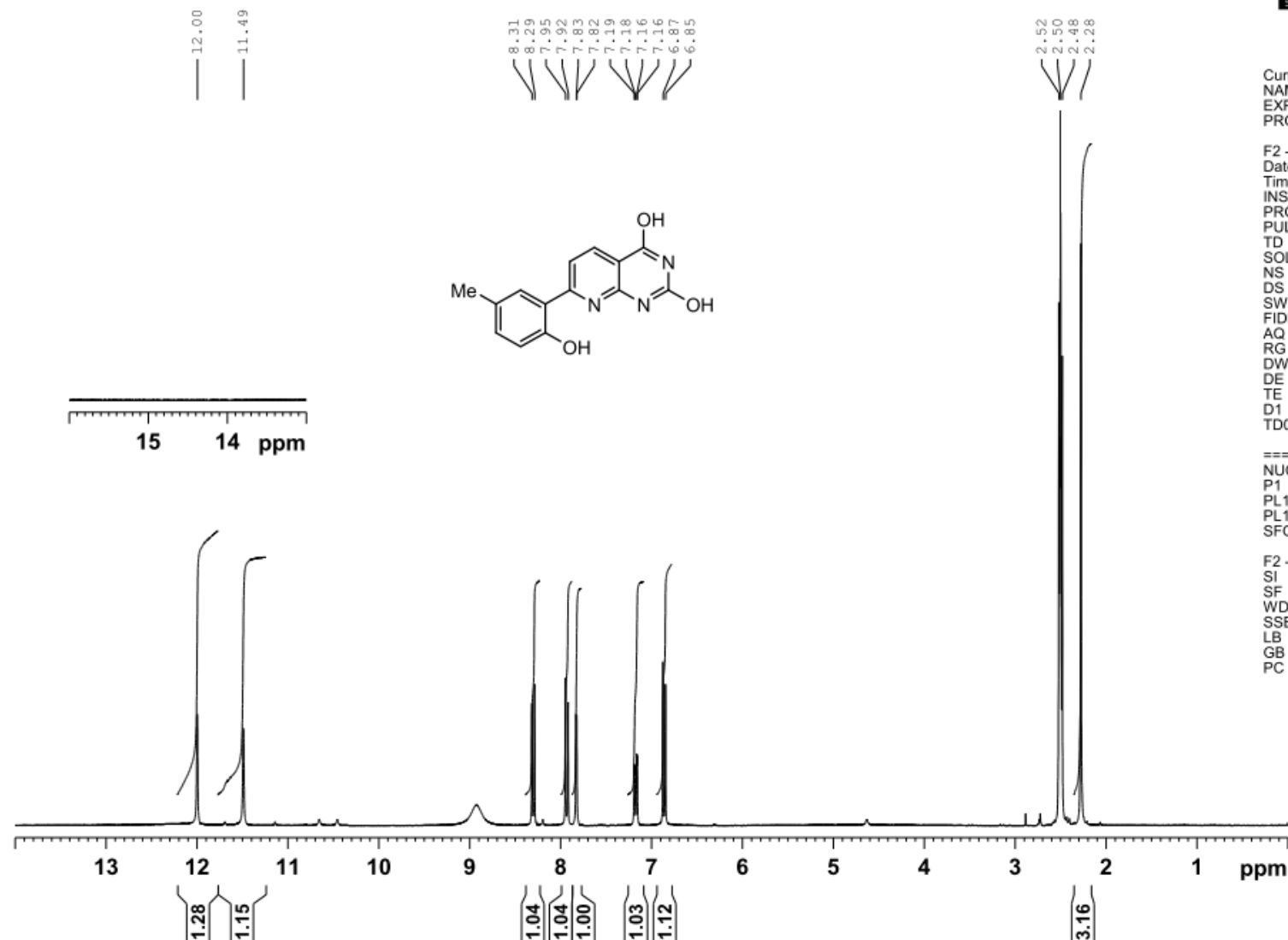
F2 - Acquisition Parameters
Date_ 20101221
Time 22.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228862 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 295.9 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952683 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG164 1H DMSO



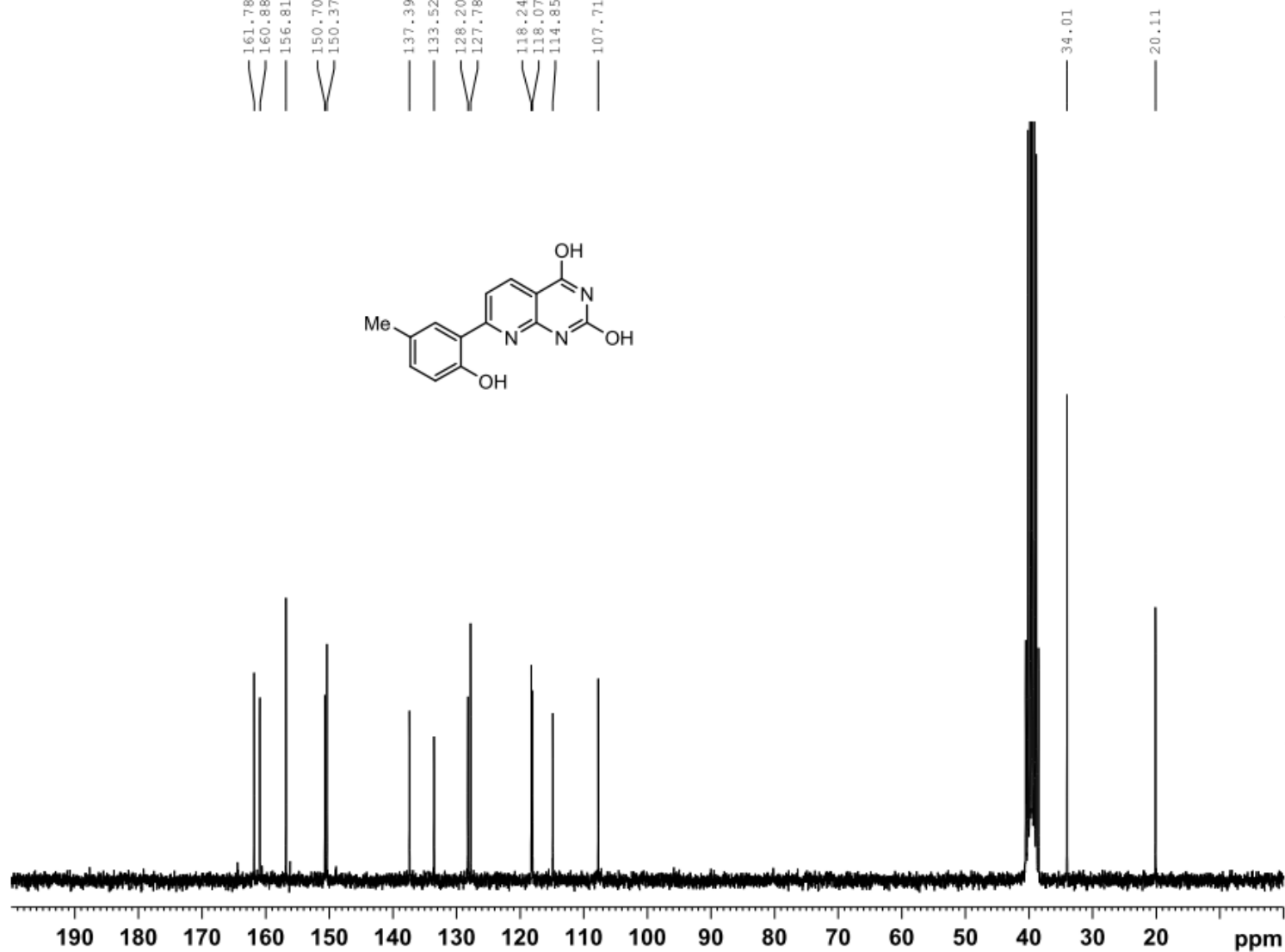
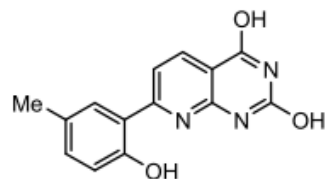
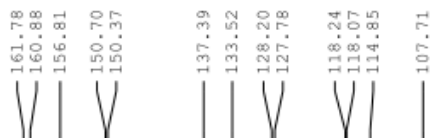
Current Data Parameters
NAME 110131.u325 ag 164
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110131
Time 11.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 90.5
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300041 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG164 13C DMSO



Current Data Parameters
NAME 110202.204 ag 164 C
EXPNO 10
PROCNO 1

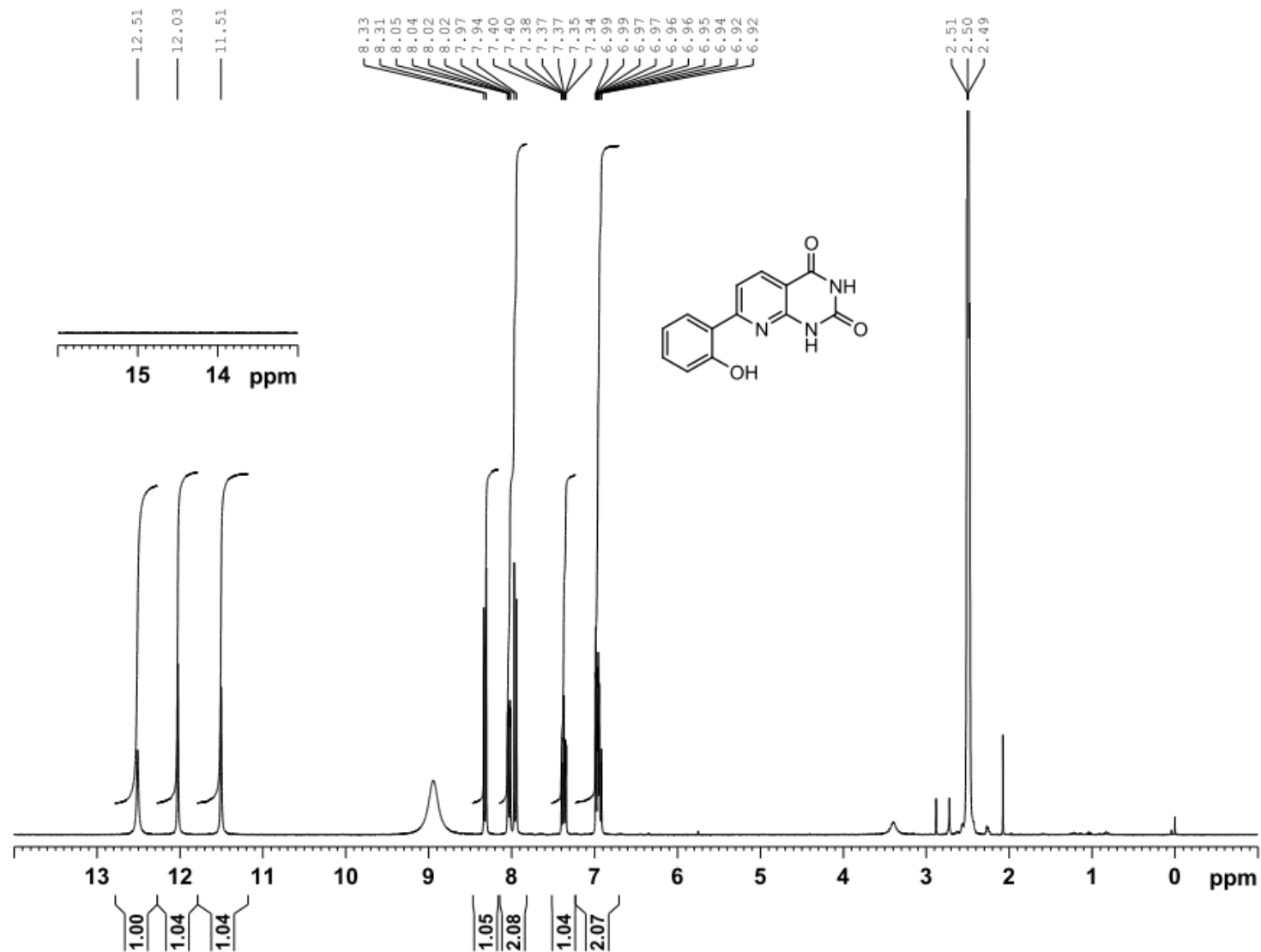
F2 - Acquisition Parameters
Date_ 20110202
Time 19.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952678 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG168 1H DMSO



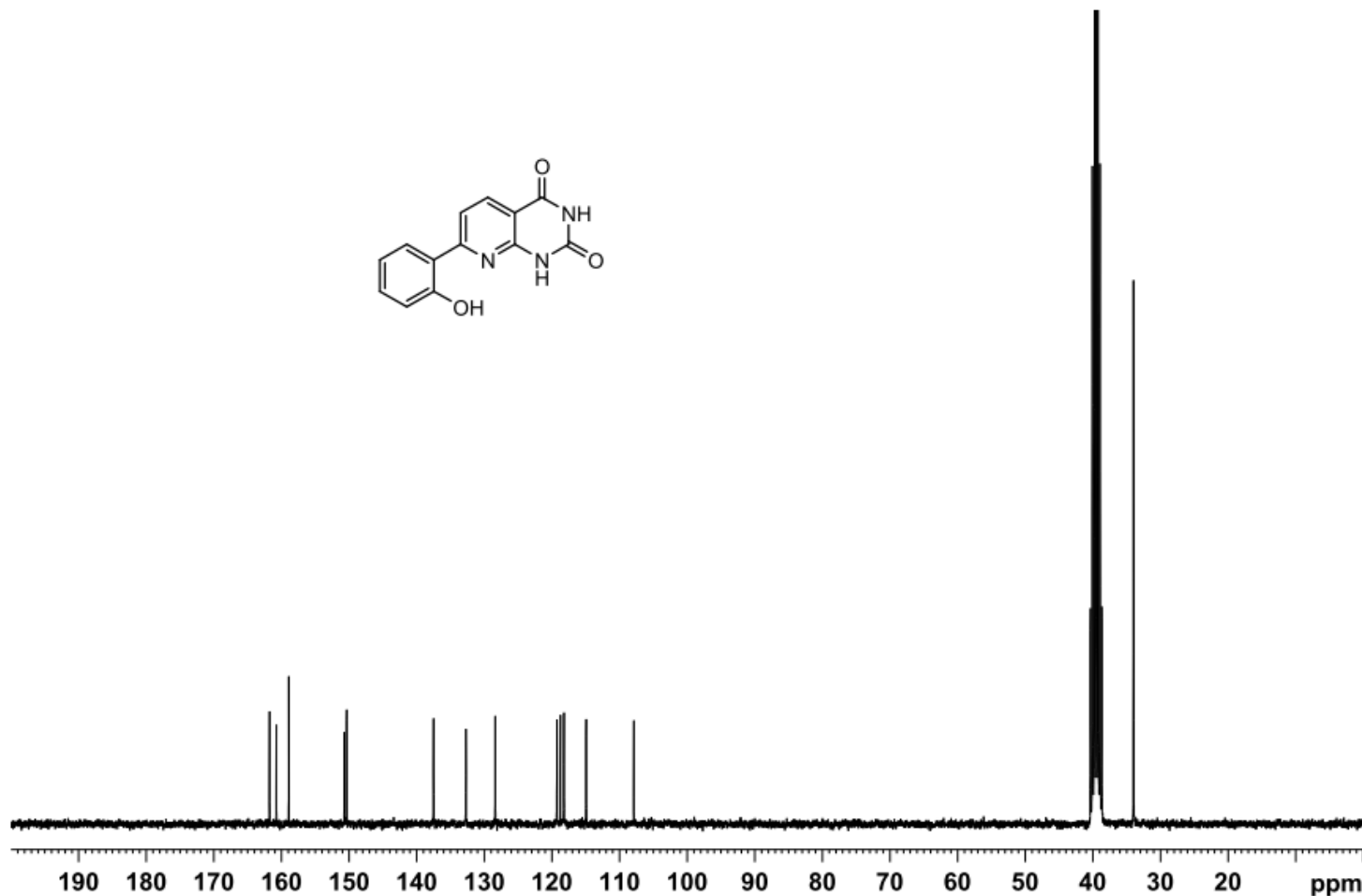
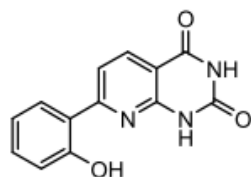
Current Data Parameters
NAME 110131.u328 ag 168
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110131
Time 11.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 101
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 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 300.1300048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG168 (A) 13C DMSO



Current Data Parameters
NAME 110324.u336 ag 168 C
EXPNO 10
PROCNO 1

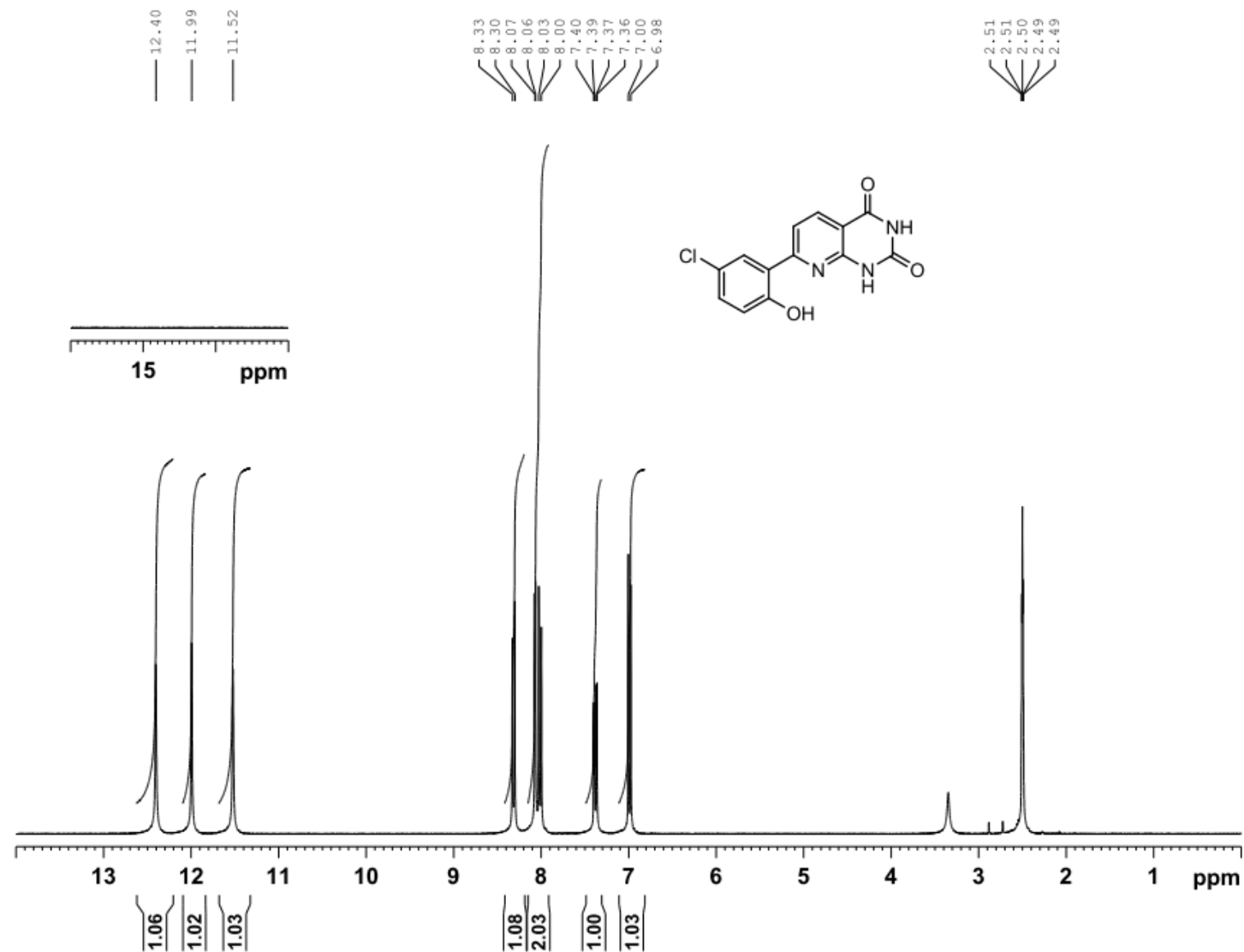
F2 - Acquisition Parameters
Date_ 20110325
Time 4.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1600
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 75.4677865 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan, AG 146, DMSO, 1H



Current Data Parameters
NAME 110114.u302 ag 146
EXPNO 10
PROCNO 1

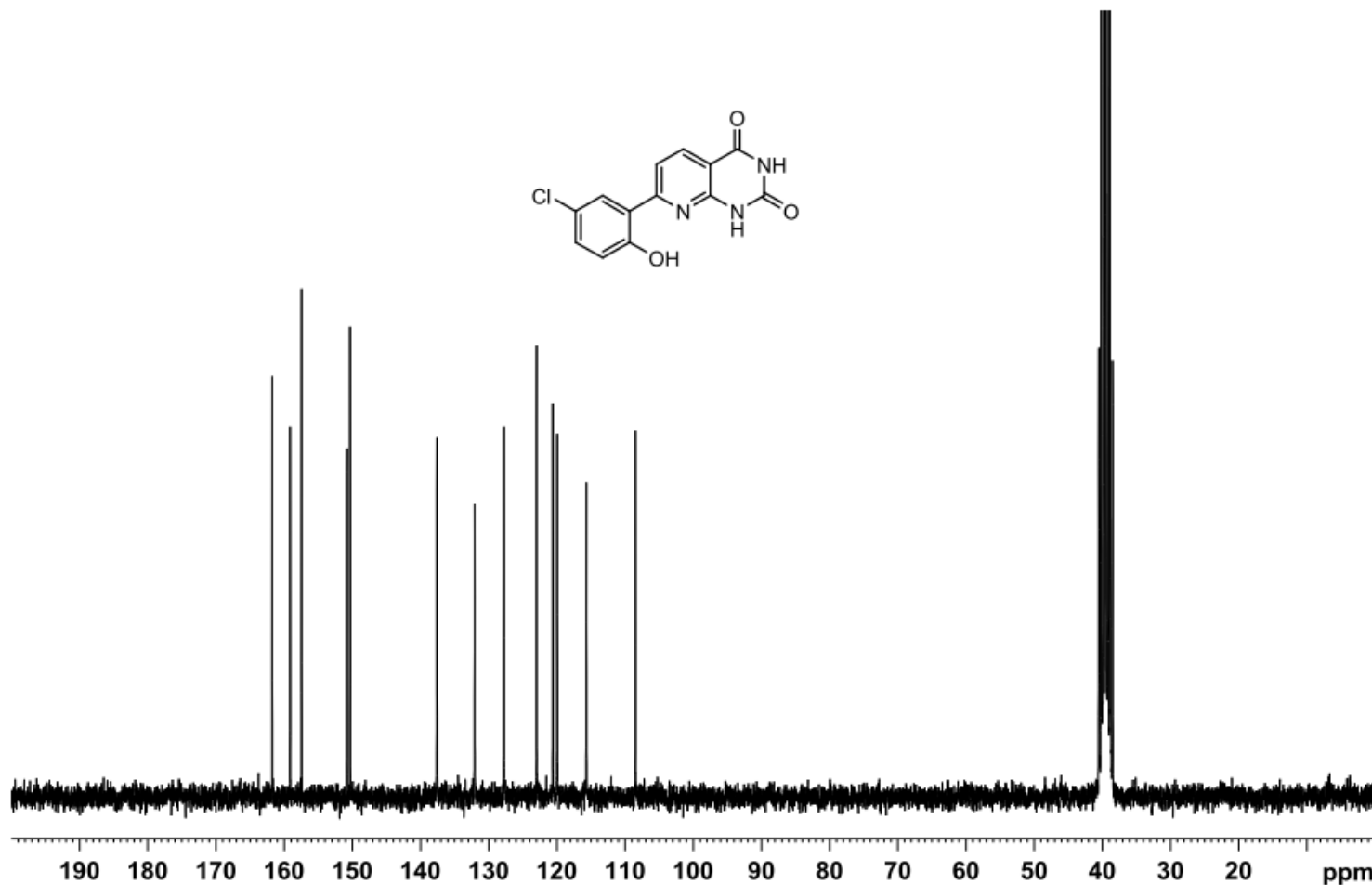
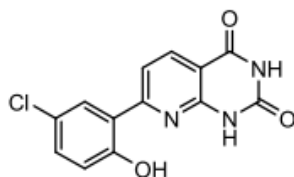
F2 - Acquisition Parameters
Date_ 20110114
Time 8.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 161
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

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

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

Gevorgyan AG146 13C DMSO

161.72
159.10
157.41
150.79
150.33
137.60
132.06
127.76
122.98
120.60
119.95
115.68
108.48



Current Data Parameters
NAME 110117.213 ag 146 C
EXPNO 10
PROCNO 1

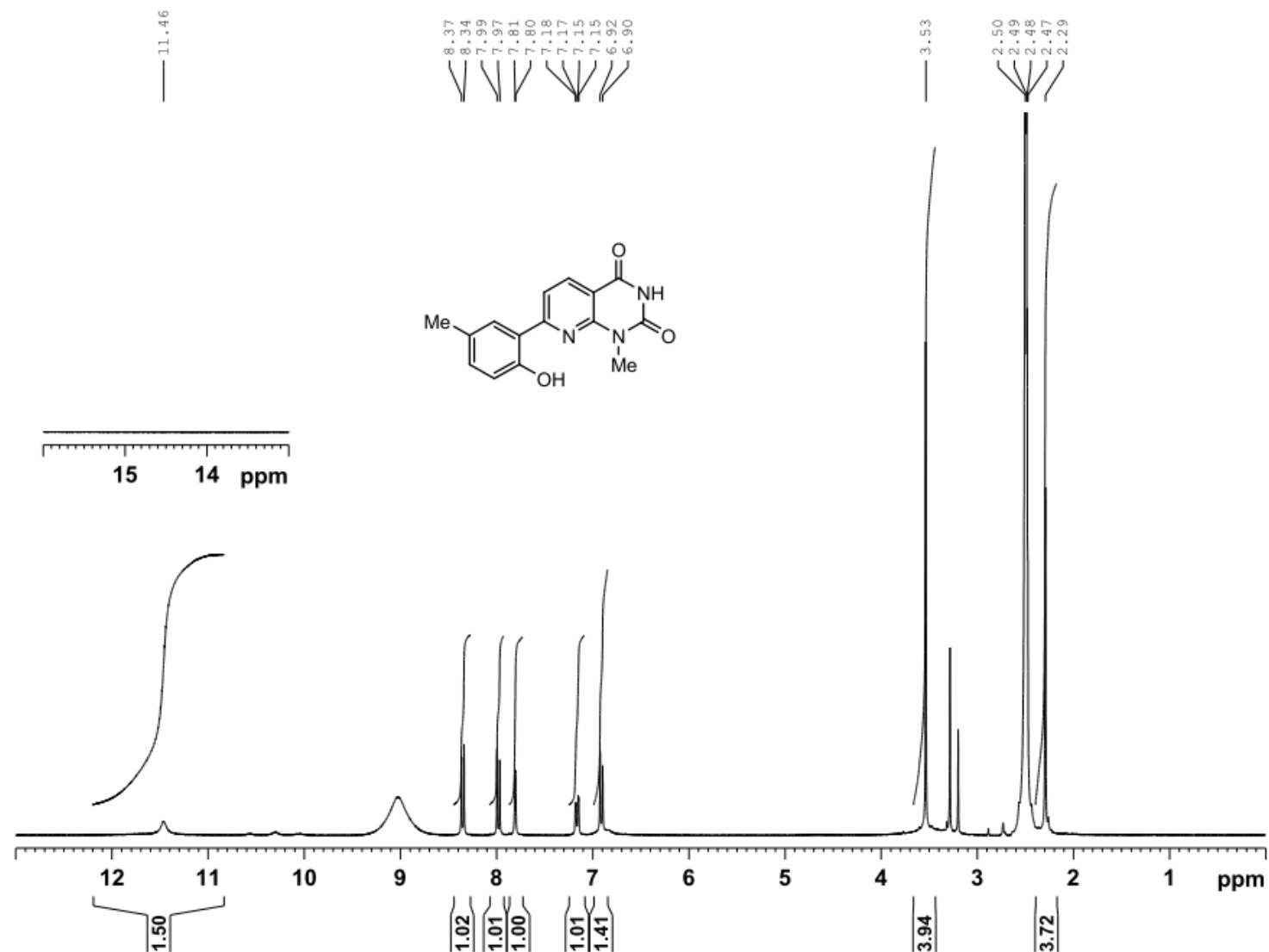
F2 - Acquisition Parameters
Date_ 20110118
Time 7.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1600
DS 4
SWH 15000.000 Hz
FIDRES 0.22882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952683 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG 161 1H DMSO 80 grd/C



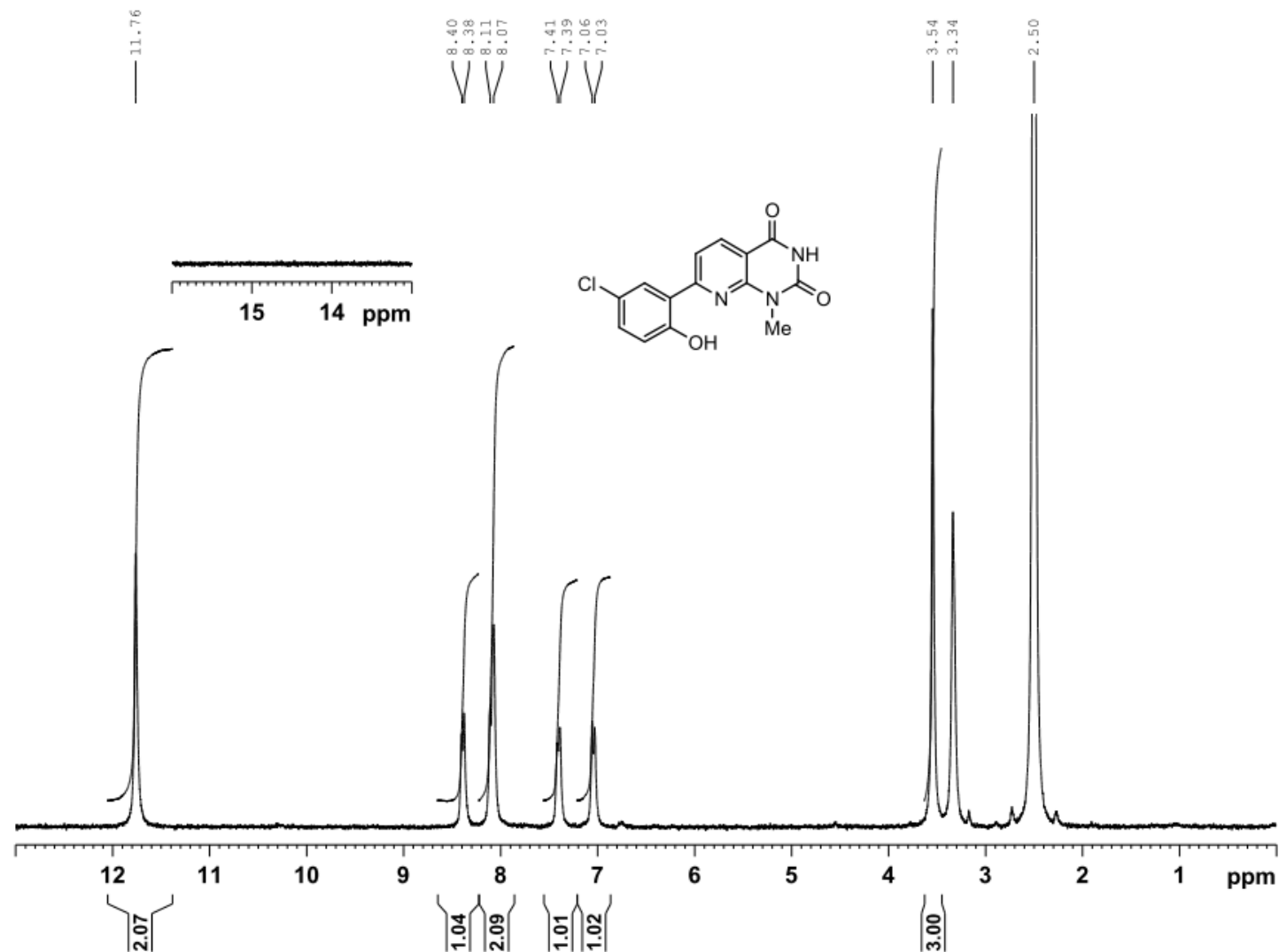
Current Data Parameters
NAME 110201.u316 ag 161
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110201
Time 14.02
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 5.2953587 sec
RG 144
DW 80.800 usec
DE 10.00 usec
TE 353.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG133 1H DMSO



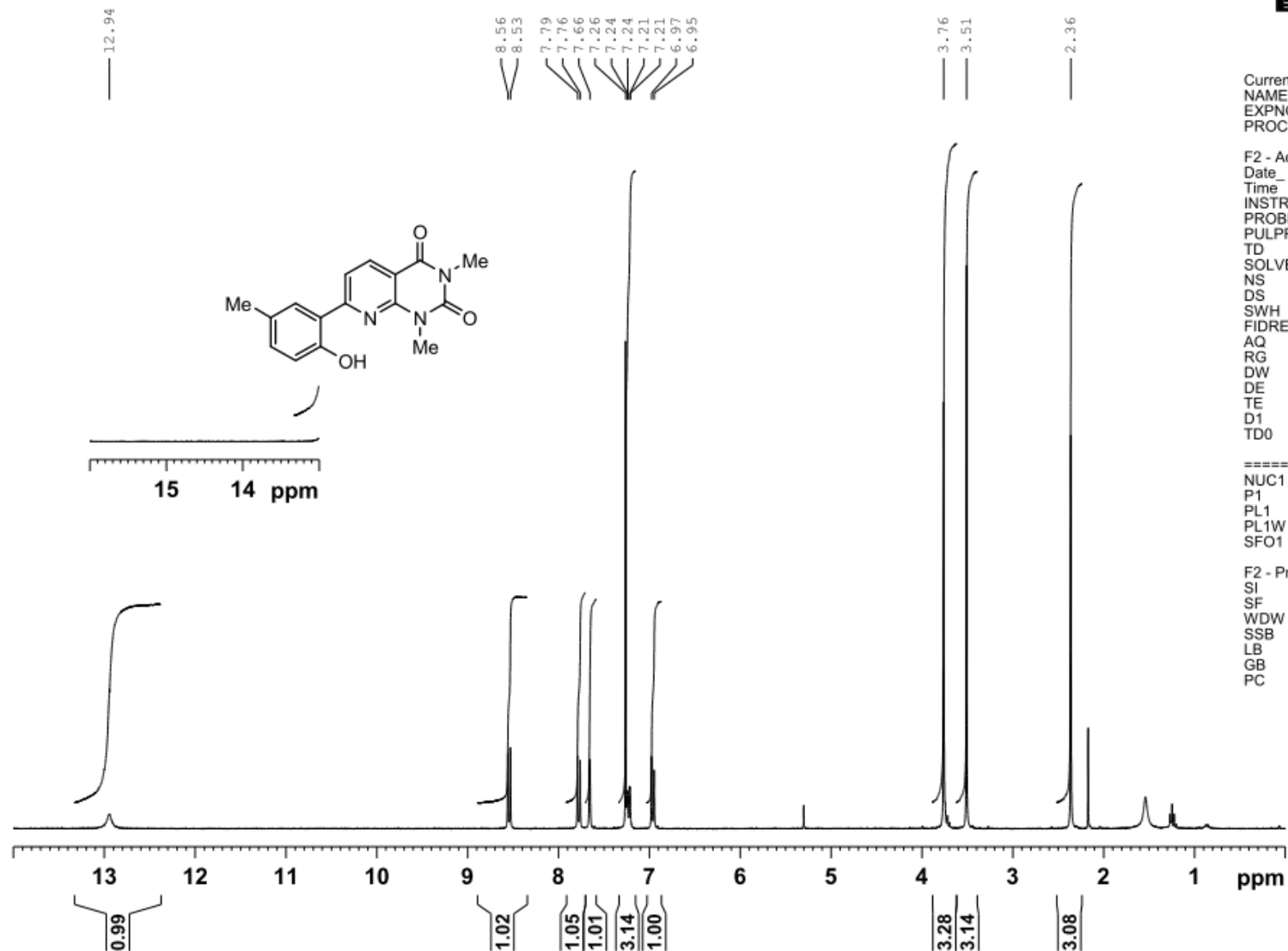
Current Data Parameters
NAME 101222.u309 ag 133
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101222
Time 10.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 181
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG139(1) 1H CDC13



Current Data Parameters
NAME 110110.u306 ag 139
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110110
Time 10.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 406
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

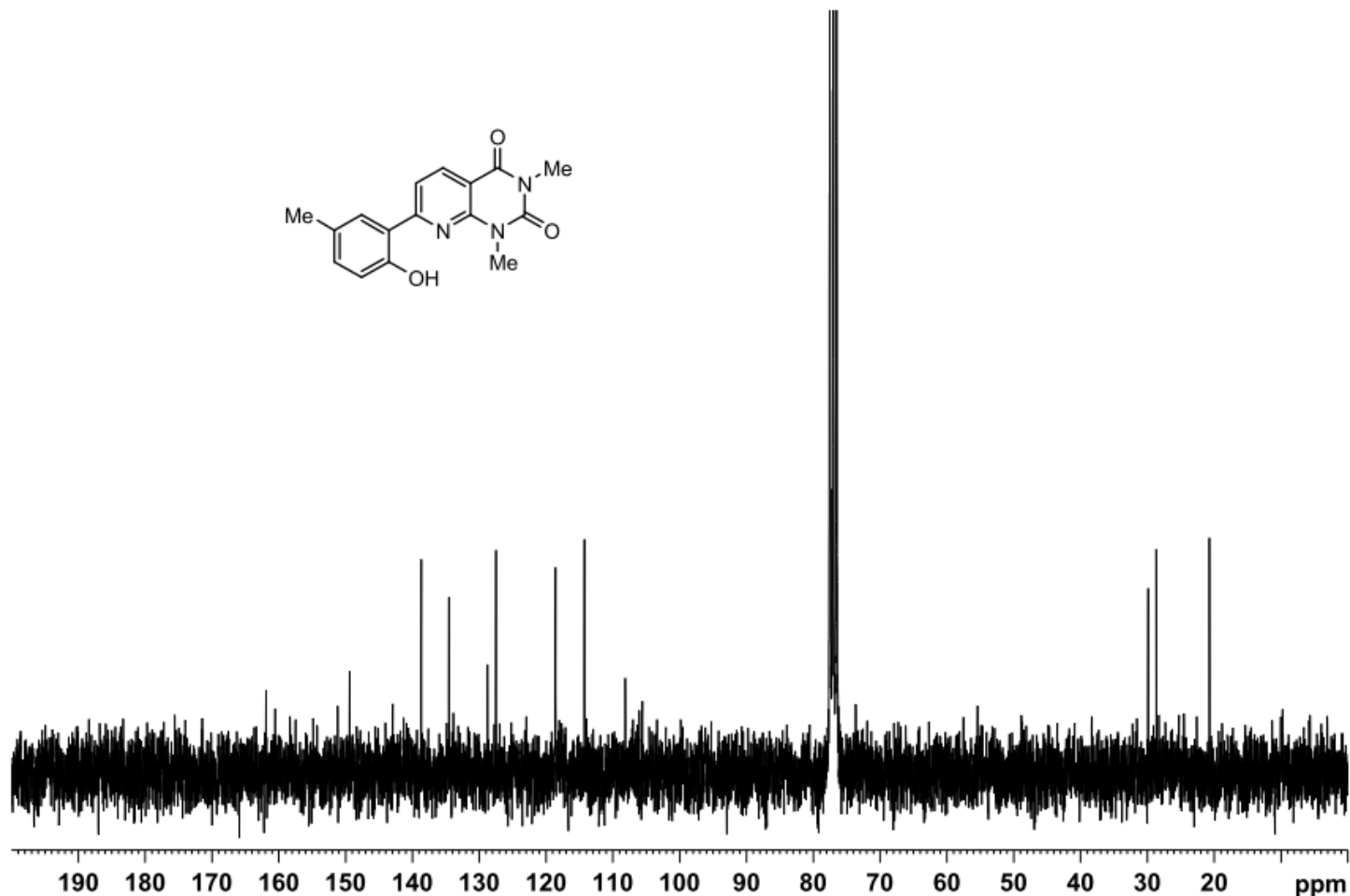
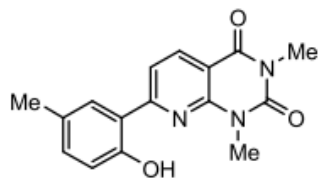
==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG139 (1) 13C CDC13

162.12
155.09
151.34
149.39
138.69
134.51
128.76
127.48
118.59
114.25
108.24
105.66

29.86
28.64
20.70



Current Data Parameters
NAME 110111.206 ag 139 C
EXPNO 10
PROCNO 1

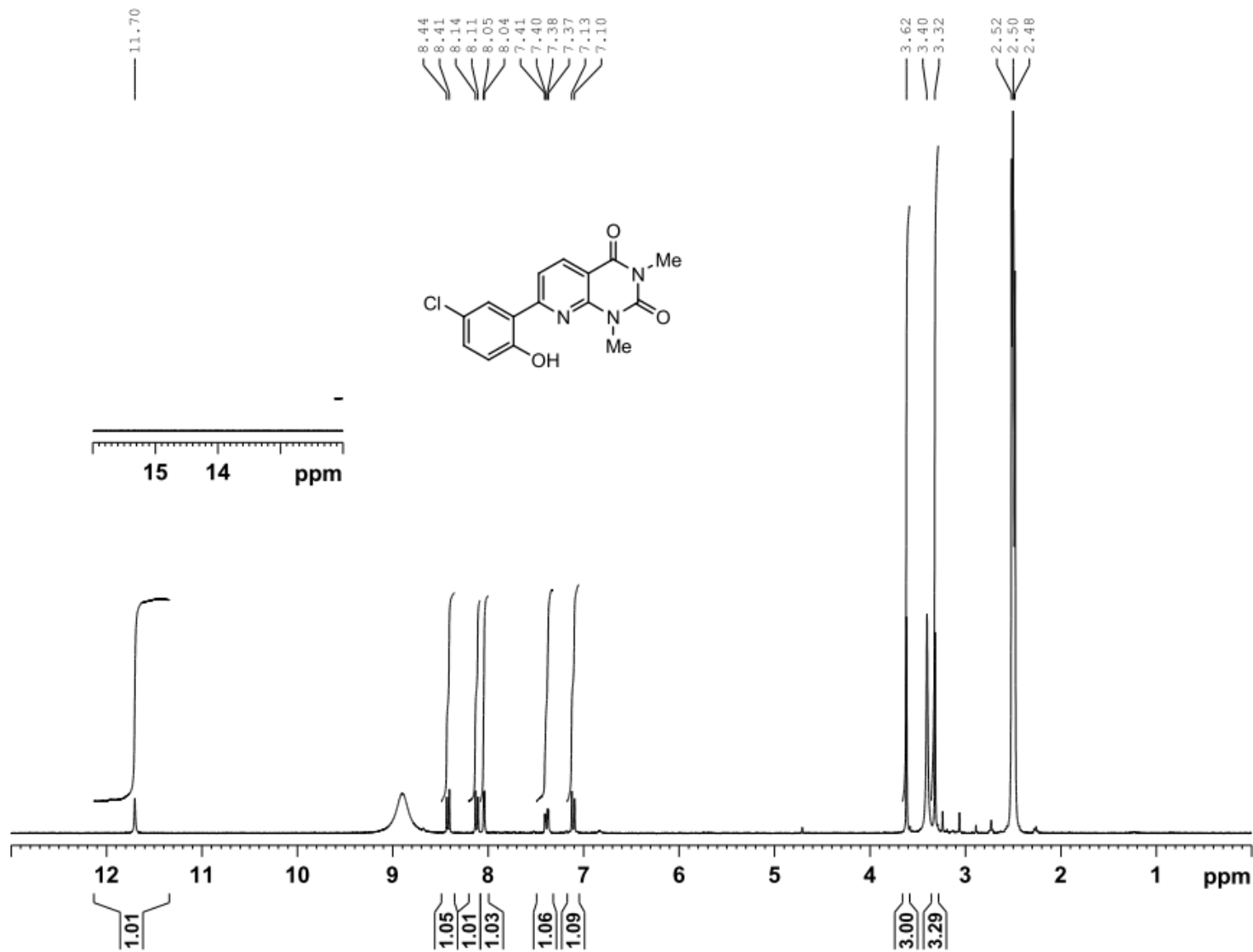
F2 - Acquisition Parameters
Date_ 20110111
Time 20.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1400
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952383 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG122 1H DMSO



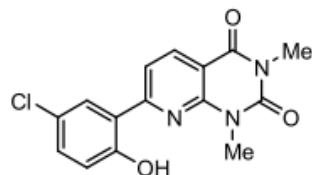
Current Data Parameters
NAME 101216.u302 ag 122
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101216
Time 7.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

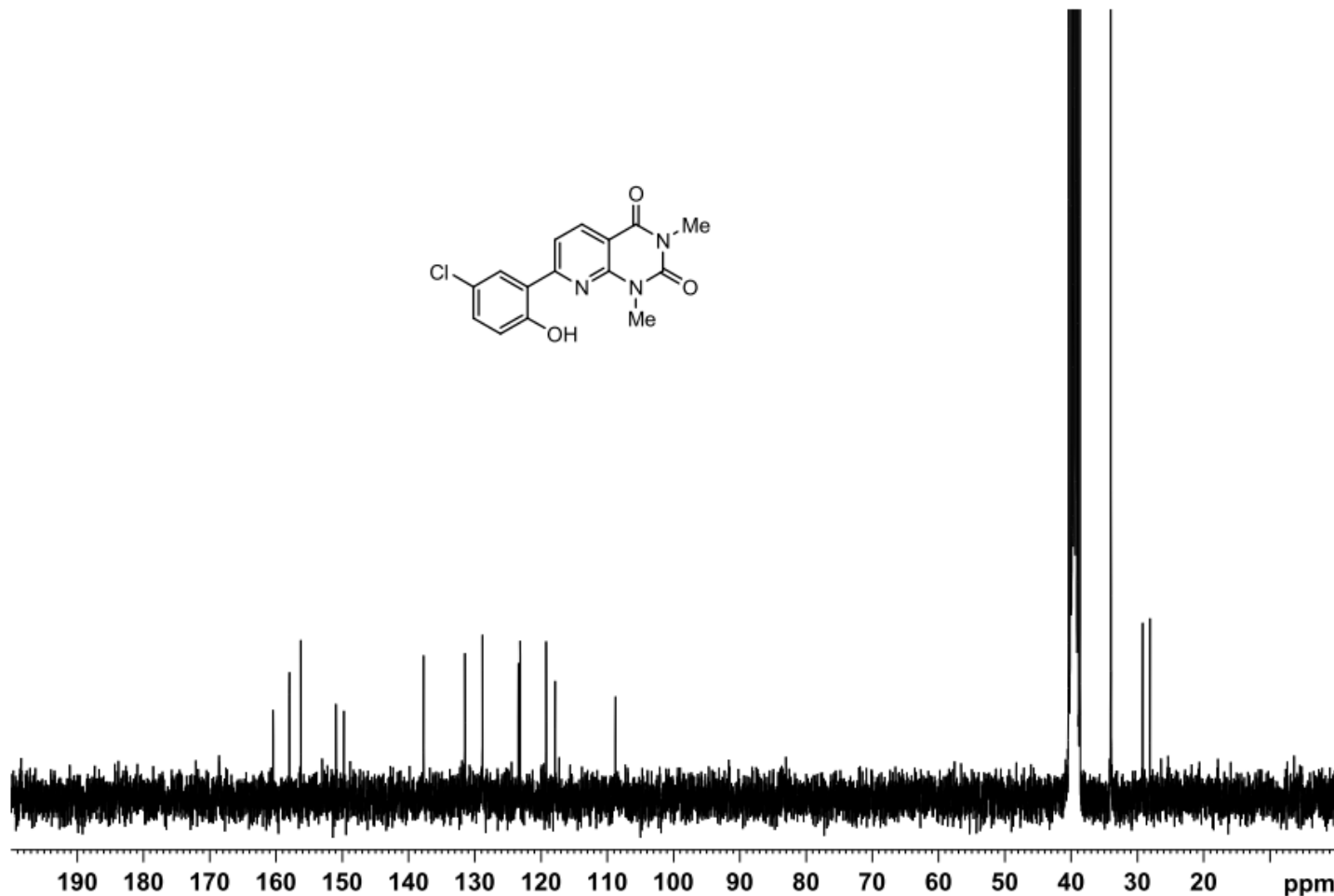
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300045 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG122 13C DMSO



29.19
28.09



Current Data Parameters
NAME 110104.u324 ag 122 C
EXPNO 10
PROCNO 1

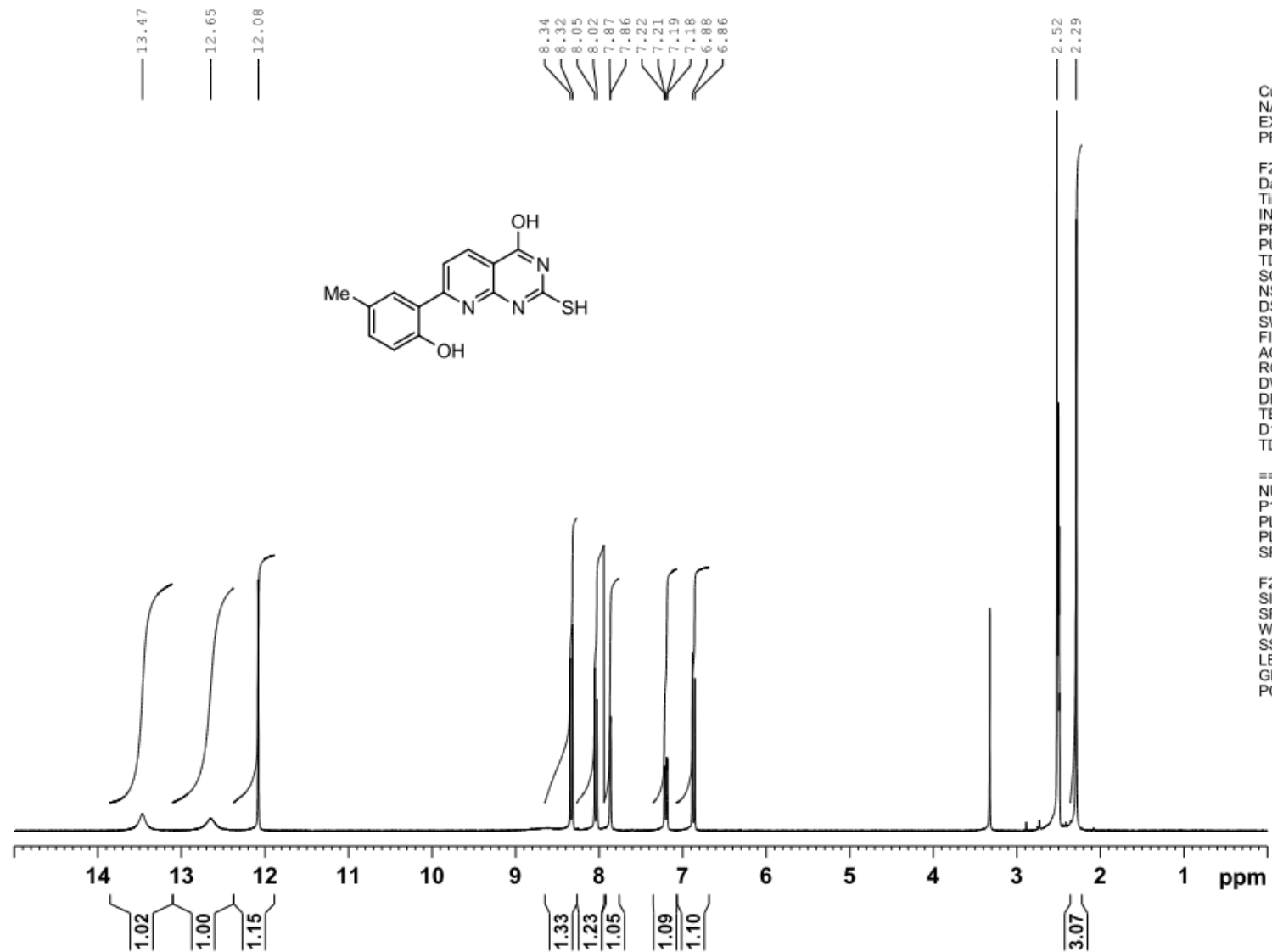
F2 - Acquisition Parameters
Date_ 20110105
Time 3.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1400
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

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

Gevorgyan AG144 1H DMSO



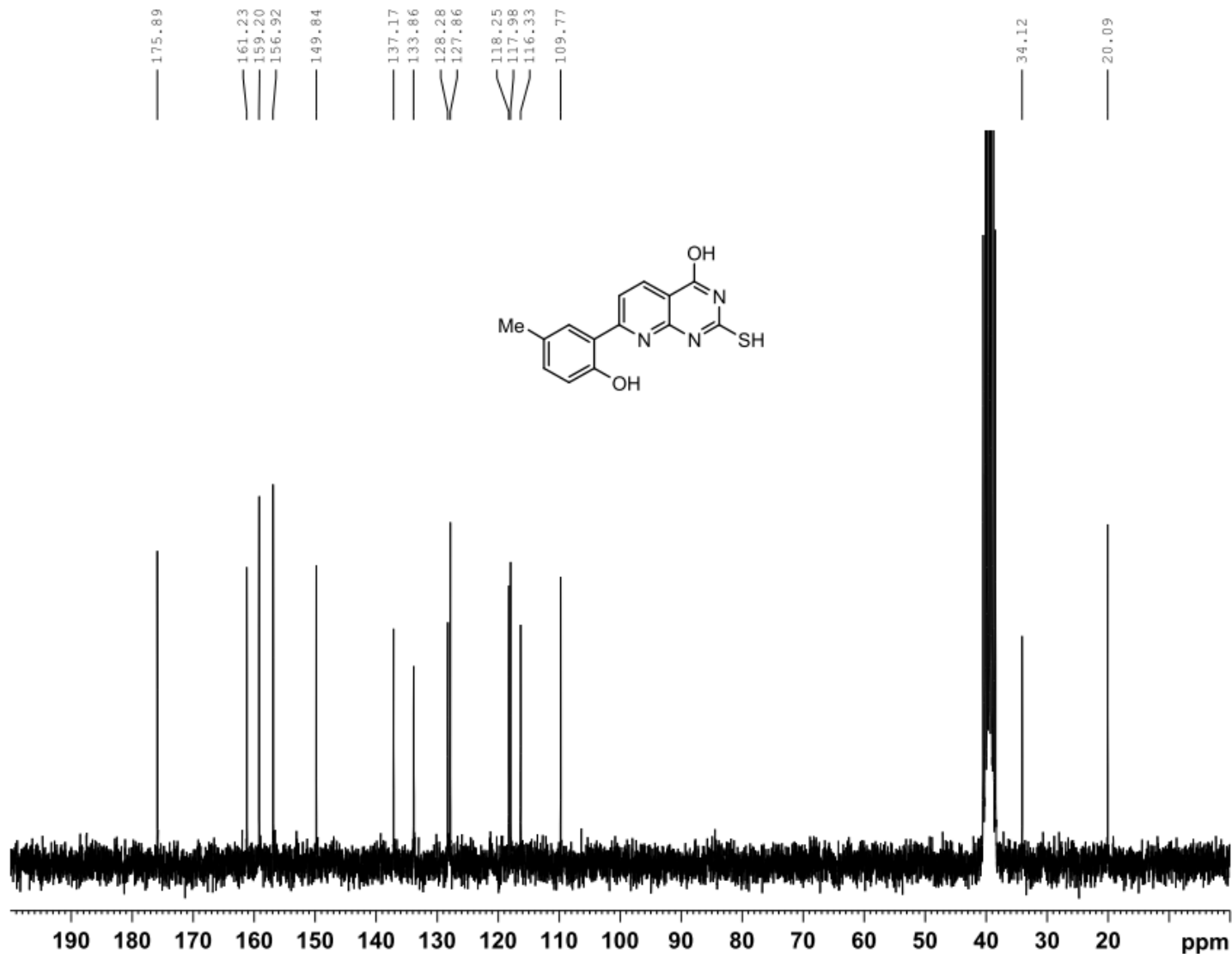
Current Data Parameters
NAME 110111.u304 ag 144
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110111
Time 8.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 144
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 300.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG144 13C DMSO



Current Data Parameters
NAME 110113.208 ag 144 C
EXPNO 10
PROCNO 1

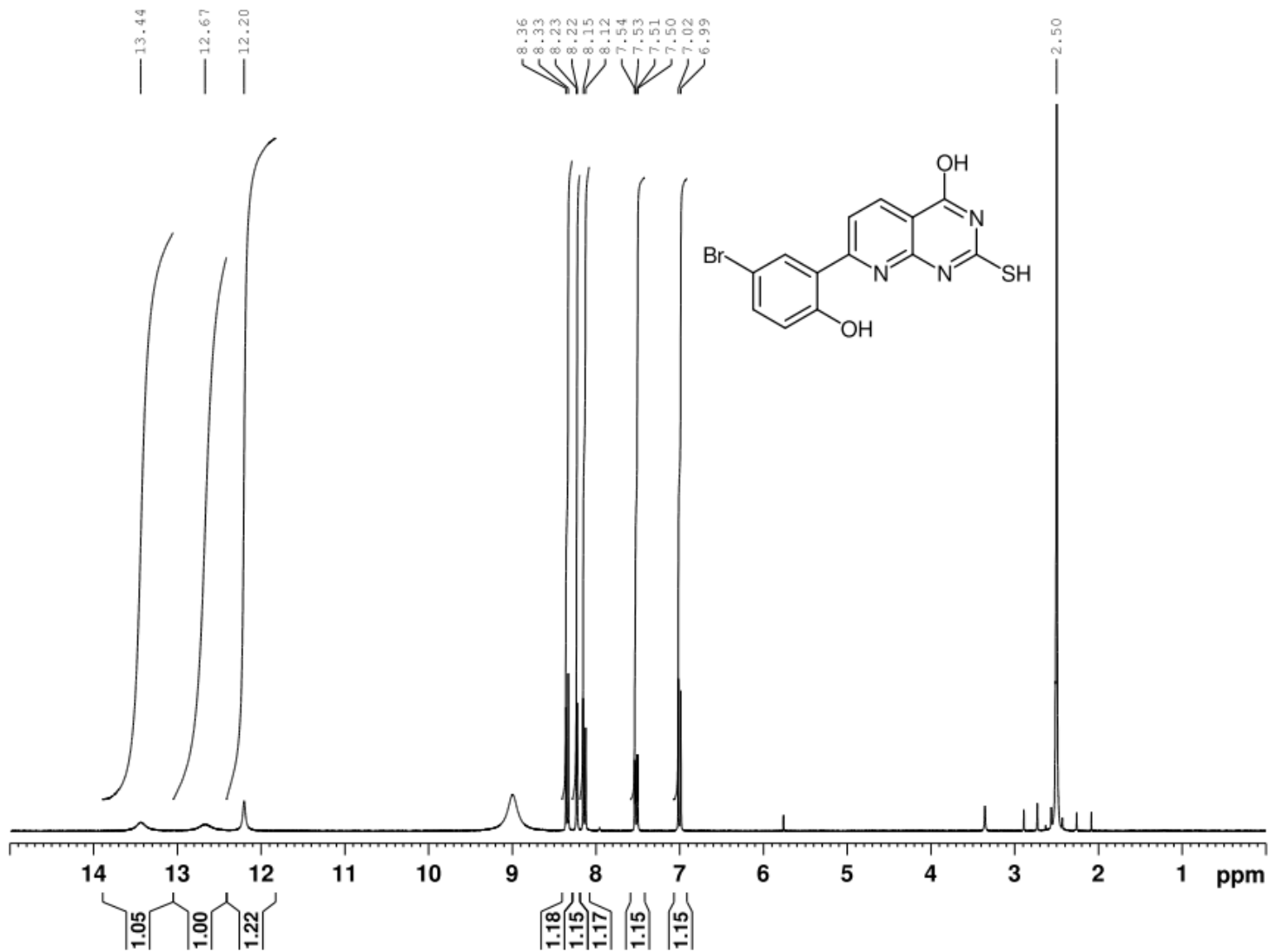
F2 - Acquisition Parameters
Date_ 20110113
Time 11.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1157
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8955672 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

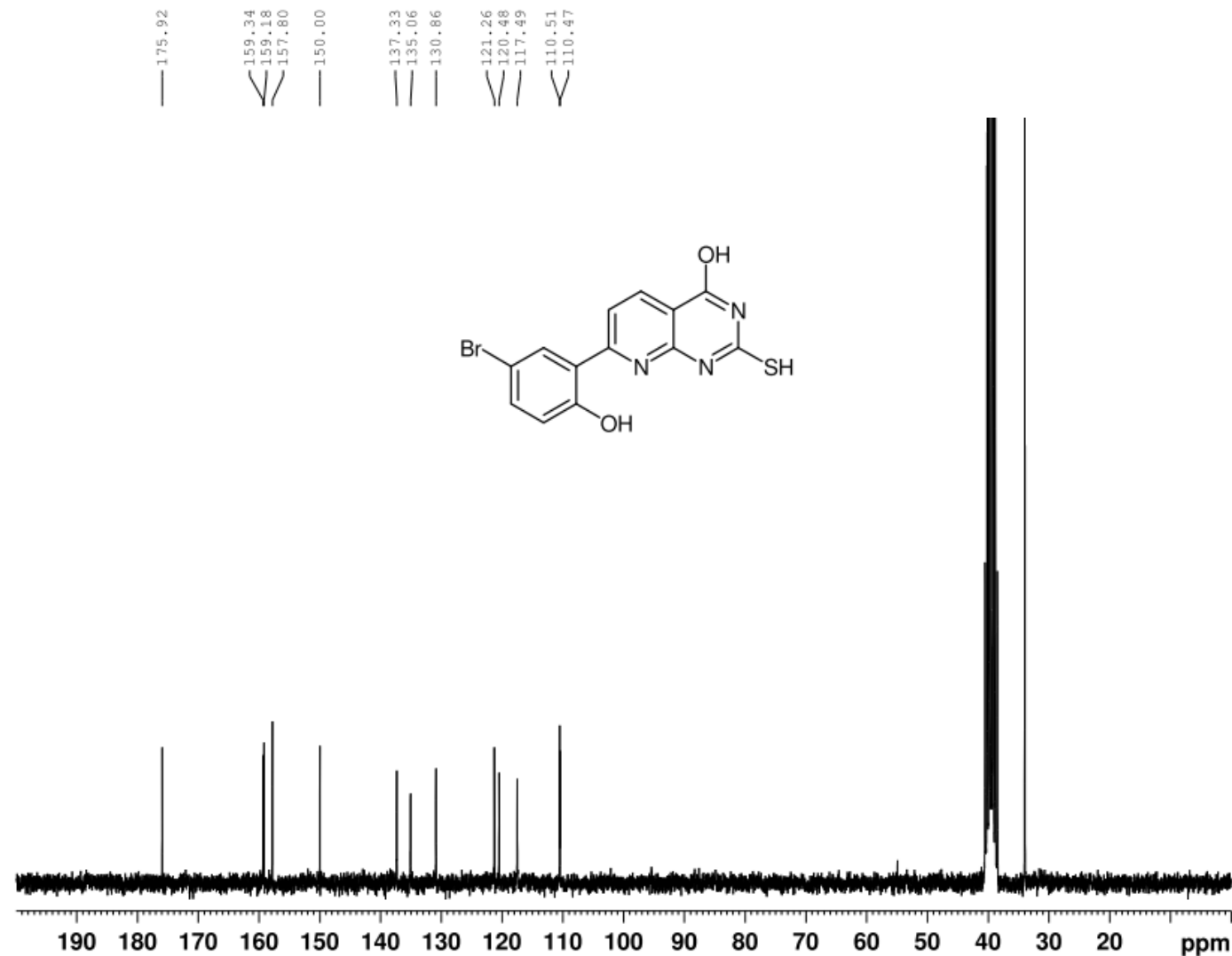
Gevorgyan AG178 (1) 1H DMSO



NAME 110218.u311 ag 178
EXPNO 10
PROCNO 1
Date_ 20110218
Time 8.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300017 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG178(1) 13C DMSO

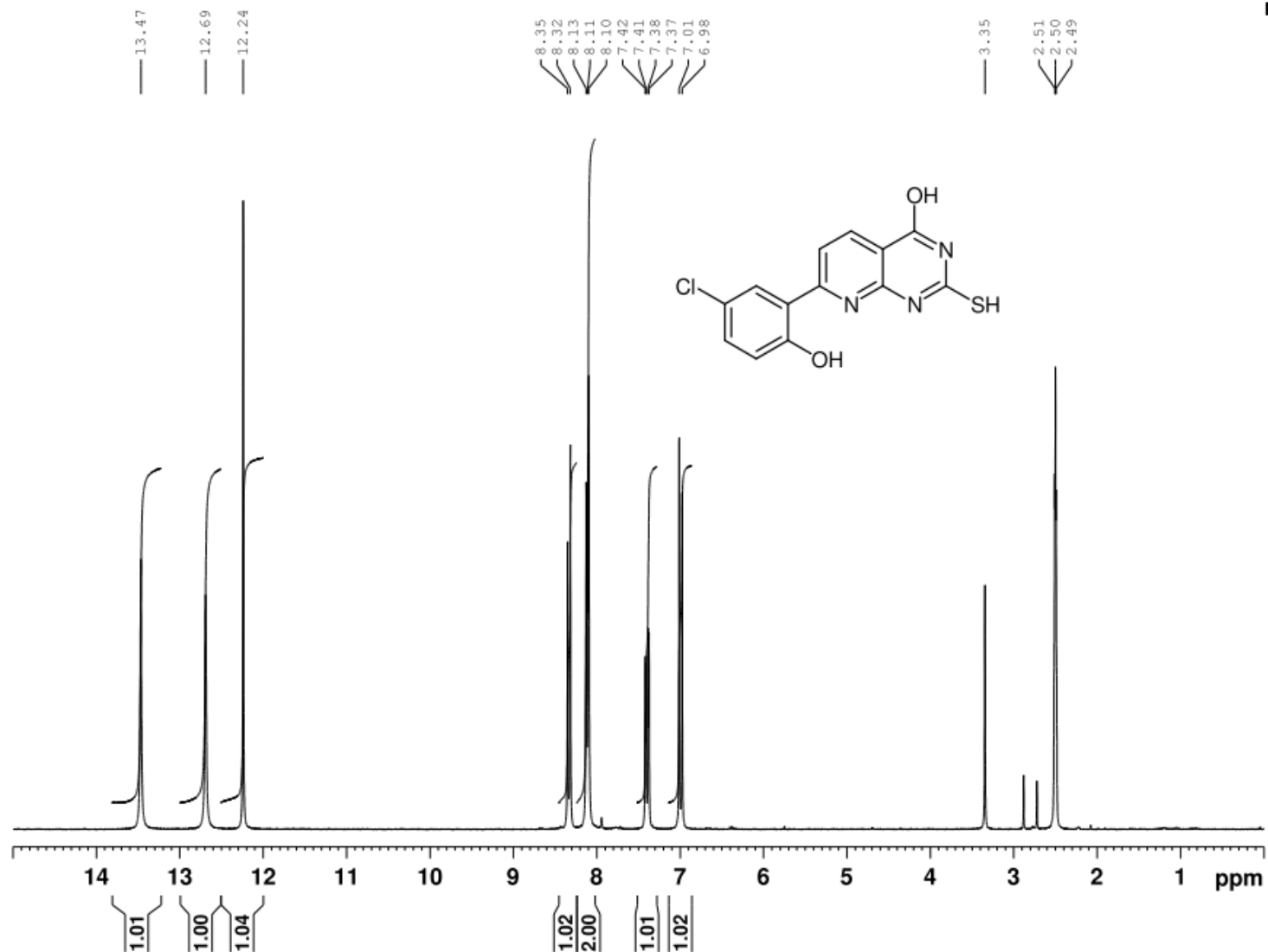


NAME 110221.206 ag 178C
EXPNO 10
PROCNO 1
Date_ 20110221
Time 17.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952692 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

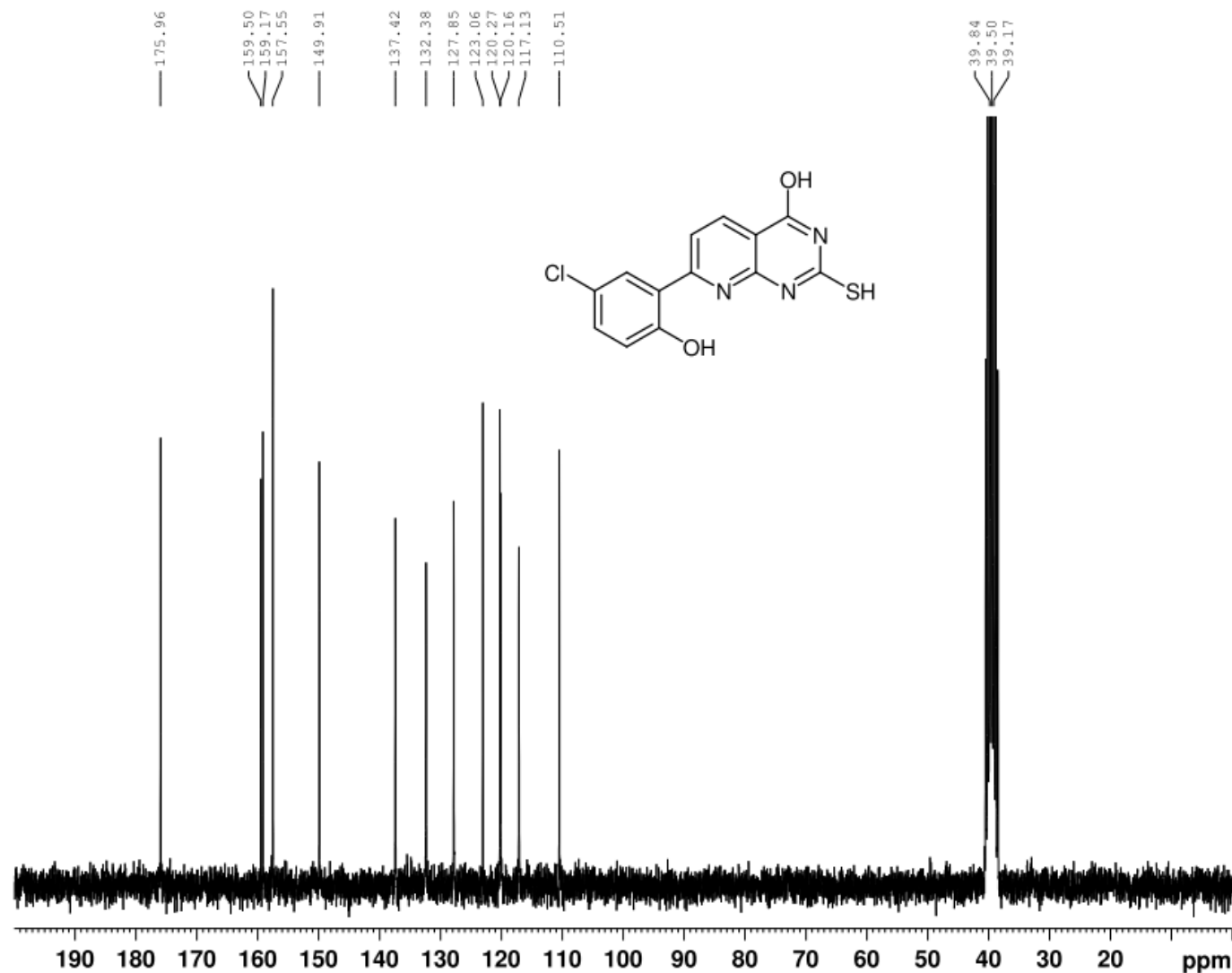
Gevorgyan AG127 1H DMSO



NAME 101220.212 ag 127
EXPNO 10
PROCNO 1
Date_ 20101220
Time 23.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 575
DW 96.800 usec
DE 10.00 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.50 dB
SFO1 250.1315447 MHz
SI 32768
SF 250.1299985 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG127 13C DMSO

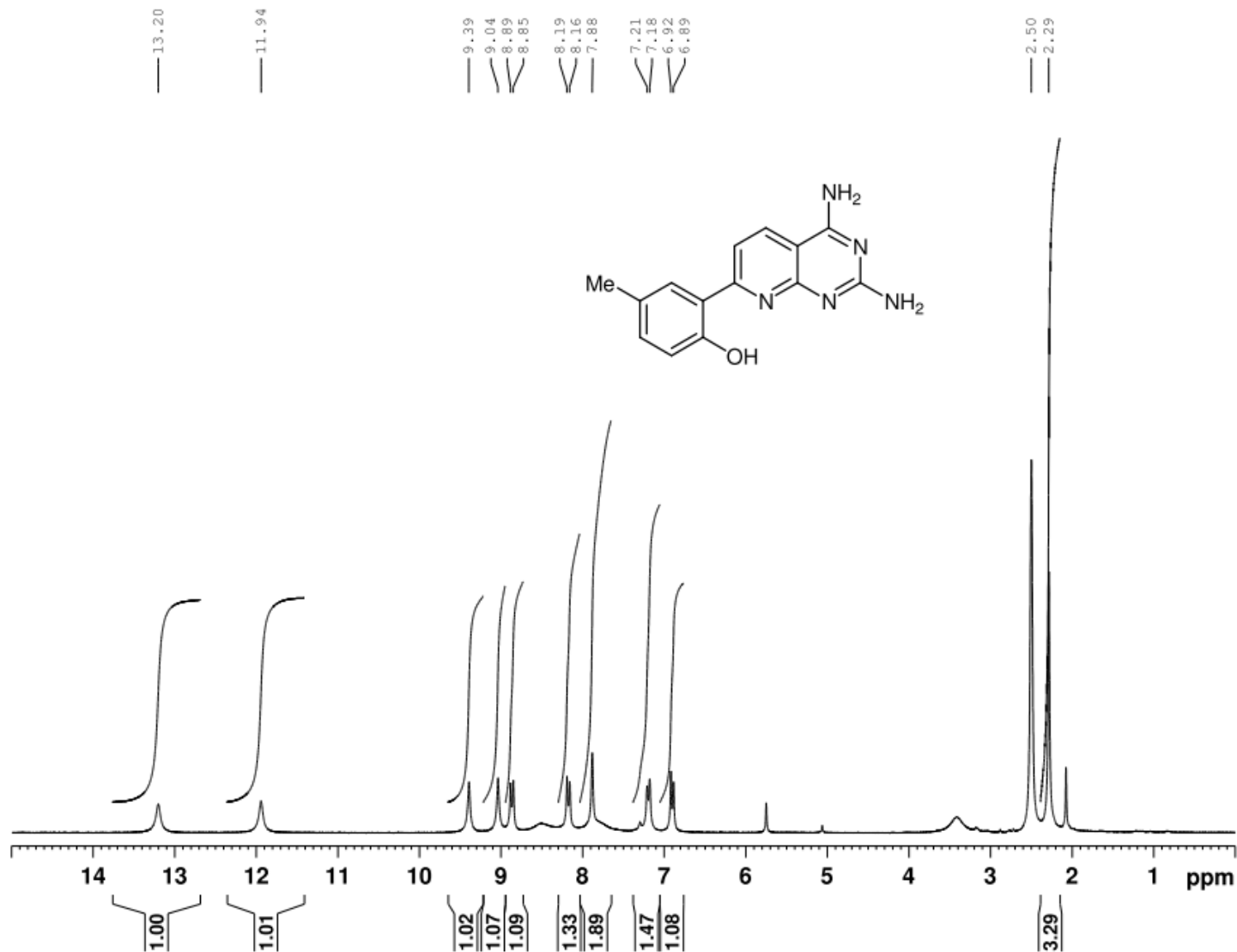


NAME 101220.212 ag 127
EXPNO 11
PROCNO 1
Date_ 20101221
Time 1.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 295.9 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952674 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

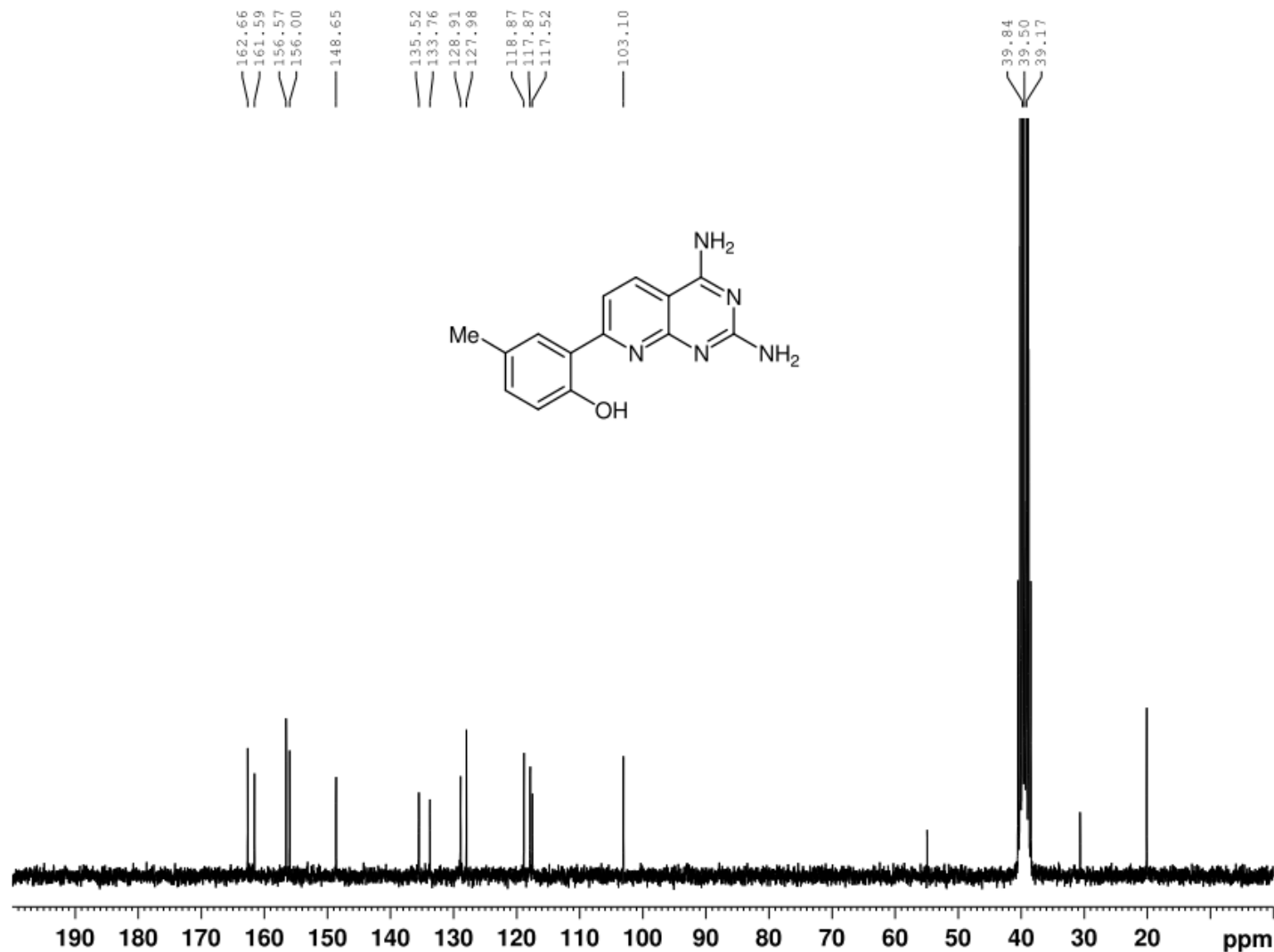
Gevorgyan AG165 (4) 1H DMSO



NAME 110216.221 ag 165
EXPNO 10
PROCNO 1
Date_ 20110216
Time 14.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 406
DW 96.800 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.50 dB
SFO1 250.1315447 MHz
SI 32768
SF 250.1299978 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG165 (4) 13C DMSO

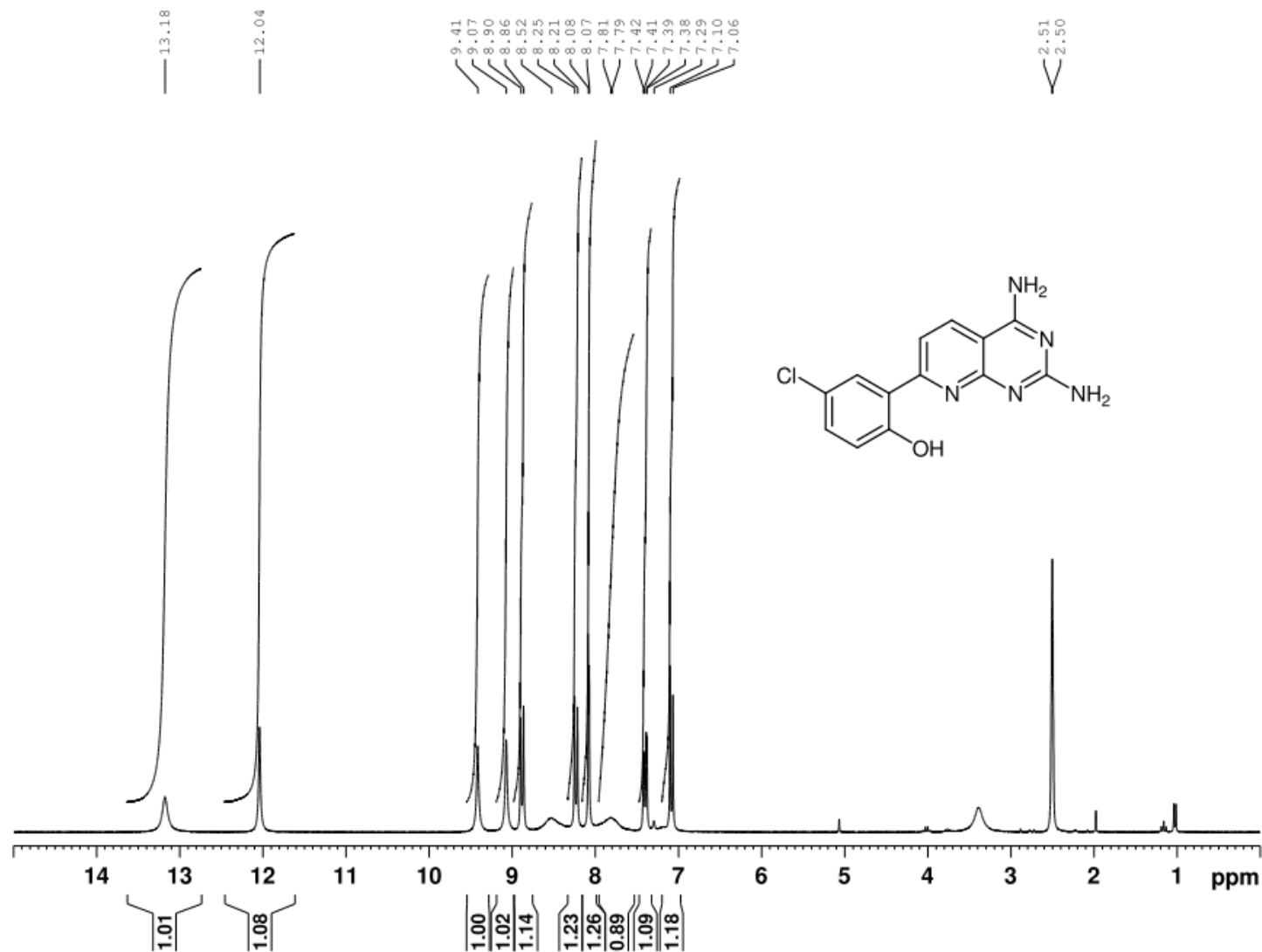


NAME 110217.210 ag 165 C
EXPNO 10
PROCNO 1
Date_ 20110218
Time 6.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952687 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG147(3) 1H DMSO

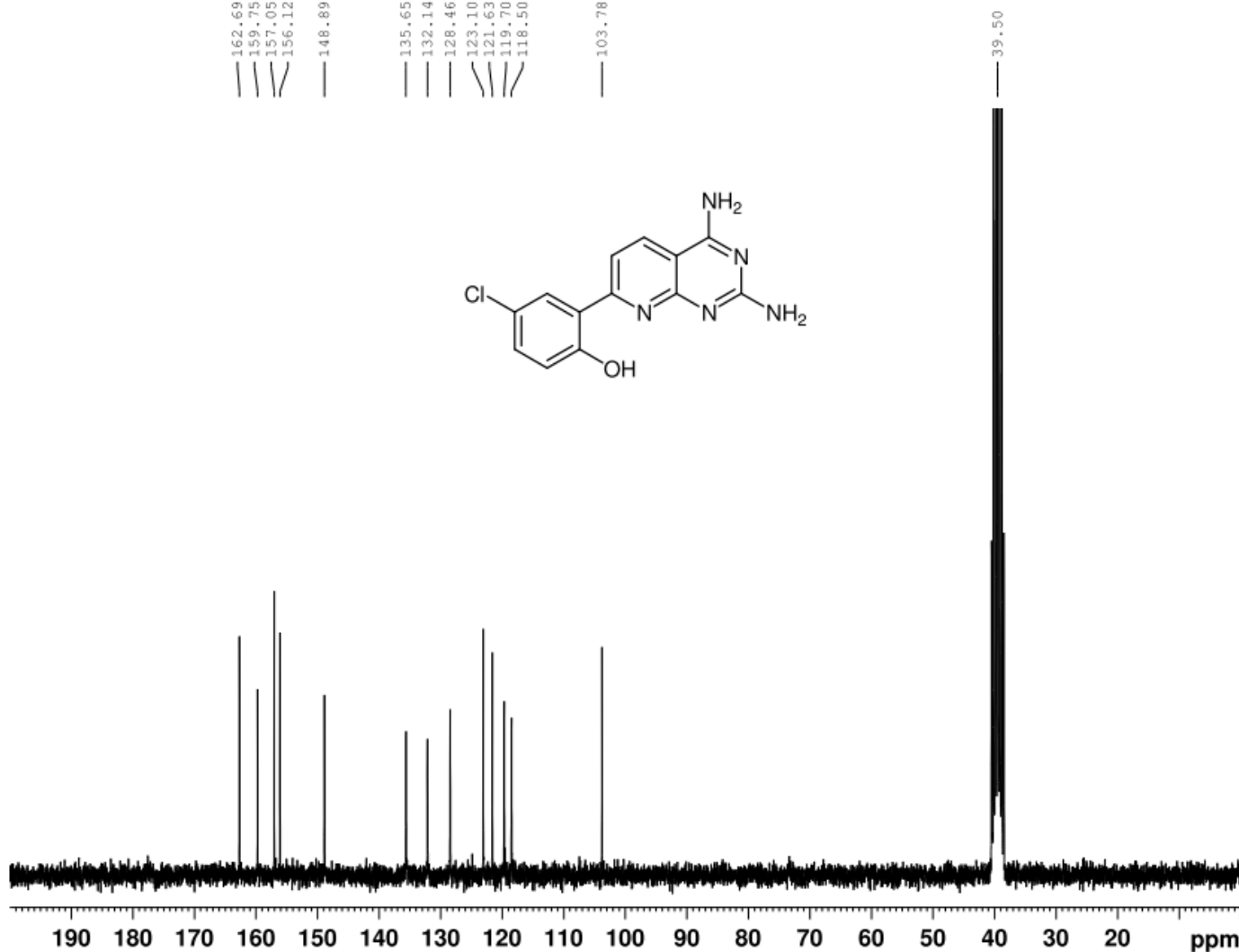
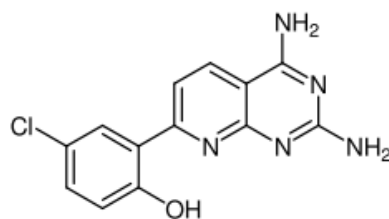


NAME 110119.207 ag 147
EXPNO 10
PROCNO 1
Date_ 20110119
Time 9.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 512
DW 96.800 usec
DE 10.00 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -2.50 dB
SFO1 250.1315447 MHz
SI 32768
SF 250.1299984 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG147(3) 13C DMSO

162.69
159.75
157.05
156.12
148.89
135.65
132.14
128.46
123.10
121.63
119.70
116.50
103.78



NAME 110121.223 ag 147 C
EXPNO 10
PROCNO 1
Date_ 20110123
Time 2.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

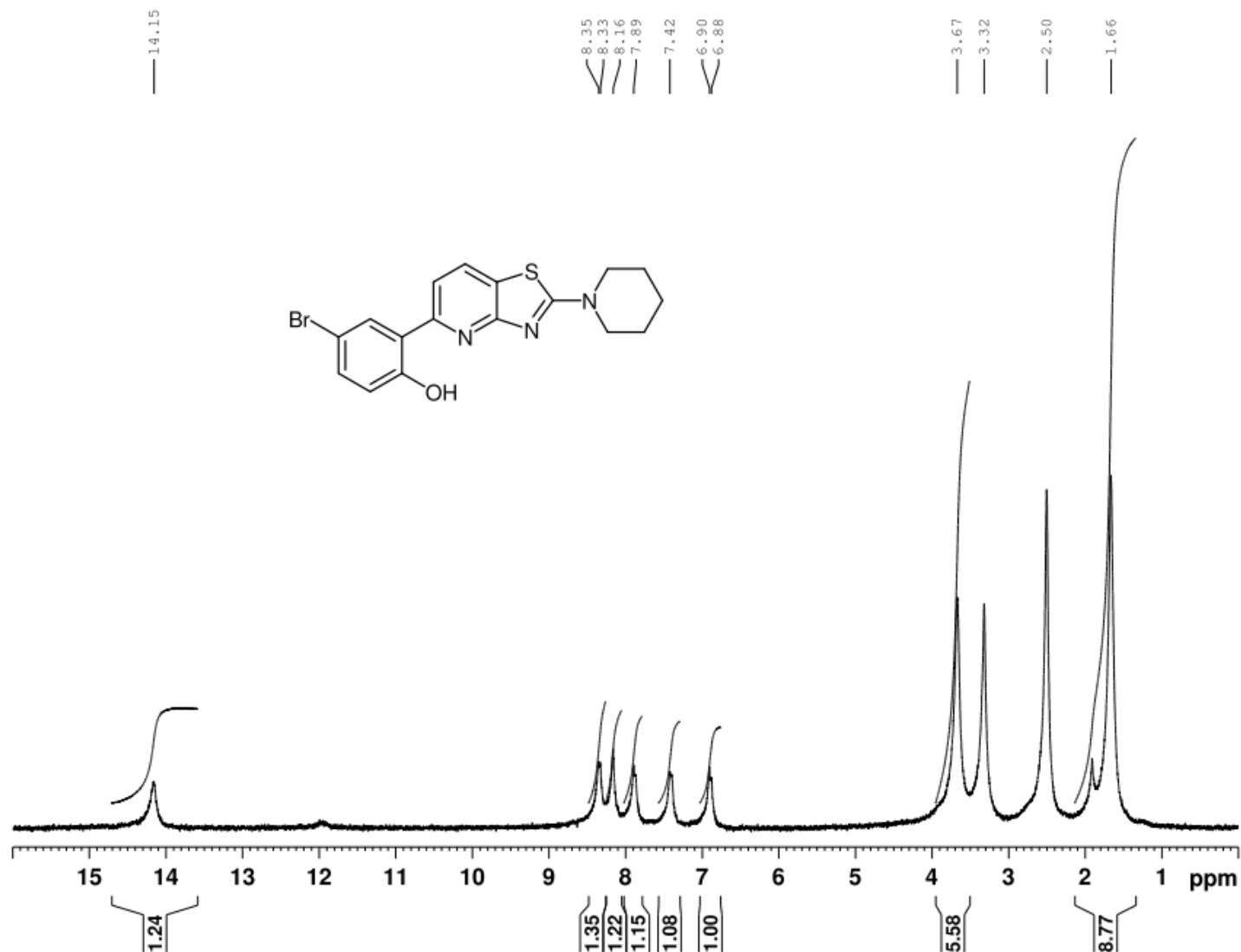
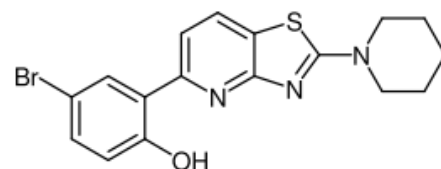
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952687 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG201 1H DMSO



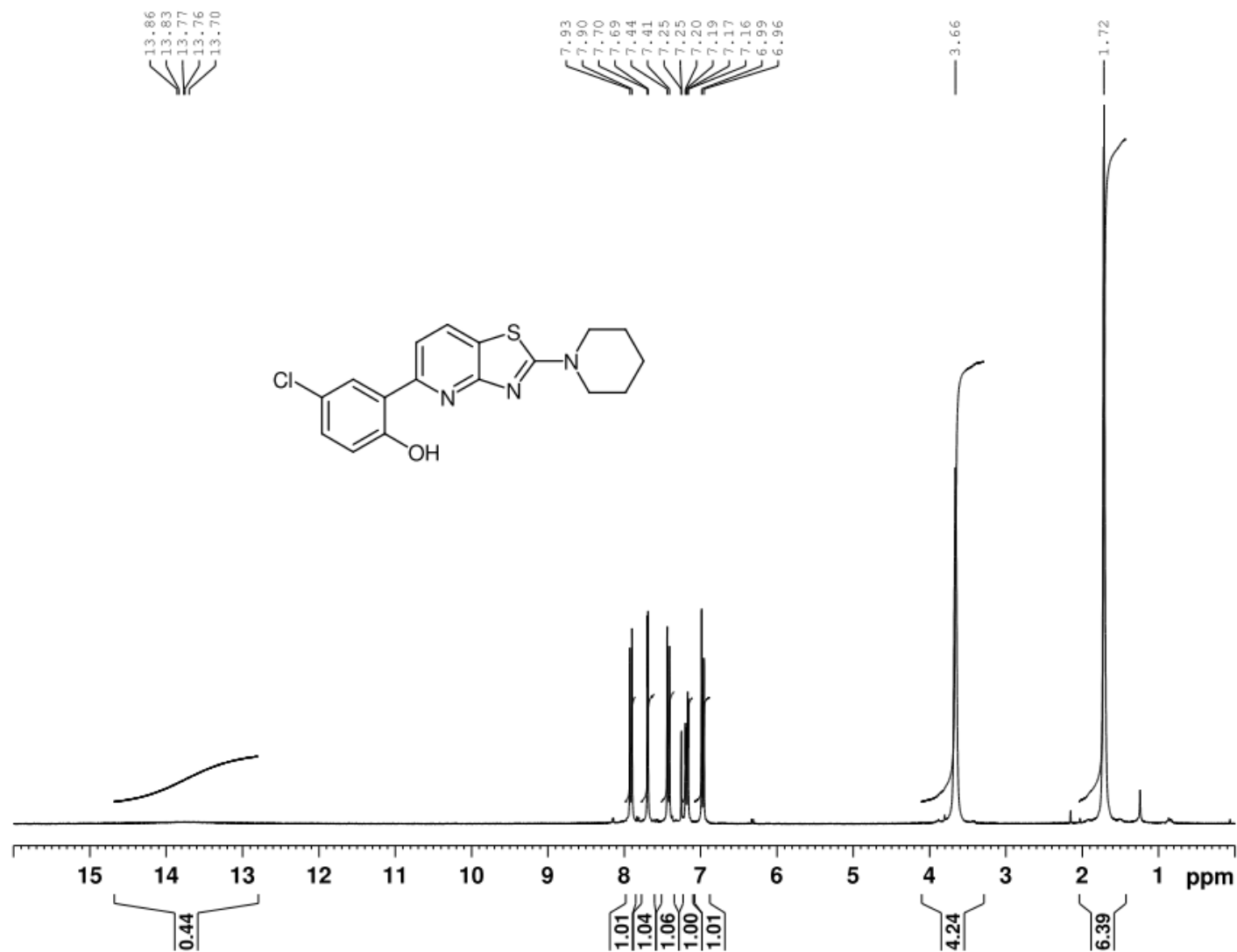
NAME 110311.u301 ag 201
EXPNO 10
PROCNO 1
Date_ 20110311
Time 8.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 181
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

100



===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300245 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG148(4) 1H CDC13

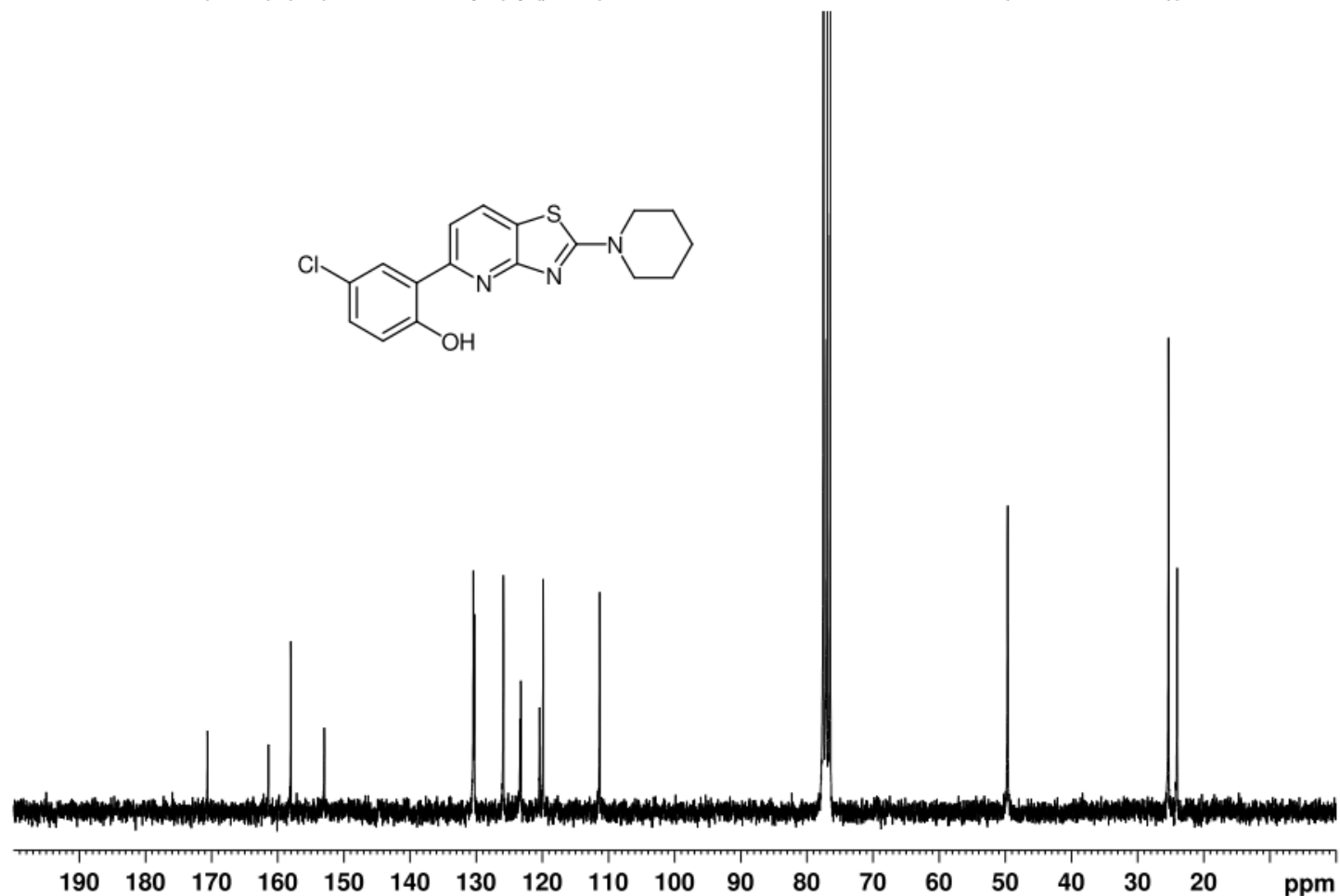
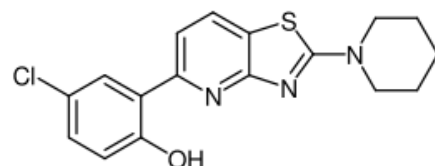


NAME 110121.u312 ag 148
EXPNO 10
PROCNO 1
Date_ 20110121
Time 9.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 114
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG148 (4) 13C CDC13

170.65
161.44
158.05
153.01
130.45
130.29
125.93
123.42
123.26
120.43
119.90
111.34

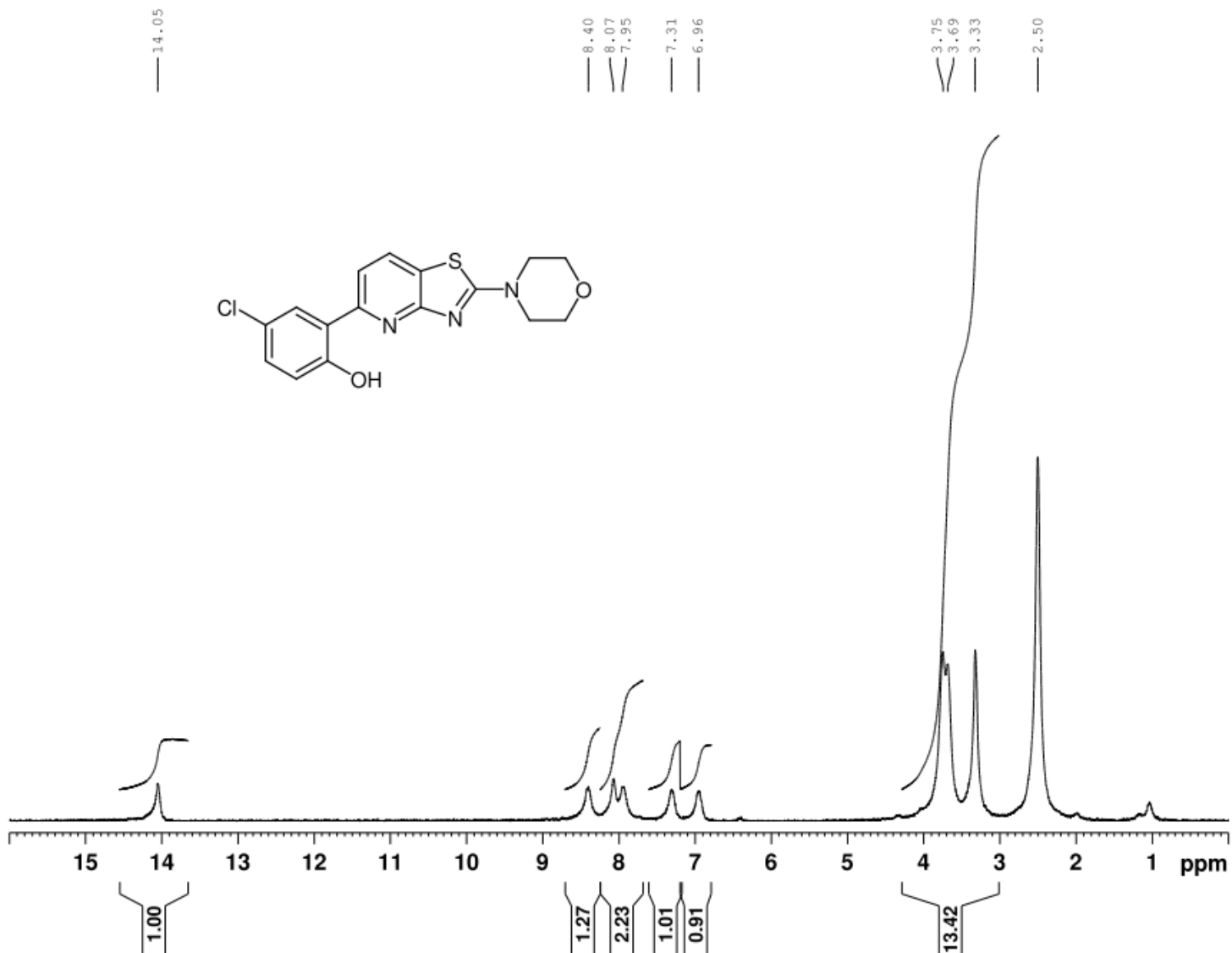


NAME 110127.209 ag 148 C
EXPNO 10
PROCNO 1
Date_ 20110128
Time 1.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1600
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952406 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

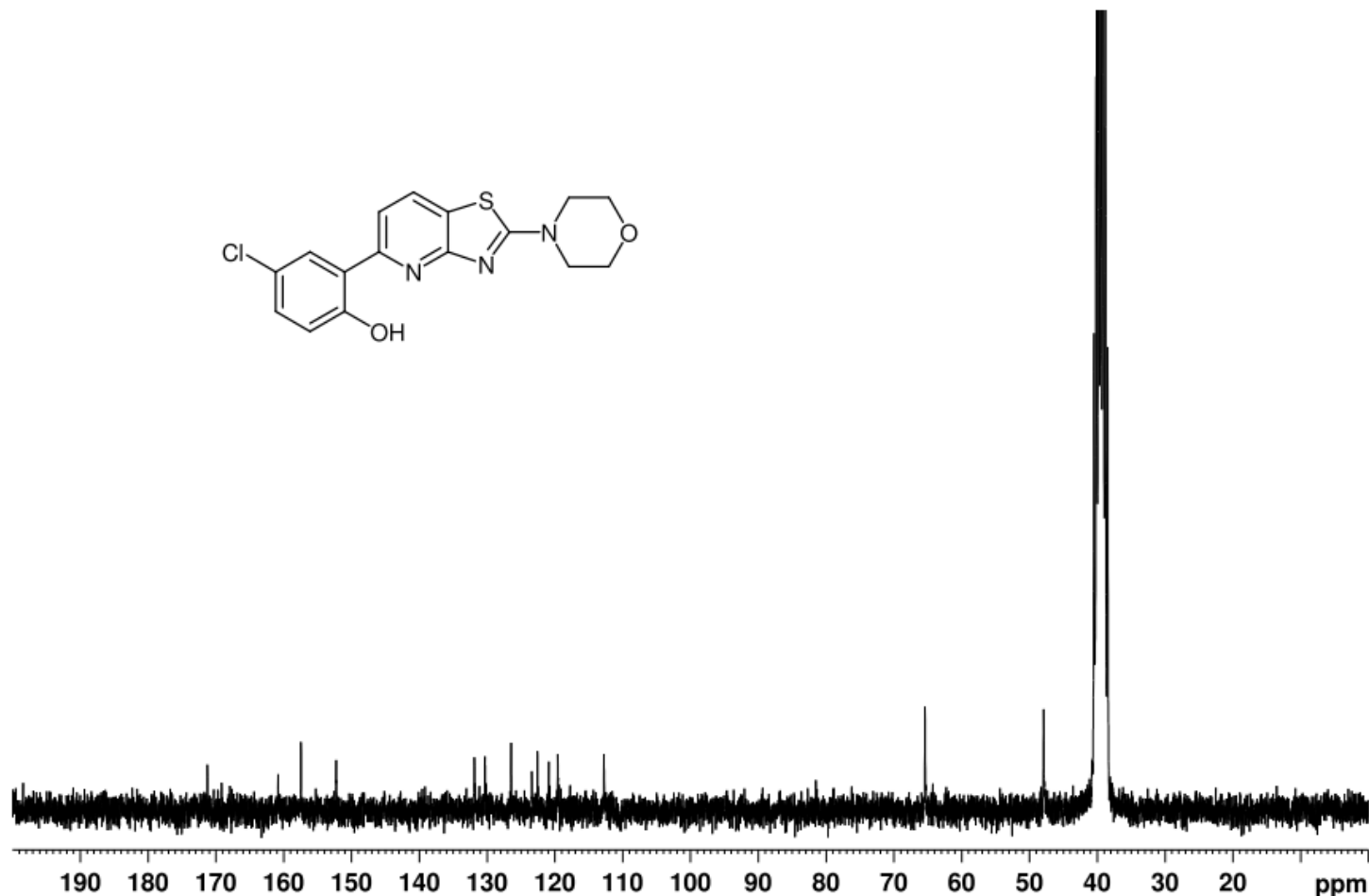
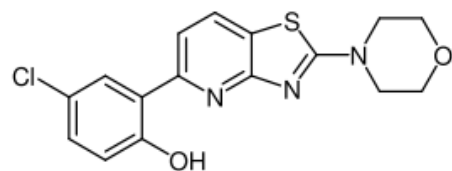
Gevorgyan AG151 1H DMSO



NAME 110118.207 ag 151
EXPNO 10
PROCNO 1
Date_ 20110118
Time 9.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 645
DW 96.800 usec
DE 10.00 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.50 dB
SFO1 250.1315447 MHz
SI 32768
SF 250.1299955 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG151 13C DMSO

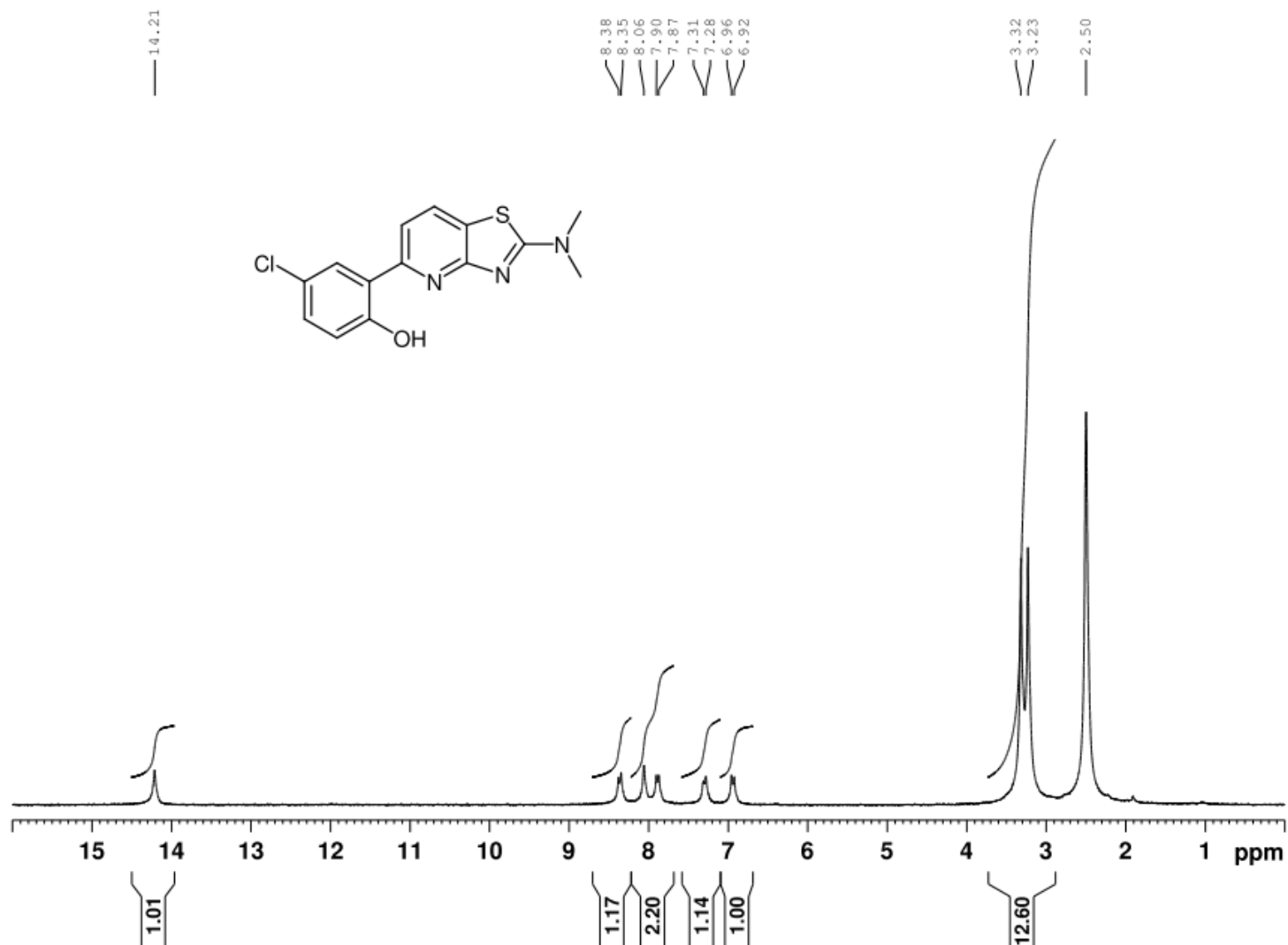


NAME 110121.224 ag 151 C
EXPNO 10
PROCNO 1
Date_ 20110123
Time 6.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952693 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG156 1H DMSO

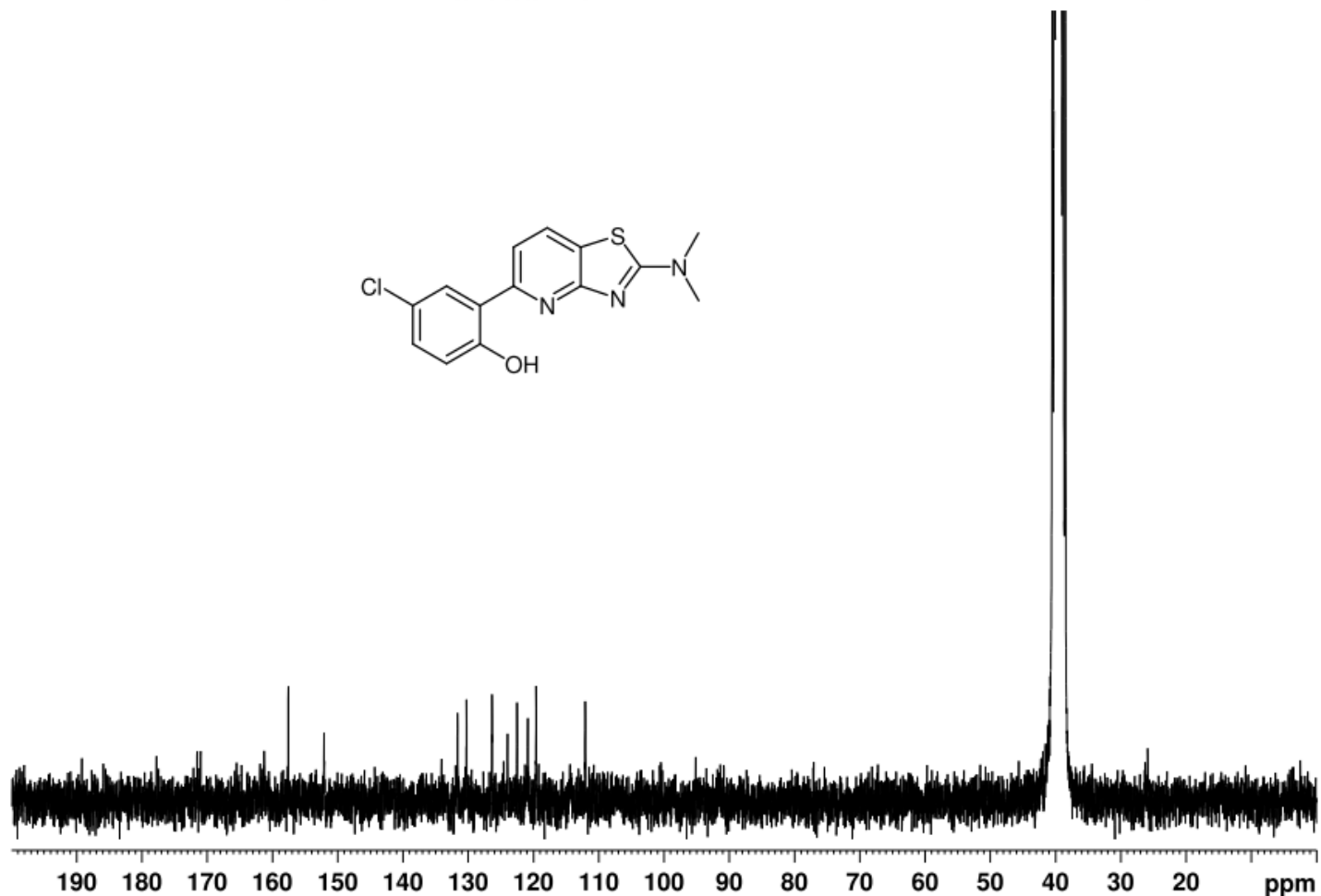
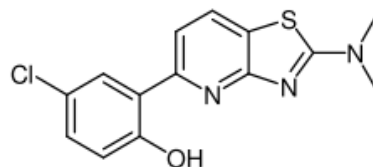


NAME 110119.209 ag 156
EXPNO 10
PROCNO 1
Date_ 20110119
Time 9.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 24
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 812
DW 96.800 usec
DE 10.00 usec
TE 298.1 K
D1 1.0000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -2.50 dB
SFO1 250.1315447 MHz
SI 32768
SF 250.1299978 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG156 13C DMSO

157.57
152.09
131.64
130.27
126.35
123.97
122.52
120.86
119.59
112.07

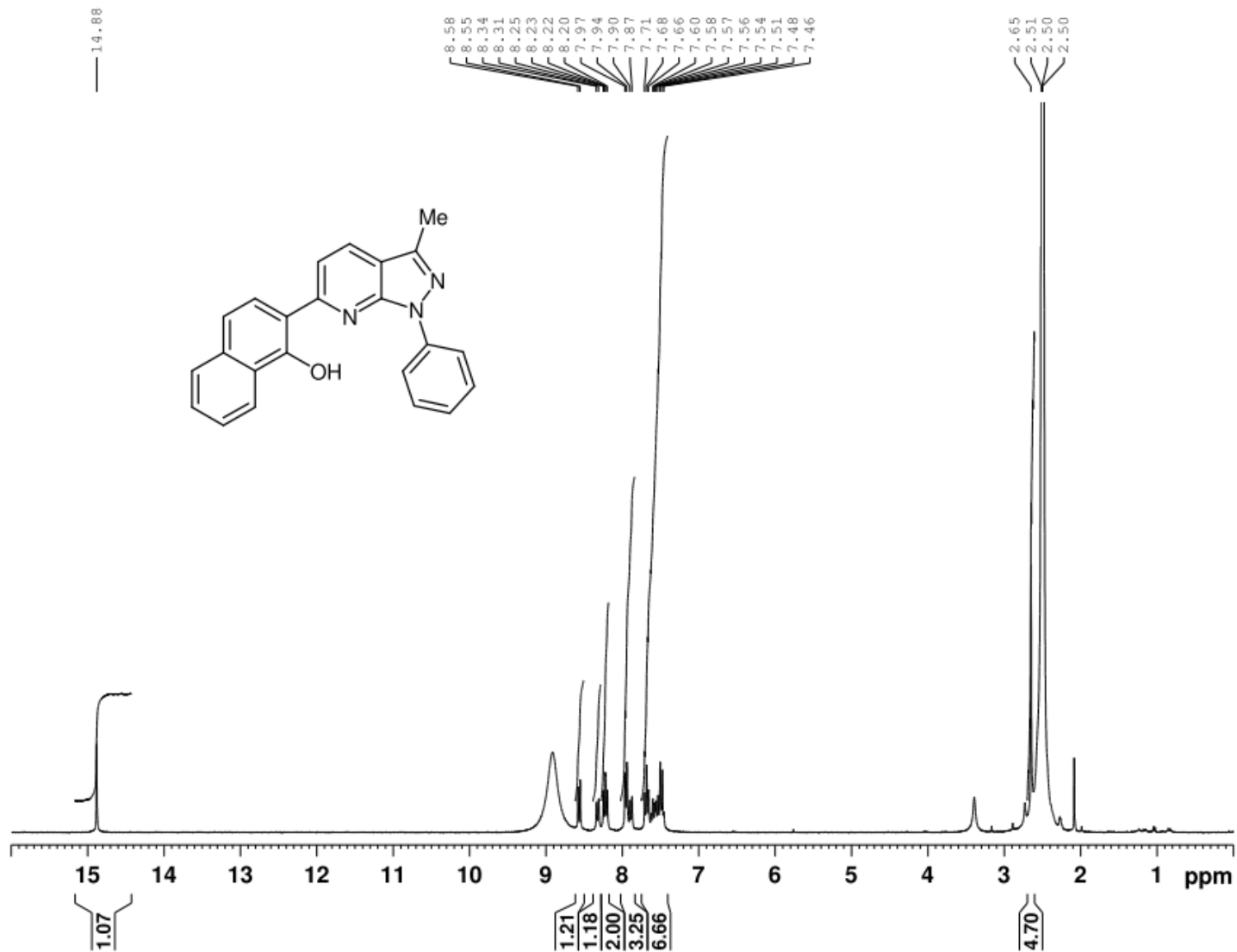


NAME 110121.225 ag 156 C
EXPNO 10
PROCNO 1
Date_ 20110123
Time 13.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 5120
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952693 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

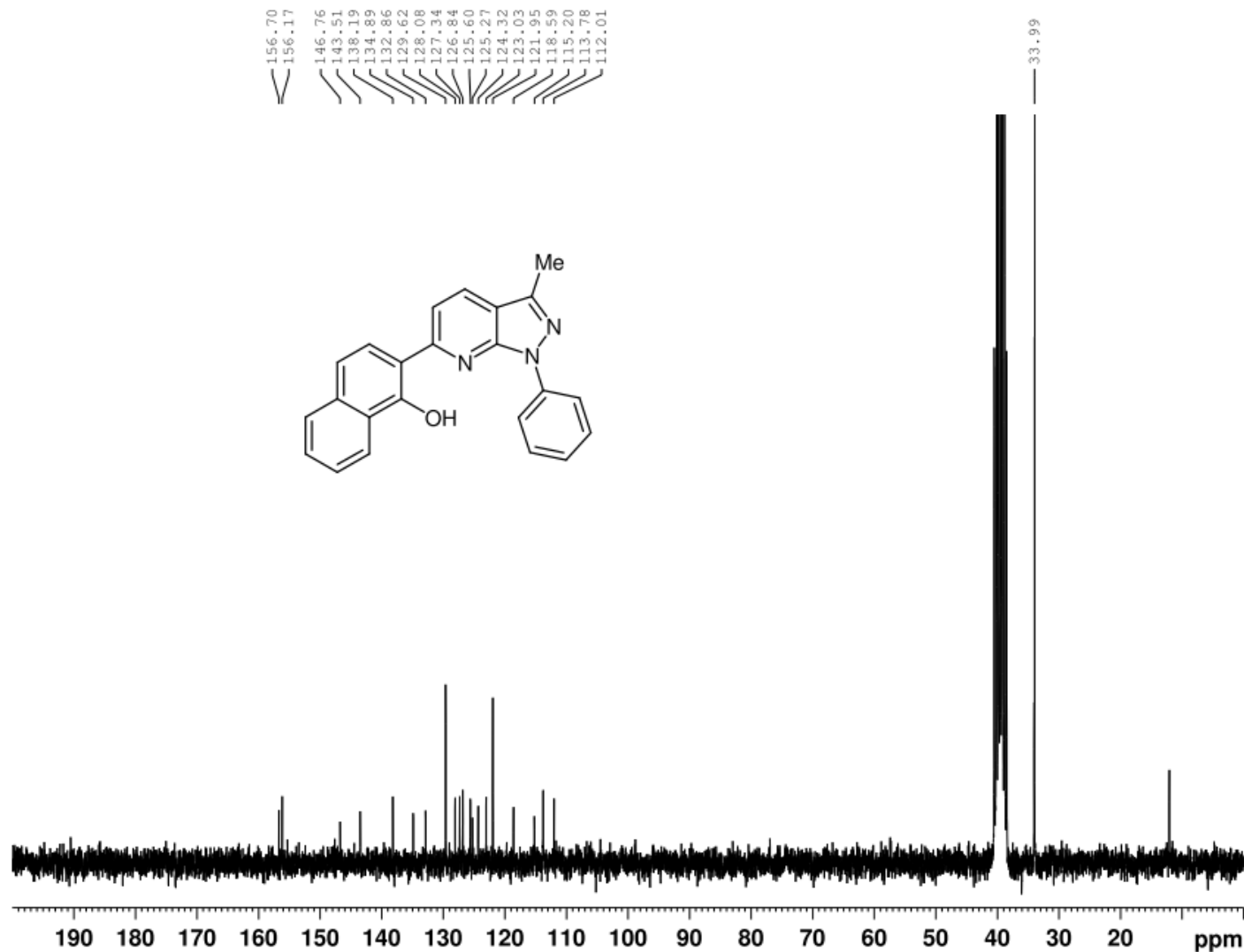
Gevorgyan AG166 1H DMSO



NAME 110131.u327 ag 166
EXPNO 10
PROCNO 1
Date_ 20110131
Time 11.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG166 (A) 13C DMSO

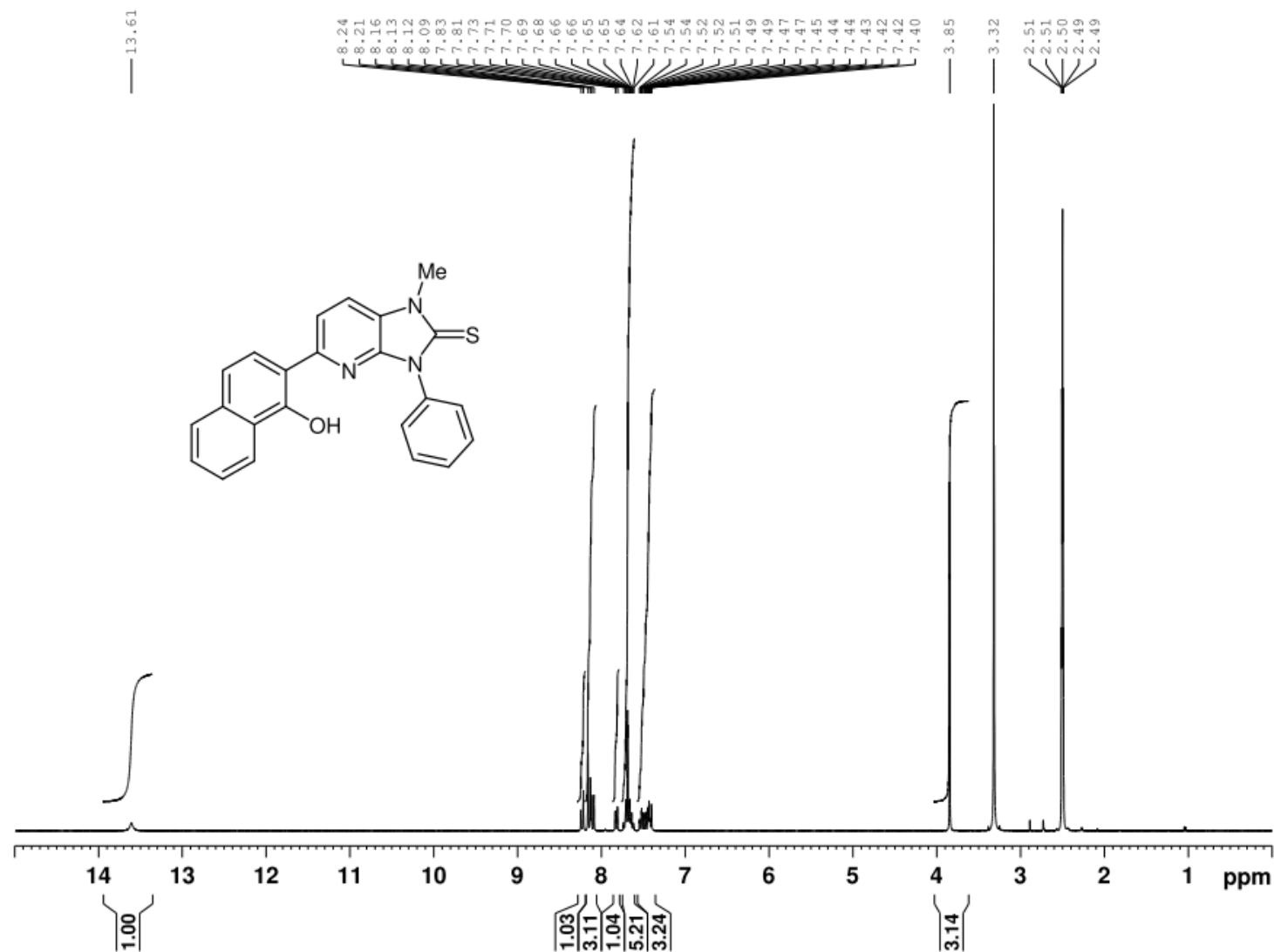


NAME 110324.212 ag 166 C
EXPNO 10
PROCNO 1
Date_ 20110325
Time 5.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1600
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952692 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

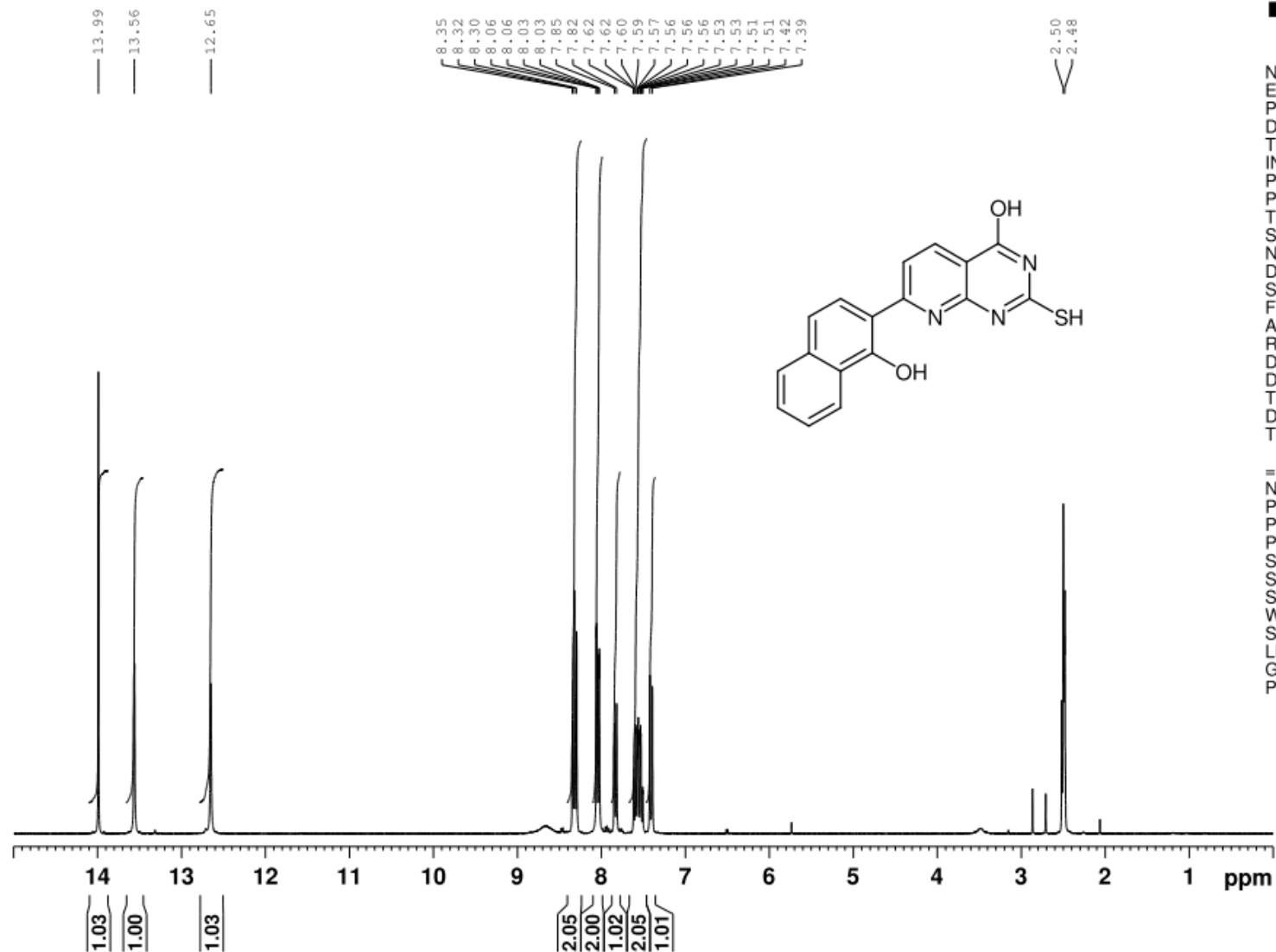
Mkrtchyan SM384 1H DMSO



NAME 101214.u338 sm 384
EXPNO 10
PROCNO 1
Date_ 20101214
Time 14.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 287
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

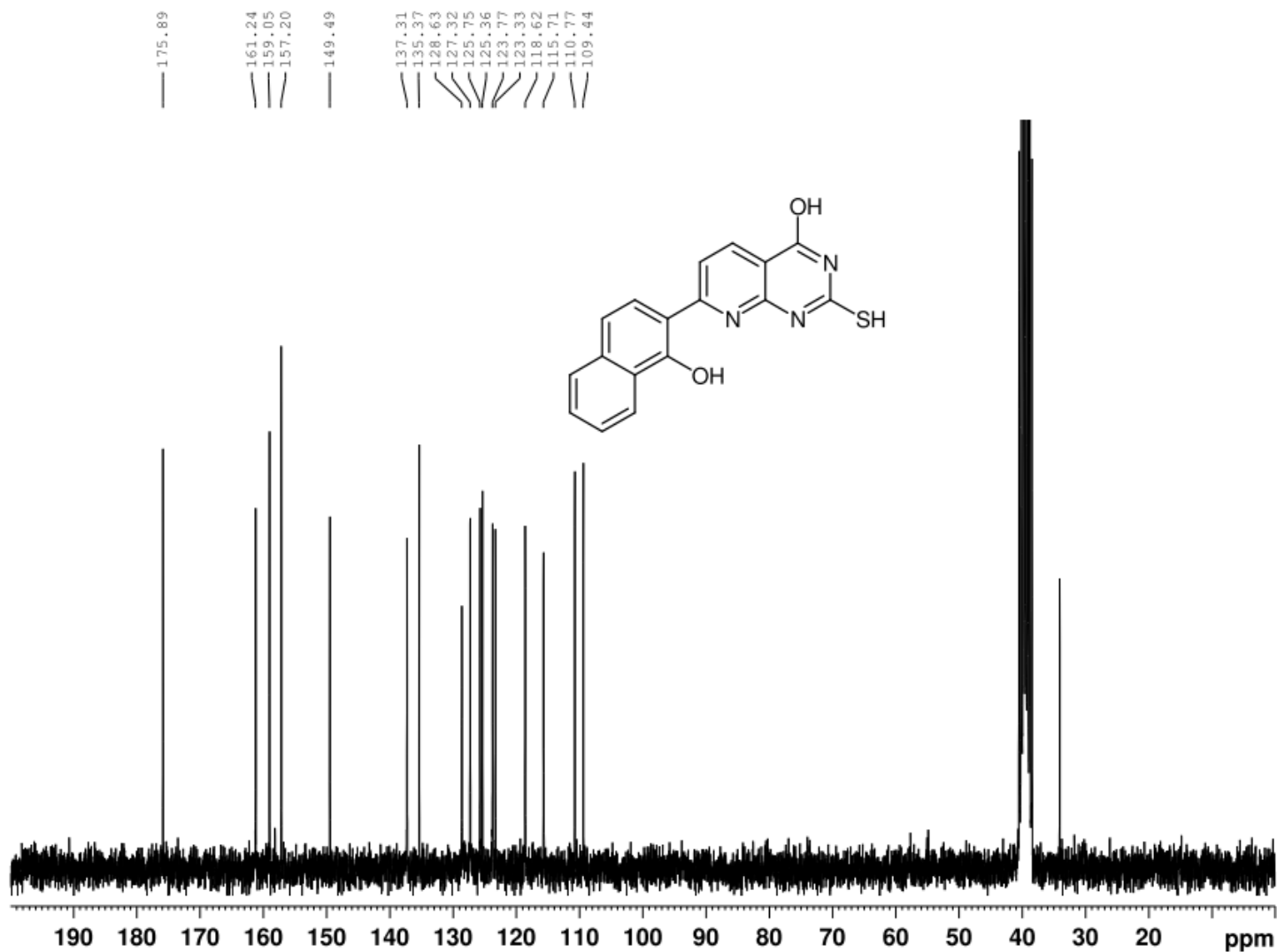
Gevorgyan AG176 (1) 1H DMSO



NAME 110218.u310 ag 176
EXPNO 10
PROCNO 1
Date_ 20110218
Time 8.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 144
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

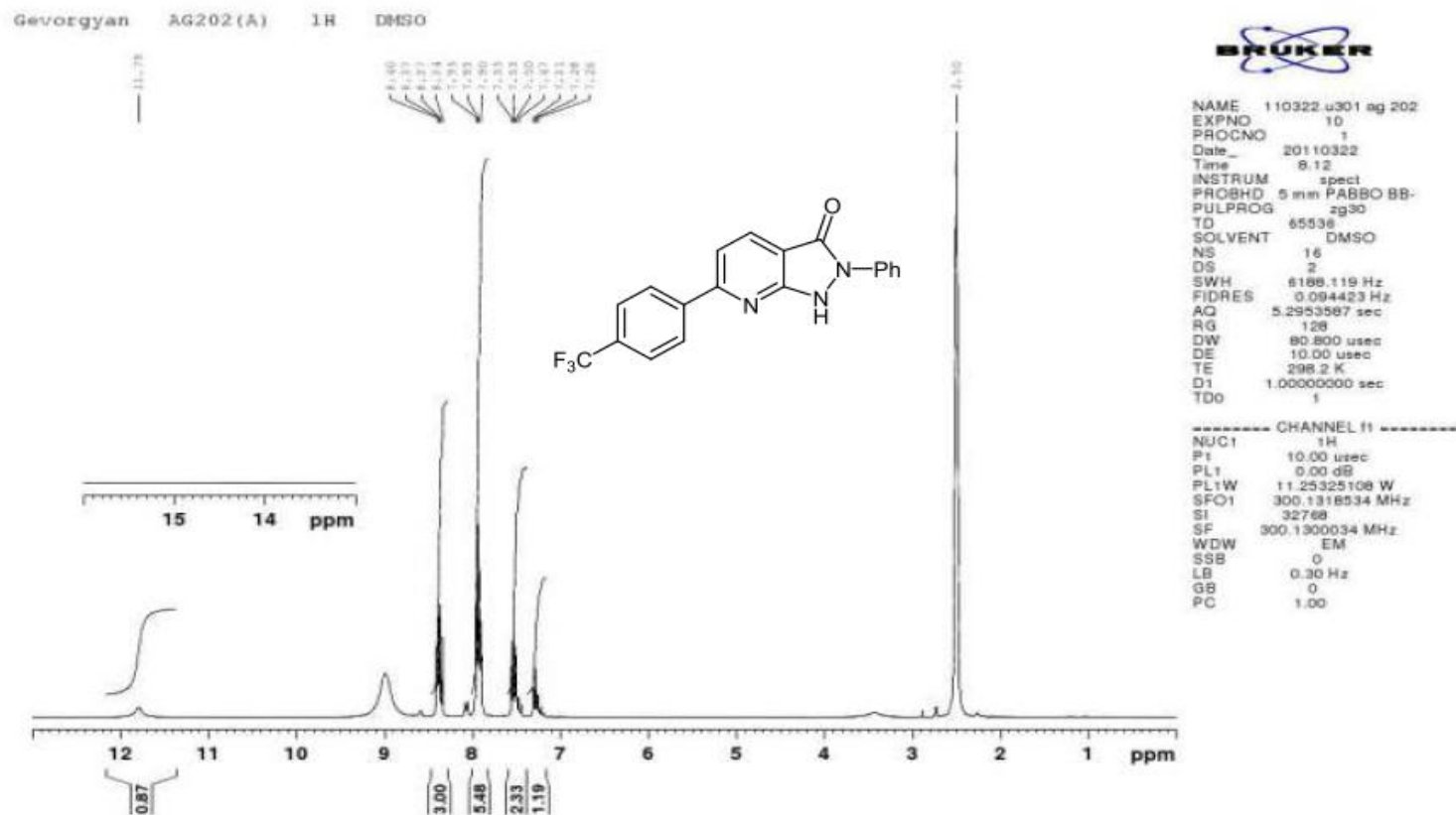
Gevorgyan AG176 (1) 13C DMSO



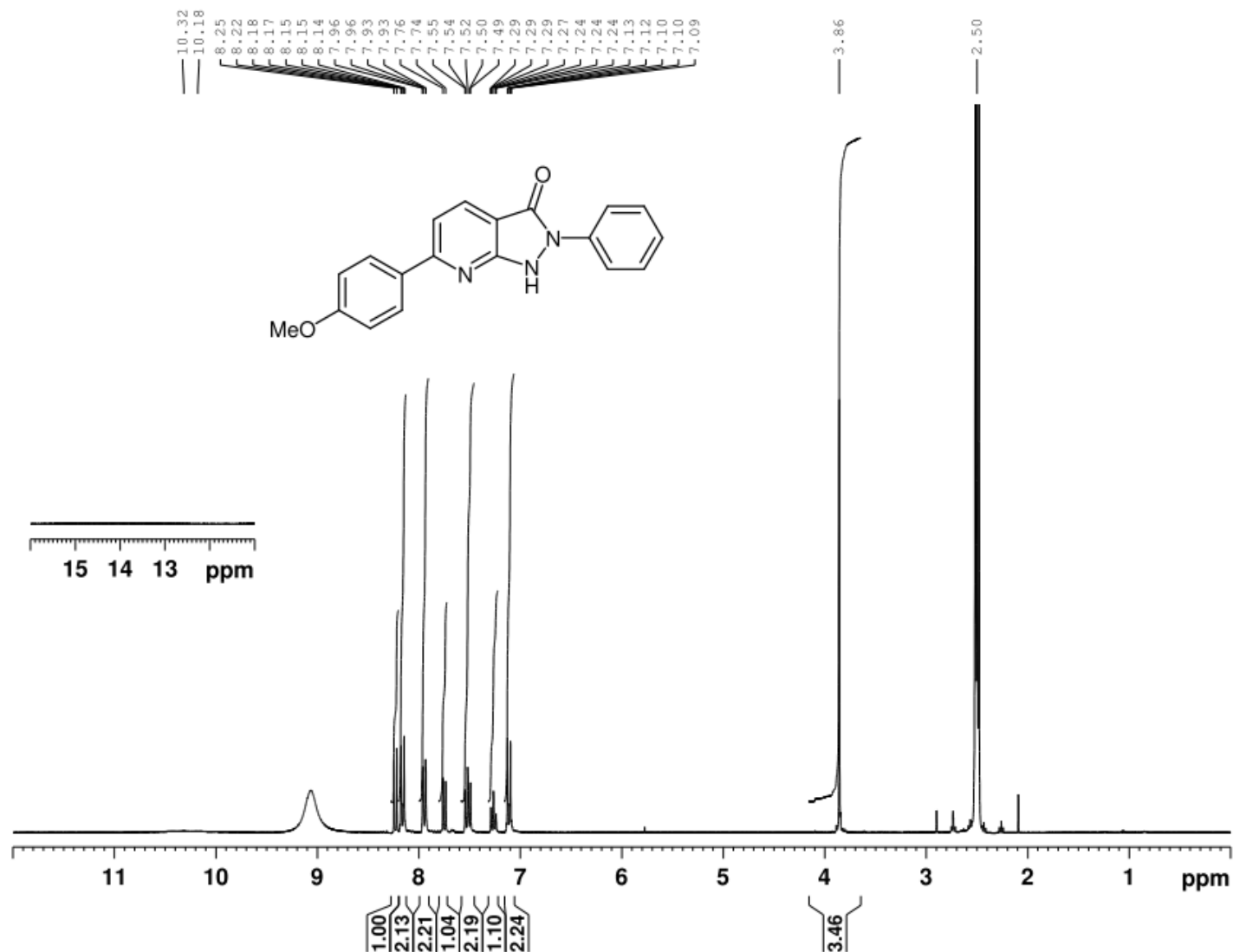
NAME 110221.205 ag 176 C
EXPNO 10
PROCNO 1
Date_ 20110221
Time 15.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.3 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952692 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Gevorgyan AG187 1H DMSO



NAME 110221.u316 ag 187
EXPNO 10
PROCNO 1
Date_ 20110221
Time 9.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 101
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

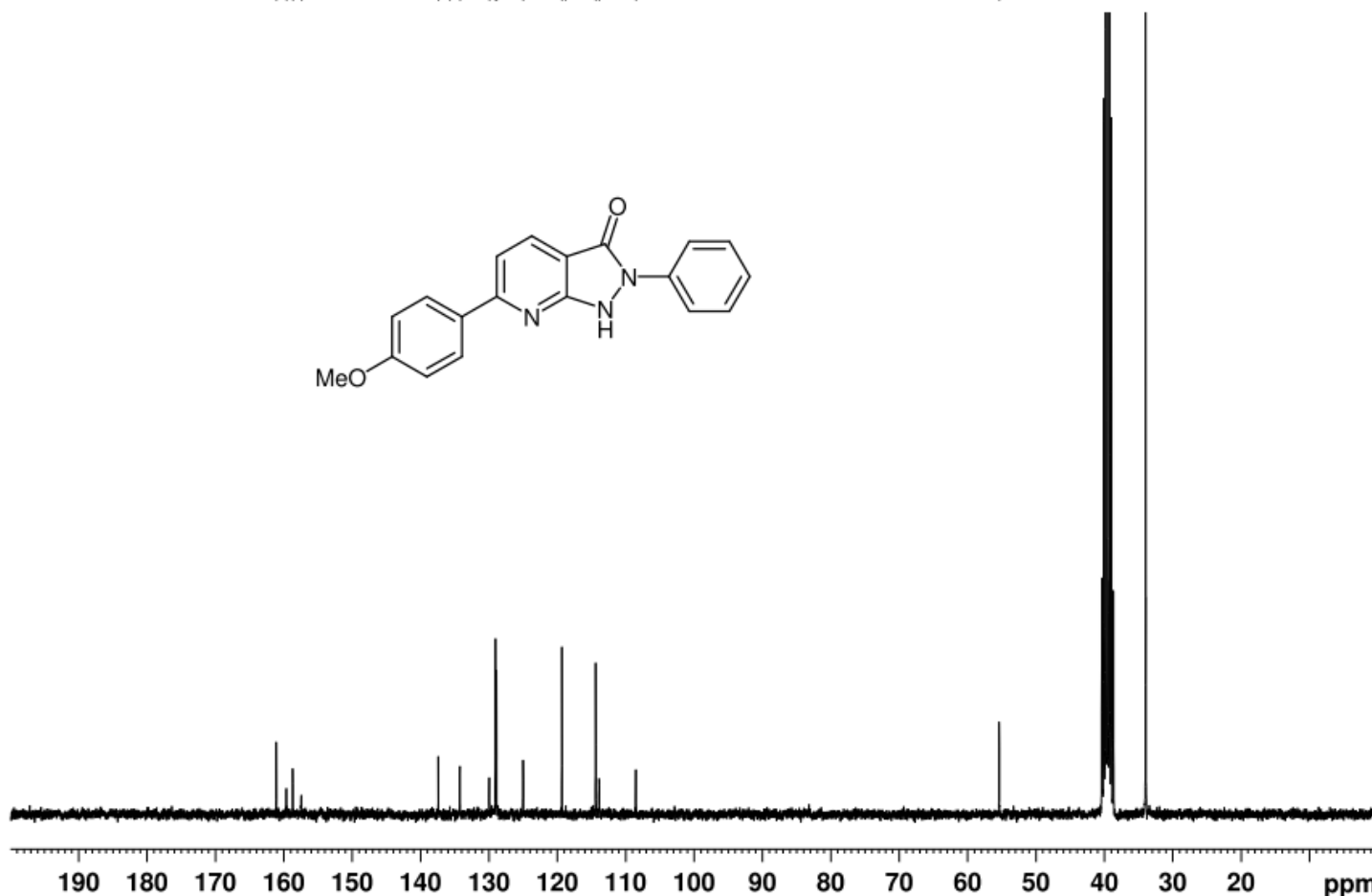
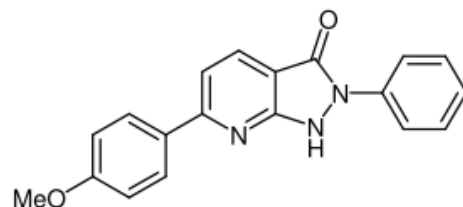
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1299994 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG187 13C DMSO



161.09
159.60
158.66
157.42
137.38
134.23
129.93
129.01
128.87
124.98
119.29
114.35
113.86
108.48
105.73
116.79

55.36

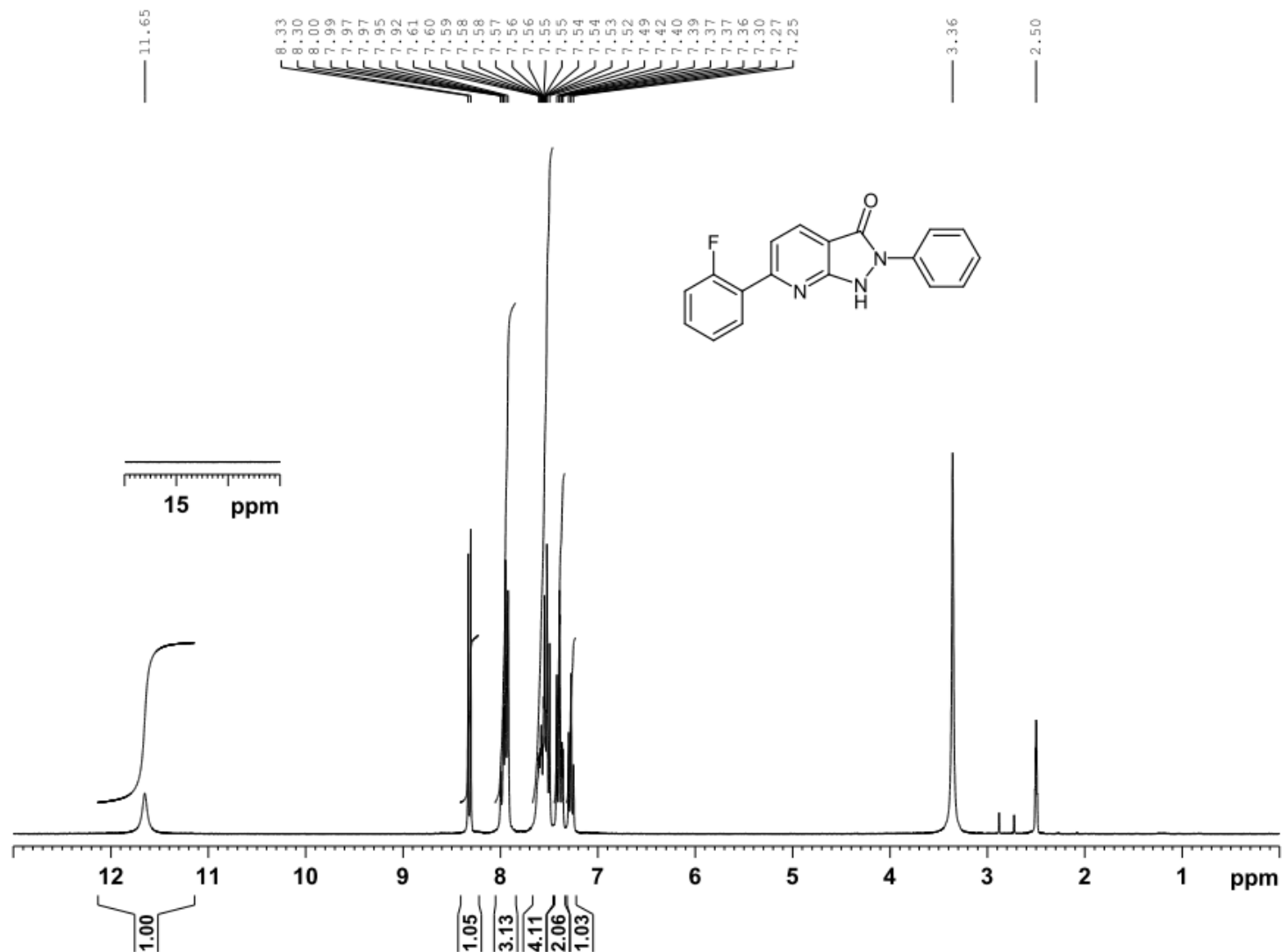


NAME 110224.u348 ag 187 C
EXPNO 10
PROCNO 1
Date_ 20110224
Time 22.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677859 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mkrtchyan, SM 508, DMSO, 1H



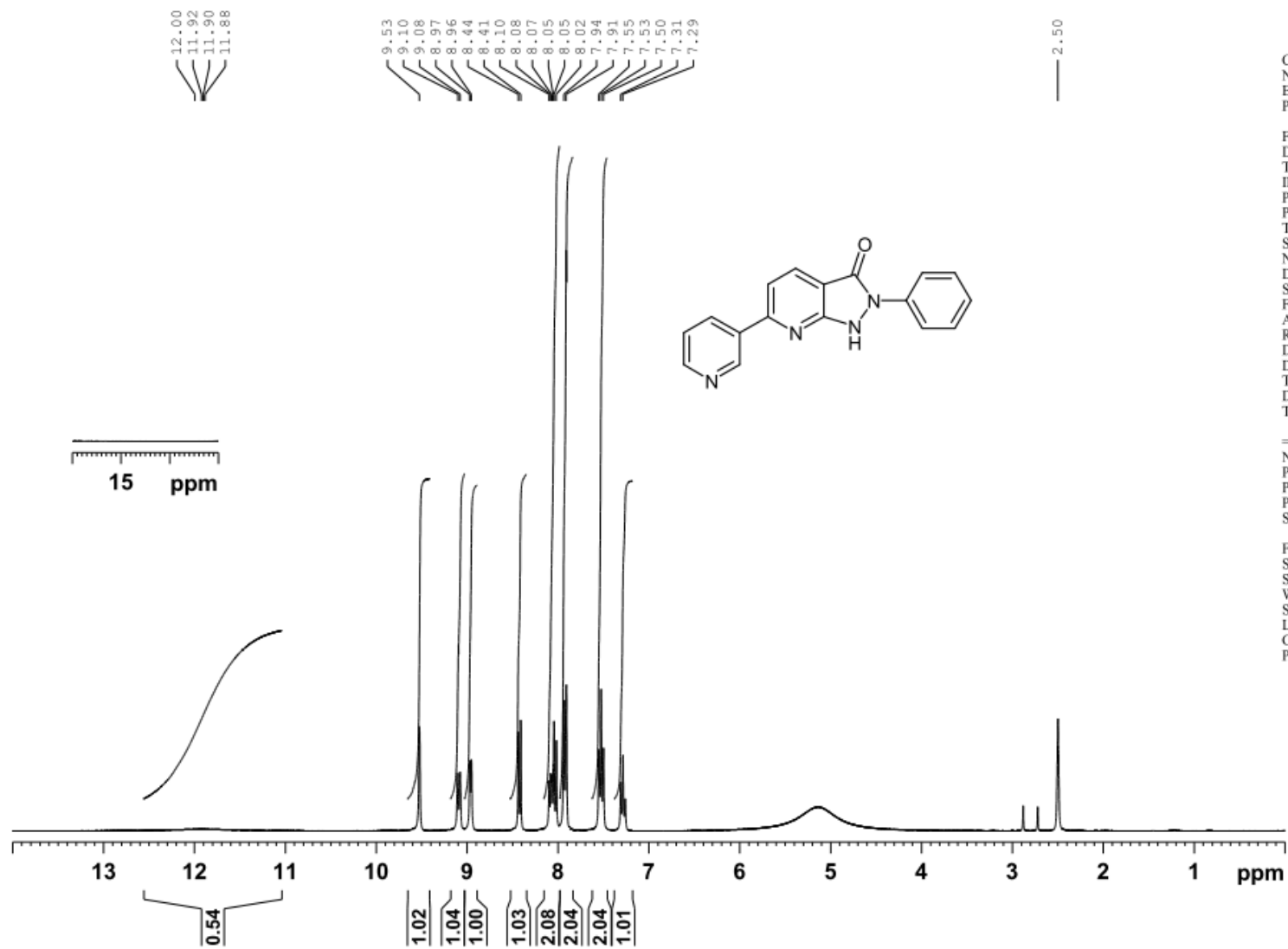
Current Data Parameters
NAME 110701.u310 sm 508
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110701
Time 9.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 114
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1300068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Mkrtchyan, SM 521, DMSO, 1H



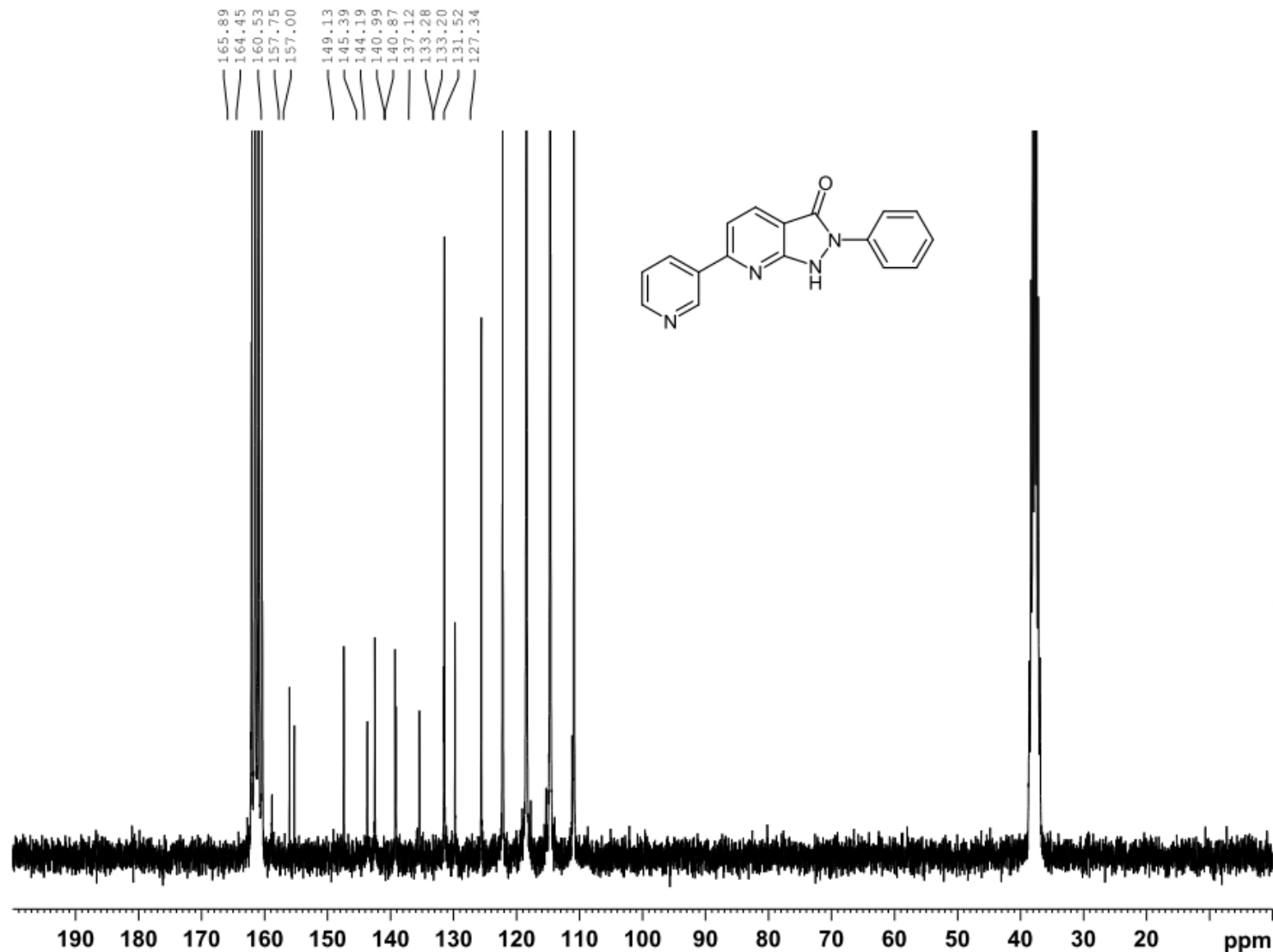
Current Data Parameters
NAME 110707.u319 sm 521
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110707
Time 11.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 144
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 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 300.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Mkrtchyan SM521 13C CF3COOD/DMSO



Current Data Parameters
NAME 110713.u321 sm 521 c
EXPNO 10
PROCNO 1

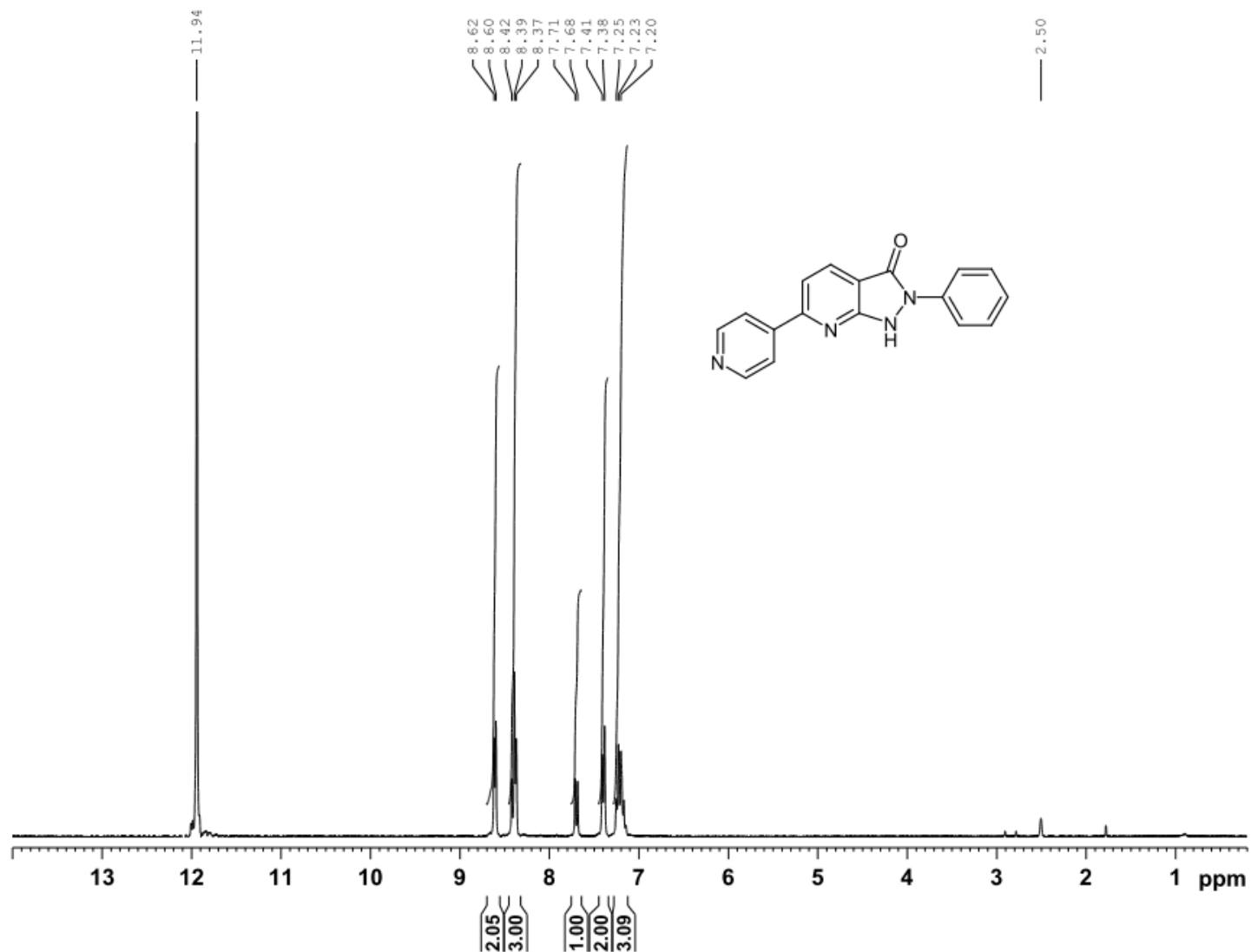
F2 - Acquisition Parameters
Date_ 20110713
Time 23.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 1600
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.5 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

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 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mkrtchyan, SM 522, CF3COOD/DMSO, 1H



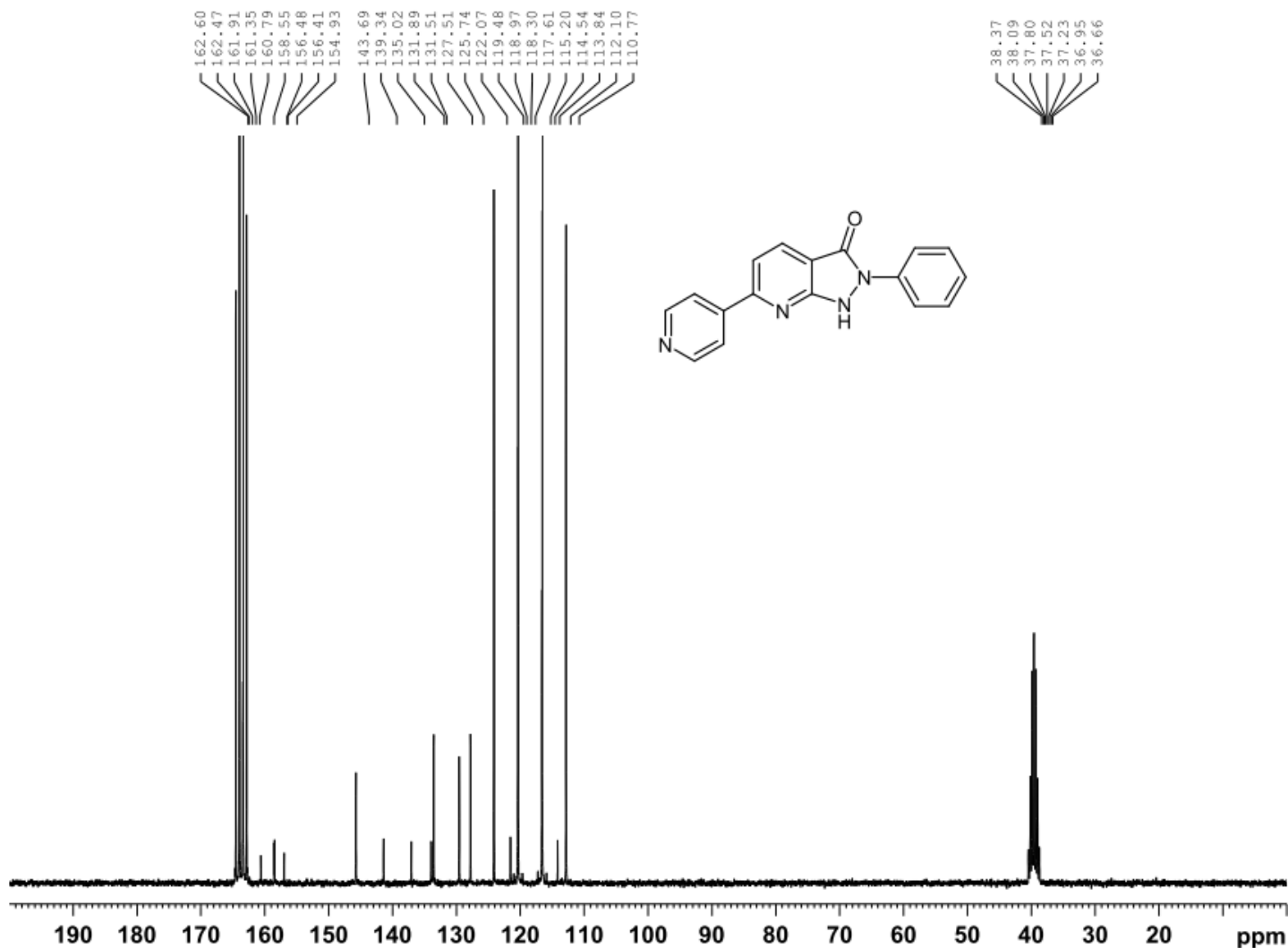
Current Data Parameters
NAME 110712.u333 sm 522
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110712
Time 22.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT D2O
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 161
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 300.1306778 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Mkrtchyan SM522 13C CF3COOD/DMSO



Current Data Parameters
NAME 110713.u322 sm 522 C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110714
Time 2.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 1600
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 0.0300000 sec
TD0 1

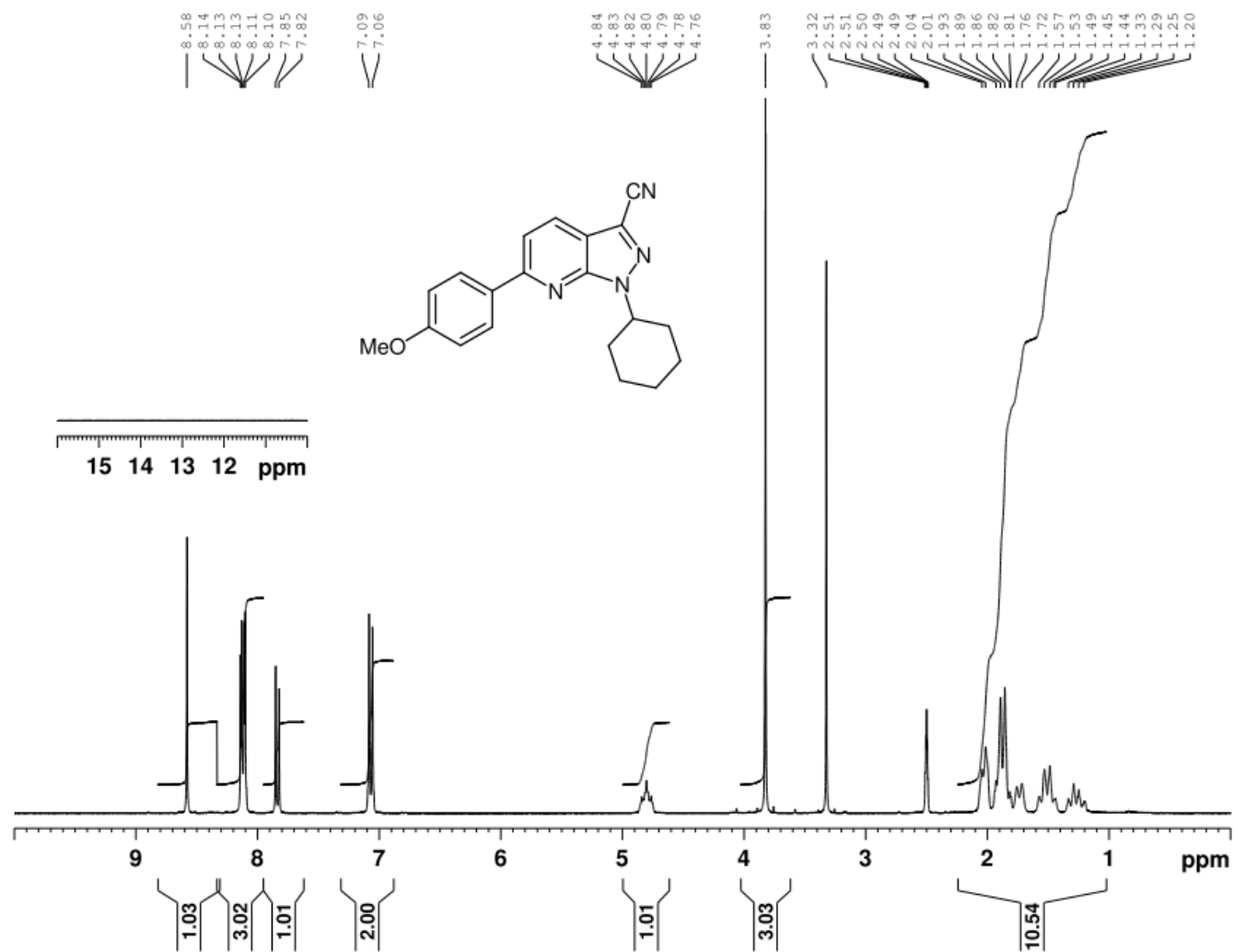
CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

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

F2 - Processing parameters
SI 32768
SF 75.4675933 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

120

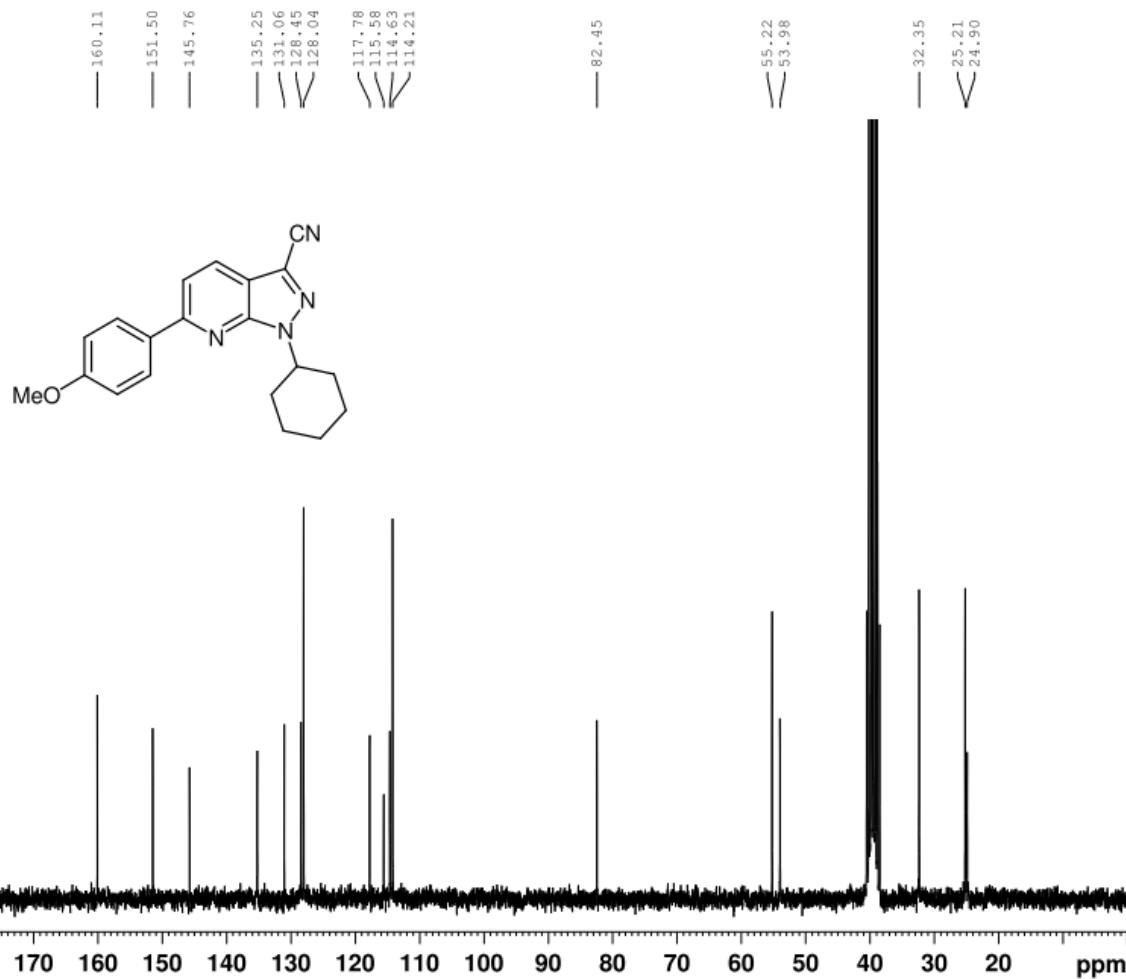
Gevorgyan AG204 1H DMSO



NAME 110316.u304 ag 204
EXPNO 10
PROCNO 1
Date_ 20110316
Time 8.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG204 13C DMSO

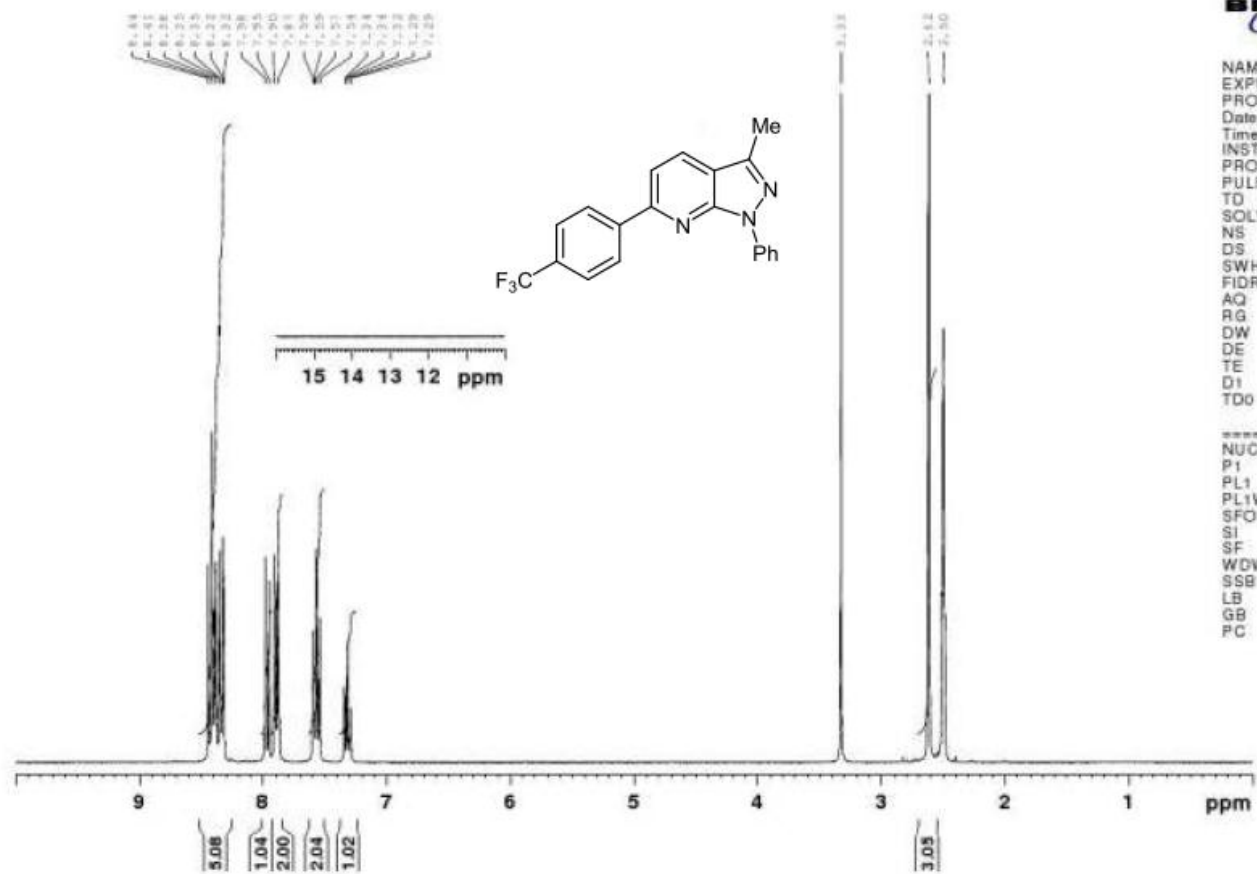


NAME 110317.210 ag 204 C
EXPNO 10
PROCNO 1
Date_ 20110318
Time 2.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952692 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

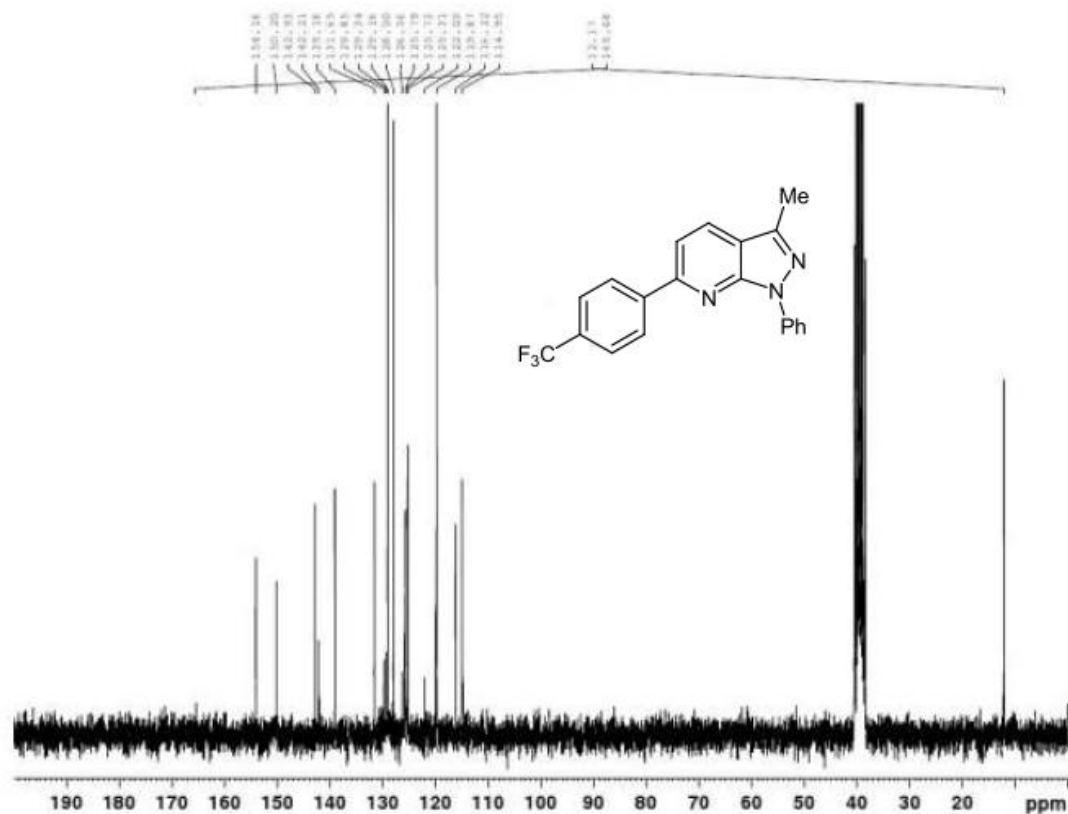
Gevorgyan AG137 1H DMSO



NAME 110120.u306.ag137
EXPNO 10
PROCNO 1
Date_ 20110120
Time 8.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 161
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1316534 MHz
SI 32768
SF 300.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG137 13C DMSO

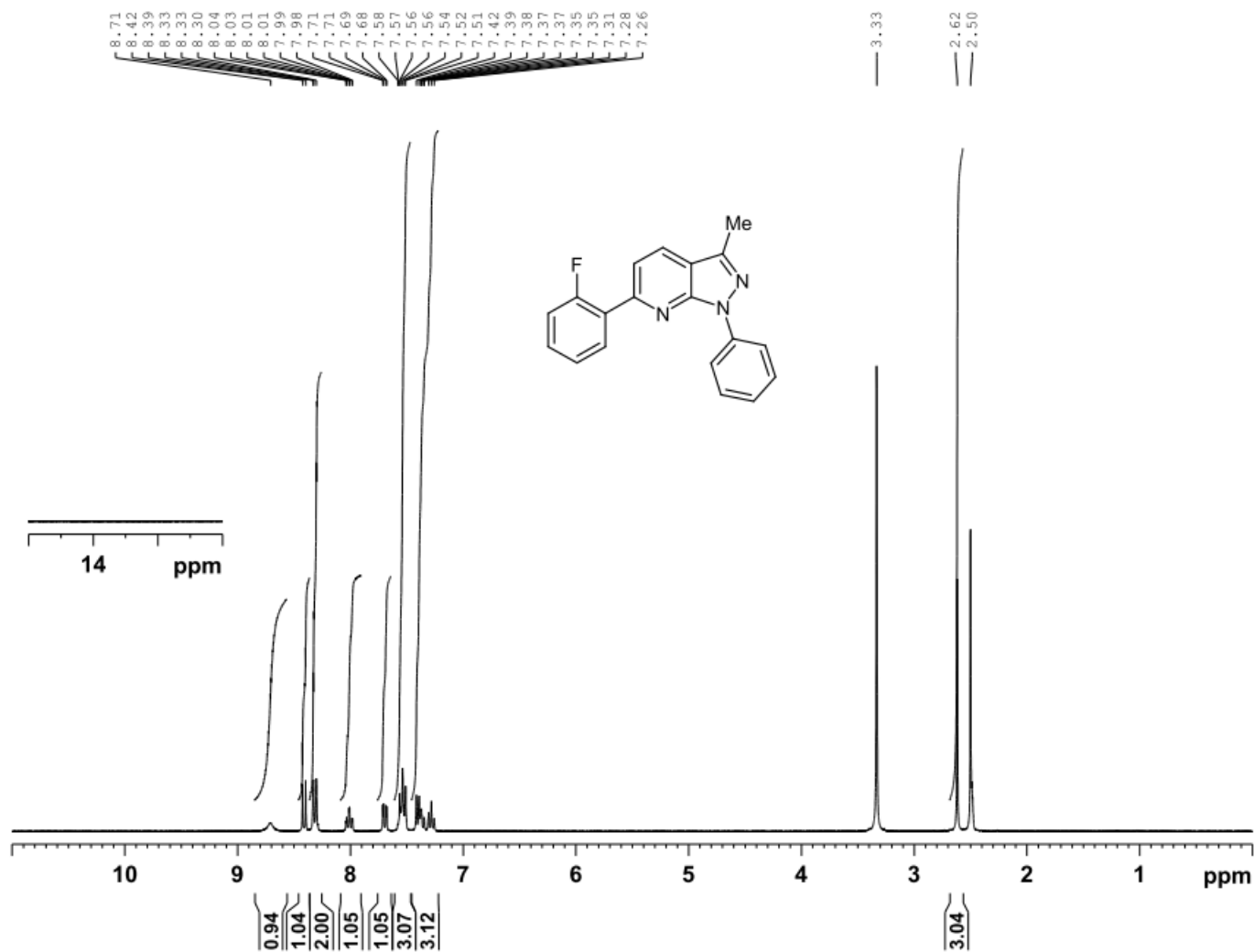


NAME 110121.222 ag 137 C
EXPNO 1
PROCNO 1
Date_ 20110123
Time 0.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228862 Hz
AQ 2.1845834 sec
RG 1620
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 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
SI 32768
SF 62.8952892 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mkrtchyan, SM 509, DMSO, 1H



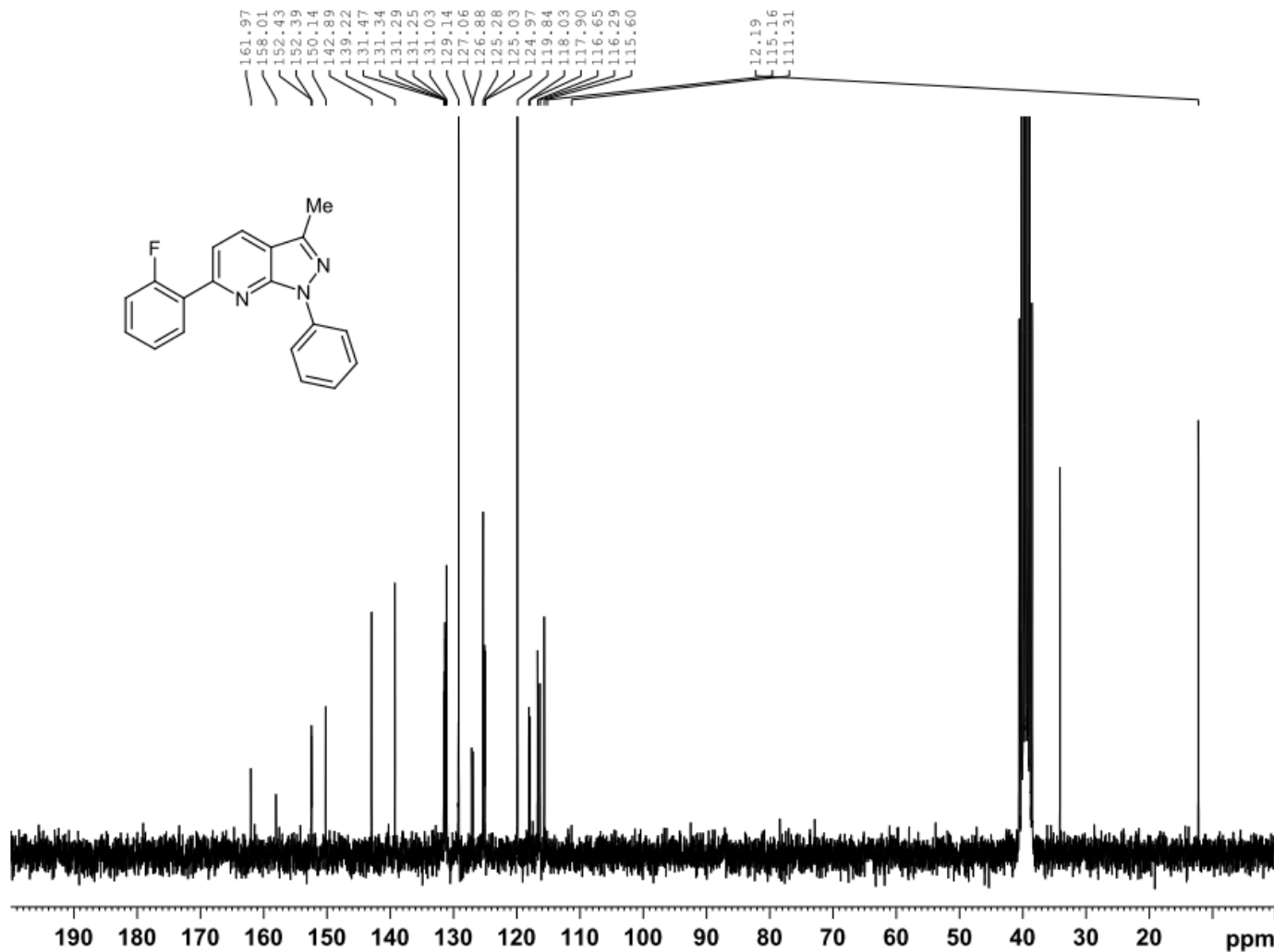
Current Data Parameters
NAME 110701.u311 sm 509
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20110701
Time 9.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
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 300.1300107 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Mkrtchyan, SM 509, DMSO, 13C

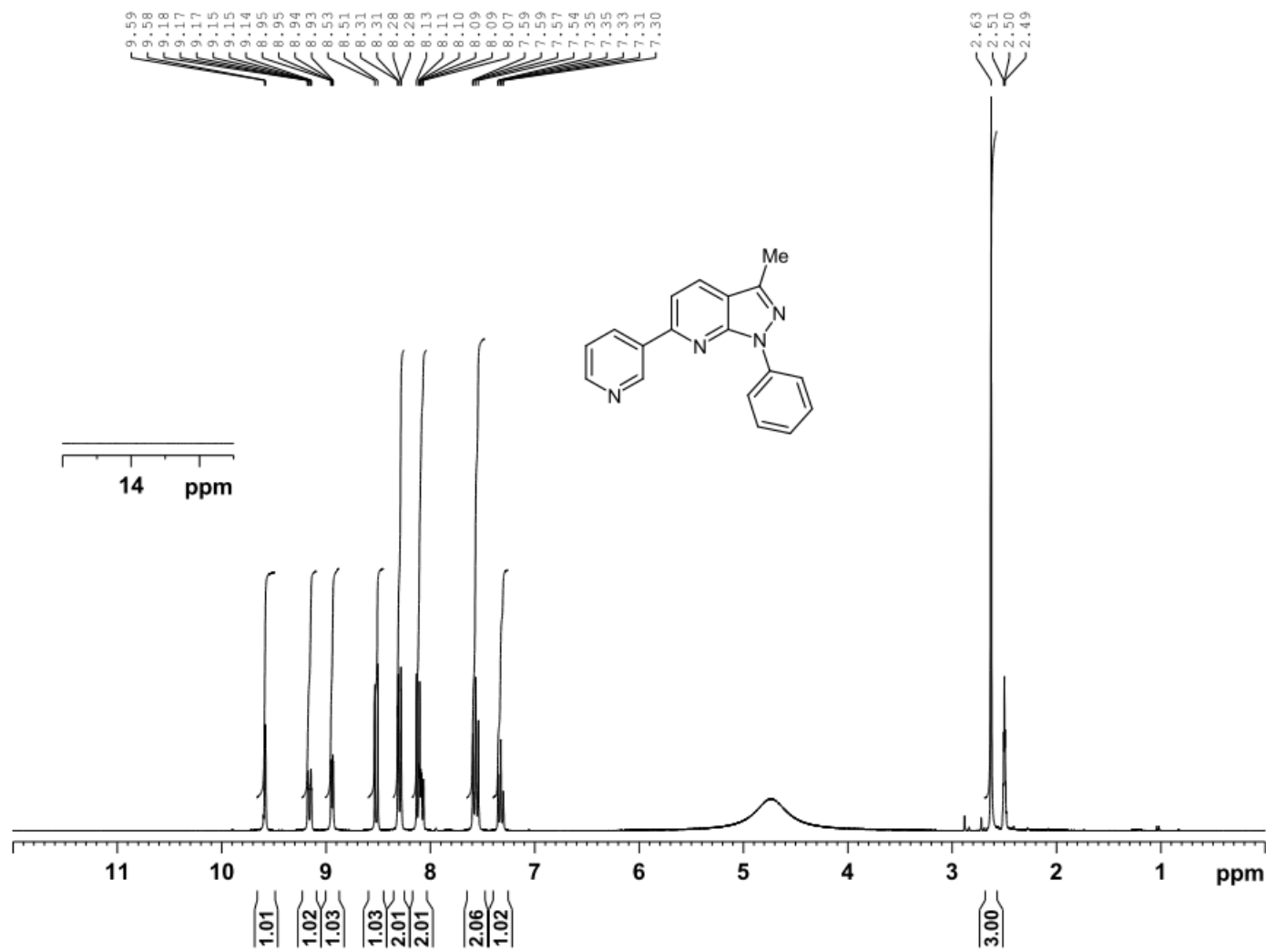


NAME 110704.204 sm 509 c
EXPNO 10
PROCNO 1
Date_ 20110704
Time 16.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952692 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mkrtchyan, SM 524, DMSO, 1H



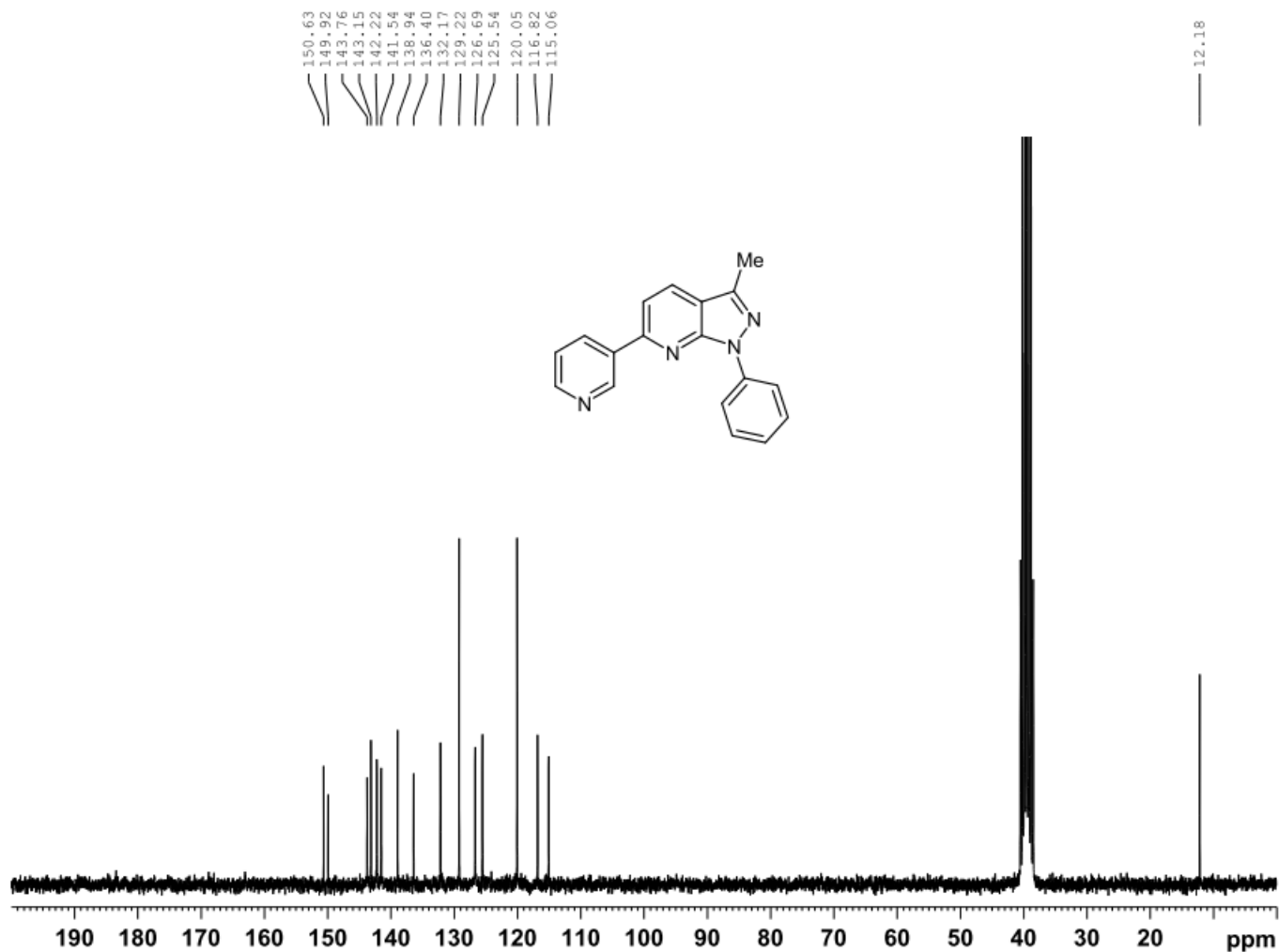
Current Data Parameters
NAME 110707.u320 sm 524
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110707
Time 11.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 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 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Mkrtchyan, SM 524, DMSO, 13C



Current Data Parameters
NAME 110708.207 sm 524 C
EXPNO 10
PROCNO 1

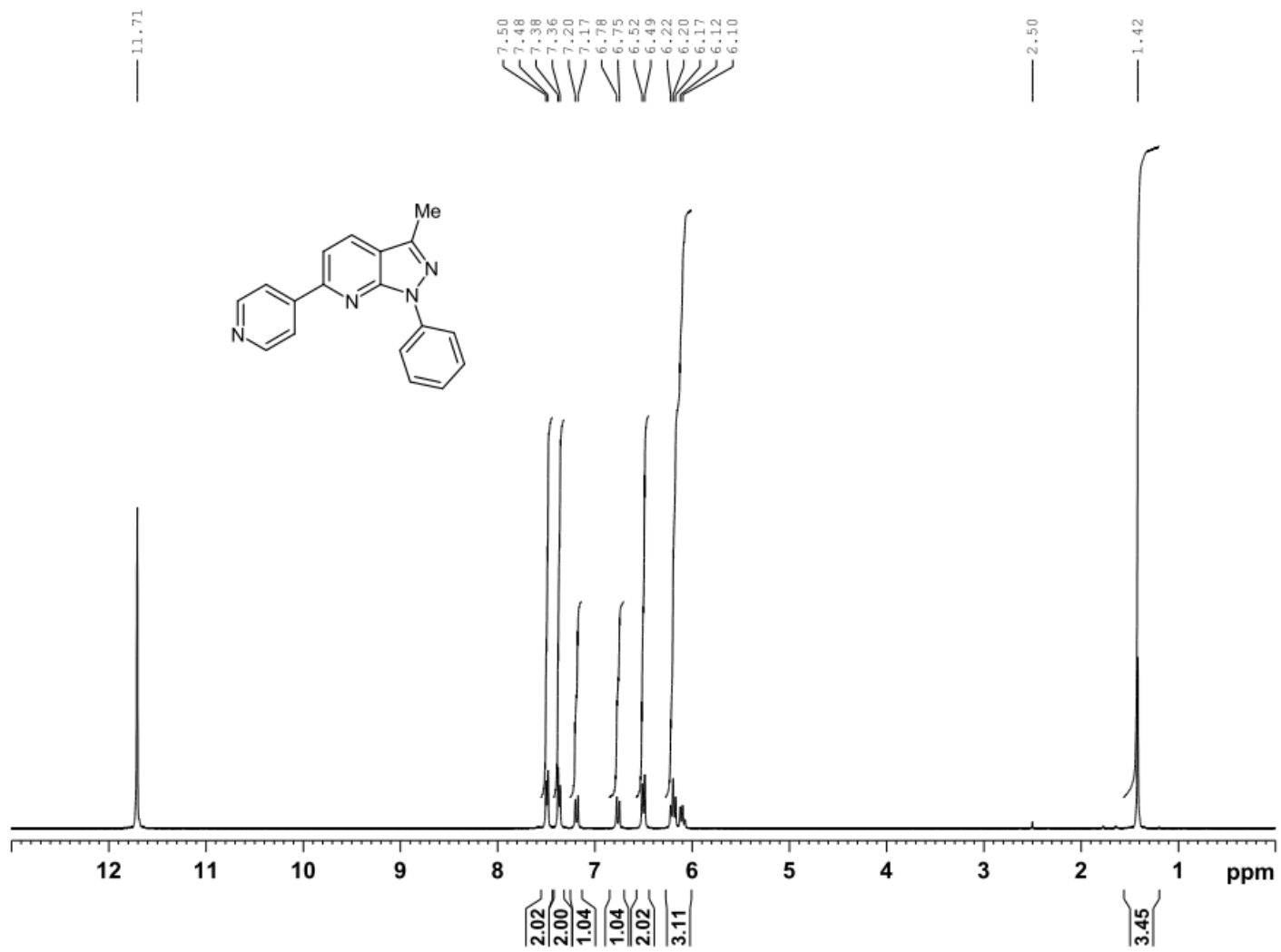
F2 - Acquisition Parameters
Date_ 20110710
Time 4.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 299.7 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952687 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mkrtchyan SM523 1H CF3COOD/DMSO



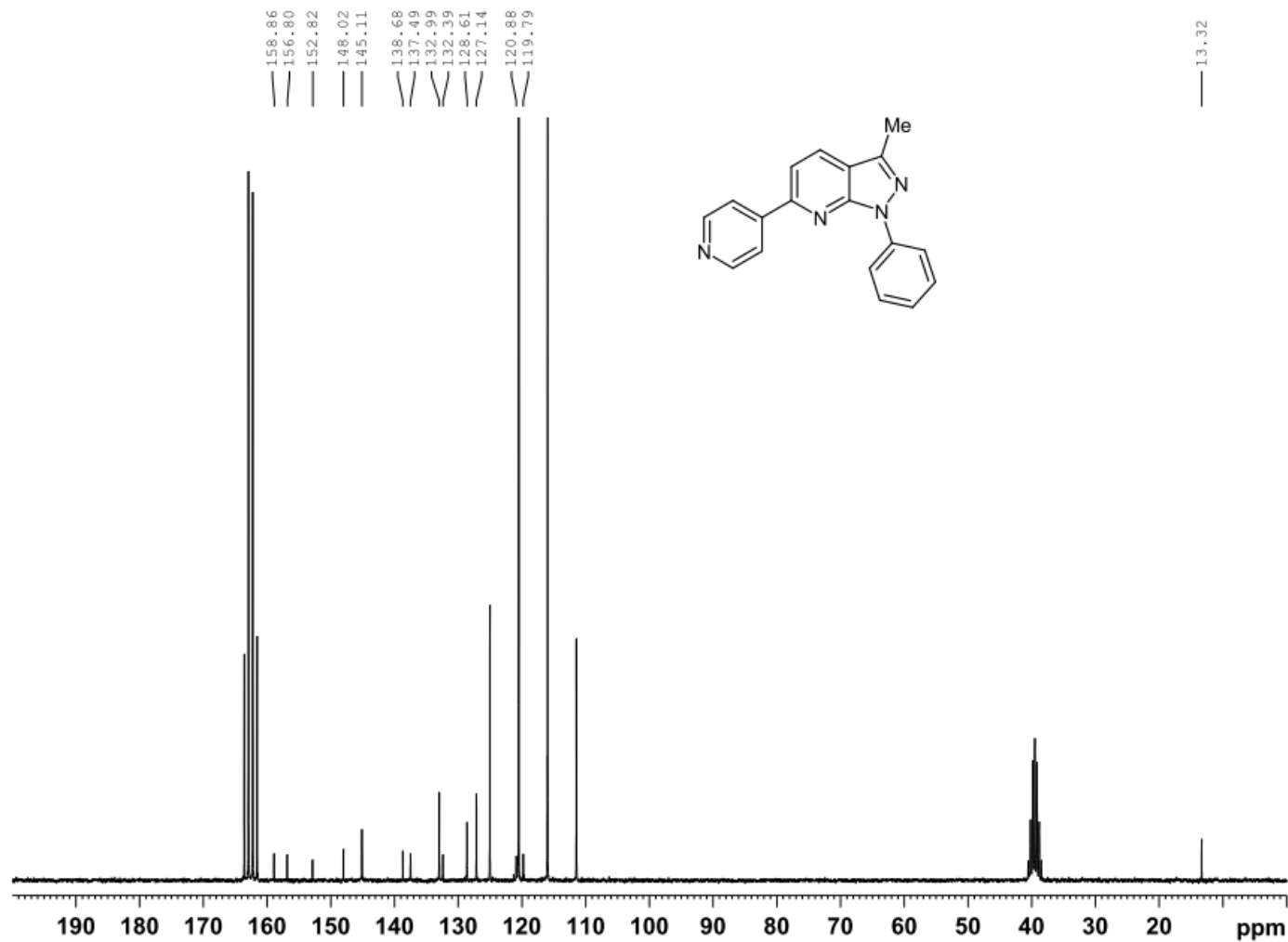
Current Data Parameters
NAME 110714.u303 sm 525
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110714
Time 8.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT D2O
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 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 300.1310072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Mkrtchyan SM525 13C CF3COOD/DMSO

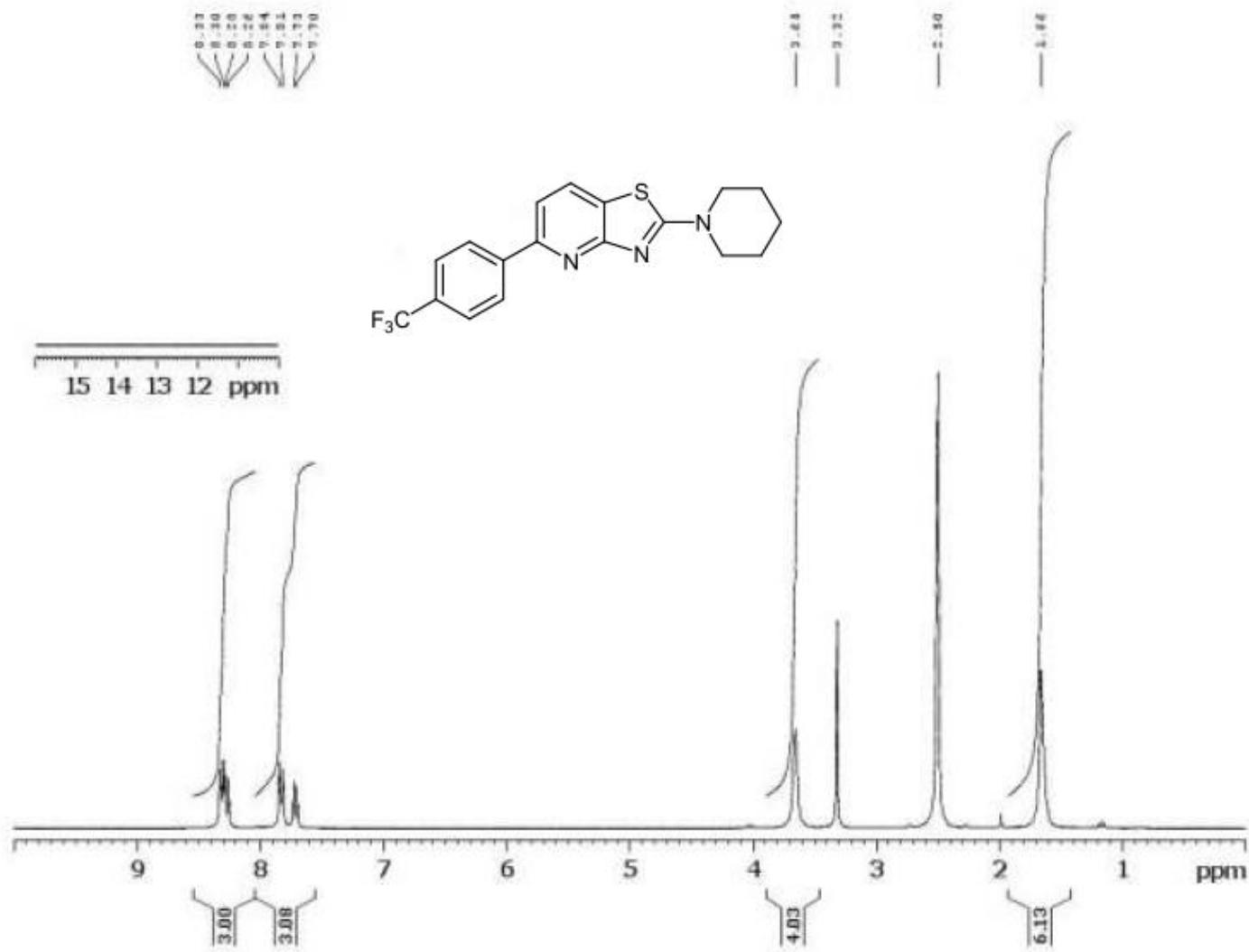


NAME 110715.212 sm 525 C
EXPNO 10
PROCNO 1
Date_ 20110717
Time 2.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8951355 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG174 1H DMSO

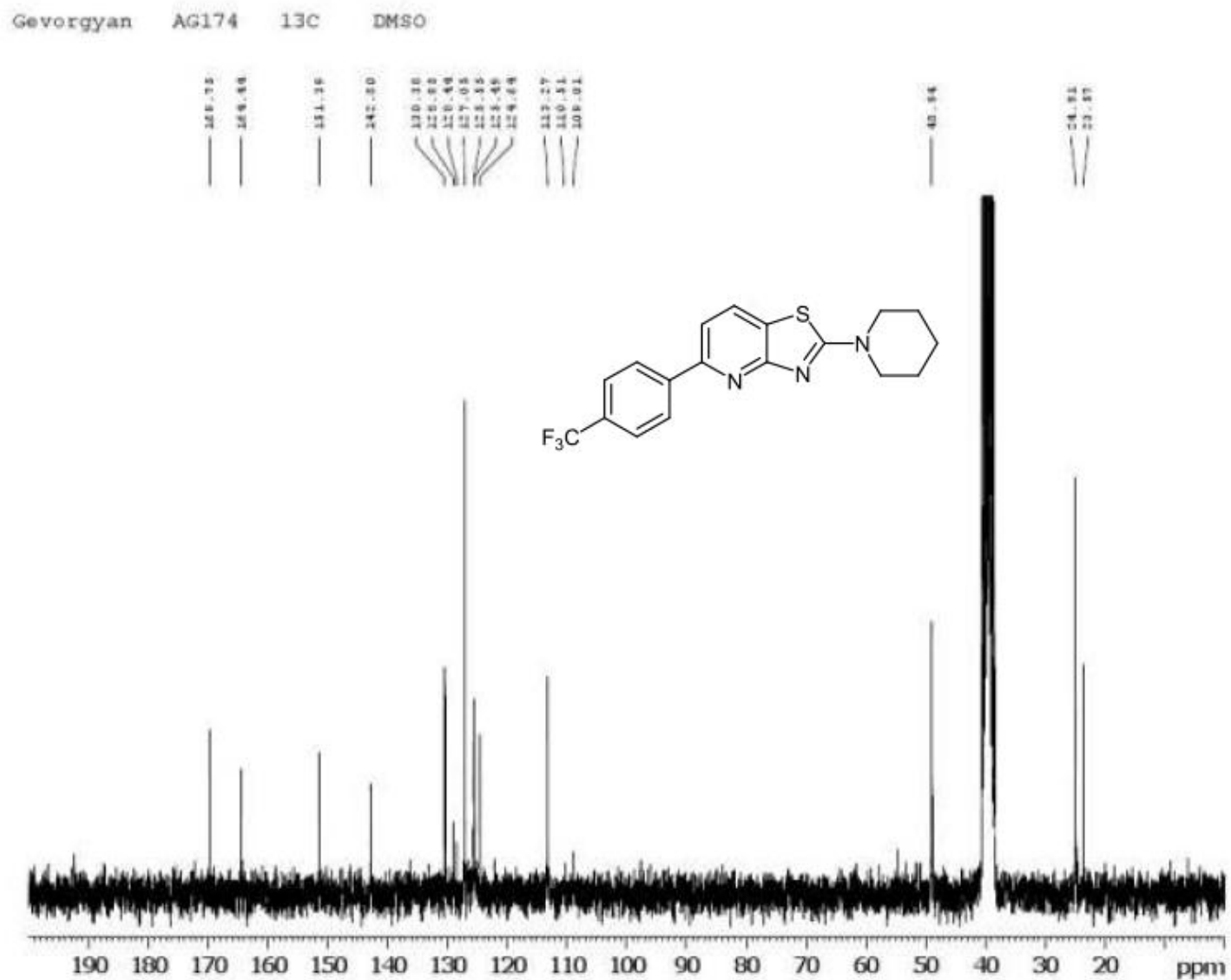


Current Data Parameters
NAME 110211.u.308 ag 174
EXPIRO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110211
Time 9.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.295387 sec
RG 144
DH 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 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.130075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 110214.212 ag 174 C
EXPHO 10
PROCNO 1

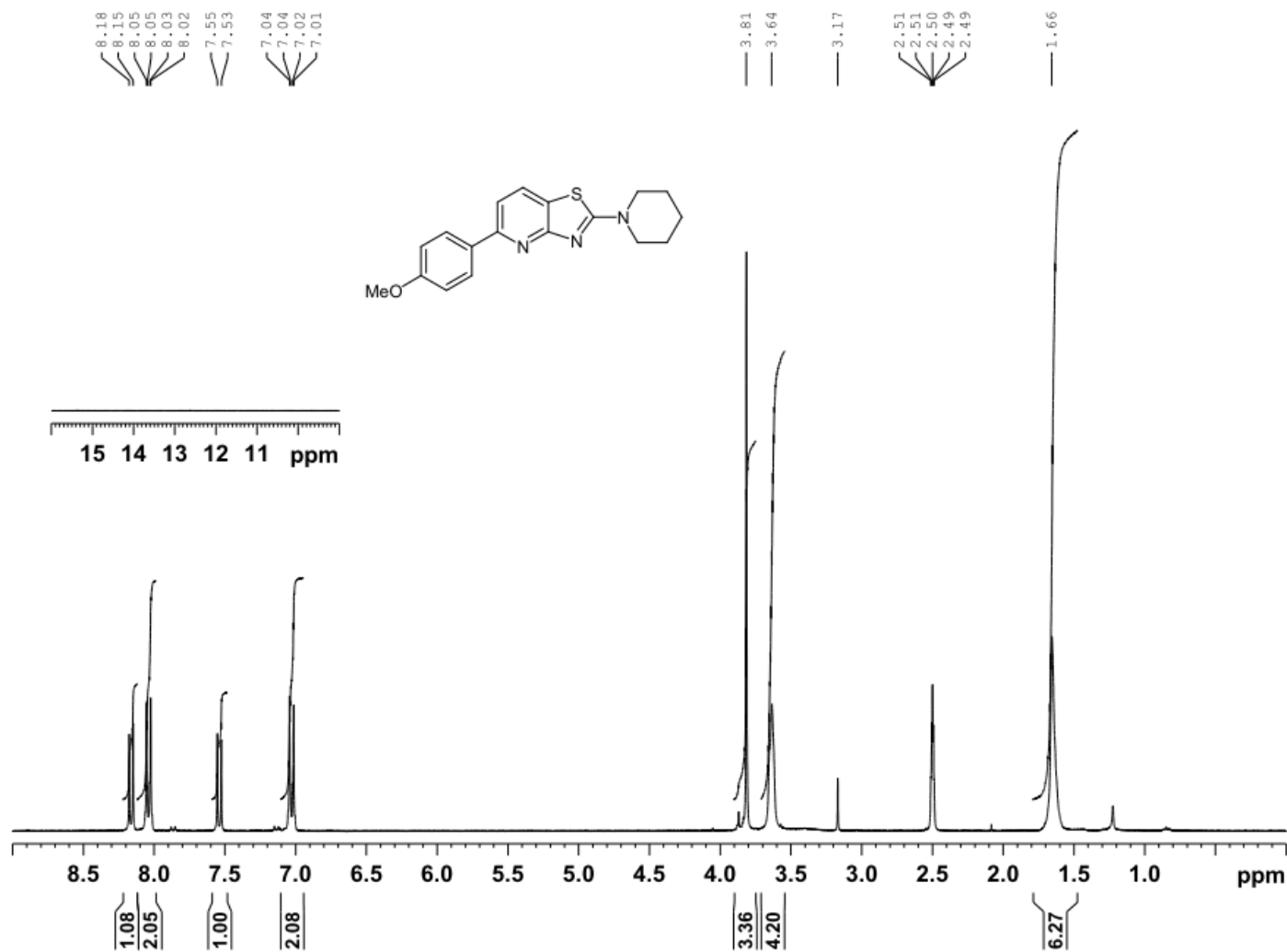
F2 - Acquisition Parameters
Date_ 20110215
Time 6:56
INSTRUM spect
PROBHD 5mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 15000.000 Hz
FIDRES 0.228802 Hz
AQ 2.1045034 sec
RG 2090
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.90150280 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 62.8902694 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG188 1H DMSO



Current Data Parameters
NAME 110303.u304 ag 188
EXPNO 10
PROCNO 1

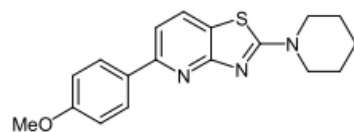
F2 - Acquisition Parameters
Date_ 20110303
Time 9.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 161
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

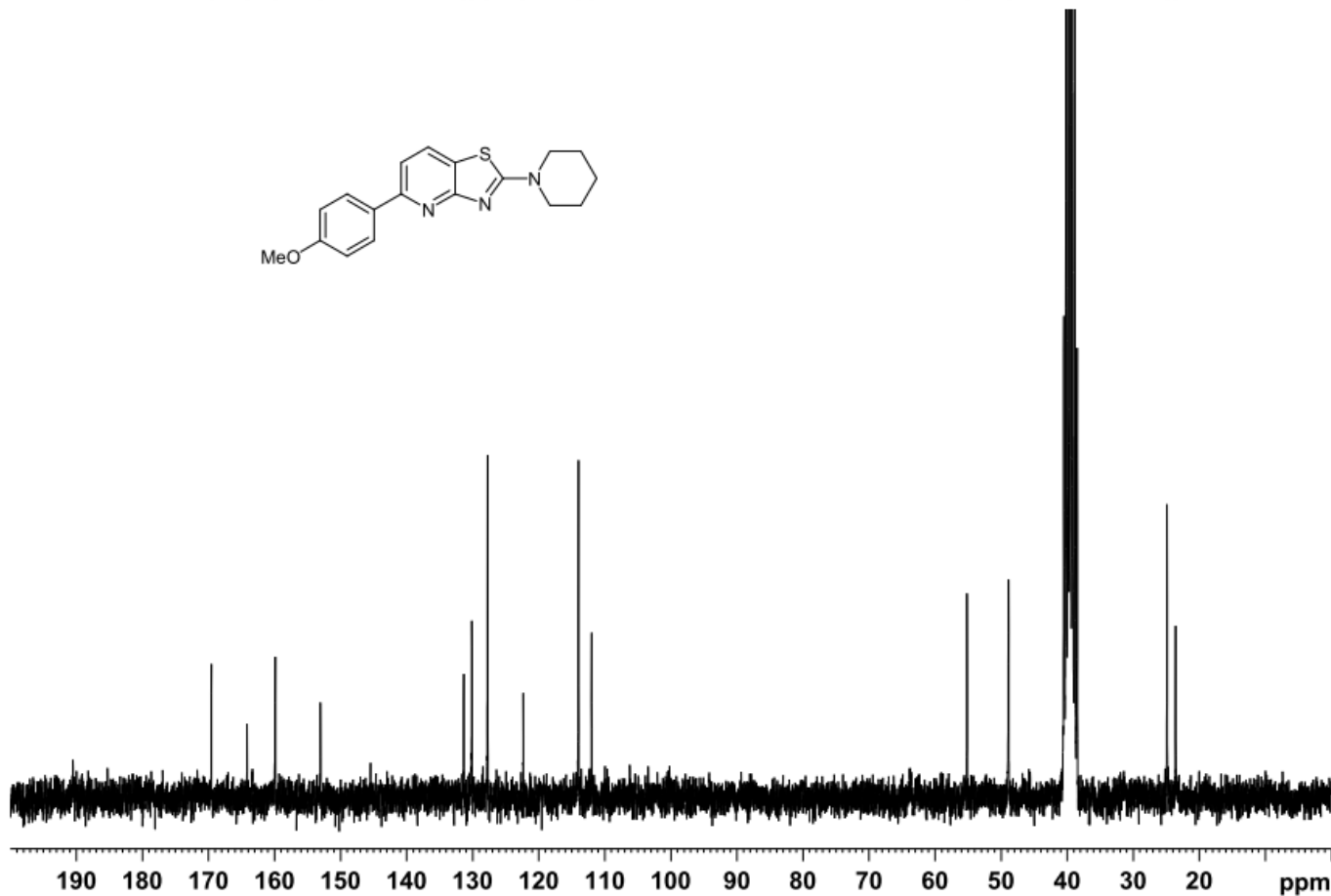
F2 - Processing parameters
SI 32768
SF 300.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG188 13C DMSO

169.54
164.13
159.86
153.02
131.36
130.13
127.74
122.33
113.99
111.99



55.17
48.89
24.89
23.59



Current Data Parameters
NAME 110304.236 ag 188
EXPNO 10
PROCNO 1

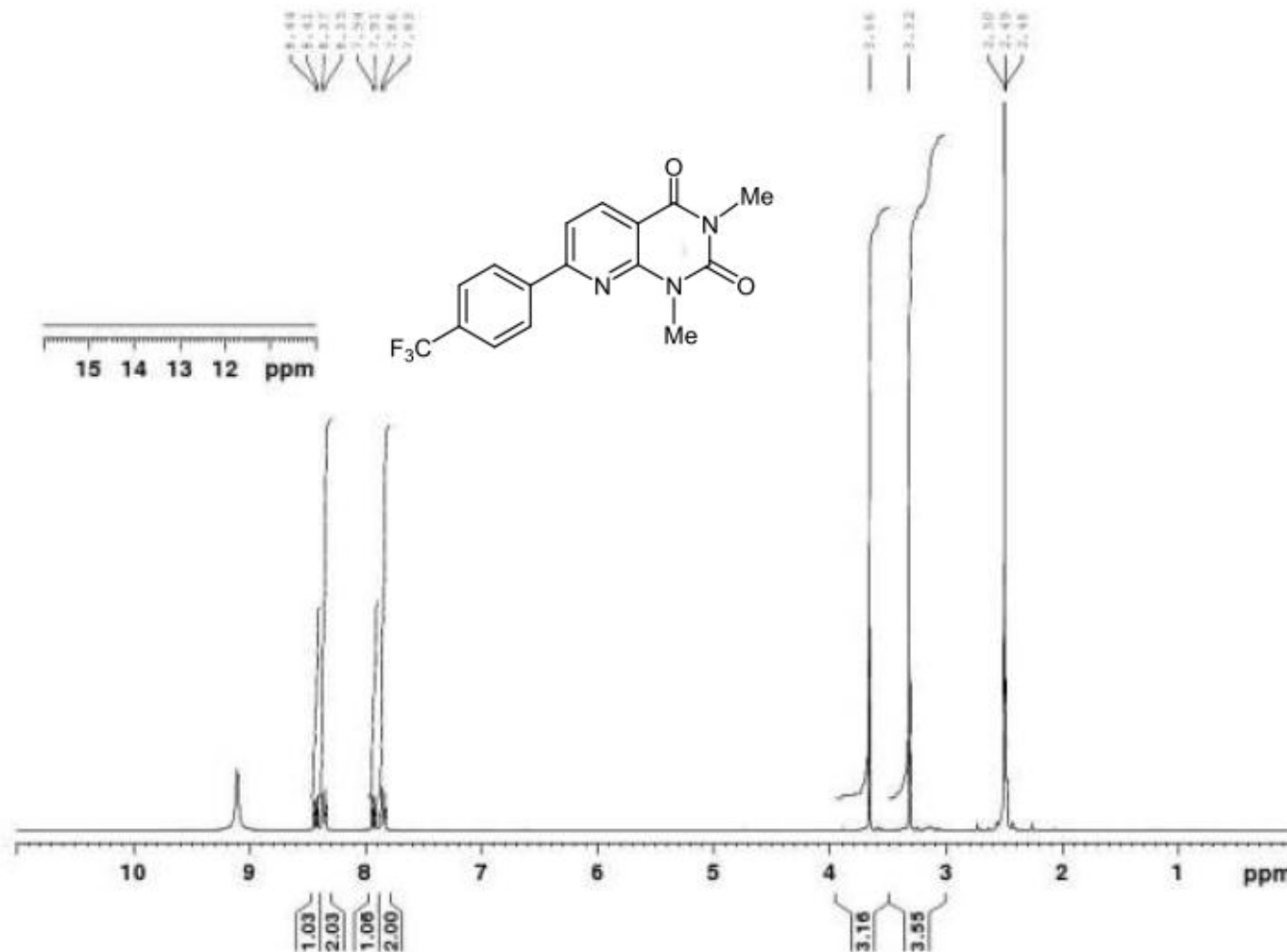
F2 - Acquisition Parameters
Date_ 20110307
Time 12.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 1440
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952696 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

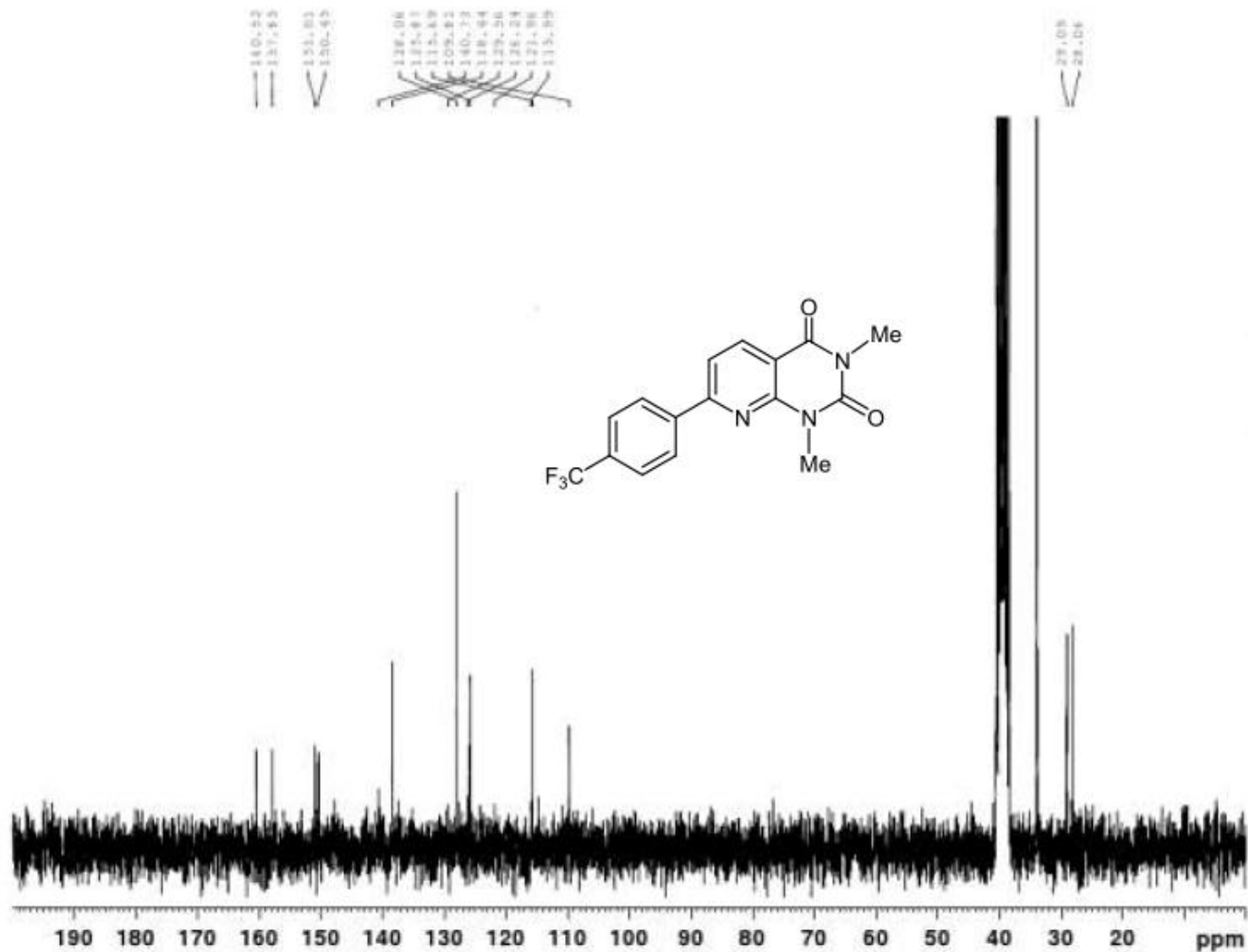
Gevorgyan AG 167 1H DMSO 80 grd/C



NAME 110201_u318 ag 167
EXPNO 10
PROCNO 1
Date_ 20110201
Time 14.47
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 5.2953567 sec
RG 114
DW 80.800 usec
DE 10.00 usec
TE 353.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1316534 MHz
SI 32768
SF 300.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG167(1) 13C DMSO

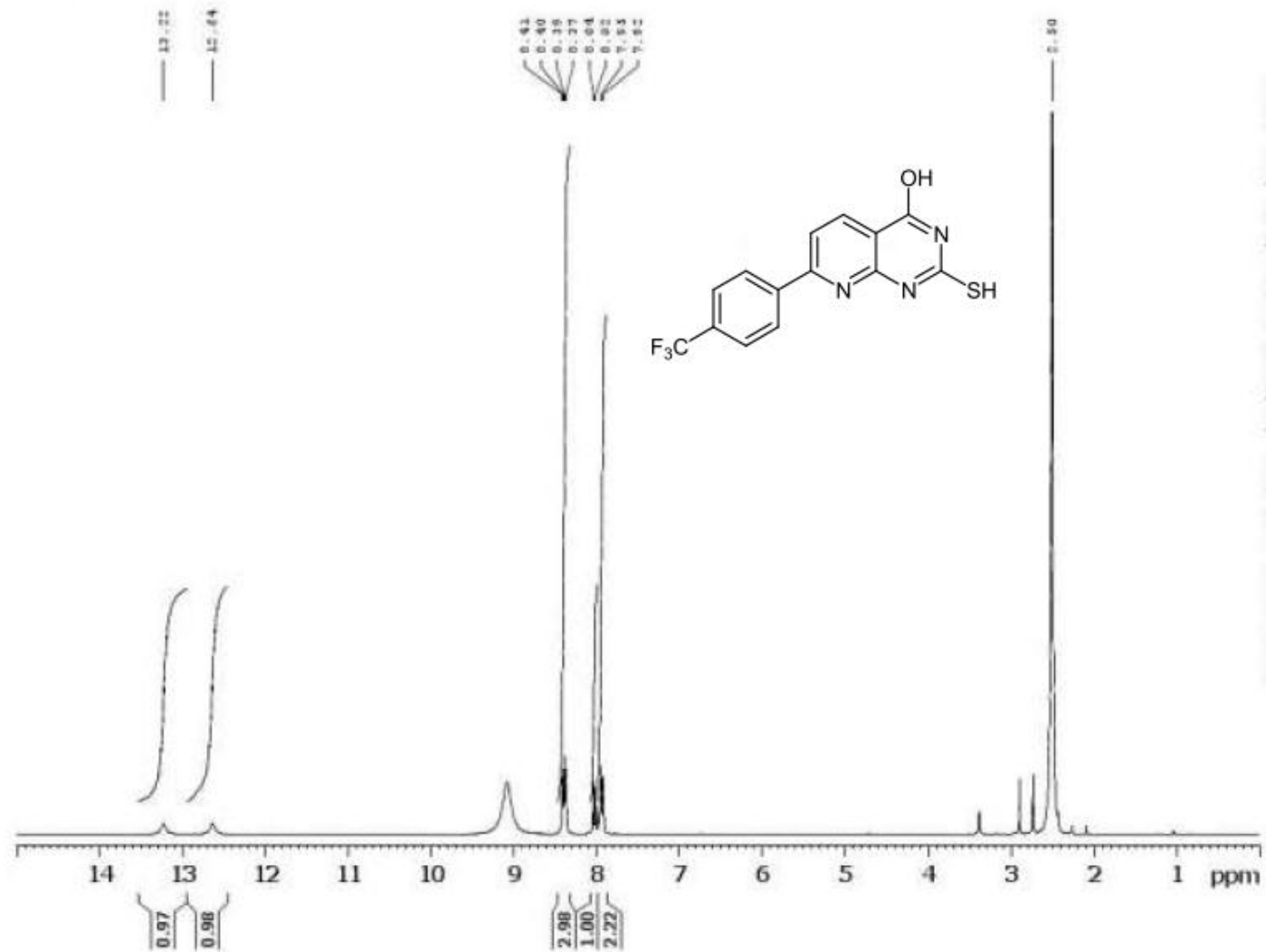


NAME 110211.226 ag 167 G
EXPNO 10
PROCNO 1
Date_ 20110213
Time 6.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952687 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG170 1H DMSO



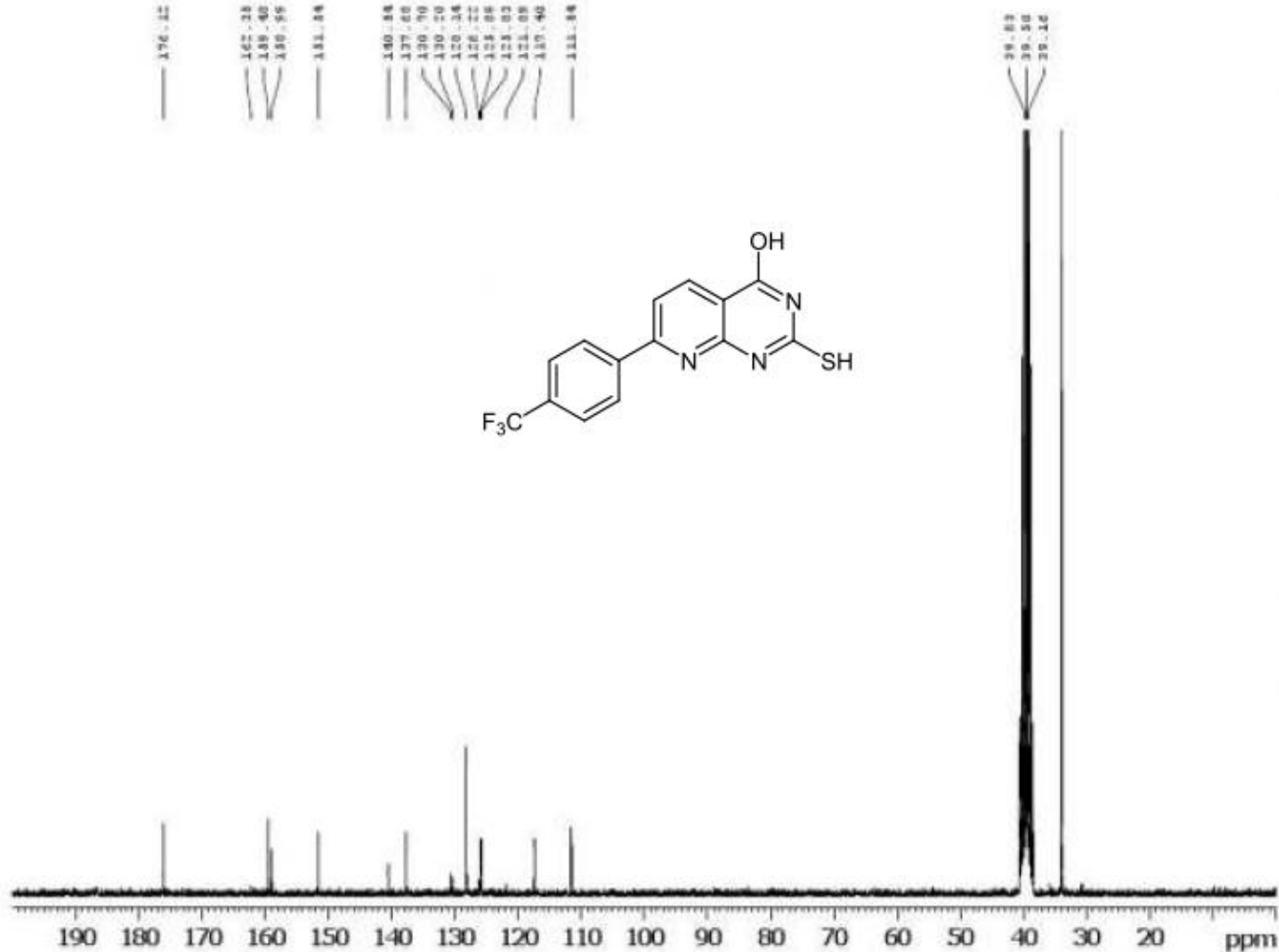
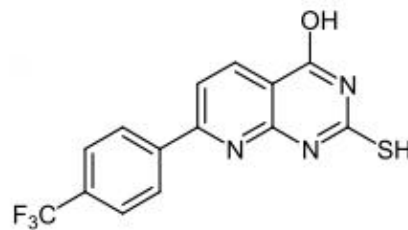
Current Data Parameters
NAME 110131.u329 ag 170
EXPHO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110131
Time 12.34
INSTRUM spect
PROBHD 5 mm PA180 MM
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6181.119 Hz
FIDRES 0.094423 Hz
AQ 5.295397 sec
RG 80.6
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 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300015 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG170 (1) 13C DMSO



Current Data Parameters
NAME 110211.227 ag 170 C
EXPNO 10
PROCNO 1

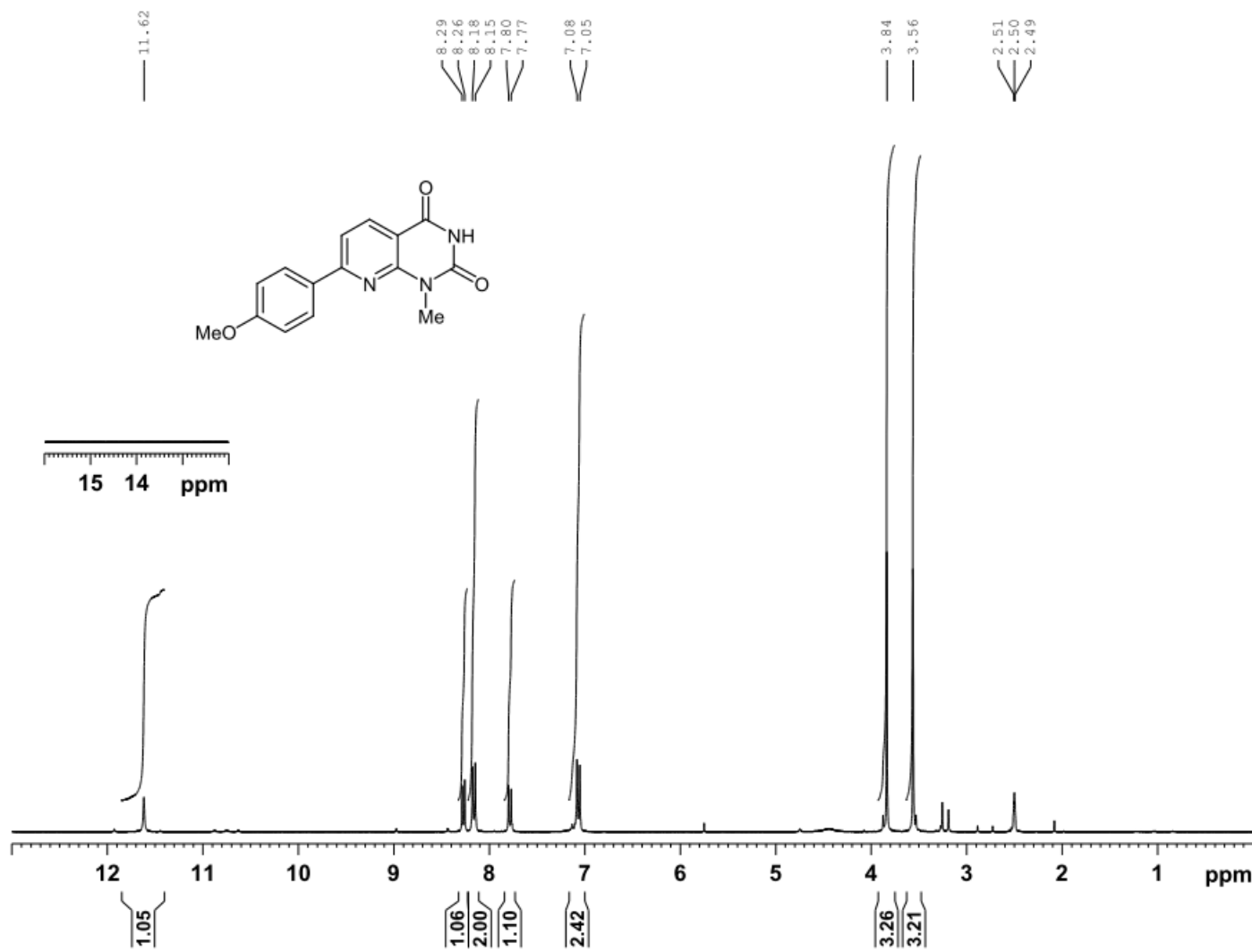
F2 - Acquisition Parameters
Date_ 20110213
Time 8.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
HS 1600
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999996 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310000 MHz

F2 - Processing parameters
SI 32768
SF 62.8952687 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Gevorgyan AG182(1) 1H DMSO



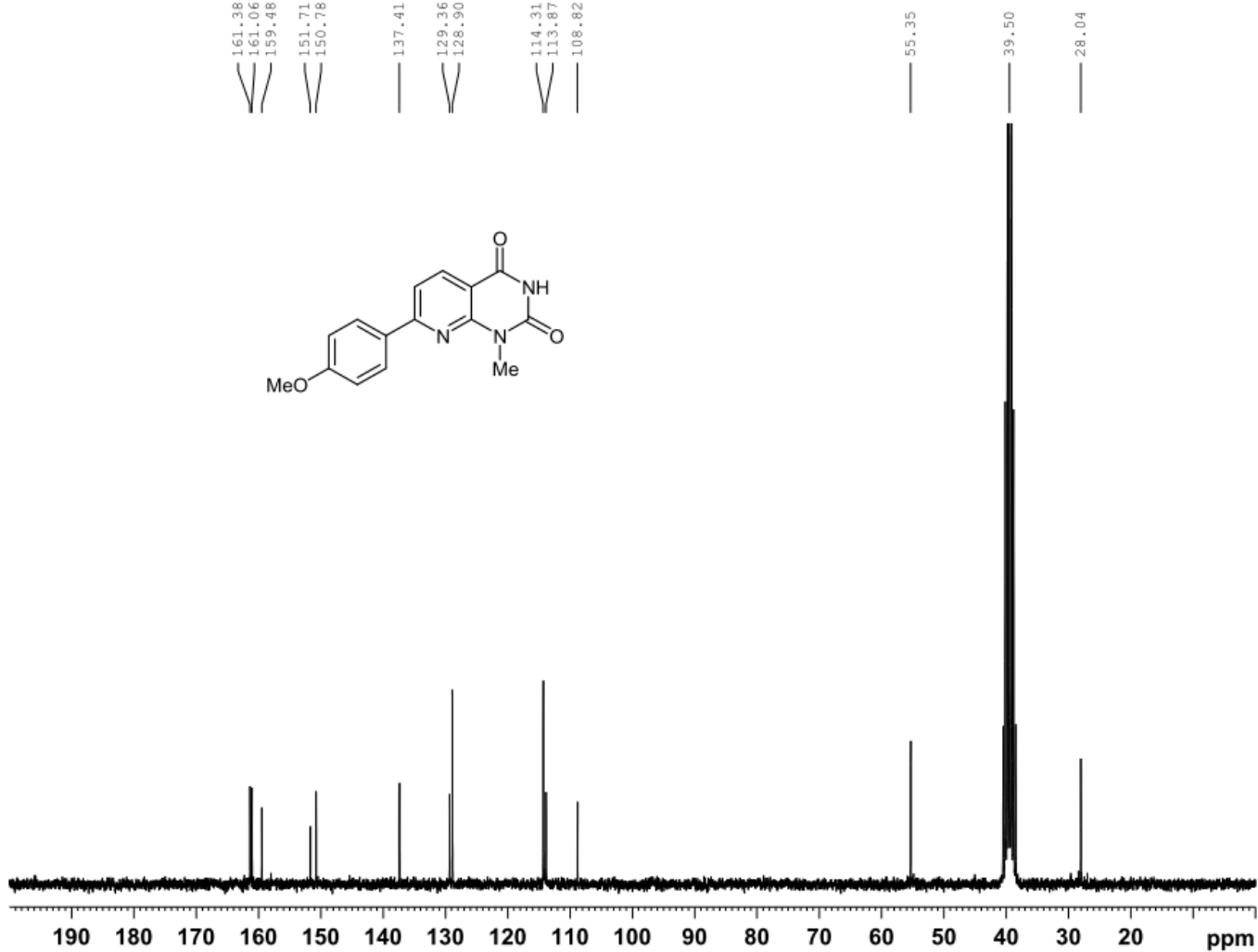
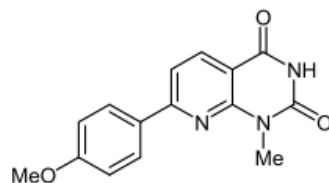
Current Data Parameters
NAME 110218.u313 ag 182
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110218
Time 8.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 144
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 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 300.1300057 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Gevorgyan AG182 (1) 13C DMSO



Current Data Parameters
NAME 110221.208 ag 182 C
EXPNO 10
PROCNO 1

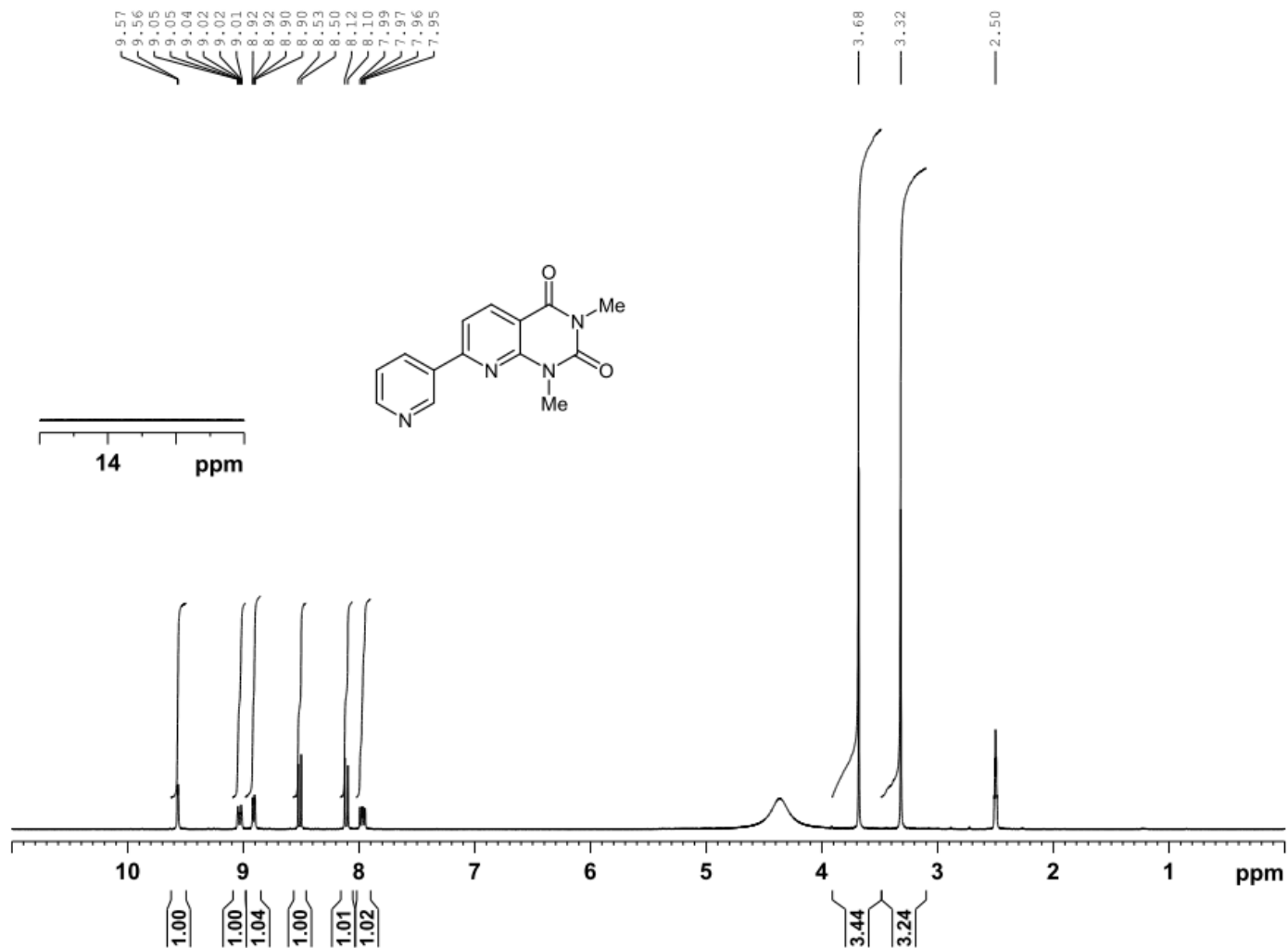
F2 - Acquisition Parameters
Date_ 20110221
Time_ 20.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 62.8952687 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Mkrtchyan SM532 1H DMSO



Current Data Parameters
NAME 110715.u321 sm 532
EXPNO 10
PROCNO 1

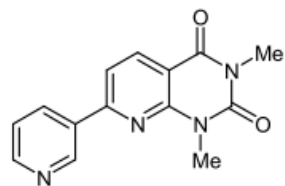
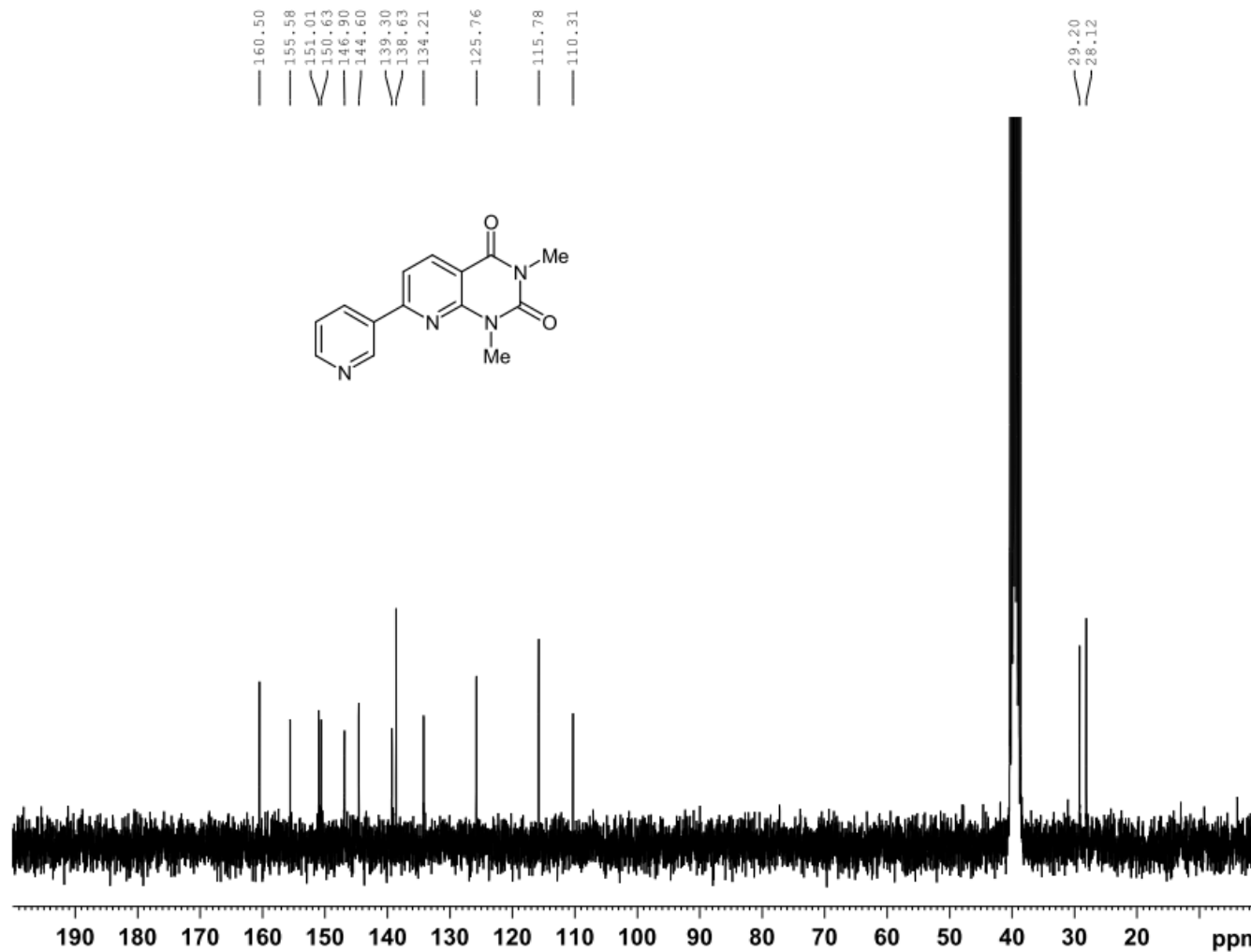
F2 - Acquisition Parameters
Date 20110715
Time 13.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 256
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

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 300.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

141

Mkrtchyan SM532 13C DMSO



NAME 110715.u321 sm 532 C
EXPNO 11
PROCNO 1
Date_ 20110717
Time 15.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677876 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

(D) X-ray single crystal analysis of compounds 15a, 15c and 17a

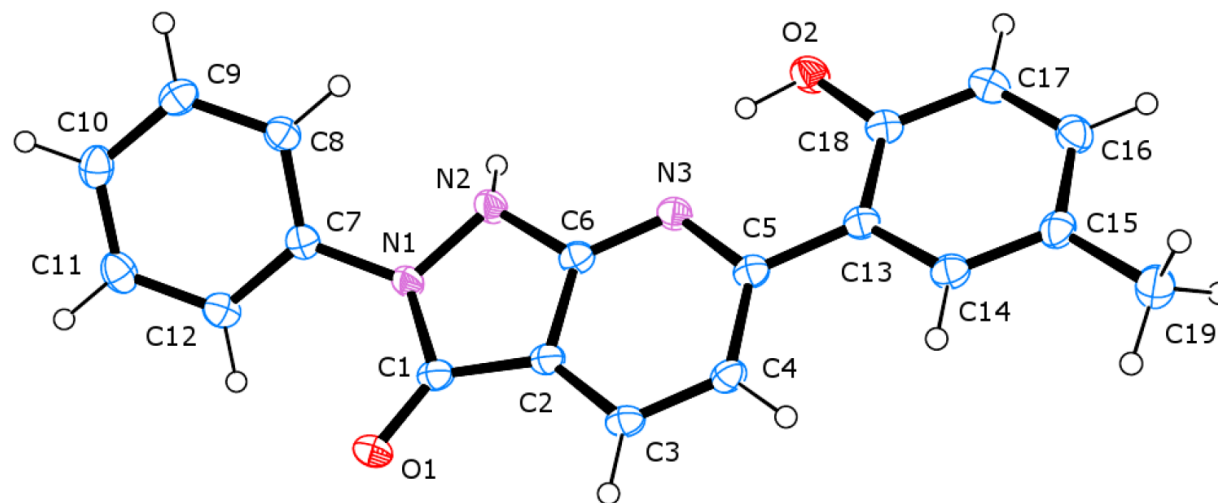


Figure 1. Molecular structure of compound **15a**

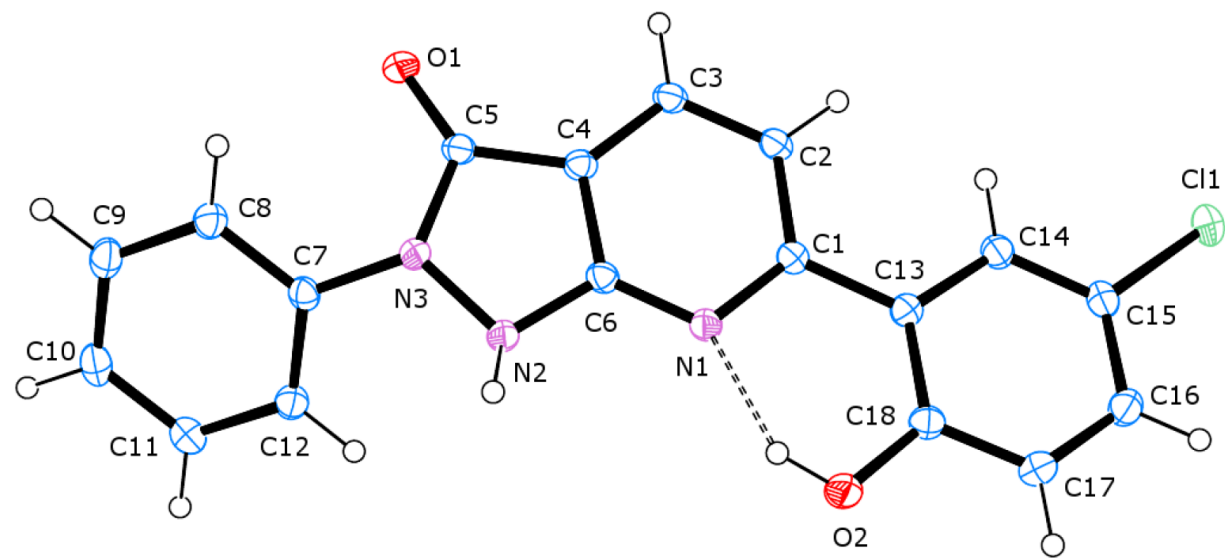


Figure 2. Molecular structure of compound **15c**

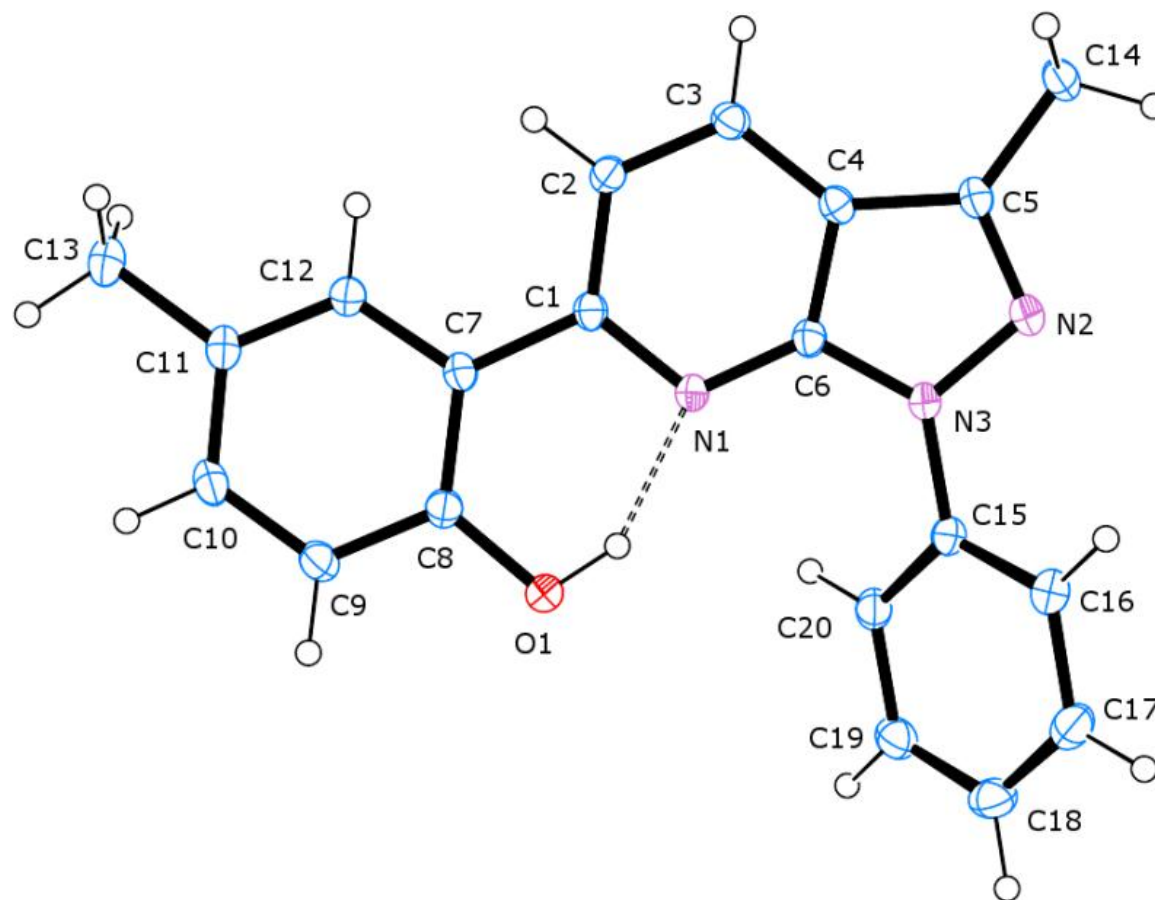


Figure 3. Molecular structure of compound **17a**