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# Pd-catalyzed oxidative C-H arylation of heterocycle embedded thiophene/furan with aryl boronic acid/ester

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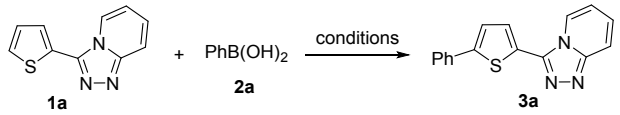
**Table 1**: Optimization of reaction condition




| Entry | Pd cat. (10 mol %) | Oxidant (2 eq) | Ligand/cooxidant (10 mol %) | Solvent | Temp ($^{o}$C) | Yield of **3a** (%)[a] |
|---|---|---|---|---|---|---|
| 1 | $Pd(OAc)_2$ | TEMPO | 2,2'-bipyridyl | DMSO | 110 | 10 |
| 2 | $Pd(OAc)_2$ | TEMPO | 2,2'-bipyridyl | DMF | 110 | 5 |
| 3 | $Pd(OAc)_2$ | $Ag_2CO_3$ | - | DMF | 120 | - |
| 4 | $Pd(OAc)_2$ | $Ag_2CO_3$ | 1,10-phen | DMF | 110 | 10 |
| 5 | $Pd(OAc)_2$ | $Ag_2CO_3$ | 1,10-phen | DMSO | 110 | 70 |
| 6 | $PdCl_2$(dppf) | $Ag_2CO_3$ | 1,10-phen | DMSO | 110 | - |
| 7 | $Pd(OAc)_2$ | $Ag_2CO_3$ | 1,10-phen | AcOH | 100 | - |
| 8 | $Pd(OAc)_2$ | $Ag_2CO_3$ | $Cu(OAc)_2$ | DMSO/t-BuOH | 110 | - |
| 9 | $Pd(OAc)_2$ | $Ag_2CO_3$ | $Cu(OAc)_2$ | DMSO/t-BuCOOH | 110 | - |
| 10 | $Pd(OAc)_2$ | $Ag_2O$ | 1,10-phen | DMSO | 110 | - |
| 11 | $Pd(OAc)_2$ | AgOTf | $Cu(OTf)_2$ | DMSO | 110 | - |
| 12 | $Pd(OAc)_2$ (5 mol %) | $Ag_2CO_3$ | 1,10-phen | DMSO | 110 | 71 |
| 13 | $Pd(OAc)_2$ (5 mol %) | $O_2$ | 1,10-phen | DMSO | 110 | traces |

Treating of 3-(thiophen-2-yl)- [1,2,4]triazolo[4,3-*a*]pyridine **1a** with phenyl boronic acid **2a** under previously reported conditions gave the arylated product **3a** (Table 1) only in trace amounts.[11] Repeated attempts by changing the solvents did not show any improvement in the yield. Further, **1a** and **2a** under 10 mol% of $Pd(OAc)_2$ and silver carbonate in DMF at 120 $^{o}$C for 24 h gave no arylated product. Meanwhile, addition of 10 mol% of 1,10-phenanthroline to the same reaction mixture showed minor amount of arylated product. Increase in the yield was observed during the trial with DMSO (70%). Changing the silver salt and copper salt gave disappointing results. Reduction in the amount of catalyst to 5 mol% of $Pd(OAc)_2$ gave the arylated product **3a** without much compromising the yield (entry 12). Under the optimized condition, molecular oxygen was used as an oxidant instead of $Ag_2CO_3$ but traces of **3a** formation was observed, major **1a** remained in the mixture (entry 13). The spectral data of purified arylated product was indeed proved to be C5-arylation **3a** and thus the outcome is 2,5-disubstituted thiophene derivative.

## 1.Experimental methods

### 1.1.General methods

All the reagents were purchased commercially and used without further purification. Solvents were used without drying. $^{1}H$ and $^{13}C$ NMR spectra were recorded on 300 or 400 MHz Bruker spectrometers in $CDCl_3$ /DMSO-$d_6$. The chemical shifts were reported in δ ppm relative to TMS. IR spectra were recorded on Nicolet 6700 instrument using a universal ATR sampling unit. UPLC was recorded on Acquity ultra performance LC instrument. Melting point was measured in BÜCKI - B545 instrument.

### 1.2. Typical experimental procedure:

**3-(5-Phenylthiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3a):** 3-(Thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (0.2 g, 1 mmol), phenylboronic acid (2 mmol), silvercarbonate (2 mmol) and 1, 10-phenanthroline (0.1 mmol) were taken in dry DMSO (5 mL). The mixture was bubbled with nitrogen for 10 mins. Then $Pd(OAc)_2$ (0.05 mmol) was added to the mixture and heated to 110 $^{o}$C for 24 h. The mixture was filtered through the celite pad and washed with DCM (20 mL). The organic layer was washed with water (2 x 20 mL), brine(20 mL) and dried over sodium sulphate. The organic layer was concentrated under reduced pressure to give a residue which was purified by silica gel column chromatography using 20% EtOAc in DCM to afford 0.19 g (70 %) of **3a** as a yellow solid. A similar procedure was followed for arylation of all other examples (Tables 2- 4).

## 2. Characterization of all the compounds.

**3-(5-Phenylthiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3a)**

mp 205-207 $^{o}$C. IR (neat) 2920, 2851, 2361, 1969, 1629, 1490, 1070, 903, 747, 684 $cm^{-1}$. **$^{1}H$ NMR (400 MHz, DMSO-$d_6$):** δ 8.82 (d, *J* = 7.04 Hz, 1H), 7.95 (d, *J* = 3.92 Hz, 1H ), 7.90 (d, *J* = 9.28 Hz, 1H), 7.80 (d, *J* = 7.88 Hz, 1H), 7.55 (d, *J* = 3.88 Hz, 1H), 7.51-7.47 (m, 3H), 7.39 (t, *J* = 7.20 Hz, 1H), 7.14 (t, *J* = 6.76 Hz, 1H); **$^{13}C$ NMR (75 MHz, $CDCl_3$):** 150.5, 145.4, 141.7, 133.3, 129.7, 128.9, 128.6, 128.1, 127.2, 126.1, 125.2, 125.0, 116.2, 115.4. UPLC: $(M + H)^+$ 278.2. Anal. Calcd. For $C_{16}H_{11}N_3S$: C, 69.29; H, 4.00; N, 15.15. Found: C, 69.47; H, 4.32; N, 15.42.

**3-(5-*p*-Tolylthiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3b)**

mp 248-250 $^{o}$C. IR (neat) 3435, 2924, 1634, 1497, 1485, 1069, 804, 749 $cm^{-1}$. **$^{1}H$ NMR (400 MHz, $CDCl_3$):** δ 8.47 (d, *J* = 7.20 Hz, 1H), 7.88 (d, *J* = 9.20 Hz, 1H),7.64 (d, *J* = 3.60 Hz, 1H), 7.58 (d, *J* = 8.00 Hz, 2H), 7.40 (d, *J* = 3.60 Hz, 1H), 7.34 (t, *J* = 7.20 Hz, 1H)), 7.26 (d, *J* = 8.00 Hz, 2H), 6.98 (t, *J* = 6.80 Hz, 1H), 2.41 (s, 3H); **$^{13}C$ NMR (100 MHz, DMSO-$d_6$):** δ 150.5, 145.7, 138.5, 130.6, 130.3, 128.6, 128.1, 126.6, 125.0, 124.7,

116.2, 115.4, 21.3. UPLC: $(M + H)^+$ 292.5. Anal. Calcd. For $C_{17}H_{13}N_3S$: C, 70.08; H, 4.50; N, 14.42. Found: C, 70.18; H, 4.45; N, 14.52.

**3-(5-(3,5-Dimethylphenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3c)**

mp 153-155 $^oC$. IR (neat) 3436, 3083, 2920, 1633, 1599, 1498, 1377, 1069, 1006, 911, 839, 818, 753 $cm^{-1}$. **$^1H$ NMR (400 MHz, DMSO-$d_6$):** δ 8.80 (d, *J* = 7.04 Hz, 1H), 7.91-7.88 (m, 2H ), 7.68 (d, *J* = 3.92 Hz, 1H), 7.49-7.45 (m, 1H), 7.40 (s, 2H), 7.13 (td, *J* = 6.72, 0.96 Hz, 1H), 7.01 (s, 1H), 2.33 (s, 6H); **$^{13}C$ NMR (100 MHz, DMSO-$d_6$):** δ 150.5, 145.8, 141.8, 138.9, 133.2, 130.4, 128.5, 128.1, 126.9, 125.0, 124.9, 123.9, 116.2, 115.4, 21.3. UPLC: $(M + H)^+$ 306.5. Anal. Calcd. For $C_{18}H_{15}N_3S$: C, 70.79; H, 4.95; N, 13.76. Found: C, 70.56; H, 5.00; N, 13.50.

**3-(5-Mesitylthiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3d)**

mp 139-137 $^oC$. IR (neat) 3435, 3114, 2923, 2853, 1743, 1634, 1612, 1497, 1076, 1061, 841, 812, 745, 733 $cm^{-1}$. **$^1H$ NMR (400 MHz, $CDCl_3$):** δ 8.47 (d, *J* = 6.80 Hz, 1H), 7.87 (d, *J* = 9.20 Hz, 1H), 7.69 (d, *J* = 3.60 Hz, 1H), 7.36-7.31 (m, 1H), 6.99 (s, 2H), 6.97(d, *J* = 3.20 Hz, 1H), 2.36 (s, 3H), 2.21 (s, 6H); **$^{13}C$ NMR (100 MHz, DMSO-$d_6$):** δ 150.4, 143.3, 141.7, 138.3, 137.7, 129.8, 128.6, 128.6, 128.5, 128.1, 127.3, 124.9, 116.2, 115.4, 21.1, 20.9. UPLC: $(M + H)^+$ 320.3. Anal. Calcd. For $C_{19}H_{17}N_3S$: C, 71.44; H, 5.36; N, 13.15. Found: C, 71.55; H, 5.67; N, 13.36.

**3-(5-(4-*tert*-Butylphenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3e)**

mp 204-206 $^oC$. IR (neat) 3107, 2957, 2361, 1632, 1572, 1450, 1378, 1264, 1114, 1069, 963, 906, 795, 757 $cm^{-1}$. **$^1H$ NMR (400 MHz, $CDCl_3$):** δ 8.47 (d, *J* = 7.04 Hz, 1H), 7.88 (d, *J* = 9.28 Hz, 1H), 7.64-7.61 (m, 3H), 7.47 (d, *J* = 8.60 Hz, 2H), 7.41 (d, *J* = 3.88 Hz, 1H), 7.36-7.32 (m, 1H), 7.00 (td, *J* = 6.86, 0.84 Hz, 1H), 1.37 (s, 9H); **$^{13}C$ NMR (100 MHz, $CDCl_3$):** δ 151.8, 147.2, 130.6, 127.8, 127.1, 126.1 125.9 (3C), 125.8 (2C), 123.3, 123.0, 116.9, 114.6, 34.7, 31.2. UPLC: $(M + H)^+$ 334.7. Anal. Calcd. For $C_{20}H_{19}N_3S$: C, 72.04; H, 5.74; N, 12.60. Found: C, 71.90; H, 5.87; N, 12.41.

**3-(5-(4-Methoxyphenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3f)**

mp 188-192 $^oC$. IR (neat) 1602, 1563, 1480, 1250, 1176, 1064, 1025, 811, 732, 686 $cm^{-1}$. **$^1H$ NMR (400 MHz, DMSO-$d_6$):** δ 8.78 (d, *J* = 7.20 Hz, 1H), 7.87 (m, 2H), 7.71 (d, *J* = 8.88 Hz, 2H), 7.59 (d, *J* = 3.60 Hz, 1H), 7.48-7.44 (m, 1H), 7.13 (td, *J* = 6.80, 0.80 Hz, 1H), 7.03 (d, *J* = 8.88 Hz, 2H), 3.80 (s, 3H); **$^{13}C$ NMR (75 MHz, DMSO-$d_6$):** δ 159.9, 150.5, 145.6, 141.8, 128.5, 128.1, 127.5, 126.0,124.9, 124.0, 116.2, 115.4, 115.1, 55.8. UPLC: $(M + H)^+$ 308.2. Anal. Calcd. For: $C_{17}H_{13}N_3OS$: C, 66.43; H, 4.26; N, 13.67. Found: C, 66.54; H, 4.06; N, 13.76.

**3-(5-(3-Methoxyphenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3g)**

mp 172-174 °C. IR (neat) 1600, 1572, 1471, 1281, 1222, 1163, 1045, 853, 807, 765, 728, 683 $cm^{-1}$. **$^1$H NMR (400 MHz, DMSO-$d_6$):** δ 8.80 (d, *J* = 7.20 Hz, 1H), 7.92 (d, *J* = 4.00 Hz, 1H), 7.88 (d, *J* = 9.20 Hz 1H), 7.75 (d, *J* = 4.00 Hz, 1H),7.49-7.45 (m, 1H), 7.40-7.31 (m, 3H), 7.12 (td, *J* = 6.80, 0.80 Hz, 1H), 6.95 (dt, *J* = 6.80, 1.2 Hz, 1H), 3.83 (s, 3H); **$^{13}$C NMR (75 MHz, DMSO-$d_6$):** δ 160.3, 150.5, 145.3, 141.7, 134.6, 130.9, 128.6, 128.0, 127.3, 125.6, 125.0, 118.6, 116.2, 115.4, 114.5, 111.4, 55.7. UPLC: $(M + H)^+$ 308.2. Anal. Calcd. For: $C_{17}H_{13}N_3OS$: C, 66.43; H, 4.26; N, 13.67. Found: C, 66.67; H, 4.34; N, 13.72.

**3-(5-(3-Ethoxyphenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3h)**

mp 177-179 °C. IR (neat) 3433, 2925, 1603, 1576, 1286, 1273, 1192, 1177, 1069, 1051, 812, 771, 748, 732 $cm^{-1}$. **$^1$H NMR (300 MHz, $CDCl_3$):** δ 8.45 (d, *J* = 6.96 Hz, 1H), 7.86 (d, *J* = 9.27 Hz, 1H), 7.63 (d, *J* = 3.84 Hz, 1H), 7.42 (d, *J* = 3.84 Hz, 1H), 7.36-7.29 (m, 2H), 7.20 (d, *J* = 1.83 Hz, 1H), 6.97 (t, *J* = 6.81 Hz, 1H), 6.90 (dd, *J* = 8.07, 1.38 Hz, 1H), 4.10 (q, *J* = 6.99 Hz, 2H), 1.46 (t, *J* = 6.99 Hz, 3H); **$^{13}$C NMR (100 MHz, DMSO-$d_6$):** δ 159.6, 150.5, 145.3, 134.6, 130.9, 128.6, 128.1, 127.7, 127.2, 125.5, 125.0, 118.5, 116.2, 115.4, 114.9, 114.7, 112.0, 63.7, 15.1. UPLC: $(M + H)^+$ 322.5. Anal. Calcd. For: $C_{18}H_{15}N_3OS$: C, 67.27; H, 4.70; N, 13.07. Found: C, 66.50; H, 4.72; N, 13.13.

**3-(5-(2-(Methylthio)phenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3i)**

mp 140-142 °C. IR (neat) 3103, 2917, 2854, 1563, 1494, 1410, 1376, 1276, 1056, 1002, 963, 794 $cm^{-1}$. **$^1$H NMR (400 MHz, $CDCl_3$):** δ 8.50 (d, *J* = 6.80 Hz, 1H), 7.89 (d, *J* = 9.20 Hz, 1H), 7.68 (d, *J* = 3.60 Hz, 1H), 7.49 (dd, *J* = 7.60, 1.60 Hz, 1H), 7.41 (d, *J* = 4.00 Hz, 1H), 7.41-7.32 (m, 3H), 7.27-7.23 (m, 1H), 6.99 (t, *J* = 6.80 Hz, 1H), 2.49 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$):** δ 144.2, 138.0, 132.0, 130.8, 129.0, 128.3, 127.4, 127.1, 126.2, 125.1, 123.0, 116.8, 114.7, 16.3. UPLC: $(M + H)^+$ 324.6.

**3-(5-(3-(Methylthio)phenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3j)**

mp 150-152 °C. IR (neat) 3112, 2915, 1632, 1587, 1561, 1495, 1478, 1068, 800, 770, 746, 691, 671 $cm^{-1}$. **$^1$H NMR (400 MHz, $CDCl_3$):** δ 8.45 (d, *J* = 6.80 Hz, 1H), 7.84 (d, *J* = 9.20 Hz, 1H), 7.62 (d, *J* = 3.60 Hz, 1H), 7.52 (s, 1H), 7.43-7.41 (m, 2H), 7.36-7.29 (m, 2H), 7.23 (d, *J* = 7.60 Hz, 1H), 7.00 (t, *J* = 6.80Hz, 1H), 2.55 (s, 3H); **$^{13}$C NMR (75 MHz, $CDCl_3$):** δ 146.1, 139.7, 133.8, 129.4, 127.6, 127.1, 126.7, 126.2, 124.0, 123.8, 122.8, 122.7, 116.8, 114.6, 15.7. UPLC: $(M + H)^+$ 324.2. Anal. Calcd. For: $C_{17}H_{13}N_3S_2$: C, 63.13; H, 4.05; N, 12.99. Found: C, 63.40; H, 4.50; N, 13.12.

**3-(5-(Biphenyl-3-yl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3k)**

mp 162-164 °C. IR (neat) 2928, 2856, 2361, 1730, 1593, 1495, 1471, 1378, 1275, 1070, 794, 690 $cm^{-1}$. **$^1$H NMR (400 MHz, CDCl3):** δ 8.50 (d, *J* = 7.20 Hz, 1H), 7.91-7.89 (m, 2H), 7.70-7.66 (m, 4H), 7.58 (d, *J*= 7.60 Hz, 1H), 7.55-7.49 (m, 4H), 7.44-7.40 (m, 1H), 7.35 (t, *J* = 7.60 Hz, 1H), 7.00 (t, *J* = 6.80 Hz, 1H); **$^{13}$C NMR (75 MHz, DMSO-$d_6$):** δ 146.9, 142.3, 140.5, 133.8, 129.6, 128.9, 128.0, 127.7, 127.4, 127.3, 127.2, 126.4, 124.9, 124.0, 123.0, 116.9, 114.8. UPLC: $(M + H)^+$ 354.7. Anal. Calcd. For: $C_{22}H_{15}N_3S$: C, 74.76; H, 4.28; N, 11.89. Found: C, 74.36; H, 4.48; N, 12.00.

**3-(5-(Naphthalen-2-yl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3l)**

mp 214-216 °C. IR (neat) 3109, 2917, 1630, 1495, 1378, 1065, 814, 745 $cm^{-1}$. **$^1$H NMR (400 MHz, CDCl3):** δ 8.52 (d, *J* = 6.80 Hz, 1H), 8.14 (s, 1H), 7.92-7.86 (m, 4H), 7.80 (d, *J* = 8.52 Hz, 1H), 7.71 (d, *J* = 3.68 Hz, 1H), 7.58 (d, *J* = 3.64 Hz, 1H), 7.55-7.50 (m, 2H), 7.37 (t, *J* = 7.40 Hz, 1H), 7.02 (t, *J* = 6.68 Hz, 1H); **$^{13}$C NMR (100 MHz, DMSO-$d_6$):** δ 150.6, 145.4, 141.7, 133.7, 133.1, 130.8, 129.3, 128.6, 128.2, 128.1, 127.5, 127.4, 127.0, 125.8, 125.0, 124.5, 124.3, 116.2, 115.5. UPLC: $(M + H)^+$ 328.3. Anal. Calcd. For: $C_{20}H_{13}N_3S$: C, 73.37; H, 4.00; N, 12.83. Found: C, 73.56; H, 3.98; N, 12.56.

**3-(5-Phenylfuran-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (4a)**

mp 135-137 °C. IR (neat) 3130, 3056, 2921, 1630, 1490, 1450, 1074, 1015, 797, 752, 687 $cm^{-1}$. **$^1$H NMR (400 MHz, DMSO-$d_6$):** δ 8.89 (d, *J* = 6.92 Hz, 1H), 7.92-7.90 (m, 3H ), 7.52-7.47 (m, 3H), 7.43 (d, *J* = 2.16 Hz, 1H), 7.38 (t, *J* = 7.72 Hz, 1H), 7.30 (d, *J* = 3.32 Hz, 1H), 7.18 (t, *J* = 6.60 Hz, 1H); **$^{13}$C NMR (100 MHz, $CDCl_3$):** 155.2, 142.1, 129.8, 129.0, 128.4, 127.4, 124.0, 116.8, 114.7, 113.2, 107.3. UPLC: $(M + H)^+$ 262.5. Anal. Calcd. For: $C_{16}H_{11}N_3O$: C, 73.55; H, 4.24; N, 16.08. Found: C, 73.70; H, 4.30; N, 16.02.

**3-(5-(4-*tert*-Butylphenyl)furan-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (4b)**

mp 167-169 °C. IR (neat) 3422, 3134, 2961, 1636, 1495, 1270, 1068, 1027, 834, 787, 749, 736 $cm^{-1}$. **$^1$H NMR (400 MHz, $CDCl_3$):** δ 8.85 (d, *J* = 7.04 Hz, 1H), 7.86 (d, *J* = 9.28 Hz, 1H), 7.71 (d, *J* = 8.40 Hz, 2H), 7.51 (d, *J* = 8.40 Hz, 2H), 7.36 (d, *J* = 3.52 Hz, 1H), 7.34-7.32 (m, 1H), 7.00 (t, *J* = 6.80 Hz, 1H), 6.86 (d, *J* = 3.56 Hz, 1H), 1.38 (s, 9H); **$^{13}$C NMR (75 MHz, $CDCl_3$):** δ 155.3, 151.6, 141.8, 127.2, 127.1, 125.9, 124.0, 123.8, 116.7, 114.6, 113.2, 106.7, 34.7, 31.2. UPLC: $(M + H)^+$ 318.3. Anal. Calcd. For: $C_{20}H_{19}N_3O$: C, 75.69; H, 6.03; N, 13.24. Found: C, 76.00; H, 5.98; N, 13.41.

**3-(5-Mesitylfuran-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (4c)**

mp 140-142 °C. IR (neat) 3142, 2922, 1656, 1610, 1573, 1374, 1180, 1130, 1033, 1016, 757 $cm^{-1}$. **$^1$H NMR (400 MHz, $CDCl_3$):** δ 8.72 (d, *J* = 7.12 Hz, 1H), 7.83 (d, *J* = 9.31 Hz, 1H), 7.43 (d, *J* = 3.44 Hz, 1H), 7.31-7.27 (m, 1H), 7.02 (s, 2H), 6.90-6.86 (m, 1H), 6.54 (d, *J* = 3.44 Hz, 1H), 2.38 (s, 3H), 2.27 (s, 6H); **$^{13}$C NMR (75**

**MHz, $CDCl_3$):** δ 153.7, 149.8, 142.0, 139.7, 139.3, 138.5, 128.4, 127.1, 127.0, 124.3, 116.5, 114.3, 112.0, 111.7, 21.1, 20.5. UPLC: $(M + H)^+$ 304.3. Anal. Calcd. For: $C_{20}H_{19}N_3O$: C, 75.23; H, 5.65; N, 13.85. Found: C, 75.37; H, 5.29; N, 13.54.

**3-(5-(3-Methoxyphenyl)furan-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (4d)**

mp 128-130 °C. IR (neat) 1583, 1488, 1378, 1290, 1222, 1079, 1042, 1034, 796, 776, 753 $cm^{-1}$. **$^1$H NMR (400 MHz, $CDCl_3$):** δ 8.83 (d, *J* = 6.80 Hz, 1H), 7.86 (d, *J* = 9.20 Hz, 1H), 7.42-7.33 (m, 4H), 7.29-7.28 (m, 1H), 7.01 (t, *J* = 6.80 Hz, 1H), 6.93-6.90 (m, 2H), 3.91 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$):** δ 160.0, 155.0, 142.2, 131.1, 130.1, 127.4, 124.0, 116.7, 116.6, 114.8, 113.5, 113.2, 110.0, 107.7, 55.4. UPLC: $(M + H)^+$ 292.2. Anal. Calcd. For: $C_{17}H_{13}N_3O_2$: C, 70.09; H, 4.50; N, 14.42. Found: C, 70.22; H, 4.45; N, 14.53.

**3-(5-(4-Methoxyphenyl)furan-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (4e)**

mp 168-170 °C. IR (neat) 2933, 2362, 1549, 1255, 1009, 813, 794 $cm^{-1}$. **$^1$H NMR (400 MHz, CDCl3):** δ 8.81 (d, *J* = 7.04 Hz, 1H), 7.86 (d, *J* = 9.24 Hz, 1H), 7.70 (dd, *J* = 6.86, 1.96 Hz, 2H), 7.36-7.32 (m, 2H), 7.02-6.99 (m, 3H), 6.77 (d, *J* = 3.56 Hz, 1H), 3.88 (s, 3H); **$^{13}$C NMR (100 MHz, CDCl3):** δ 159.8, 155.4, 141.4, 127.4, 125.6, 124.0, 12.8, 116.7, 114.7, 114.5, 113.4, 105.8, 55.4. UPLC: $(M + H)^+$ 292.6. Anal. Calcd. For: $C_{17}H_{13}N_3O_2$: C, 70.09; H, 4.50; N, 14.42. Found: C, 70.12; H, 4.54; N, 14.34.

**3-(5-(3-(Methylthio)phenyl)furan-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (4f)**

Low melting solid. IR (neat) 2931, 2231, 1689, 1638, 1401, 1265, 1145, 792, 753 $cm^{-1}$. **$^1$H NMR (400 MHz, $CDCl_3$):** δ 8.85 (d, *J* = 6.88 Hz, 1H), 7.96-7.94 (m, 1H), 7.64 (s, 1H), 7.54 (d, *J* = 7.72 Hz, 1H), 7.43-7.38 (m, 3H), 7.27-7.25 (m, 1H), 7.08 (t, J = 6.80 Hz, 1H), 6.92 (d, *J* = 3.52 Hz, 1H), 2.55 (s, 3H) ; **$^{13}$C NMR (100 MHz, $CDCl_3$):** δ 154.9, 142.0, 139.7, 130.3, 129.4, 128.1, 126.3, 124.1, 122.1, 120.8, 116.6, 115.2, 113.7, 107.9, 15.8. UPLC: $(M + H)^+$ 308.2.

**3-(5-(4-*tert*-Butylphenyl)thiophen-2-yl)-[1,2,4]triazolo[3,4-a]isoquinoline (5a)**

mp 285-287 °C. IR (neat) 3430, 2958, 1515, 1483, 1474, 1426, 1385, 1360, 819, 786 $cm^{-1}$. **$^1$H NMR (400 MHz, $CDCl_3$):** δ 8.86 (d, *J* = 7.20 Hz, 1H), 8.22 (d, *J* = 7.20 Hz, 1H), 7.81-7.71 (m, 3H), 7.67 (d, *J* = 4.0 Hz, 1H), 7.64 (d, *J* = 6.80 Hz, 2H), 7.49 (dd, *J* = 6.40, 2.00 Hz, 2H), 7.43 (d, *J* = 3.60 Hz, 1H), 7.22 (d, *J* = 7.60 Hz, 1H), 1.37 (s, 9H); **$^{13}$C NMR (100 MHz, $CDCl_3$):** δ 151.7, 149.1, 147.5, 143.7, 130.6, 130.3, 129.7, 129.4, 128.5, 127.1, 126.1, 125.9, 125.7, 124.3, 123.4, 121.6, 119.7, 115.9, 34.7, 31.2. UPLC: $(M + H)^+$ 384.3.

**3-(5-(3-Methoxyphenyl)thiophen-2-yl)-[1,2,4]triazolo[3,4-a]isoquinoline (5b)**

mp 173-175 °C. IR (neat) 3422, 1601, 1576, 1567, 1521, 1471, 1424, 1289, 1165, 1053, 786, 761, 700 $cm^{-1}$. **$^1$H NMR (400 MHz, $CDCl_3$):** δ 8.86 (d, *J* = 7.6 Hz, 1H), 8.22 (d, *J* = 7.2 Hz, 1H), 7.81-7.73 (m, 3H), 7.68 (d, *J* =

3.60 Hz, 1H), 7.46 (d, *J* = 3.60 Hz, 1H), 7.37 (t, *J* = 7.60 Hz, 1H), 7.31-7.29 (m, 1H), 7.22 (d, *J* = 7.60 Hz, 2H), 6.94 (dd, *J* = 2.40, 8.0 Hz, 1H), 3.90 (s, 3H); **$^{13}$C NMR (75 MHz, $CDCl_3$):** δ 160.0, 147.1, 134.5, 130.2, 130.1, 129.6, 129.3, 128.4, 127.0, 126.2, 124.2, 123.9, 119.5, 118.6, 115.9, 113.9, 111.7, 55.3. UPLC: $(M + H)^+$ 358.3. Anal. Calcd. For: $C_{21}H_{15}N_3OS$: C, 70.57; H, 4.23; N, 11.76. Found: C, 70.71; H, 4.09; N, 11.45.

**3-(5-Mesitylthiophen-2-yl)-[1,2,4]triazolo[3,4-a]isoquinoline (5c)**

mp 180-184 $^{o}$C. IR (neat) 2929, 2850, 1720, 1603, 1560, 1518, 1252, 793 cm$^{-1}$. **$^1$H NMR (400 MHz, $CDCl_3$):** δ 8.83 (d, *J* = 8.20 Hz, 1H), 8.21 (d, *J* = 7.40 Hz, 1H), 7.80-7.72 (m, 3H), 7.71 (d, *J* = 3.60 Hz, 1H), 7.19 (d, *J* = 7.44 Hz, 1H), 6.99-6.98 (m, 1H), 2.35 (s, 3H), 2.21 (s, 6H); **$^{13}$C NMR (100 MHz, $CDCl_3$):** δ 149.1, 145.2, 143.8, 138.5, 138.1, 130.2, 129.7, 129.7, 129.3, 128.3, 128.0, 127.6, 127.2, 127.1, 124.3, 121.7, 119.7, 115.8, 21.1, 20.8. UPLC: $(M + H)^+$ 370.7. Anal. Calcd. For: $C_{23}H_{19}N_3S$: C, 74.77; H, 5.18; N, 11.37. Found: C, 75.03; H, 5.21; N, 11.49.

**2-(5-Mesitylthiophen-2-yl)pyridine (6a)**

IR (neat) 2918, 1582, 1464, 1430, 772 cm$^{-1.}$ **$^1$H NMR (400 MHz, $CDCl_3$):** δ 8.60-8.58 (m, 2H), 7.74-7.68 (m, 2H), 7.62 (d, *J* = 3.64 Hz, 1H), 7.18-7.15 (m, 1H),6.98 (s, 2H), 6.84 (d, *J* = 3.64 Hz, 1H), 2.35 (s, 3H), 2.21 (s, 6H). **$^{13}$C NMR (100 MHz, $CDCl_3$):** δ 152.7, 149.5, 144.2, 138.1, 138.0, 136.8, 130.9, 128.2, 127.8, 124.9, 121.7, 118.7, 21.1, 20.8. Anal. Calcd. For: C, 77.38; H, 6.13; N, 5.01. Found: C, 77.65; H, 5.94; N, 5.20.

**1-(5-Mesitylthiophen-2-yl)-1H-pyrazole (6b)**

IR (neat) 2916, 1565, 1521, 1386, 1043, 922, 791, 744 cm$^{-1.}$ **$^1$H NMR (400 MHz, $CDCl_3$):** δ 7.85 (d, *J* = 2.40 Hz, 1H), 7.71 (d, *J* = 2.00 Hz, 1H), 7.06 (d, *J* = 3.60 Hz, 1H), 6.98 (s, 2H), 6.66 (d, *J* = 3.60 Hz, 1H), 6.47 (t, *J* = 2.00 Hz, 1H), 2.35 (s, 3H), 2.22 (s, 6H). Anal. Calcd. For: C, 71.61; H, 6.01; N, 10.44. Found: C, 71.74; H, 6.25; N, 10.56.

**2-(5-Mesitylthiophen-2-yl)benzo[d]oxazole (6c)**

**$^1$H NMR (400 MHz, $CDCl_3$):** δ 7.83 (d, *J* = 3.72 Hz, 1H), 7.66-7.64 (m, 1H), 7.48-7.45 (m, 1H), 7.26-7.23 (m, 2H), 6.88 (s, 2H), 6.81 (d, *J* = 3.68 Hz, 1H), 2.25 (s, 3H), 2.09 (s, 6H); **$^{13}$C NMR (100 MHz, $CDCl_3$):** δ 159.0, 150.5, 147.3, 142.1, 138.6, 138.0, 130.3, 129.8, 129.4, 128.3, 128.1, 125.0, 124.7, 119.7, 110.4, 21.1, 20.7. Anal. Calcd. For: C, 75.20; H, 5.36; N, 4.39. Found: C, 75.5; H, 5.19; N, 4.15.

**2-(5-Mesitylfuran-2-yl)benzo[d]oxazole (6d)**

IR (neat) 2918, 1638, 1564, 1240, 1088, 796, 741 cm$^{-1}$. **$^1$H NMR (300 MHz, $CDCl_3$):** δ 7.77-7.73 (m,1H), 7.57-7.54 (m, 1H), 7.40 (d, *J* = 3.45 Hz, 1H), 7.80-7.72 (m, 2H), 6.95 (s, 2H), 6.49 (d, *J* = 3.42 Hz, 1H), 2.33 (s, 3H), 2.24 (s, 6H); **$^{13}$C NMR (100 MHz, $CDCl_3$):** δ 156.5, 155.6, 150.2, 141.8, 141.6, 138.4, 128.4, 126.9,

125.1, 124.8, 120.0, 115.4, 112.0, 110.5, 21.2, 20.5. Anal. Calcd. For: C, 79.19; H, 5.65; N, 4.62. Found: C, 79.42; H, 5.45; N, 4.76.

**2-(5-Mesitylthiophen-2-yl)benzo[d]thiazole (6e)**

IR (neat) 2914, 1440,1228, 894, 812, 723 $cm^{-1}$. **$^1$H NMR (400 MHz, $CDCl_3$):** δ 8.03 (d, *J* = 8.00 Hz, 1H), 7.87 (d, *J* = 8.00 Hz, 1H), 7.68 (d, *J* = 3.60 Hz, 1H), 7.48 (t, *J* = 7.20 Hz, 1H), 7.38 (t, *J* = 7.20 Hz, 1H), 6.98 (s, 2H), 6.87 (d, *J* = 3.60 Hz, 1H), 2.35 (s, 3H), 2.20 (s, 6H); **$^{13}$C NMR (75 MHz, $CDCl_3$):** δ 161.5, 153.6, 146.2, 138.4, 137.9, 136.9, 134.5, 130.0, 128.9, 128.2, 127.8, 126.3, 125.0, 122.8, 121.4, 21.0, 20.6. Anal. Calcd. For: C, 71.60; H, 5.11; N, 4.18. Found: C, 71.30; H, 5.31; N, 4.00.

**2-(5-Mesitylfuran-2-yl)benzo[d]thiazole (6f)**

**$^1$H NMR (400 MHz, $CDCl_3$):** δ 8.06 (d, *J* = 8.00 Hz, 1H), 7.89 (d, *J* = 8.00 Hz, 1H), 7.50 (t, *J* = 7.20 Hz, 1H), 7.38 (t, *J* = 7.20 Hz, 1H), 6.88 (s, 2H), 6.50 (d, *J* = 3.20 Hz, 1H), 2.35 (s, 3H), 2.29 (s, 6H); **$^{13}$C NMR (75 MHz, $CDCl_3$):** δ 157.9, 155.2, 153.8, 147.8, 139.1, 138.2, 134.2, 128.5, 127.0, 126.3, 124.9, 122.8, 121.5, 112.4, 112.3, 21.1, 20.6. Anal. Calcd. For: C, 75.20; H, 5.36; N, 4.39. Found: C, 75.42; H, 5.16; N, 4.45.

**2-Mesityl-5-(4-methoxyphenyl)thiophene (6g)**

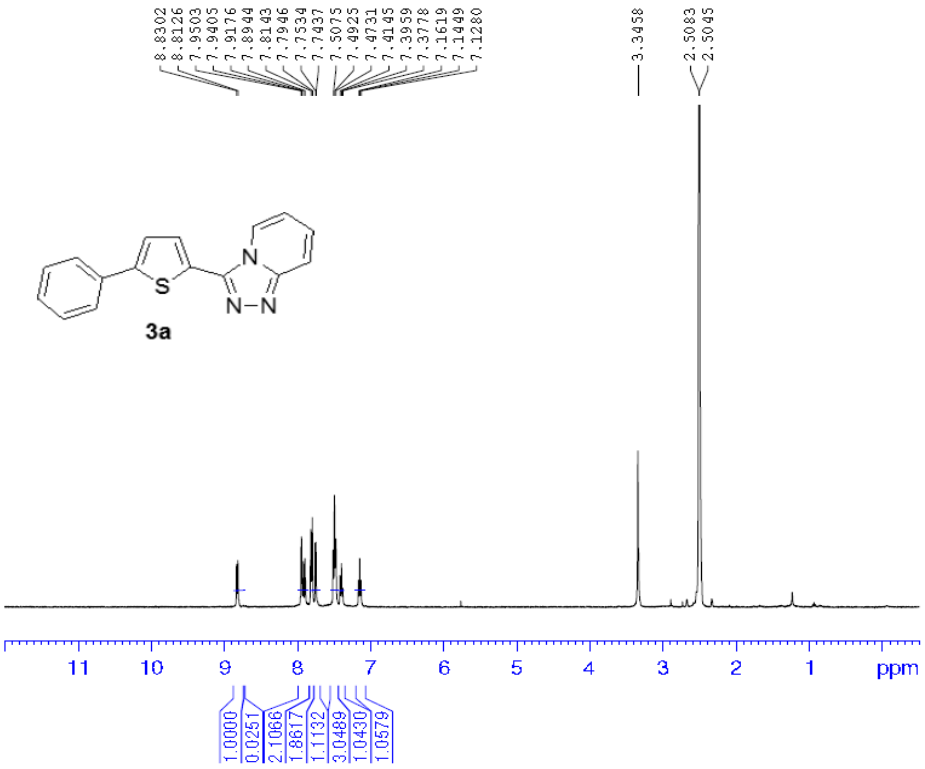
mp 78-80 $^oC$ . IR (neat) 2921, 1454, 1243, 1174, 1028, 825, 795 $cm^{-1.}$ **$^1$H NMR (400 MHz, $CDCl_3$):** δ 7.58 (d, *J* = 8.80 Hz, 2H), 7.22 (d, *J* = 3.20 Hz, 1H), 6.97 (s, 2H), 6.94 (d, *J* = 8.80 Hz, 2H), 6.76 (d, *J* = 3.60 Hz, 1H), 3.86 (s, 3H), 2.35 (s, 3H), 2.20 (s, 6H). **$^{13}$C NMR (100 MHz, $CDCl_3$):** δ 159.0, 144.0, 140.0, 138.3, 137.9, 131.1, 128.1, 127.5, 126.9, 121.9, 114.3, 55.4, 21.1, 20.8. Anal. Calcd. For: C, 78.88; H, 6.54. Found: C, 77.93; H, 6.33.

**2-mesityl-5-methylfuran (6h)**

IR (neat) 2920, 1569, 1443, 1218, 1046, 1017, 849, 781 $cm^{-1.}$ **$^1$H NMR (400 MHz, $CDCl_3$):** δ 7.27 (s, 2H), 6.14 (d, *J* = 3.20 Hz, 1H), 6.08-6.07 (m, 1H), 2.36 (s, 3H), 2.32 (s, 3H), 2.22 (s, 6H). **$^{13}$C NMR (100 MHz, $CDCl_3$):** δ 151.0, 150.4, 138.2, 138.0, 128.5, 128.3, 128.0, 109.8, 106.2, 21.1, 20.6, 13.6. Anal. Calcd. For: C, 83.96; H, 8.05; Found: C, 83.81; H, 8.21.

**3. $^1$H and $^{13}$C NMR spectrum of compounds (3a-3l), (4a-4f), (5a-5c) and (6a-6h).**

1. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-Phenylthiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3a)

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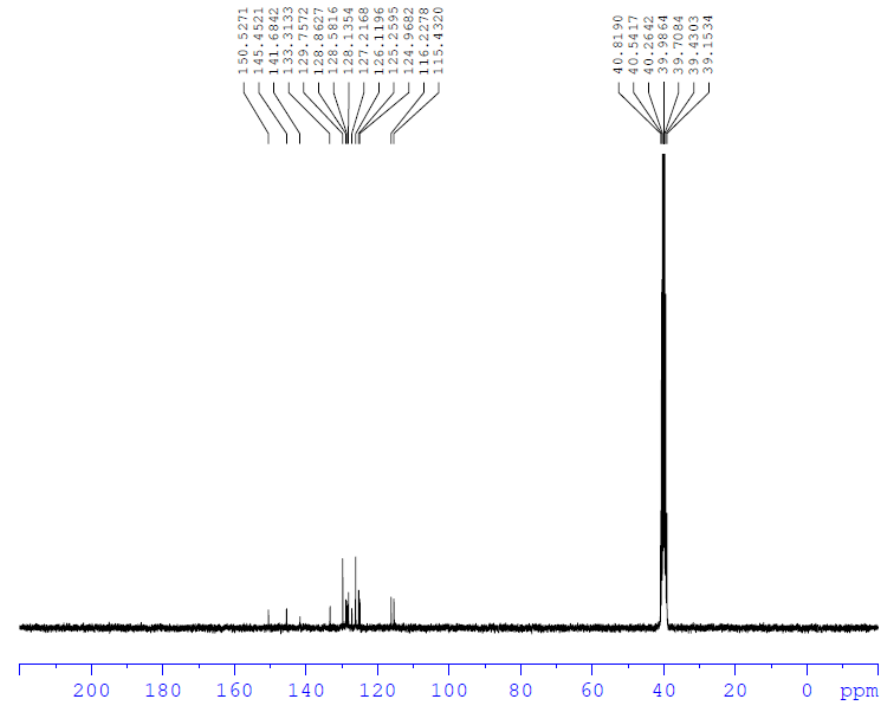


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F2 - Processing parameters
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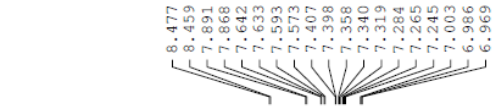
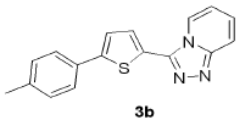
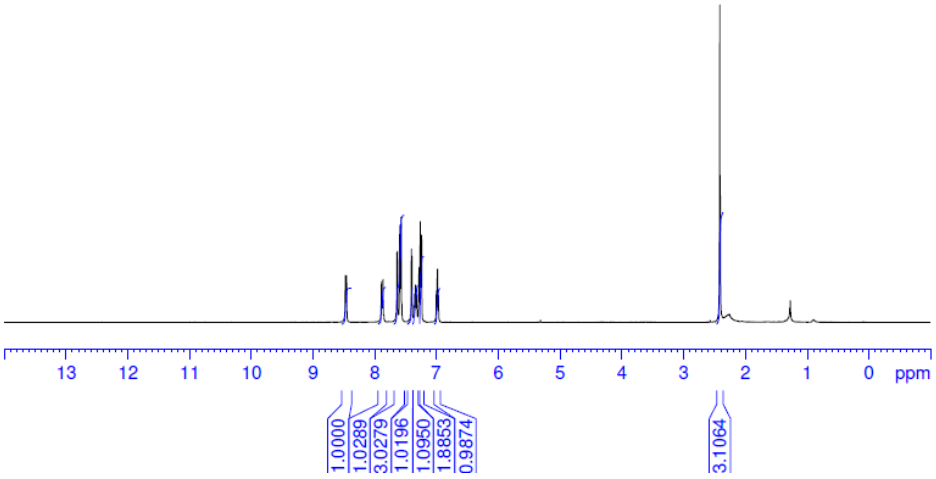
2. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-*p*-Tolylthiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3b)



3b

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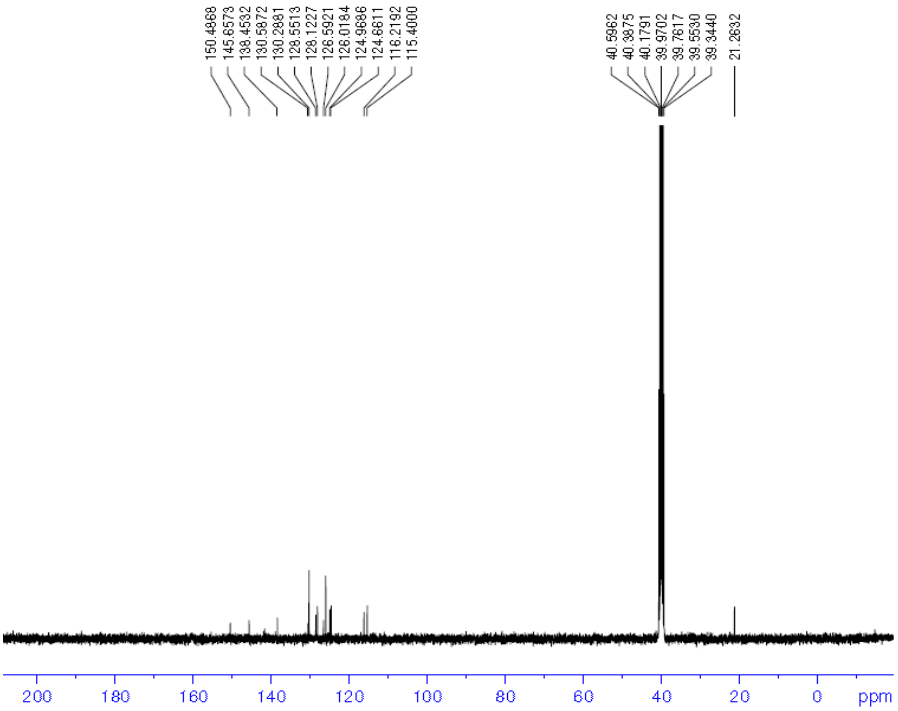


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F2 - Processing parameters
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LB                 1.00 Hz
GB                    0
PC                 1.40
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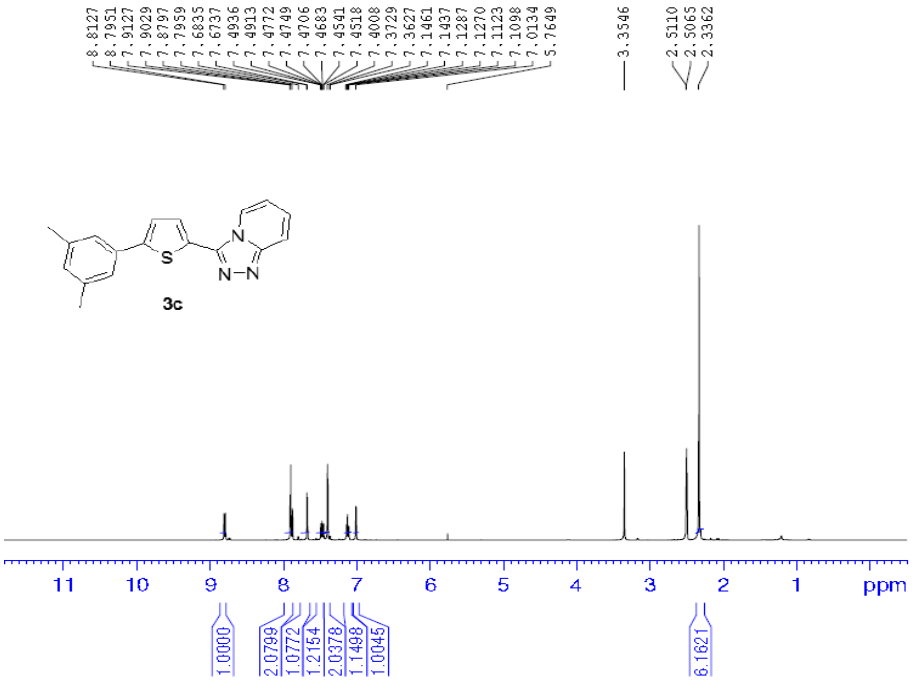
3. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(3,5-Dimethylphenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3c)

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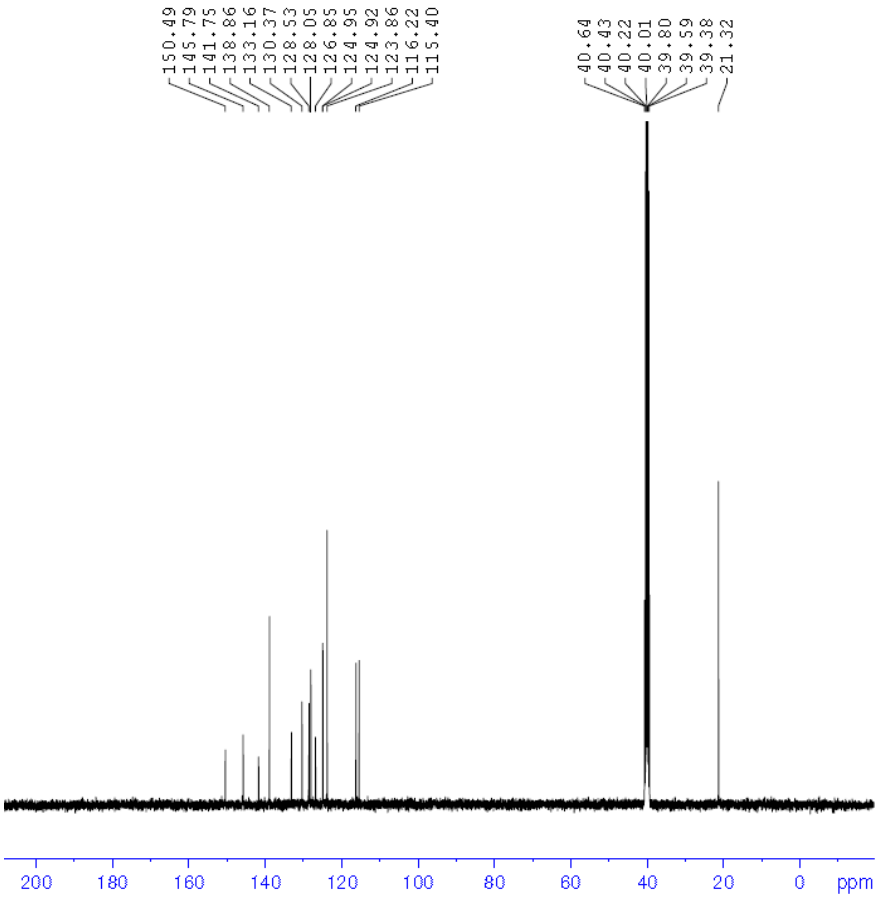


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FIDRES          0.733596 Hz
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RG                  2050
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DE                 6.50 usec
TE                293.0 K
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TD0                    1

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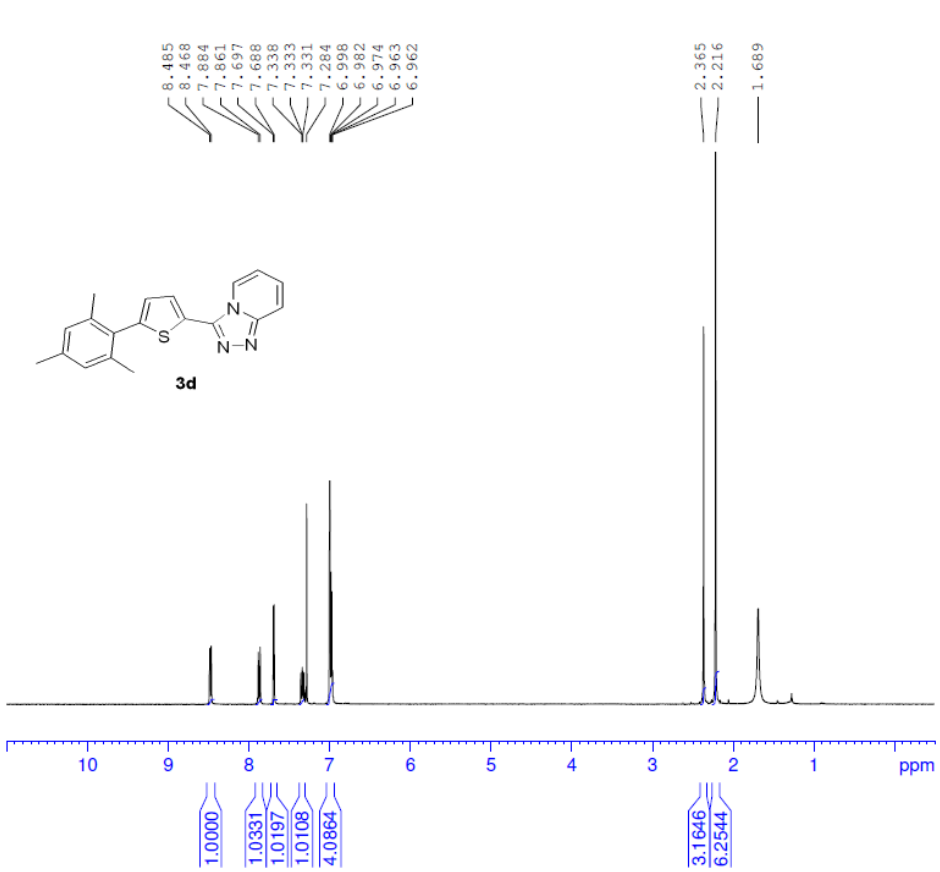
4. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-Mesitylthiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3d)

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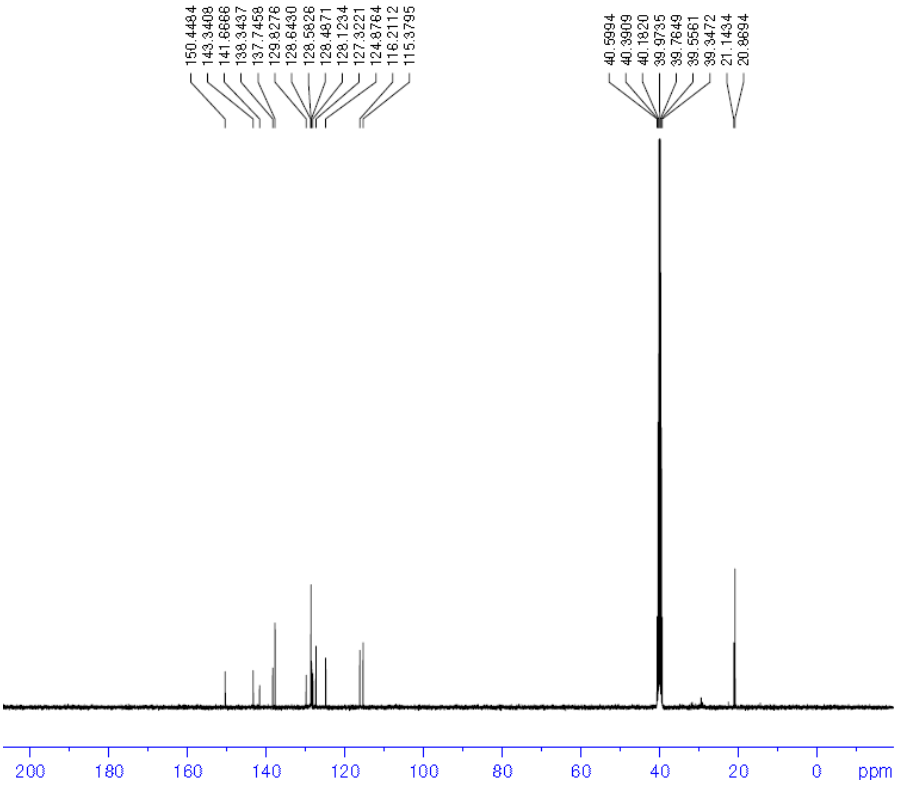
======== CHANNEL f1 =======
NUC1                  1H
P1                 13.75 use
PL1                -2.00 dB
SFO1         400.3754725 MHz

F2 - Processing parameters
SI                 32768
SF           400.3730000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters

EXPNO                  2
PROCNO                 1

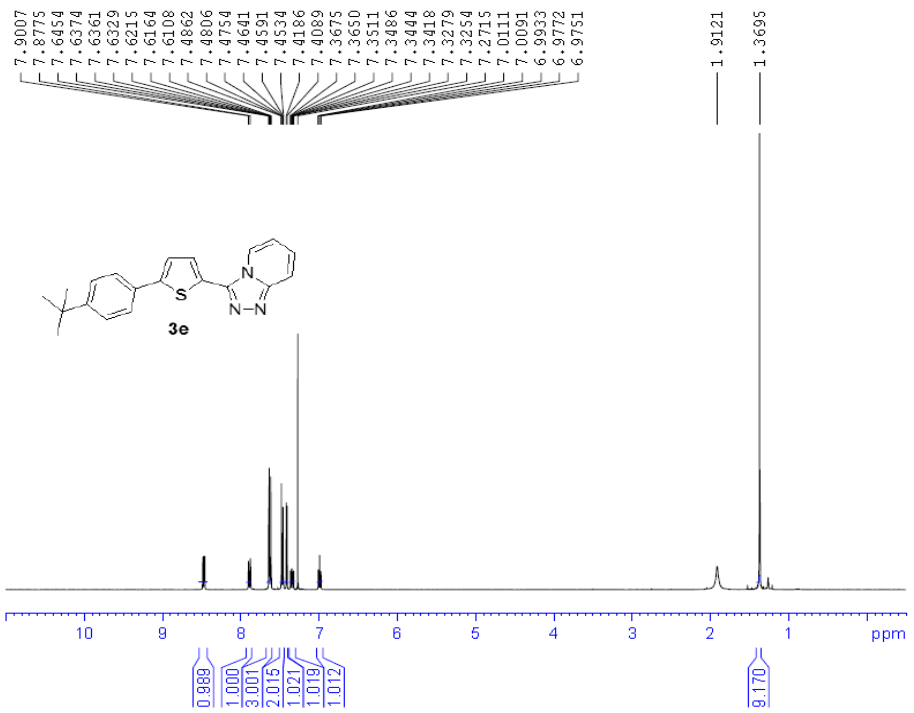
F2 - Acquisition Parameters
Date_           20130717
Time               7.15
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816244 sec
RG                   114
DW                20.800 usec
DE                 6.00 usec
TE                295.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 8.10 usec
PL1                -3.00 dB
SFO1         100.6278593 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL12               14.04 dB
PL13               15.00 dB
PL2                -0.50 dB
SFO2         400.1516006 MHz

F2 - Processing parameters
SI                 32768
SF           100.6177980 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

5. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(4-*tert*-Butylphenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3e)



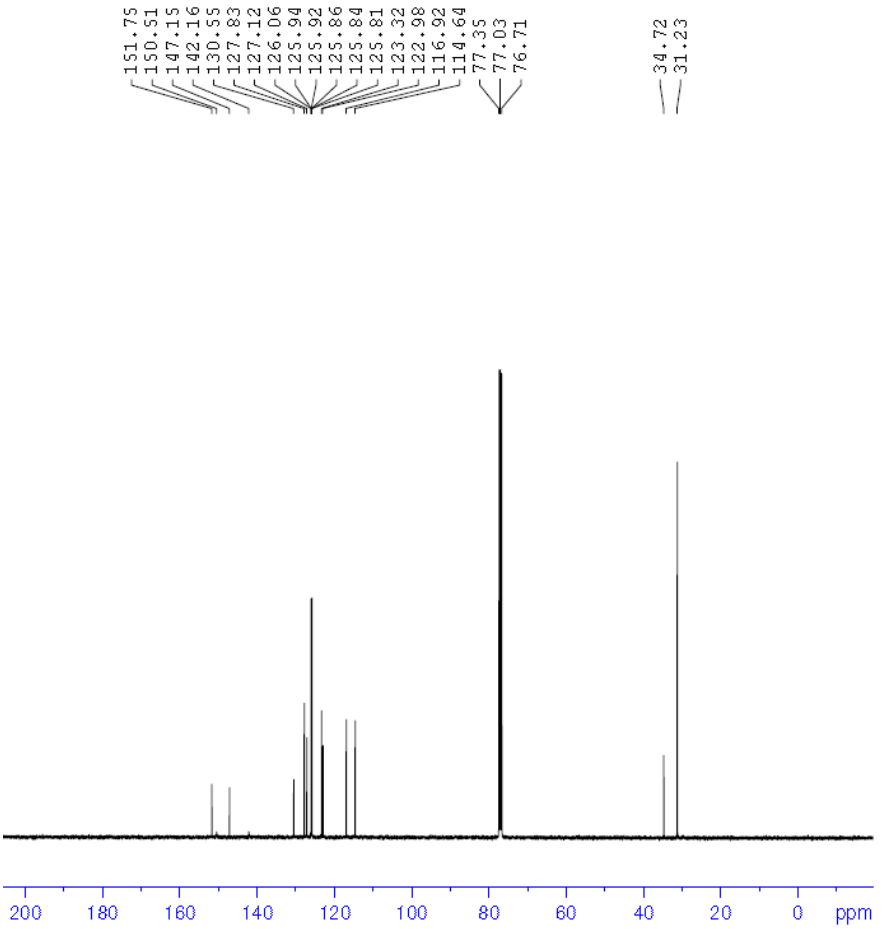

```
Current Data Parameters

EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20131016
Time              10.06
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9923444 sec
RG                 575
DW              60.800 usec
DE               6.00 usec
TE              295.3 K
D1            2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               15.00 usec
PL1              -0.50 dB
SFO1        400.1524711 MHz

F2 - Processing parameters
SI               32768
SF          400.1500000 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.40
```

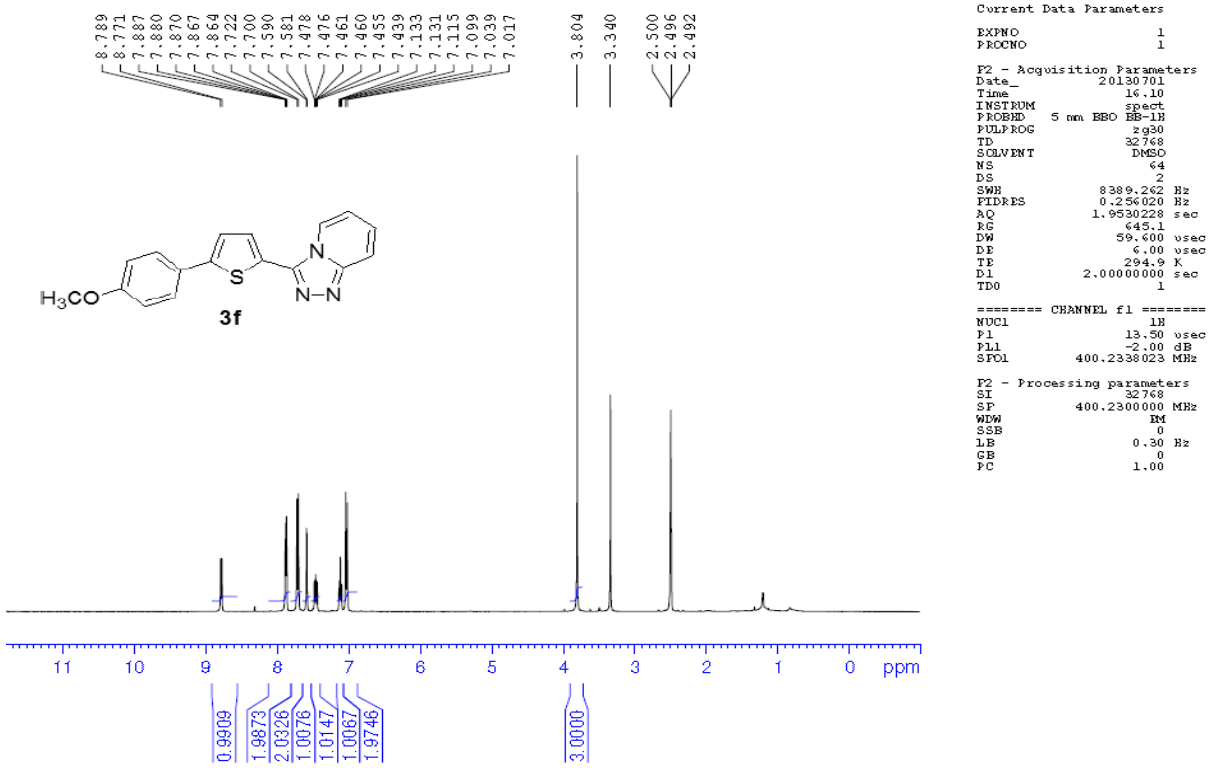



```
EXPNO                  2
PROCNO                 1
Date_           20131017
Time               0.04
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD               32768
SOLVENT          CDCl3
NS                3000
DS                   4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816244 sec
RG                2050
DW              20.800 usec
DE               6.50 usec
TE              293.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               13C
P1                8.50 usec
PL1              -2.00 dB
PL1W        57.32743073 W
SFO1       100.6680954 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2               1H
PCPD2            80.00 usec
PL2              -1.00 dB
PL12             13.69 dB
PL13             14.18 dB
PL2W        11.92178631 W
PL12W        0.40489405 W
PL13W        0.36169401 W
SFO2       400.3116012 MHz
SI               32768
SF         100.6580300 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

6. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(4-Methoxyphenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3f)



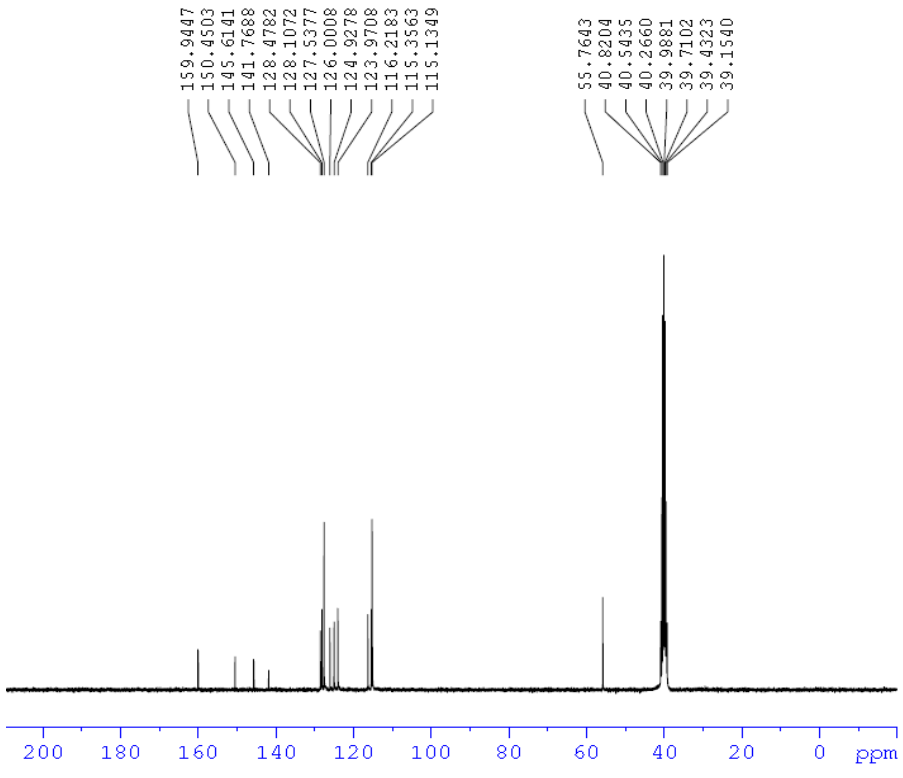

```
Current Data Parameters

EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130701
Time                16.10
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    64
DS                     2
SWH             8389.262 Hz
FIDRES          0.256020 Hz
AQ              1.9530228 sec
RG                 645.1
DW                59.600 usec
DE                 6.00 usec
TE                294.9 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                13.50 usec
PL1               -2.00 dB
SFO1         400.2338023 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters

EXPNO                  2
PROCNO                 1

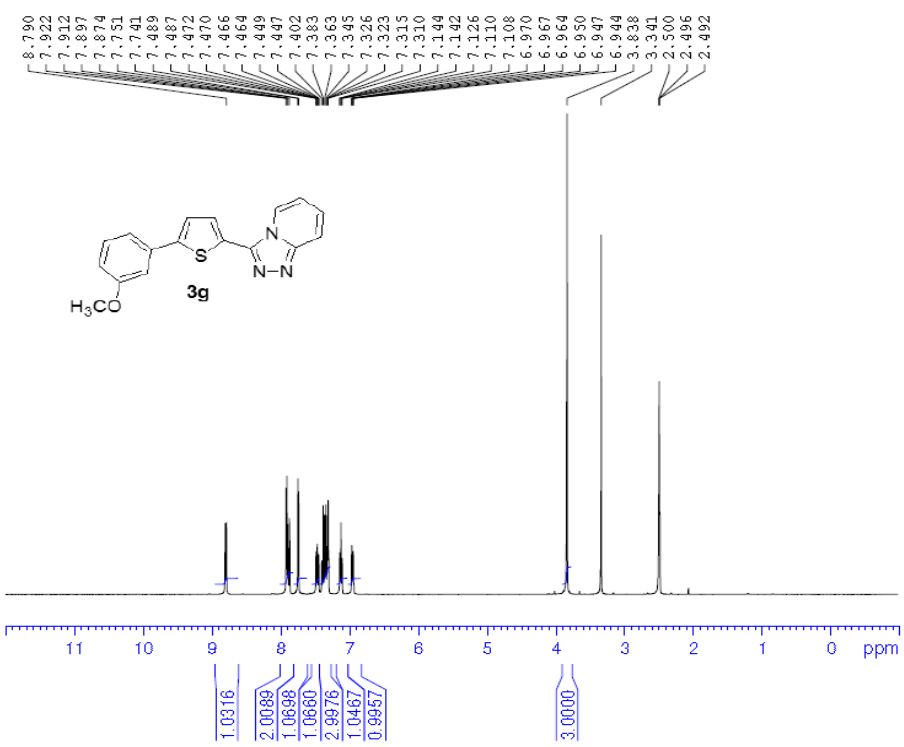
F2 - Acquisition Parameters
Date_           20130702
Time                0.18
INSTRUM             spect
PROBHD   5 mm DUL BB-1H
PULPROG             zgpg
TD                 32768
SOLVENT             DMSO
NS                  3000
DS                     0
SWH            18115.941 Hz
FIDRES          0.552855 Hz
AQ              0.9044468 sec
RG                 11585.2
DW                27.600 usec
DE                 6.00 usec
TE                 0.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 8.50 usec
PL1                0.00 dB
SFO1         75.4752958 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12              14.75 dB
PL13              18.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                131072
SF          75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

7. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(3-Methoxyphenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3g)



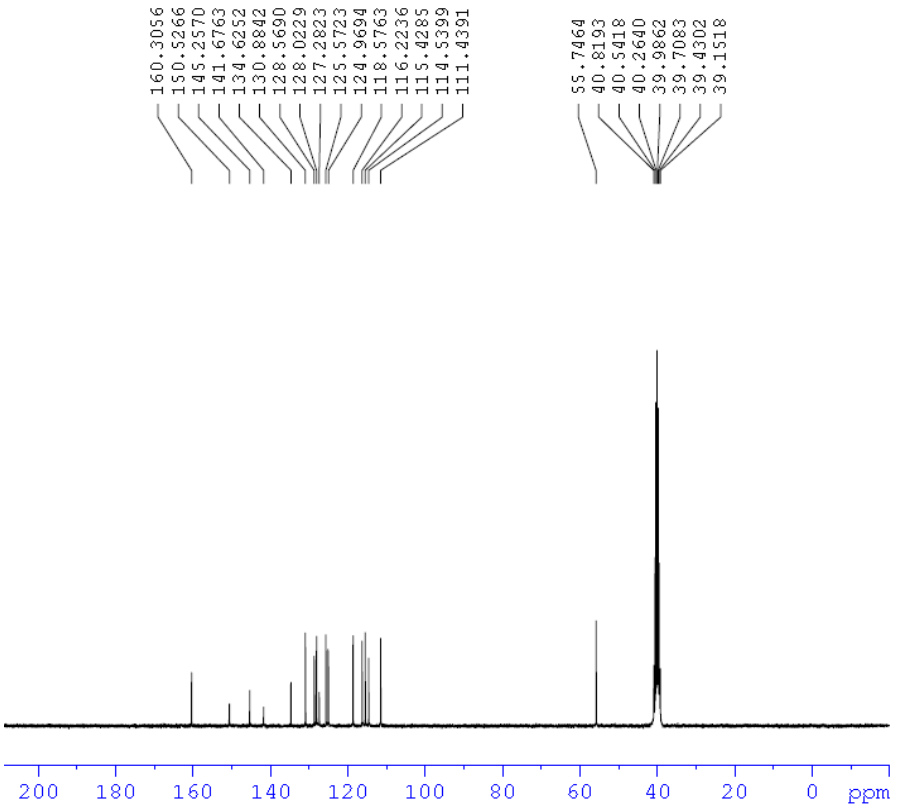

```
Current Data Parameters

EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130701
Time               16.29
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8389.262 Hz
FIDRES          0.256020 Hz
AQ            1.9530228 sec
RG                574.7
DW                59.600 usec
DE                 6.00 usec
TE                295.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                13.50 usec
PL1               -2.00 dB
SFO1        400.2338023 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```




```
Current Data Parameters

EXPNO                  2
PROCNO                 1

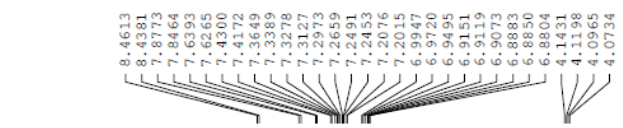
F2 - Acquisition Parameters
Date_           20130701
Time               21.44
INSTRUM            spect
PROBHD   5 mm DUL BB-1H
PULPROG             zgpg
TD                 32768
SOLVENT             DMSO
NS                  3000
DS                     0
SWH            18115.941 Hz
FIDRES          0.552855 Hz
AQ             0.9044468 sec
RG                10321.3
DW                27.600 usec
DE                 6.00 usec
TE                 0.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

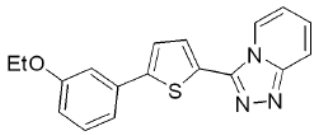
======== CHANNEL f1 ========
NUC1                 13C
P1                 8.50 usec
PL1                0.00 dB
SFO1         75.4752958 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              14.75 dB
PL13              18.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                131072
SF          75.4677490 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

8. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(3-Ethoxyphenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3h)



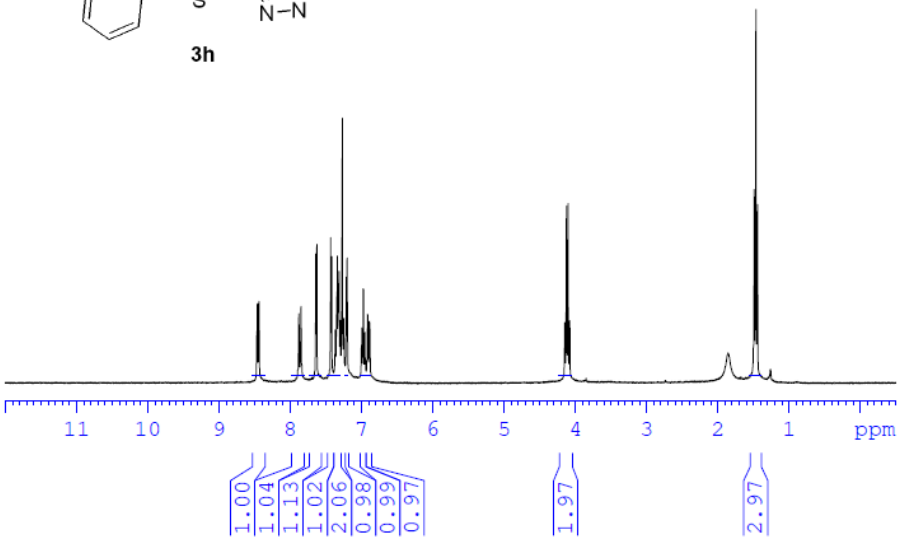

**3h**

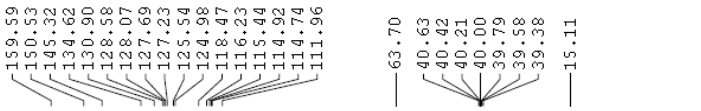
```
EXPNO                 1
PROCNO                1

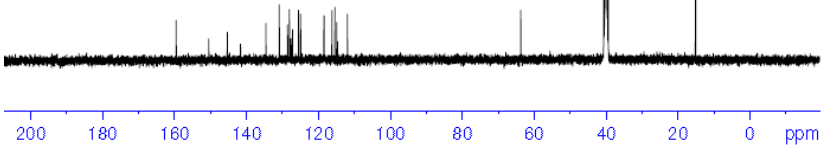
F2 - Acquisition Parameters
Date_          20140819
Time              18.05
INSTRUM           spect
PROBHD   5 mm DUL BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             5995.204 Hz
FIDRES          0.182959 Hz
AQ             2.7329011 sec
RG                   512
DW                83.400 usec
DE                 6.00 usec
TE                  0.0 K
D1           2.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                14.65 usec
PL1                0.00 dB
SFO1         300.1318008 MHz

F2 - Processing parameters
SI                 32768
SF          300.1298168 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```



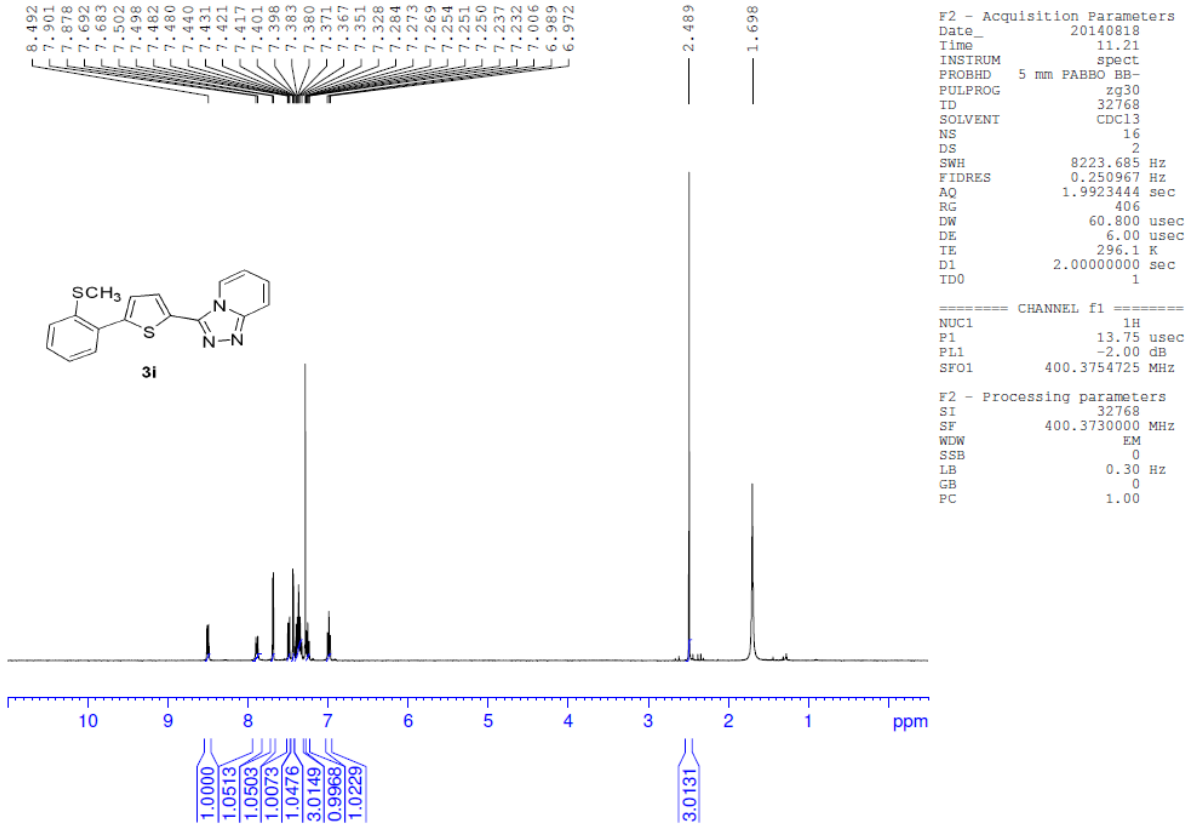




```
EXPNO                 2
PROCNO                1
Date_          20130716
Time               0.38
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT              DMSO
NS                   1024
DS                      4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816244 sec
RG                   2050
DW                20.800 usec
DE                 6.50 usec
TE                293.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1                 8.50 usec
PL1               -2.00 dB
PL1W        57.32743073 W
SFO1       100.6680954 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2           80.00 usec
PL2              -1.00 dB
PL12             13.69 dB
PL13             14.18 dB
PL2W        11.92178631 W
PL12W        0.40489405 W
PL13W        0.36169401 W
SFO2       400.3116012 MHz
SI                 32768
SF         100.6580300 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

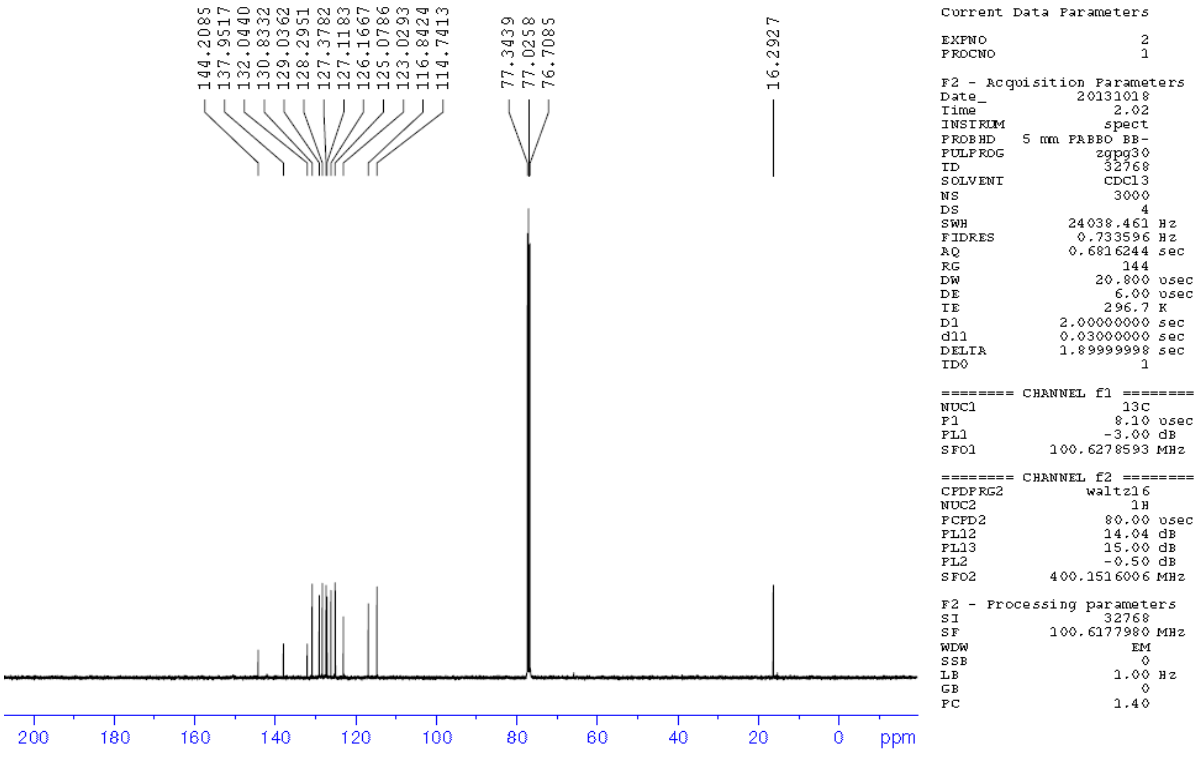
9. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(2-(Methylthio)phenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3i)




F2 - Acquisition Parameters
Date_ 20140818
Time 11.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 406
DW 60.800 usec
DE 6.00 usec
TE 296.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.75 usec
PL1 -2.00 dB
SFO1 400.3754725 MHz

F2 - Processing parameters
SI 32768
SF 400.3730000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




Current Data Parameters

EXPNO 2
PROCNO 1

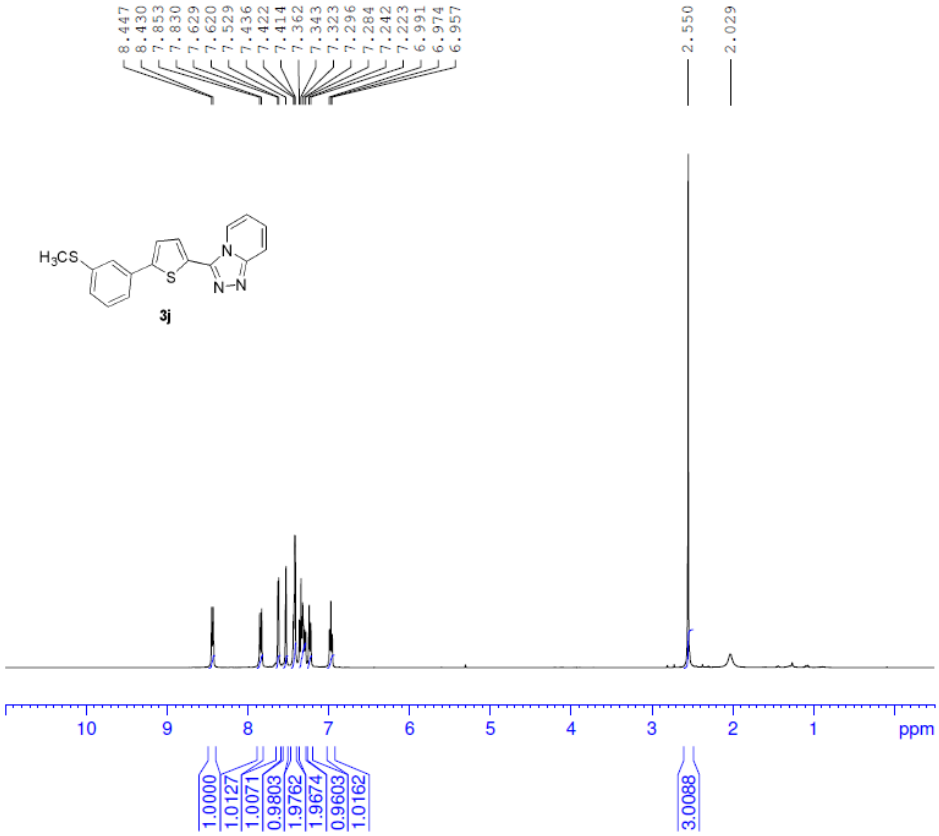
F2 - Acquisition Parameters
Date_ 20131018
Time 2.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 3000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 144
DW 20.800 usec
DE 6.00 usec
TE 296.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.10 usec
PL1 -3.00 dB
SFO1 100.6278593 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.04 dB
PL13 15.00 dB
PL2 -0.50 dB
SFO2 400.1516006 MHz

F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

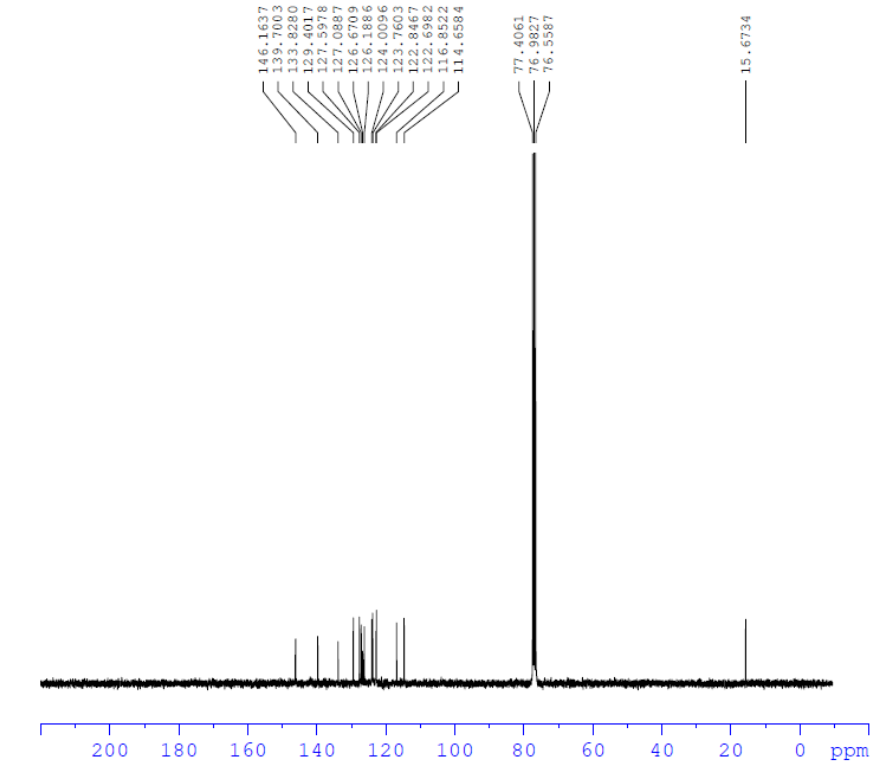
10. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(3-(Methylthio)phenyl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3j)




```
F2 - Acquisition Parameters
Date_              20140818
Time                  11.32
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.250967 Hz
AQ                 1.9923444 sec
RG                       181
DW                    60.800 usec
DE                     6.00 usec
TE                    296.0 K
D1                 2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.75 usec
PL1                    -2.00 dB
SFO1            400.3754725 MHz

F2 - Processing parameters
SI                    32768
SF              400.3730000 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```




```
EXPNO                     2
PROCNO                    1

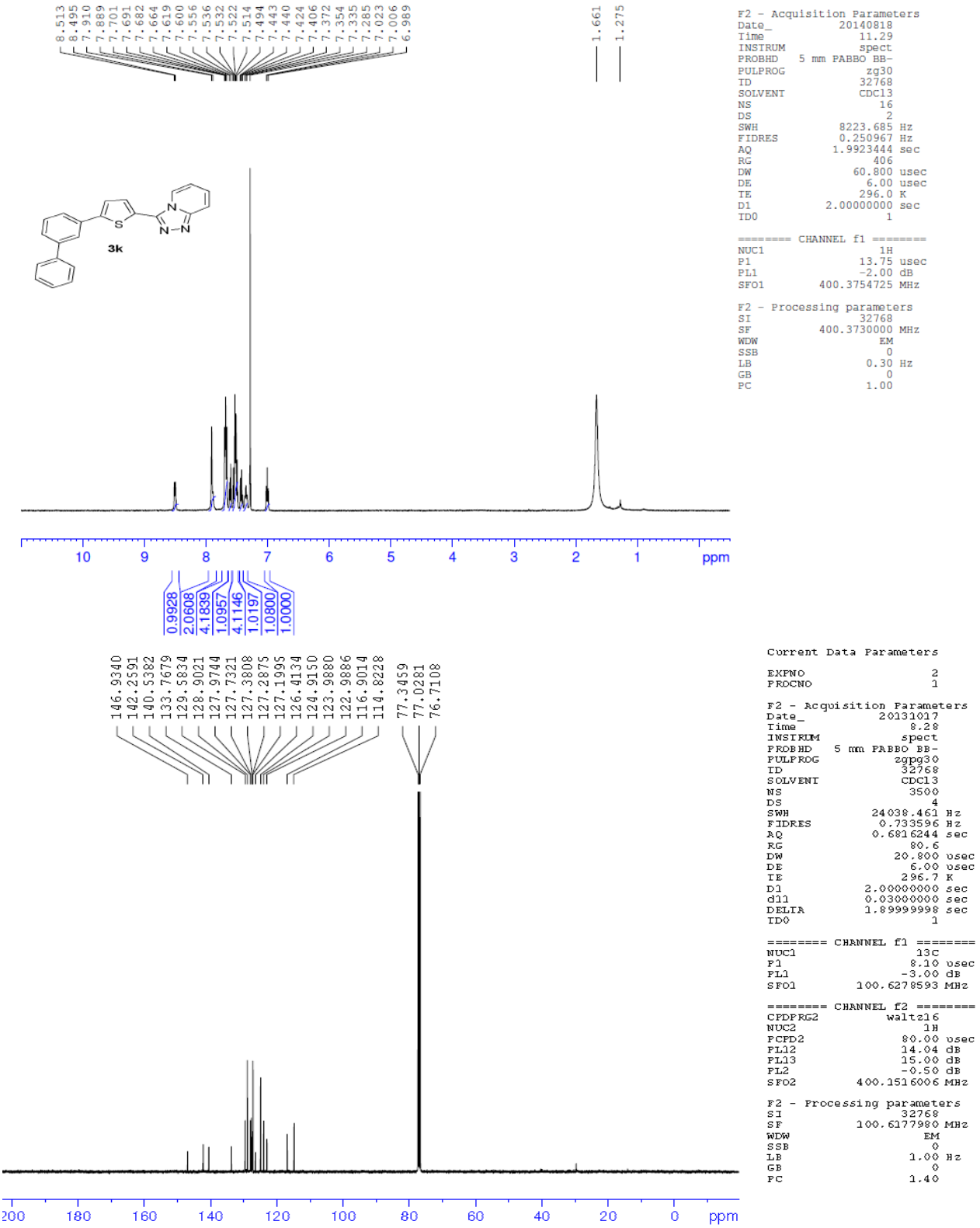
F2 - Acquisition Parameters
Date_              20140819
Time                  7.51
INSTRUM              spect
PROBHD   5 mm DUL BB-1H
PULPROG            zgpg30
TD                    32768
SOLVENT               CDCl3
NS                     3000
DS                        0
SWH               20325.203 Hz
FIDRES             0.620276 Hz
AQ                 0.8061428 sec
RG                   14596.5
DW                    24.600 usec
DE                     6.00 usec
TE                     0.0 K
D1                 3.00000000 sec
d11                0.03000000 sec
DELTA              2.90000010 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     8.50 usec
PL1                    0.00 dB
SFO1            75.4771525 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                    0.00 dB
PL12                  14.75 dB
PL13                  18.00 dB
SFO2           300.1315007 MHz

F2 - Processing parameters
SI                    32768
SF              75.4677079 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.70
```

11. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(Biphenyl-3-yl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3k)




```
F2 - Acquisition Parameters
Date_            20140818
Time                11.29
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                   406
DW                60.800 usec
DE                 6.00 usec
TE                296.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 1H
P1                13.75 usec
PL1               -2.00 dB
SFO1         400.3754725 MHz

F2 - Processing parameters
SI                 32768
SF           400.3730000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

```
Current Data Parameters

EXPNO                  2
PROCNO                 1

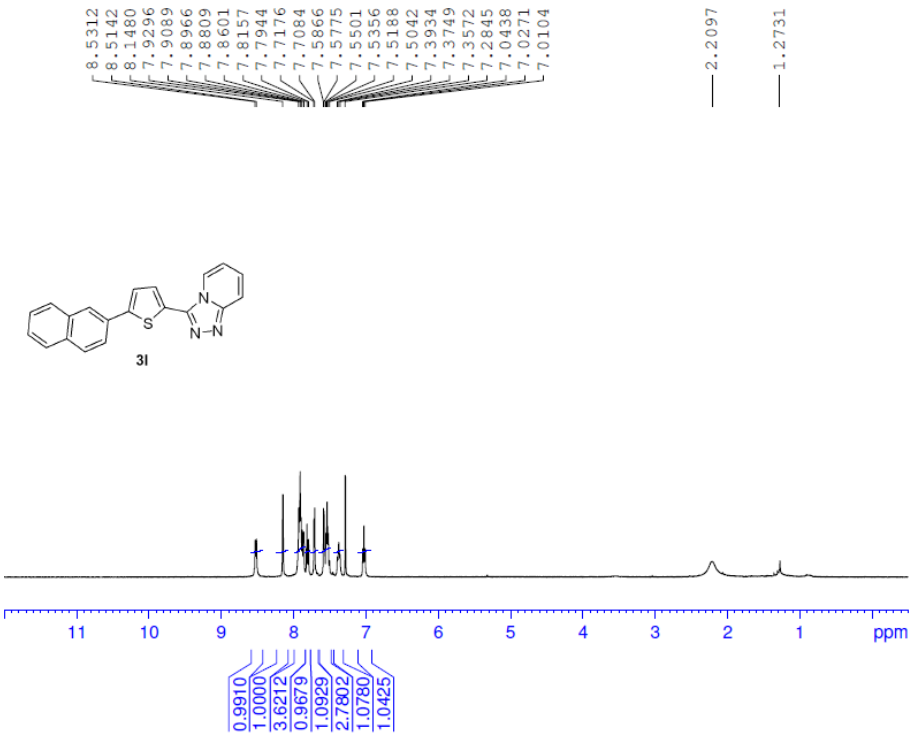
F2 - Acquisition Parameters
Date_           20131017
Time                8.28
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  3500
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816244 sec
RG                  80.6
DW                20.800 usec
DE                 6.00 usec
TE                296.7 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.10 usec
PL1               -3.00 dB
SFO1         100.6278593 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL12               14.04 dB
PL13               15.00 dB
PL2                -0.50 dB
SFO2         400.1516006 MHz

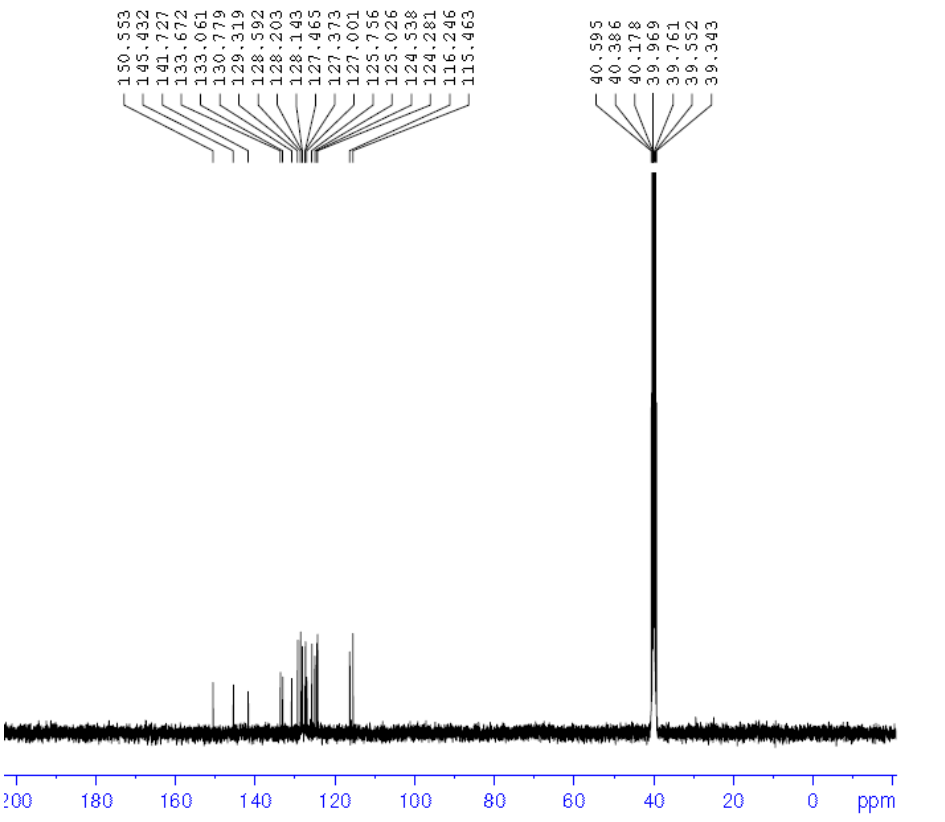
F2 - Processing parameters
SI                 32768
SF           100.6177980 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

12. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(Naphthalen-2-yl)thiophen-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (3l)




```
EXPNO                  1
PROCNO                 1
Date_           20140821
Time               12.16
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             9615.385 Hz
FIDRES          0.293438 Hz
AQ             1.7039860 sec
RG                   456
DW                52.000 usec
DE                 6.50 usec
TE                293.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.35 usec
PL1                -2.00 dB
PL1W        15.00864029 W
SFO1        400.3136028 MHz
SI                131072
SF          400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters

EXPNO                  2
PROCNO                 1

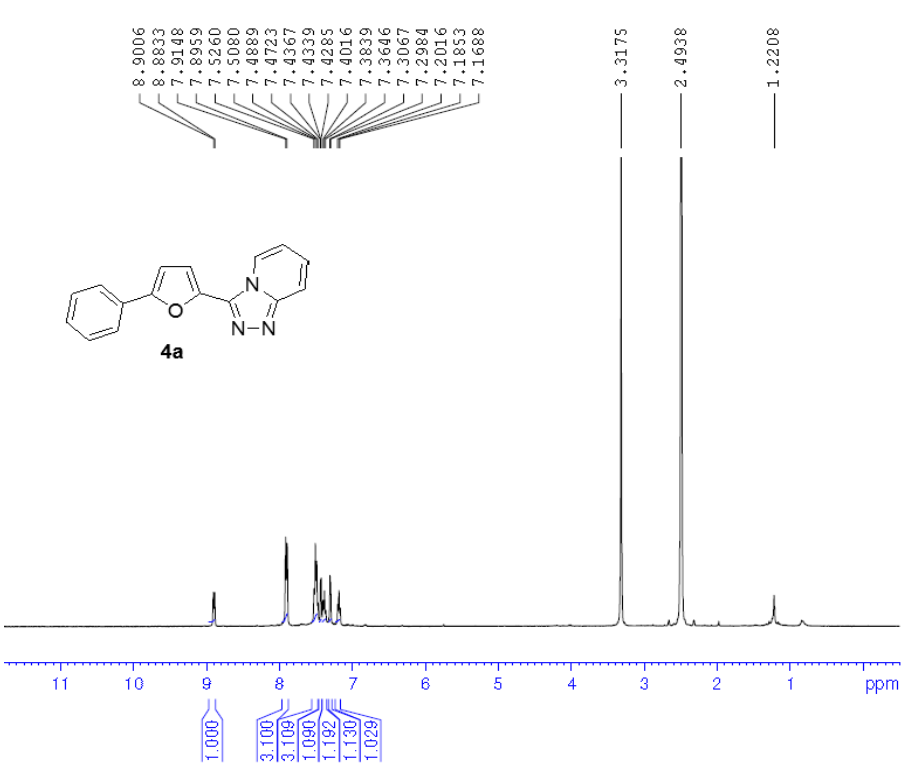
F2 - Acquisition Parameters
Date_           20130702
Time               11.07
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                  1024
DS                     2
SWH            24154.590 Hz
FIDRES          0.737140 Hz
AQ              0.6783476 sec
RG                1448.2
DW                20.700 usec
DE                 6.00 usec
TE                295.7 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.30 usec
PL1                -1.00 dB
SFO1        100.6478930 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               13.46 dB
PL13               15.00 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                 32768
SF          100.6379140 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

13. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-Phenylfuran-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (4a)



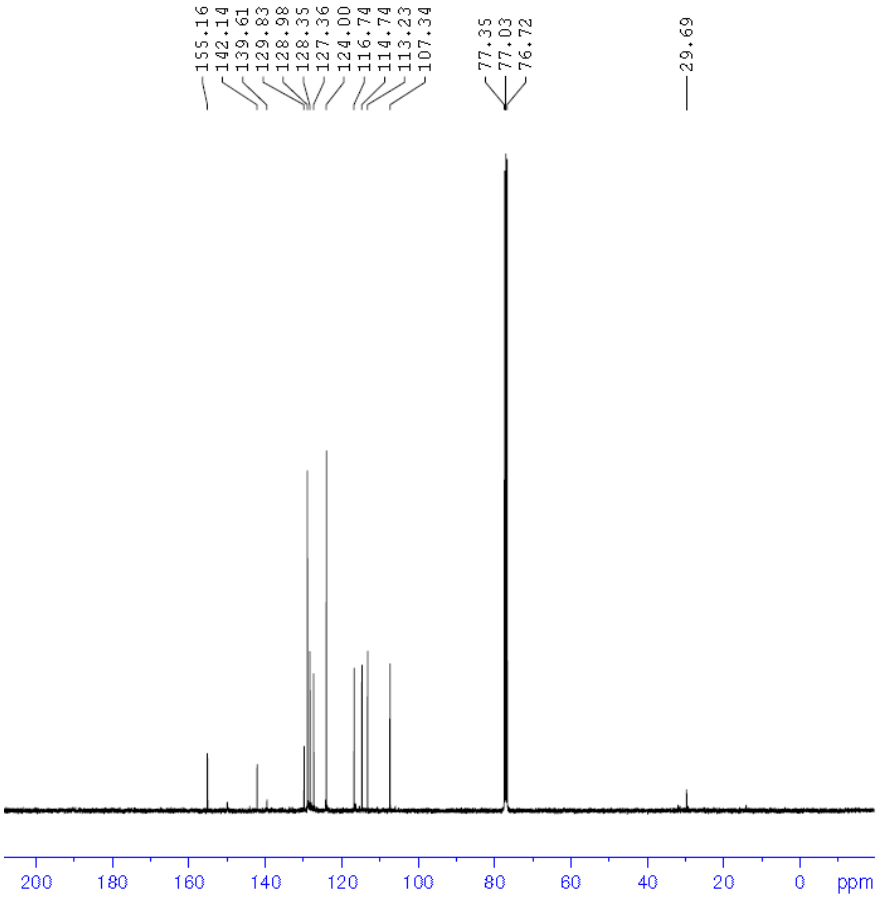

```
Current Data Parameters

EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130309
Time               12.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    32
DS                     2
SWH              8802.817 Hz
FIDRES           0.268641 Hz
AQ               1.8612725 sec
RG                   724
DW                56.800 usec
DE                 6.00 usec
TE                296.8 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.00 usec
PL1                 0.00 dB
SFO1         400.1532012 MHz

F2 - Processing parameters
SI                 32768
SF           400.1500000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

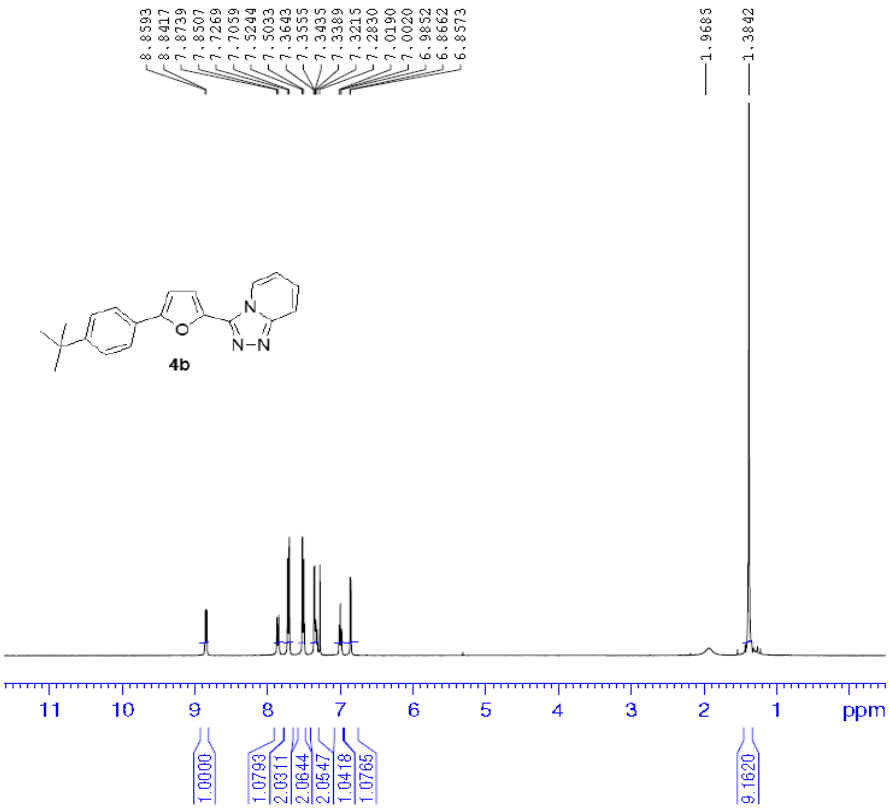



```
EXPNO                  3
PROCNO                 1
Date_           20131001
Time               4.26
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  3000
DS                     4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6816244 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                293.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 8.50 usec
PL1                -2.00 dB
PL1W        57.32743073 W
SFO1        100.6680954 MHz

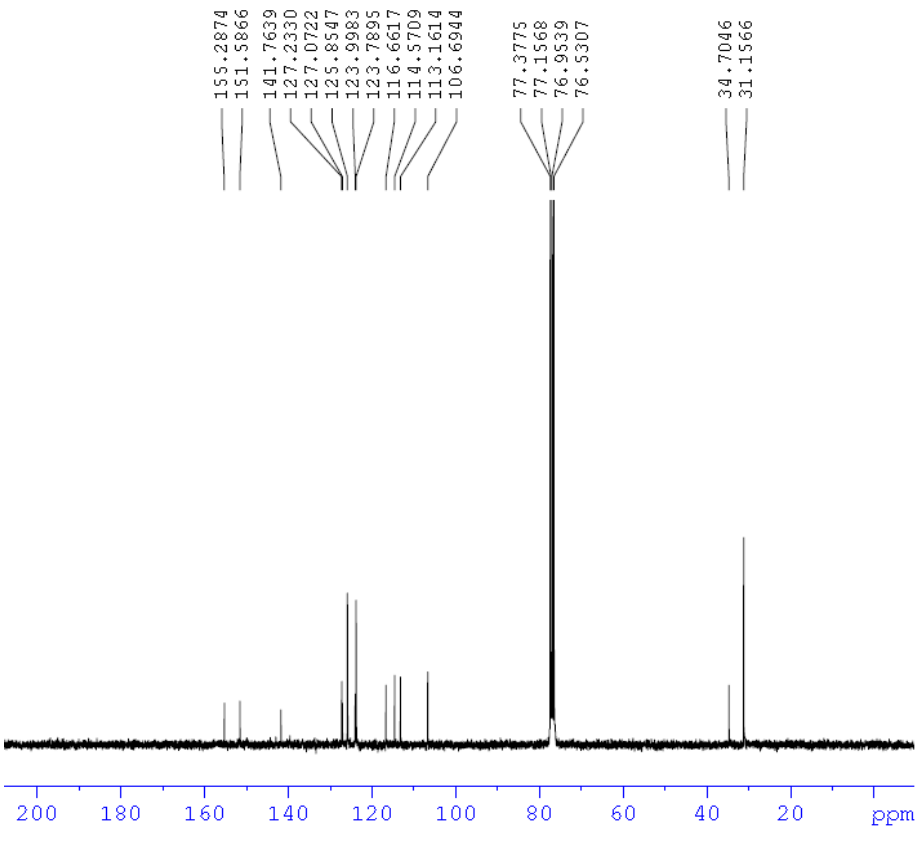
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               13.69 dB
PL13               14.18 dB
PL2W        11.92178631 W
PL12W        0.40489405 W
PL13W        0.36169401 W
SFO2        400.3116012 MHz
SI                 32768
SF          100.6580300 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

14. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(4-*tert*-Butylphenyl)furan-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (4b)




```
EXPNO                  1
PROCNO                 1
Date_           20130904
Time               11.14
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             9615.385 Hz
FIDRES          0.293438 Hz
AQ              1.7039860 sec
RG                   228
DW                52.000 usec
DE                 6.50 usec
TE                293.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.25 usec
PL1                -2.00 dB
PL1W         15.00864029 W
SFO1         400.3136028 MHz
SI                131072
SF           400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters

EXPNO                  2
PROCNO                 1

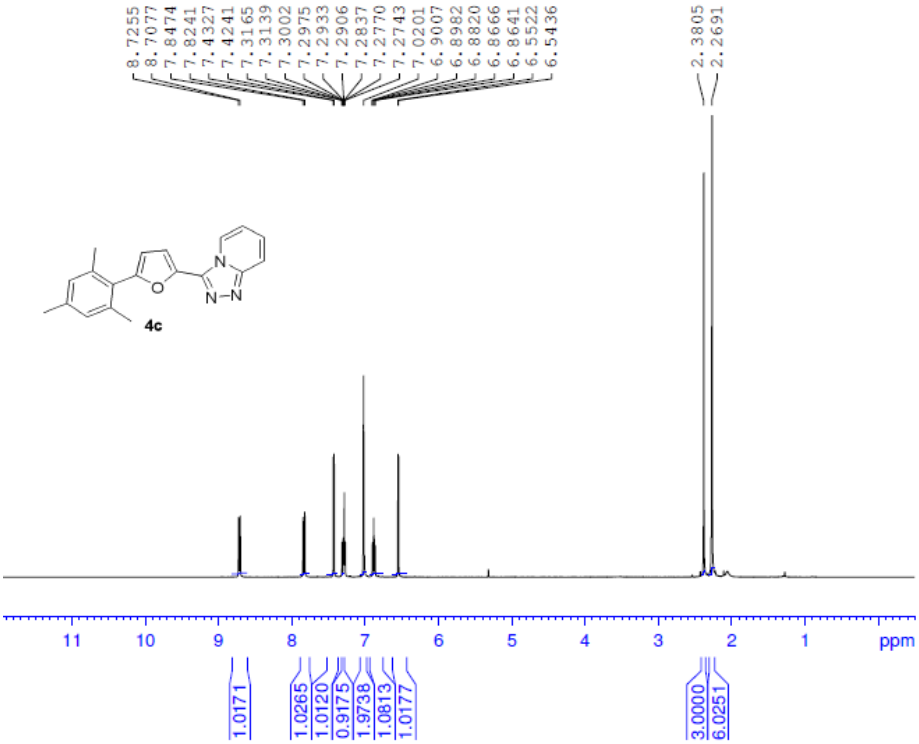
F2 - Acquisition Parameters
Date_           20130904
Time               23.12
INSTRUM            spect
PROBHD   5 mm DUL BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2000
DS                     0
SWH            20325.203 Hz
FIDRES          0.620276 Hz
AQ              0.8061428 sec
RG                 16384
DW                24.600 usec
DE                 6.00 usec
TE                 0.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 8.50 usec
PL1                0.00 dB
SFO1         75.4771525 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              14.75 dB
PL13              18.00 dB
SFO2         300.1315007 MHz

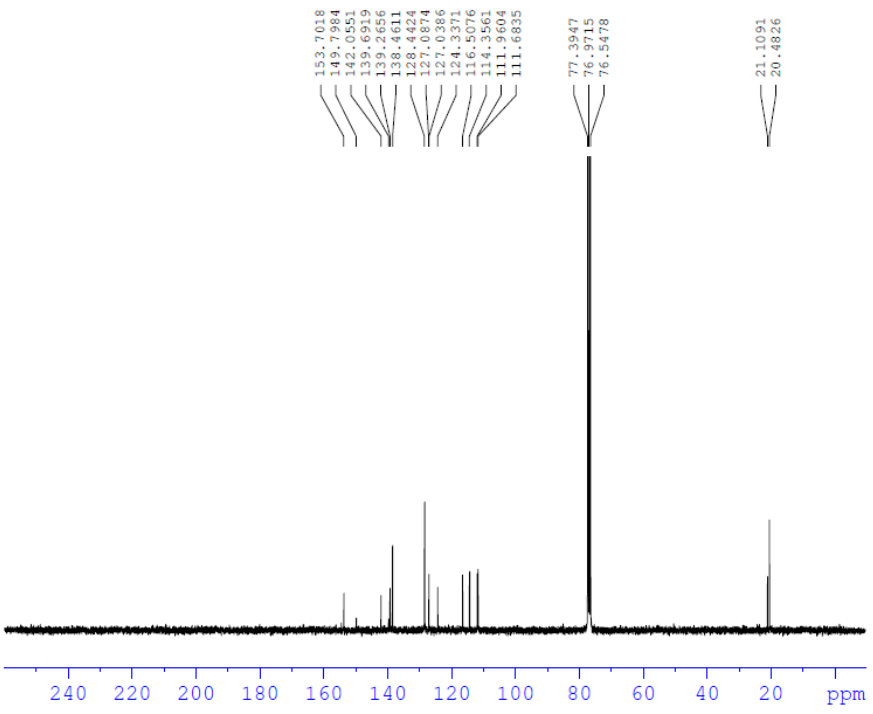
F2 - Processing parameters
SI                 32768
SF           75.4677079 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.70
```

15. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-Mesitylfuran-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (4c)




```
EXPNO                  1
PROCNO                 1
Date_           20140808
Time               14.14
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             9615.385 Hz
FIDRES          0.293438 Hz
AQ             1.7039860 sec
RG                   322
DW                52.000 usec
DE                 6.50 usec
TE                293.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.35 usec
PL1                -2.00 dB
PL1W         15.00864029 W
SFO1         400.3136028 MHz
SI                131072
SF           400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```




```
EXPNO                  2
PROCNO                 1

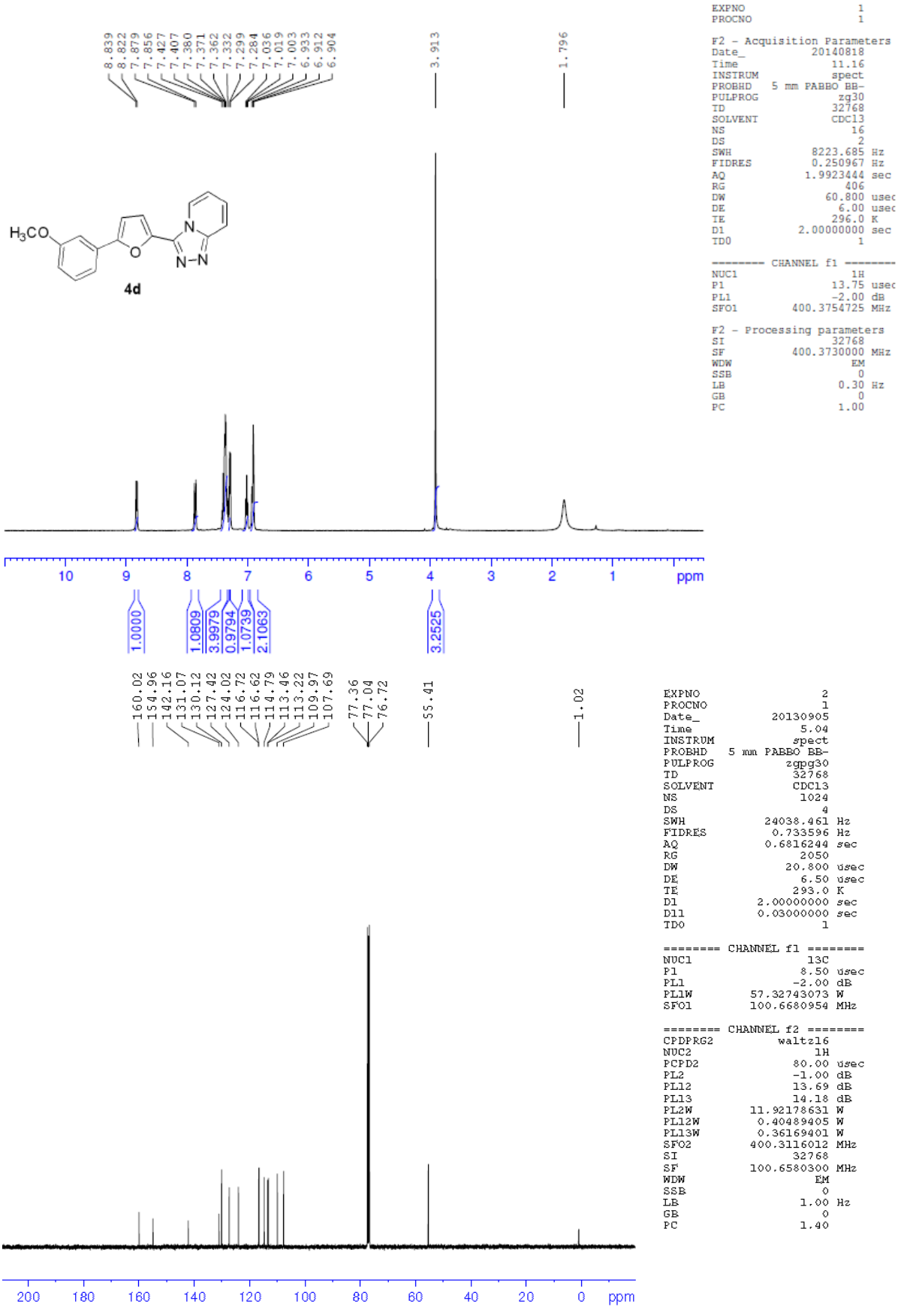
F2 - Acquisition Parameters
Date_           20140808
Time               22.04
INSTRUM            spect
PROBHD   5 mm DUL BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2500
DS                     0
SWH            20325.203 Hz
FIDRES          0.620276 Hz
AQ             0.8061428 sec
RG                5792.6
DW                24.600 usec
DE                 6.00 usec
TE                 0.0 K
D1           3.00000000 sec
d11          0.03000000 sec
DELTA        2.90000010 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.50 usec
PL1                0.00 dB
SFO1         75.4771525 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              14.75 dB
PL13              18.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677079 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.70
```

16. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(3-Methoxyphenyl)furan-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (4d)




```
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140818
Time                11.16
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ             1.9923444 sec
RG                   406
DW                60.800 usec
DE                 6.00 usec
TE                296.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.75 usec
PL1                -2.00 dB
SFO1         400.3754725 MHz

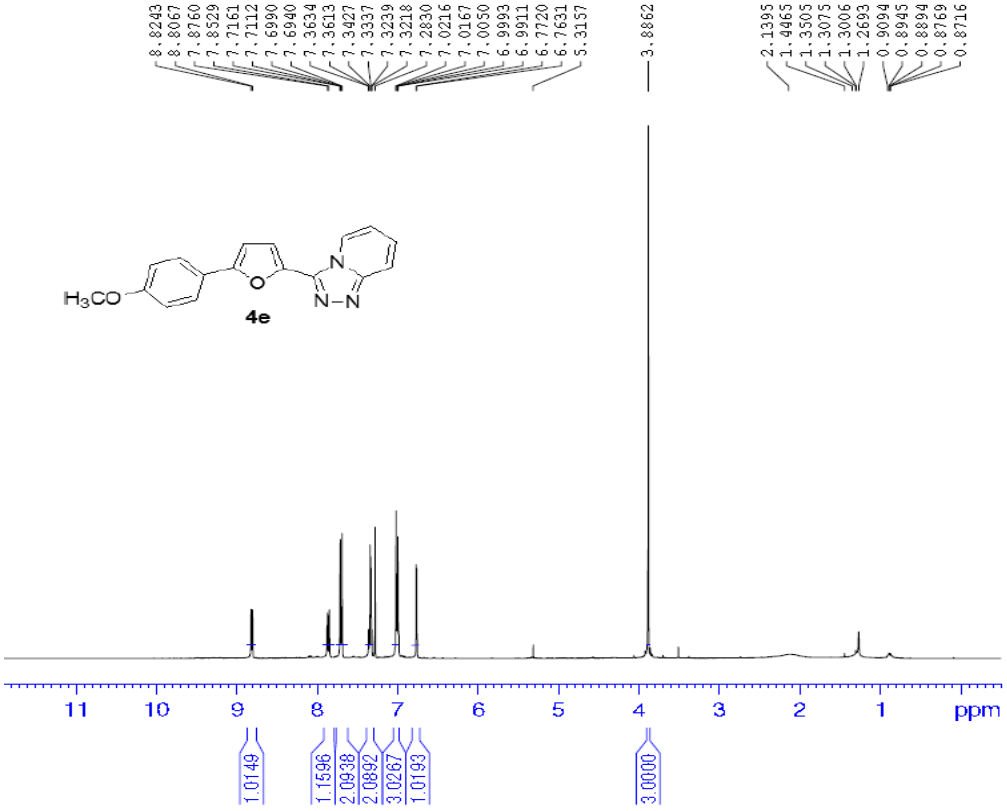
F2 - Processing parameters
SI                 32768
SF          400.3730000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

```
EXPNO                  2
PROCNO                 1
Date_           20130905
Time                5.04
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ             0.6816244 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                293.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.50 usec
PL1                -2.00 dB
PL1W          57.32743073 W
SFO1         100.6680954 MHz

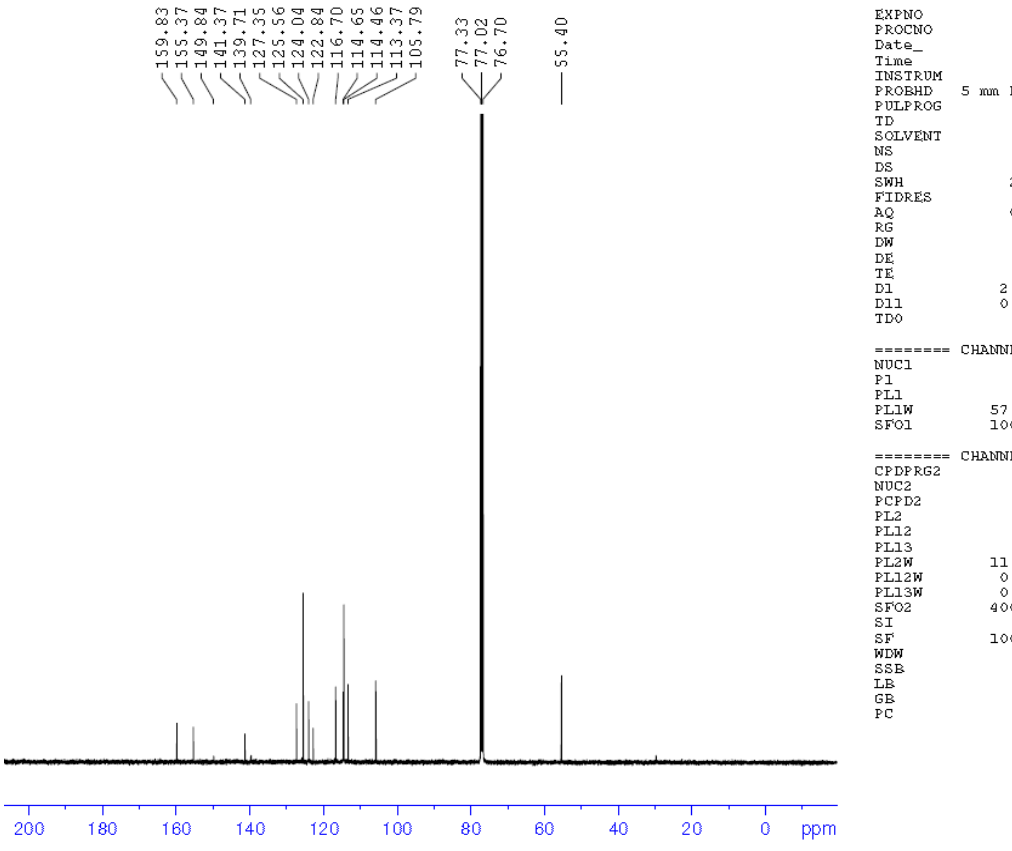
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               13.69 dB
PL13               14.18 dB
PL2W          11.92178631 W
PL12W          0.40489405 W
PL13W          0.36169401 W
SFO2         400.3116012 MHz
SI                 32768
SF          100.6580300 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

17. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(4-Methoxyphenyl)furan-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (4e)




```
EXPNO                  1
PROCNO                 1
Date_           20131015
Time                20.39
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                293.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.75 usec
PL1                -1.00 dB
PL1W        11.92178631 W
SFO1        400.3124721 MHz
SI                 32768
SF          400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```

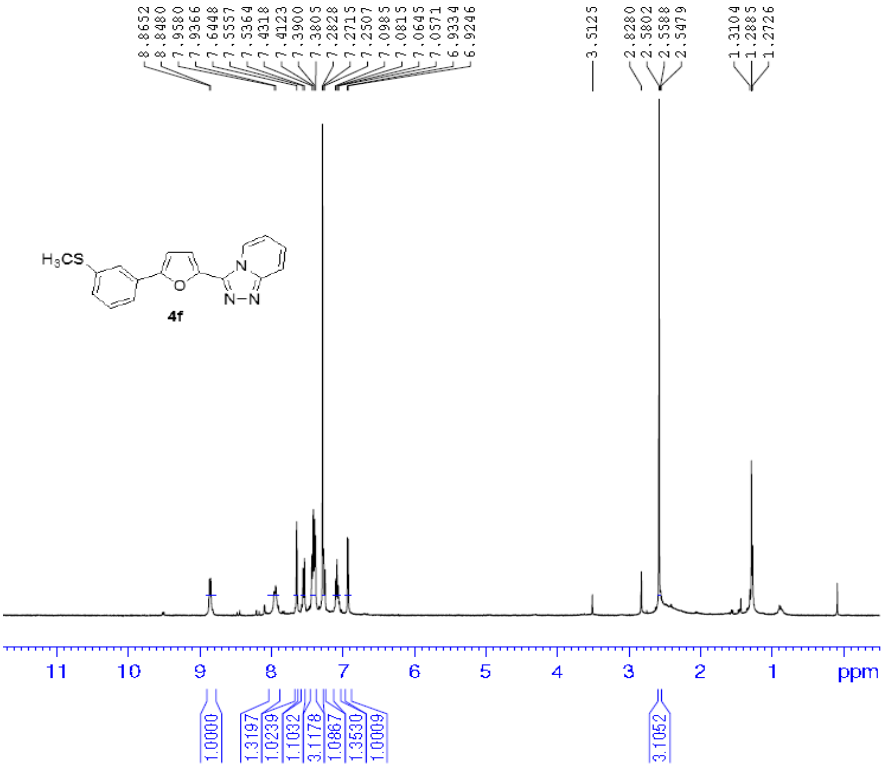



```
EXPNO                  2
PROCNO                 1
Date_           20131015
Time                22.58
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  3000
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816244 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                293.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 8.50 usec
PL1                -2.00 dB
PL1W        57.32743073 W
SFO1        100.6680954 MHz

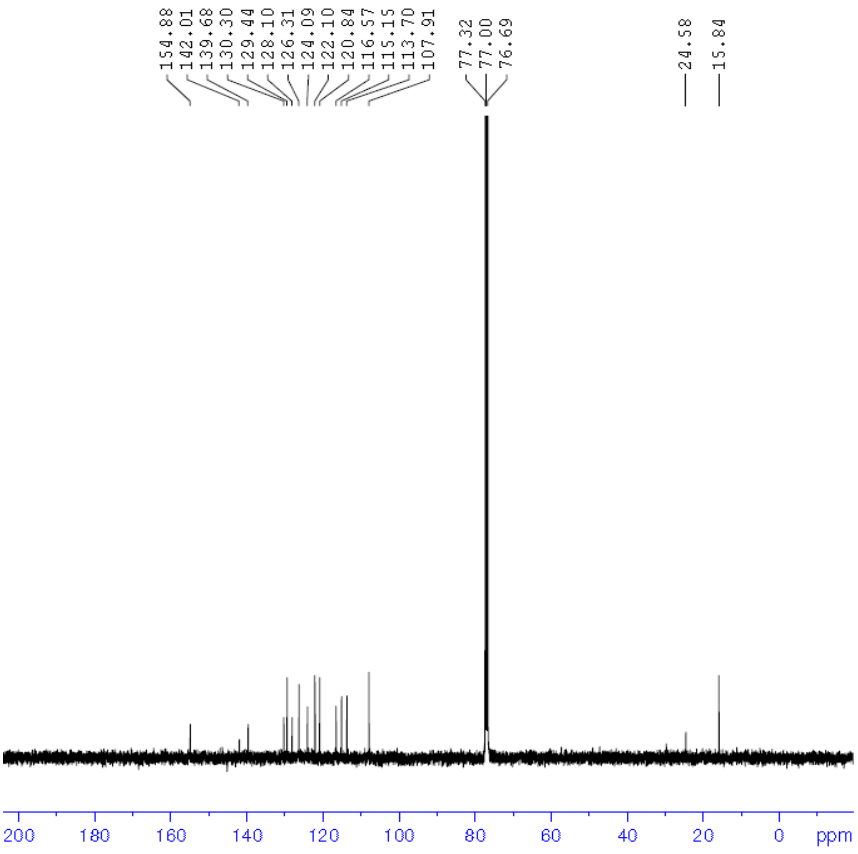
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               13.69 dB
PL13               14.18 dB
PL2W        11.92178631 W
PL12W        0.40489405 W
PL13W        0.36169401 W
SFO2        400.3116012 MHz
SI                 32768
SF          100.6580300 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

18. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(3-(Methylthio)phenyl)furan-2-yl)-[1,2,4]triazolo[4,3-a]pyridine (4f)




```
EXPNO                  3
PROCNO                 1
Date_           20131018
Time                8.37
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                   362
DW                60.800 usec
DE                 6.50 usec
TE                293.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.75 usec
PL1               -1.00 dB
PL1W         11.92178631 W
SFO1         400.3124721 MHz
SI                 32768
SF           400.3100000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.40
```

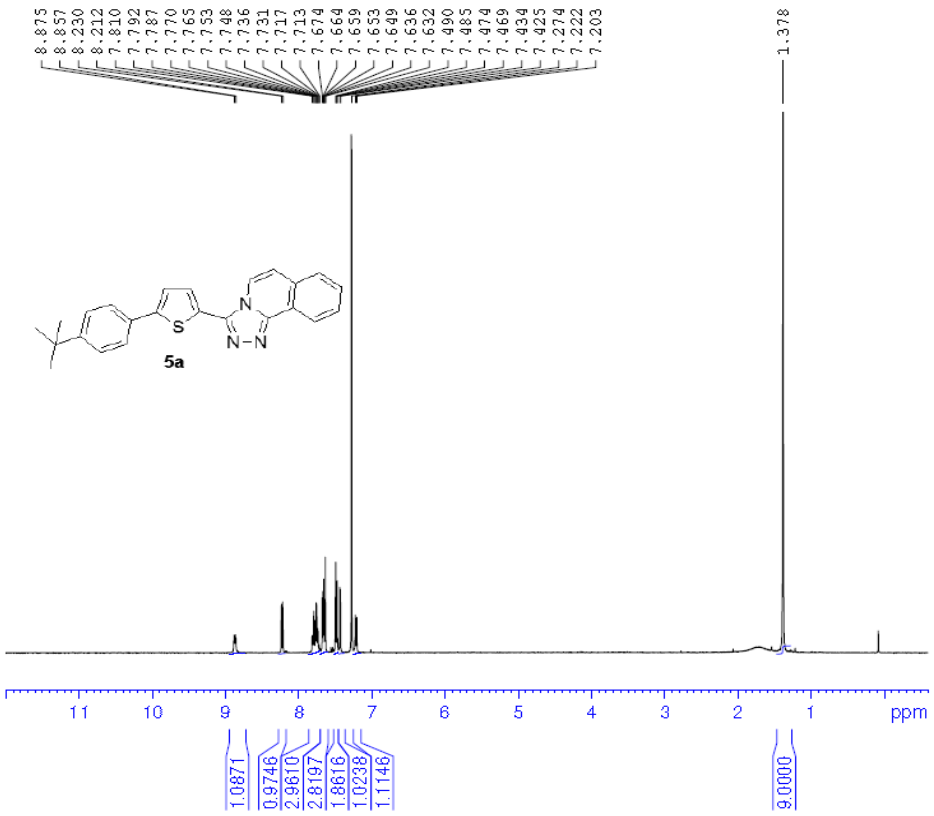



```
EXPNO                  2
PROCNO                 1
Date_           20131018
Time                3.56
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  3000
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816244 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                293.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.50 usec
PL1               -2.00 dB
PL1W         57.32743073 W
SFO1         100.6680954 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              13.69 dB
PL13              14.18 dB
PL2W         11.92178631 W
PL12W         0.40489405 W
PL13W         0.36169401 W
SFO2         400.3116012 MHz
SI                 32768
SF           100.6580300 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

19. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-(4-*tert*-Butylphenyl)thiophen-2-yl)-[1,2,4]triazolo[3,4-a]isoquinoline (5a)



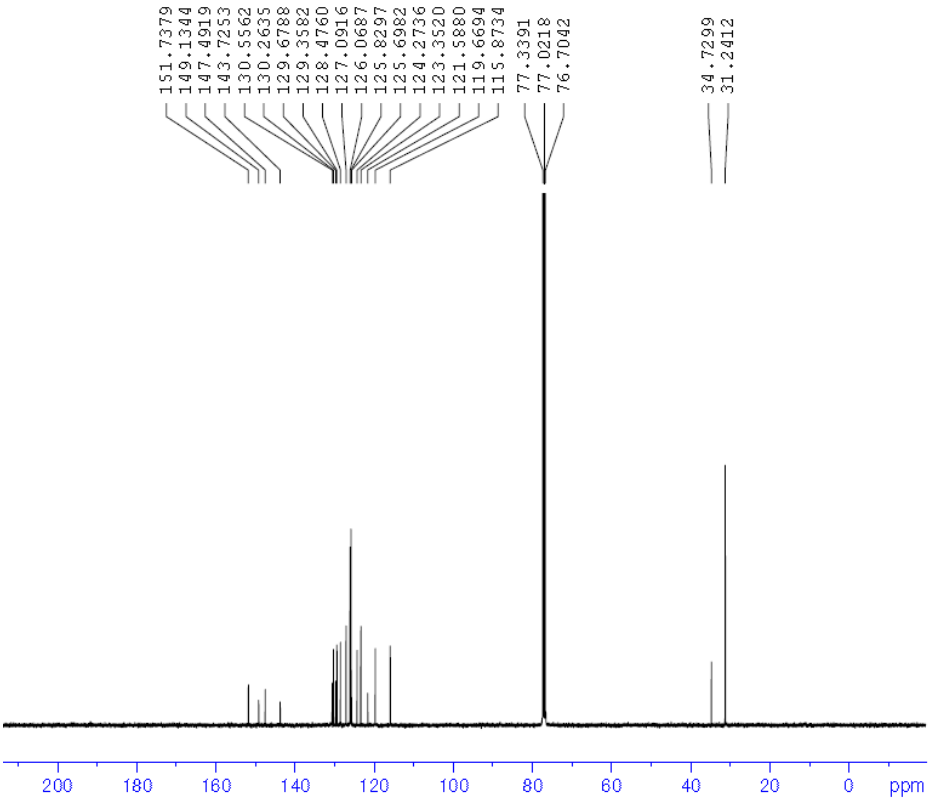

```
Current Data Parameters

EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130725
Time               12.24
INSTRUM            spect
PROBHD    5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8741.259 Hz
FIDRES          0.266762 Hz
AQ              1.8743796 sec
RG                  1024
DW                57.200 usec
DE                 6.00 usec
TE                295.2 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.20 usec
PL1                -2.00 dB
SFO1         400.2336755 MHz

F2 - Processing parameters
SI                 32768
SF           400.2300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters

EXPNO                  2
PROCNO                 1

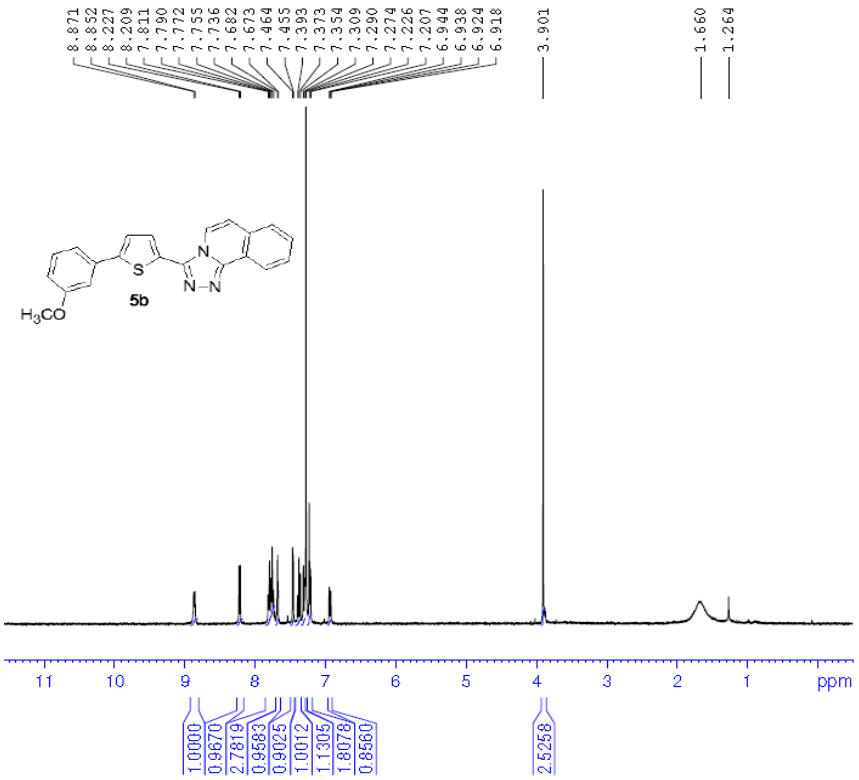
F2 - Acquisition Parameters
Date_           20130728
Time               4.45
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  4000
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816244 sec
RG                  80.6
DW                20.800 usec
DE                 6.00 usec
TE                295.8 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  8.10 usec
PL1                -3.00 dB
SFO1         100.6278593 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL12               14.04 dB
PL13               15.00 dB
PL2                -0.50 dB
SFO2         400.1516006 MHz

F2 - Processing parameters
SI                 32768
SF           100.6177980 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

20.[1]H and [13]C NMR spectrum of 3-(5-(3-Methoxyphenyl)thiophen-2-yl)-[1,2,4]triazolo[3,4-a]isoquinoline (5b)



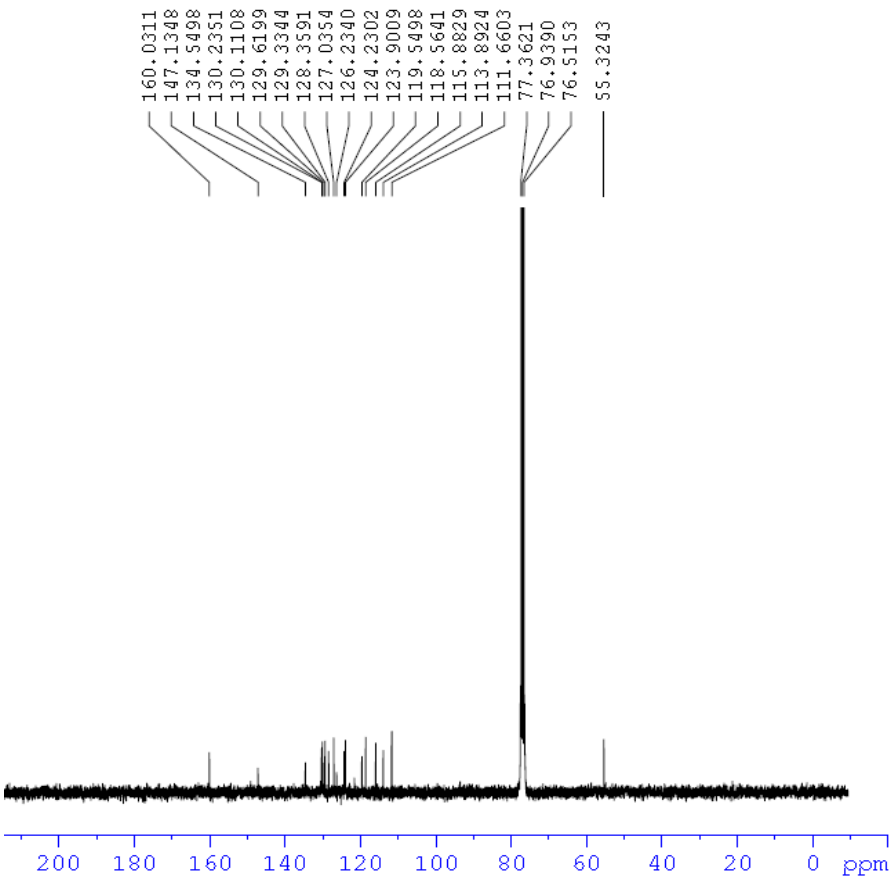

```
Current Data Parameters

EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130905
Time               17.14
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                1149.4
DW                60.800 usec
DE                 6.00 usec
TE                294.9 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.20 usec
PL1                -2.00 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters

EXPNO                  5
PROCNO                 1

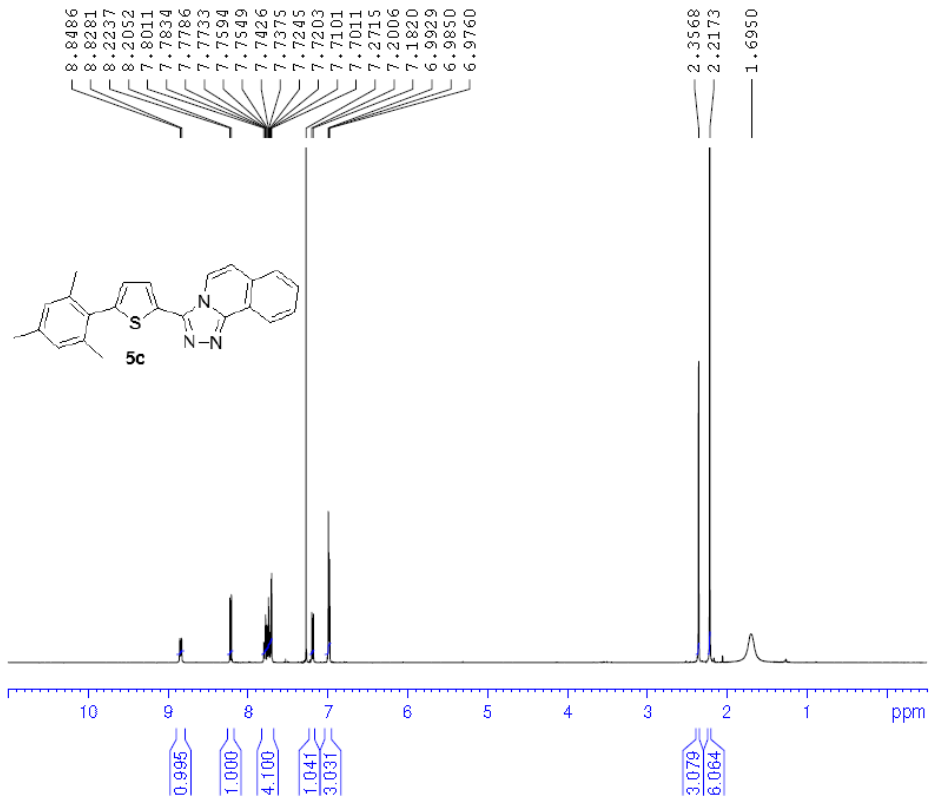
F2 - Acquisition Parameters
Date_           20130911
Time               1.26
INSTRUM            spect
PROBHD   5 mm DUL BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  3000
DS                     0
SWH            20325.203 Hz
FIDRES          0.620276 Hz
AQ              0.8061428 sec
RG                10321.3
DW                24.600 usec
DE                 6.00 usec
TE                 0.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 8.50 usec
PL1                0.00 dB
SFO1         75.4771525 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12              14.75 dB
PL13              18.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677079 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.70
```

21. $^{1}H$ and $^{13}C$ NMR spectrum of 3-(5-Mesitylthiophen-2-yl)-[1,2,4]triazolo[3,4-a]isoquinoline (5c)



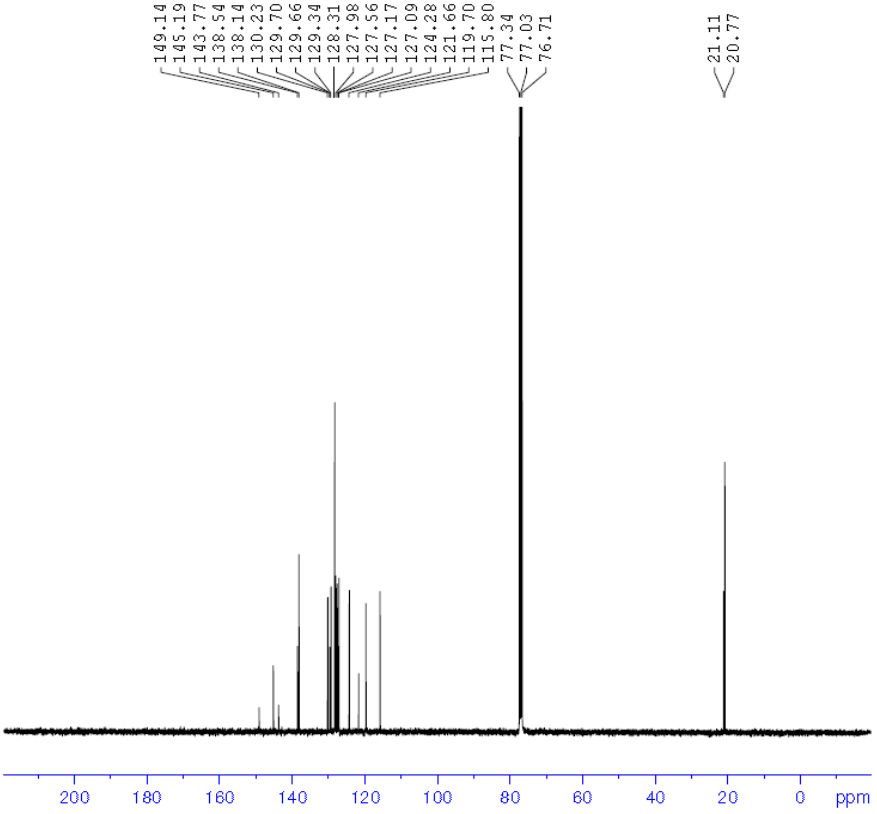

```
Current Data Parameters

EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20131016
Time               10.02
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                   575
DW                60.800 usec
DE                 6.00 usec
TE                295.2 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                -0.50 dB
SFO1         400.1524711 MHz

F2 - Processing parameters
SI                 32768
SF          400.1500000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```

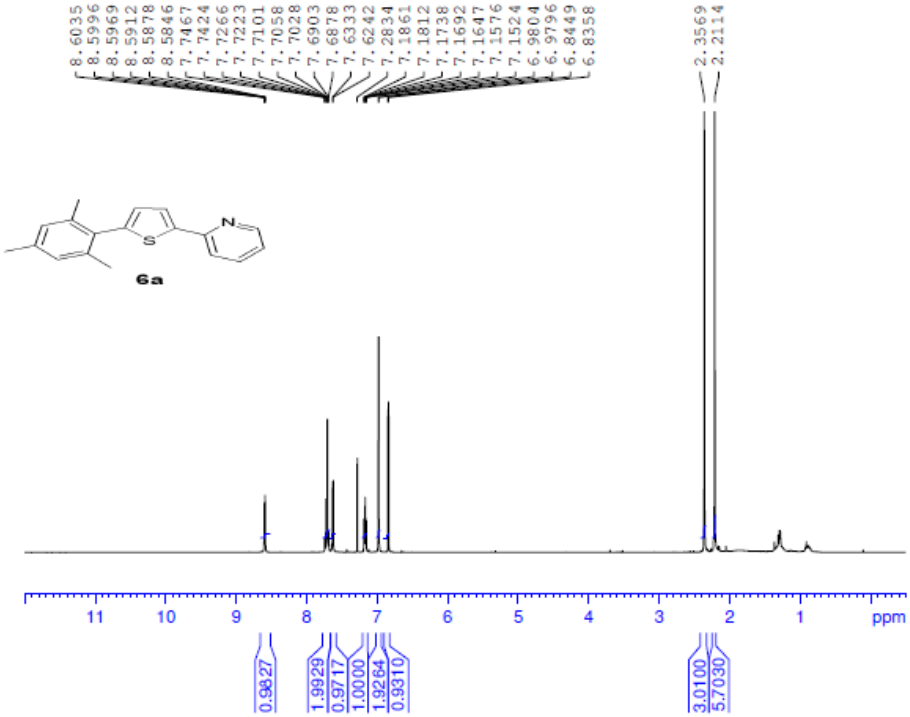



```
EXPNO                  2
PROCNO                 1
Date_           20131017
Time               4.49
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  3000
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816244 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                293.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 8.50 usec
PL1               -2.00 dB
PL1W         57.32743073 W
SFO1        100.6680954 MHz

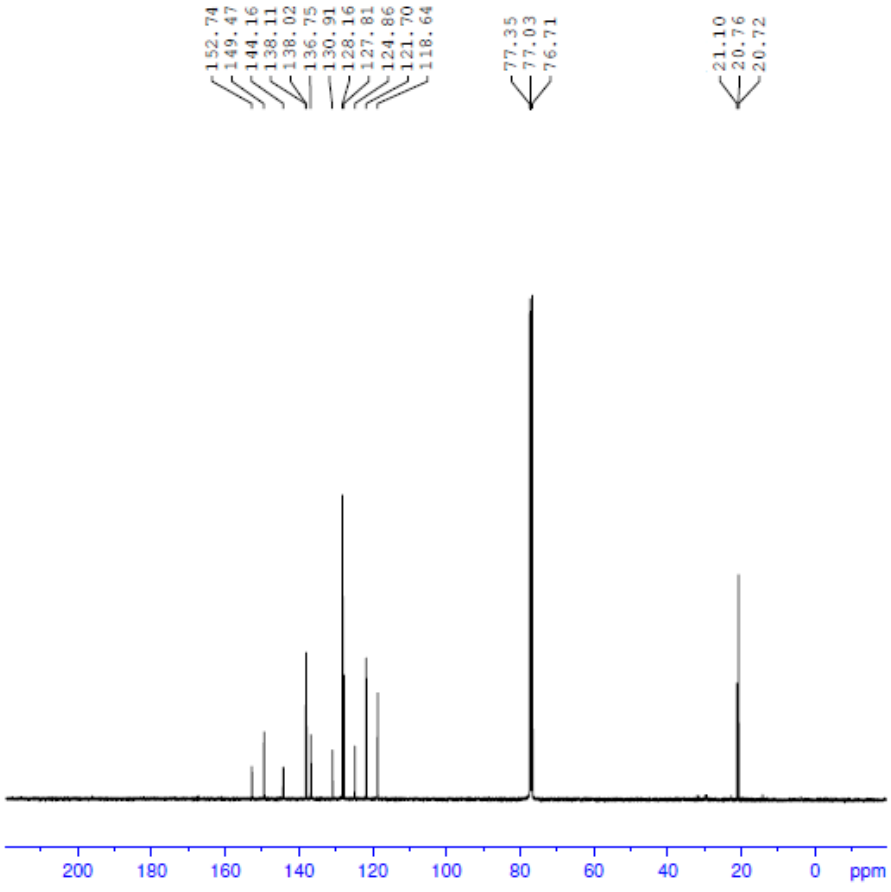
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              13.69 dB
PL13              14.18 dB
PL2W         11.92178631 W
PL12W         0.40489405 W
PL13W         0.36169401 W
SFO2        400.3116012 MHz
SI                 32768
SF          100.6580300 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

22. $^{1}H$ and $^{13}C$ NMR spectrum of 2-(5-Mesitylthiophen-2-yl)pyridine (6a)




```
EXPNO                  1
PROCNO                 1
Date_           20140812
Time               23.32
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                293.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.35 usec
PL1                -2.00 dB
PL1W          15.00864029 W
SFO1          400.3124721 MHz
SI                 32768
SF            400.3100000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```

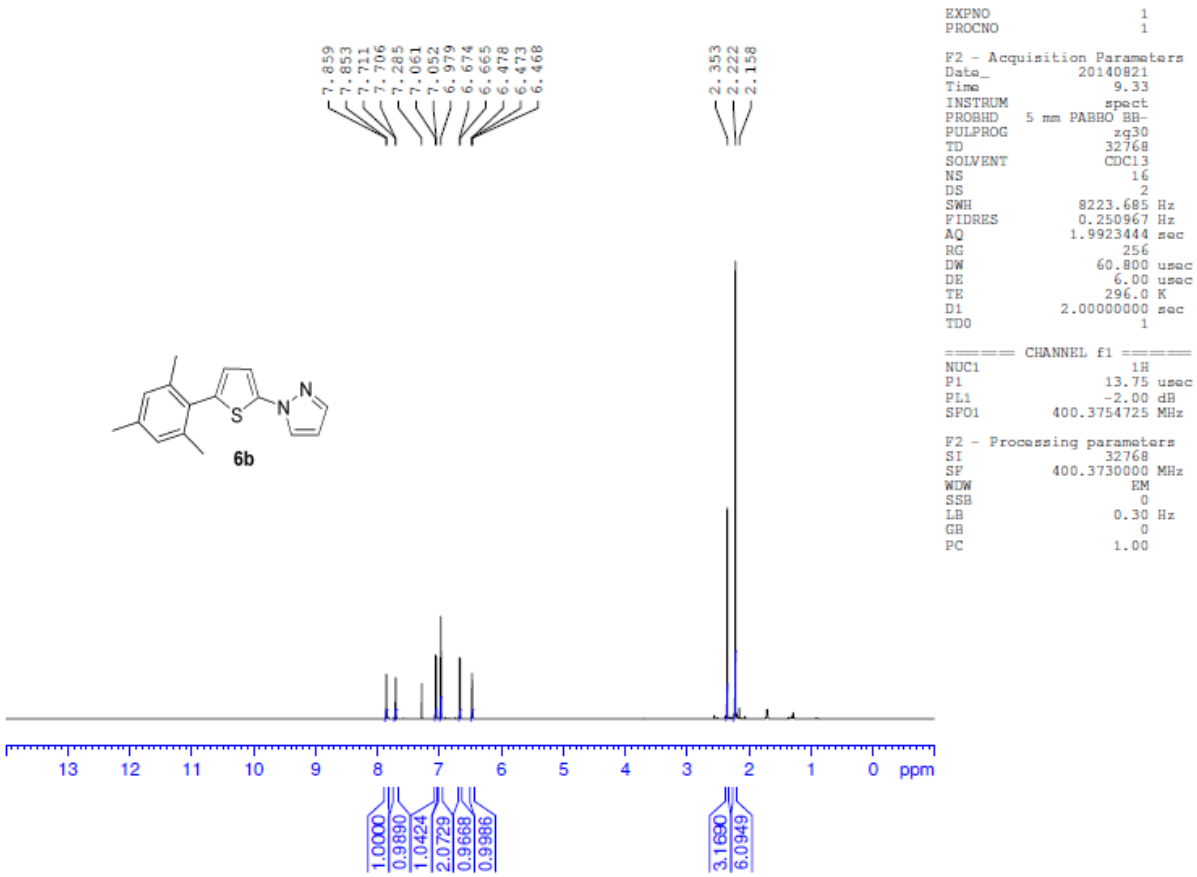



```
EXPNO                  2
PROCNO                 1
Date_           20140813
Time               3.21
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  5000
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816244 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                293.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.50 usec
PL1                -1.50 dB
PL1W          51.09312820 W
SFO1          100.6680954 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                -2.00 dB
PL12               16.17 dB
PL13               17.00 dB
PL2W          15.00864029 W
PL12W          0.22873959 W
PL13W          0.18894759 W
SFO2          400.3116012 MHz
SI                 32768
SF            100.6580300 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

23. $^{1}H$ spectrum of 1-(5-Mesitylthiophen-2-yl)-1H-pyrazole (6b)



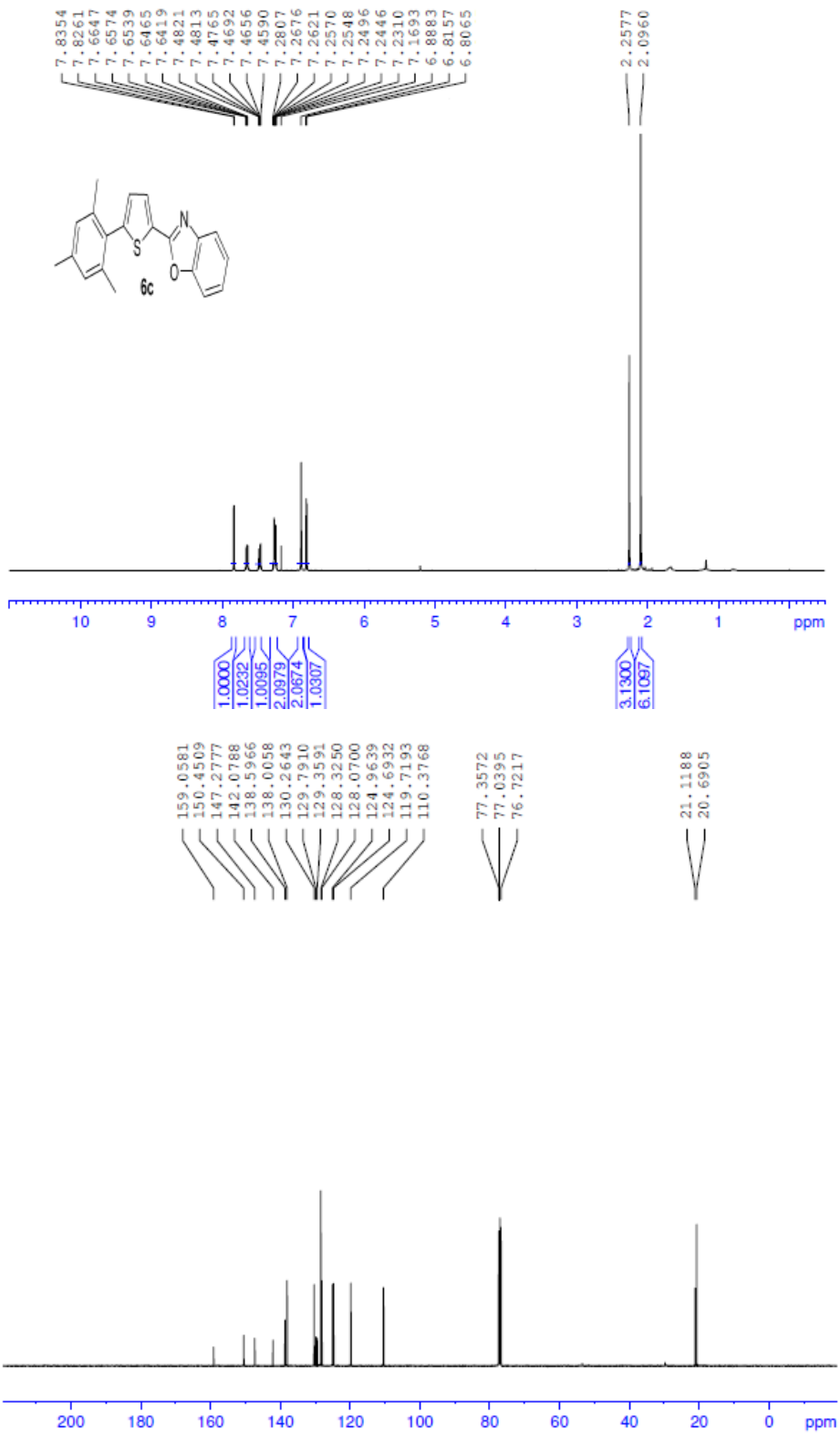

```
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140821
Time                9.33
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                   256
DW                60.800 usec
DE                 6.00 usec
TE                296.0 K
D1           2.00000000 sec
TD0                    1

====== CHANNEL f1 ======
NUC1                  1H
P1                 13.75 usec
PL1                -2.00 dB
SFO1         400.3754725 MHz

F2 - Processing parameters
SI                 32768
SF           400.3730000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

24. $^{1}H$ and $^{13}C$ NMR spectrum of 2-(5-Mesitylthiophen-2-yl)benzo[d]oxazole (6c)




```
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140812
Time               21.58
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT             CDC13
NS                    32
DS                     2
SWH              8223.685 Hz
FIDRES           0.250967 Hz
AQ               1.9923444 sec
RG                   128
DW                60.800 usec
DE                 6.00 usec
TE                295.6 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.25 usec
PL1                -0.50 dB
SFO1         400.1524711 MHz

F2 - Processing parameters
SI                 32768
SF           400.1500411 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

```
EXPNO                  2
PROCNO                 1

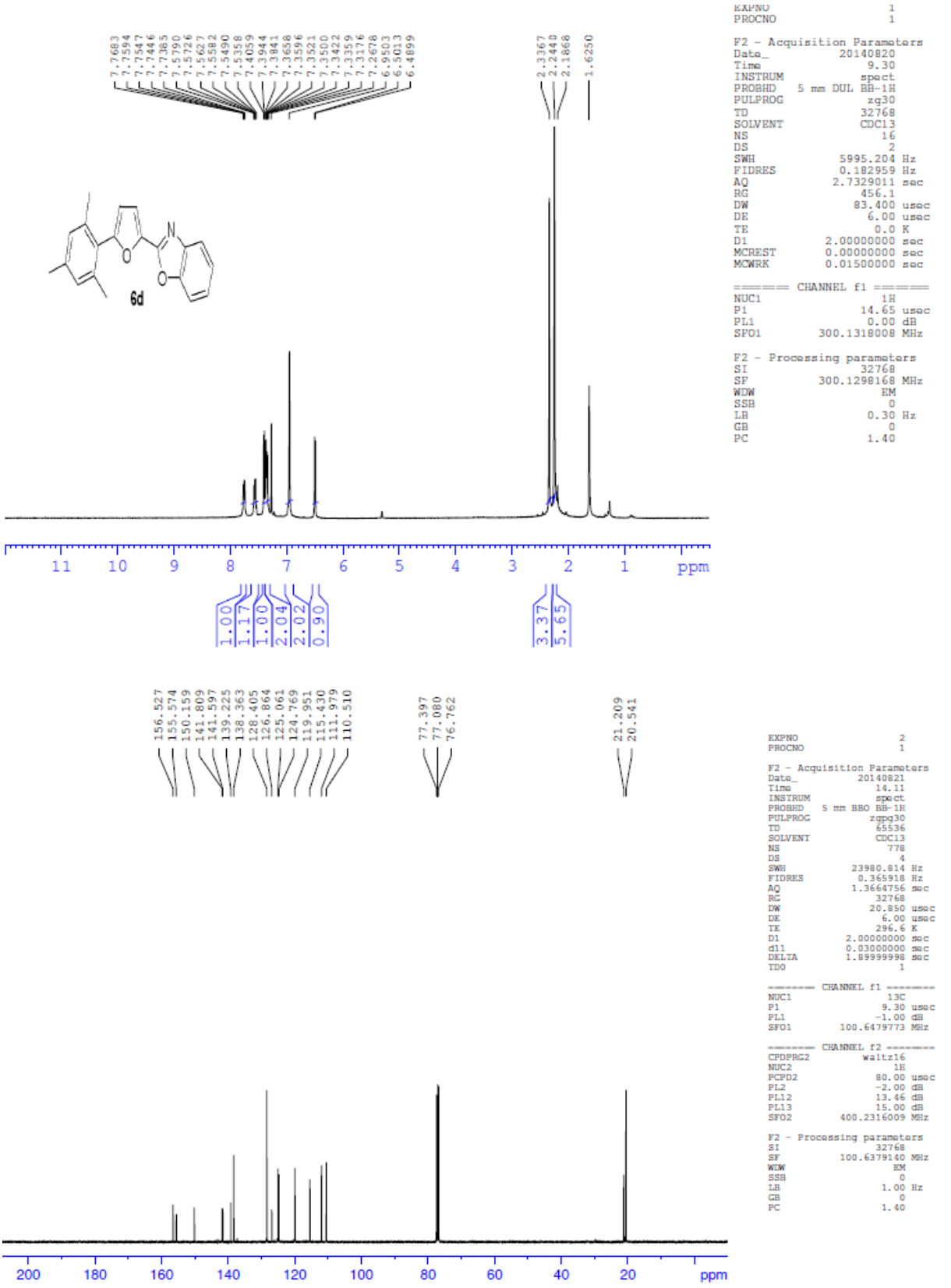
F2 - Acquisition Parameters
Date_           20140813
Time               0.40
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT             CDC13
NS                  3500
DS                     4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6816244 sec
RG                   128
DW                20.800 usec
DE                 6.00 usec
TE                296.5 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  8.75 usec
PL1                -3.00 dB
SFO1         100.6278593 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL12               14.49 dB
PL13               15.00 dB
PL2                -0.50 dB
SFO2         400.1516006 MHz

F2 - Processing parameters
SI                 32768
SF           100.6177980 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

25. $^{1}H$ and $^{13}C$ NMR spectrum of 2-(5-Mesitylfuran-2-yl)benzo[d]oxazole (6d)




EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140820
Time 9.30
INSTRUM spect
PROBHD 5 mm DUL BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 456.1
DW 83.400 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======= CHANNEL f1 =======
NUC1 1H
P1 14.65 usec
PL1 0.00 dB
SFO1 300.1318008 MHz

F2 - Processing parameters
SI 32768
SF 300.1298168 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

EXPNO 2
PROCNO 1

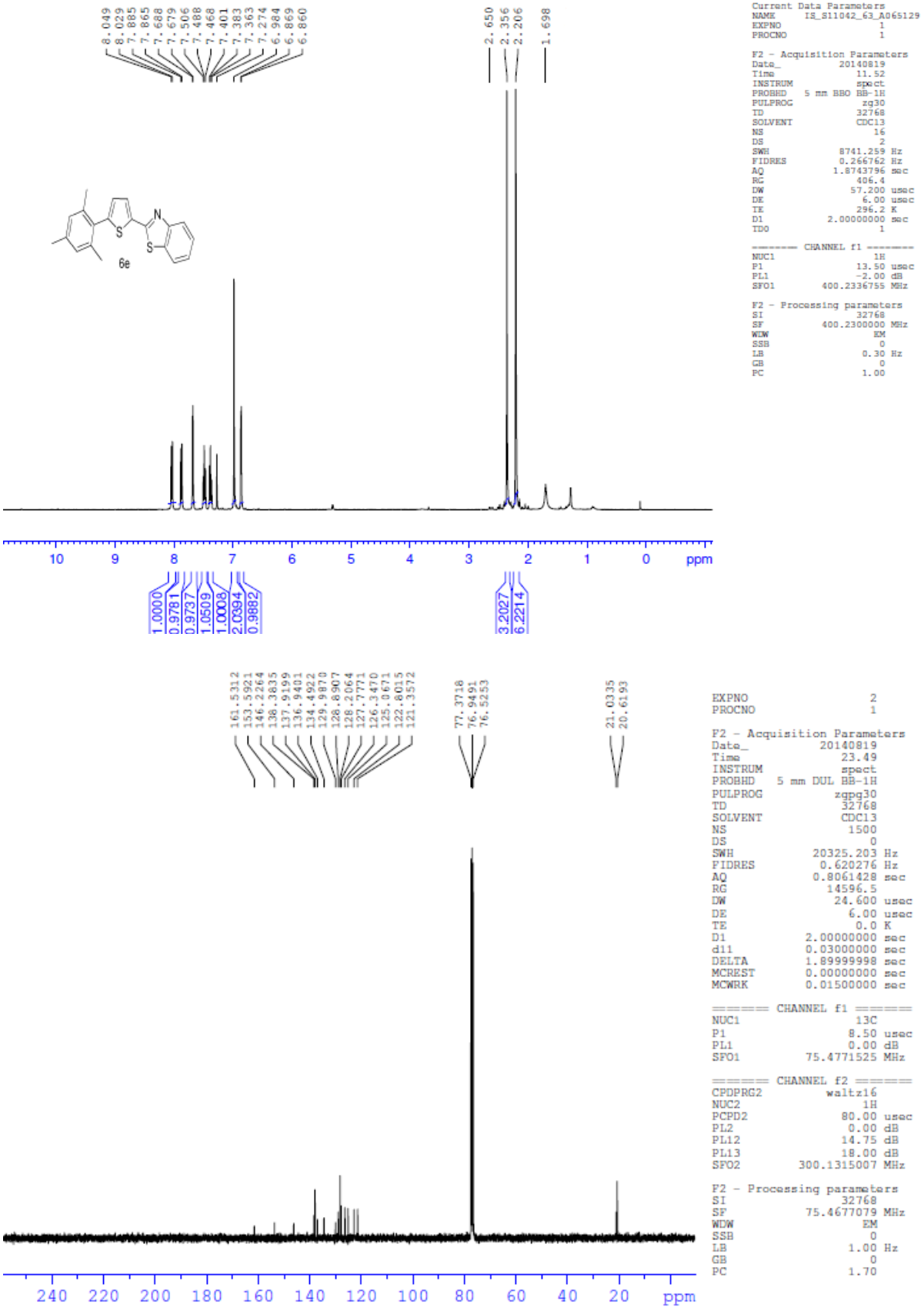
F2 - Acquisition Parameters
Date_ 20140821
Time 14.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 778
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 -1.00 dB
SFO1 100.6479773 MHz

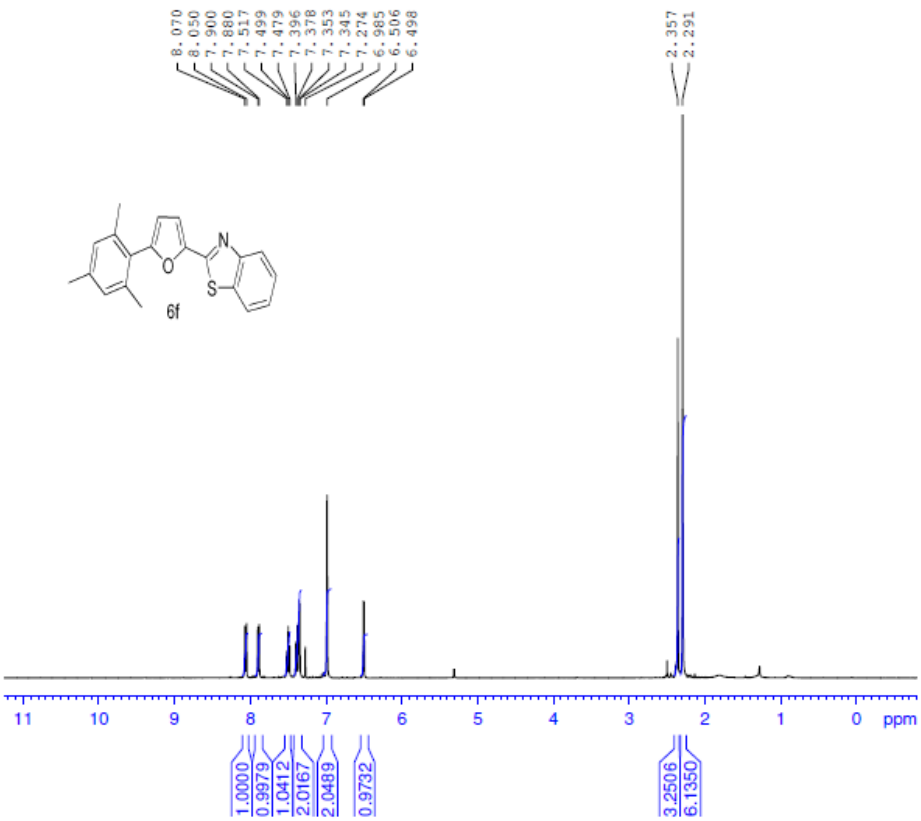
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.46 dB
PL13 15.00 dB
SFO2 400.2316009 MHz

F2 - Processing parameters
SI 32768
SF 100.6379140 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

26. $^{1}H$ and $^{13}C$ NMR spectrum of 2-(5-Mesitylthiophen-2-yl)benzo[d]thiazole (6e)




27. $^{1}H$ and $^{13}C$ NMR spectrum of 2-(5-Mesitylfuran-2-yl)benzo[d]thiazole (6f)

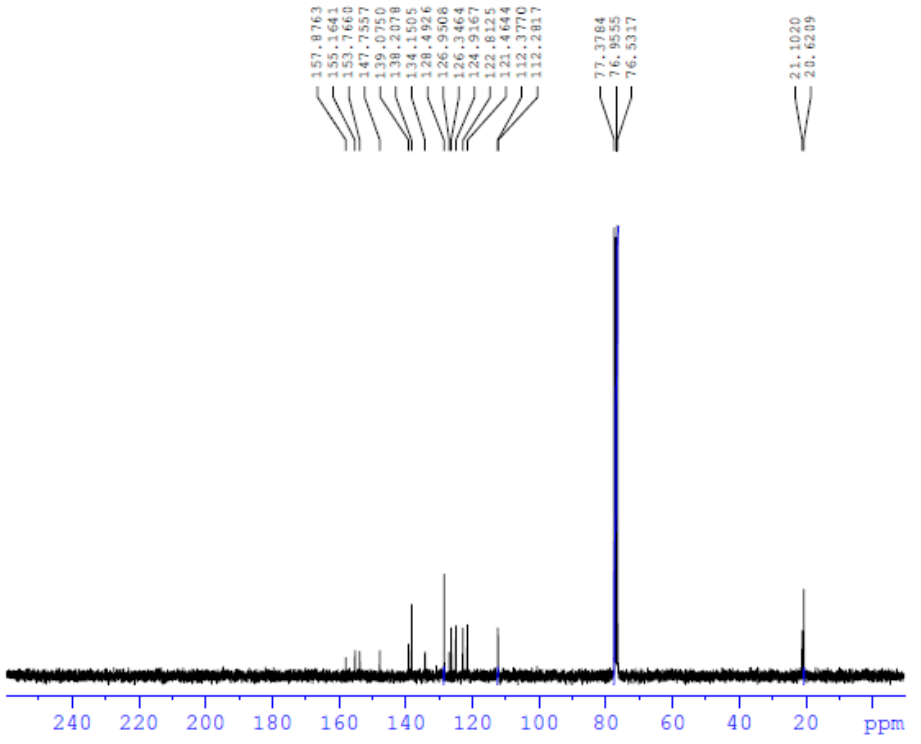



```
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140820
Time               10.24
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8741.259 Hz
FIDRES          0.266762 Hz
AQ              1.8743796 sec
RG                 322.5
DW                57.200 usec
DE                 6.00 usec
TE                296.2 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.50 usec
PL1                -2.00 dB
SFO1         400.2336755 MHz

F2 - Processing parameters
SI                 32768
SF           400.2300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
EXPNO                  2
PROCNO                 1

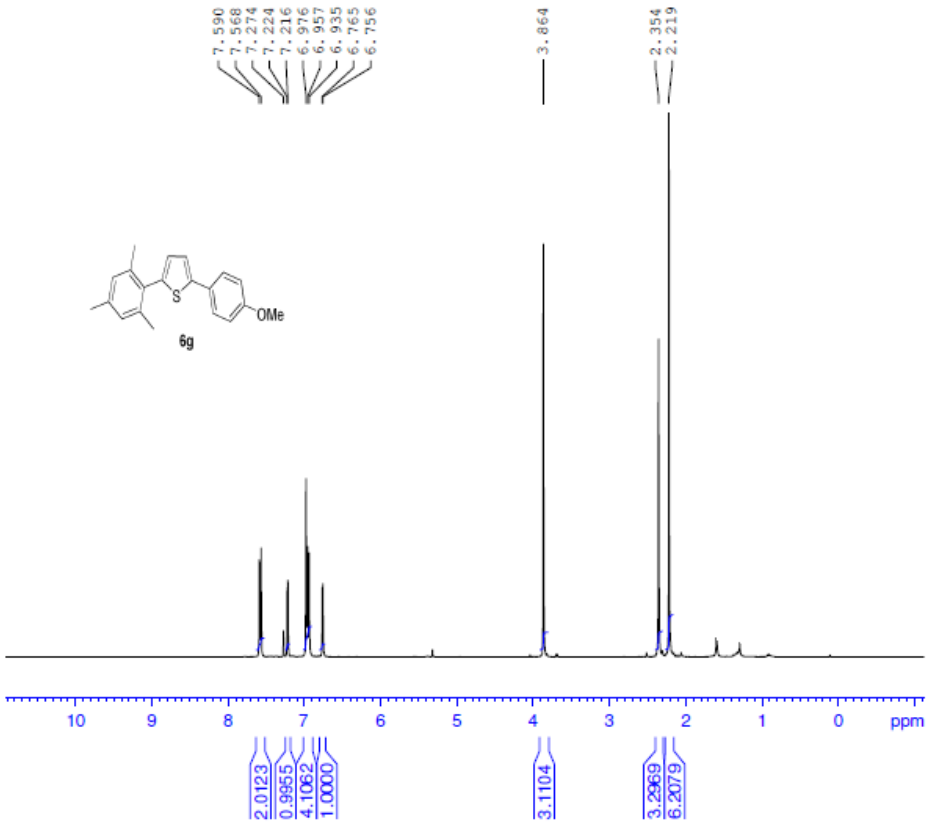
F2 - Acquisition Parameters
Date_           20140820
Time               22.35
INSTRUM            spect
PROBHD   5 mm DUL BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  1024
DS                     0
SWH            20325.203 Hz
FIDRES          0.620276 Hz
AQ              0.8061428 sec
RG                 5792.6
DW                24.600 usec
DE                 6.00 usec
TE                 0.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 8.50 usec
PL1                0.00 dB
SFO1         75.4771525 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              14.75 dB
PL13              18.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677079 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.70
```

28. $^{1}H$ and $^{13}C$ NMR spectrum of 2-Mesityl-5-(4-methoxyphenyl)thiophene (6g)

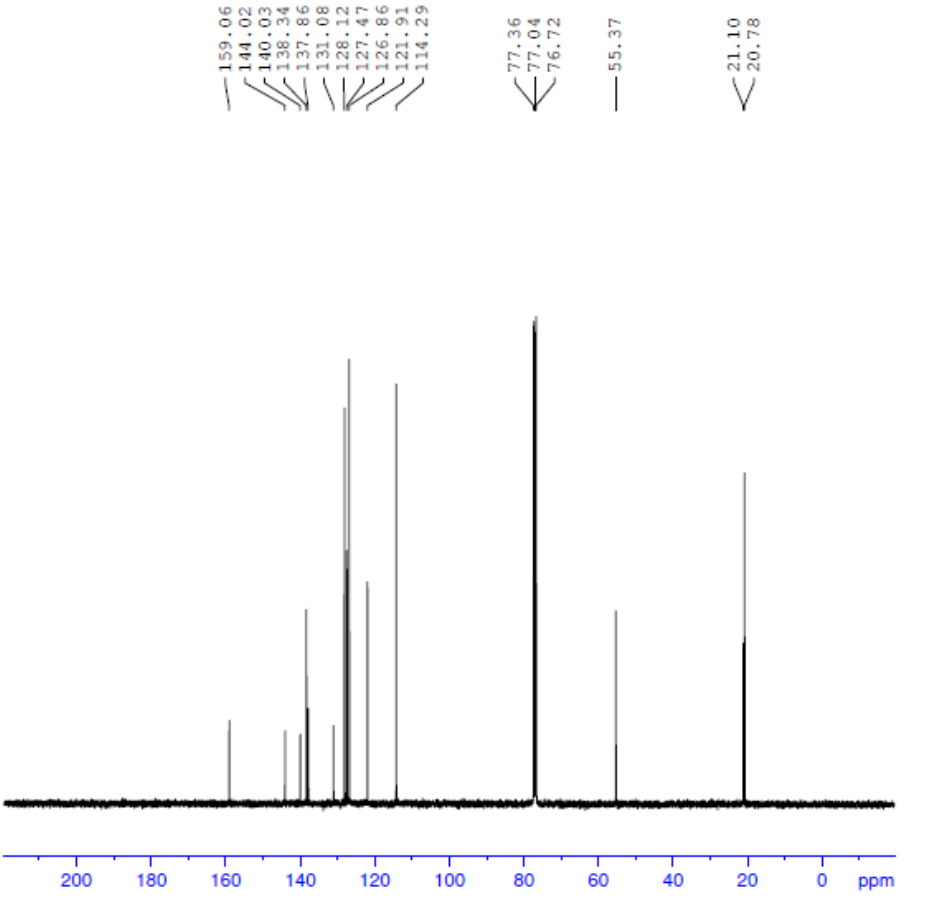



```
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140819
Time               11.41
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8741.259 Hz
FIDRES          0.266762 Hz
AQ              1.8743796 sec
RG                   256
DW                57.200 usec
DE                 6.00 usec
TE                296.2 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.50 usec
PL1                -2.00 dB
SFO1          400.2336755 MHz

F2 - Processing parameters
SI                 32768
SF            400.2300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

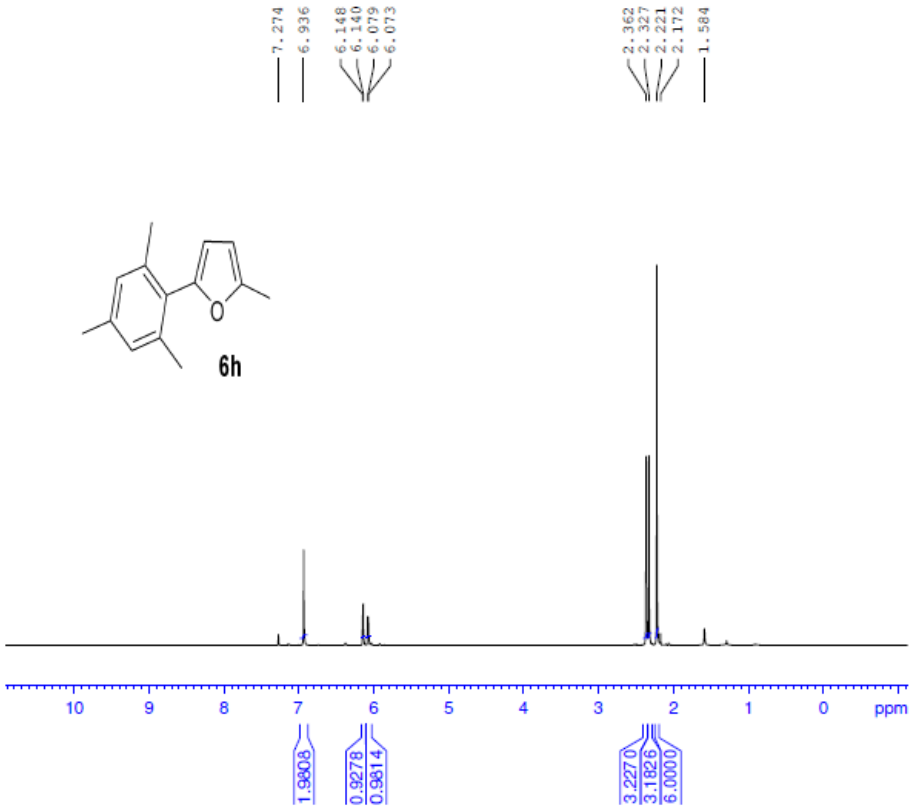



```
EXPNO                  2
PROCNO                 1
Date_           20140820
Time               6.38
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816244 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                293.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.50 usec
PL1                -1.50 dB
PL1W          51.09312820 W
SFO1         100.6680954 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                -2.00 dB
PL12               16.17 dB
PL13               17.00 dB
PL2W          15.00864029 W
PL12W          0.22873959 W
PL13W          0.18894759 W
SFO2         400.3116012 MHz
SI                 32768
SF           100.6580300 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

29. $^{1}H$ and $^{13}C$ NMR spectrum of 2-mesityl-5-methylfuran (6h)

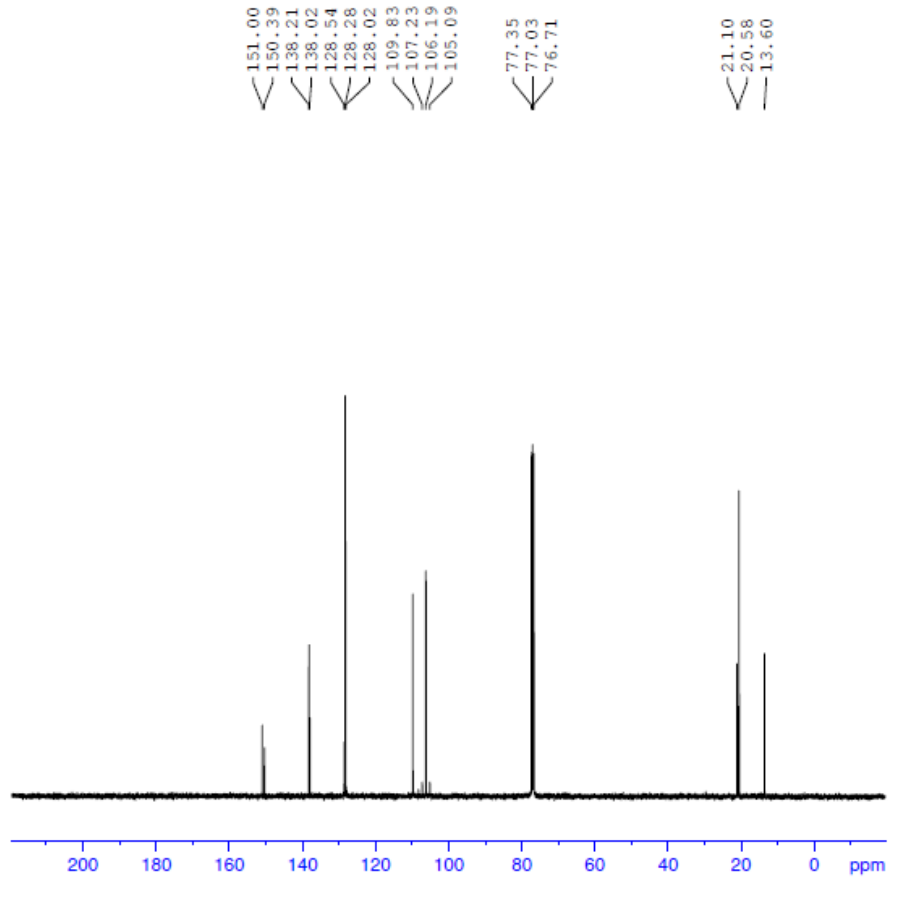



```
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140819
Time               11.44
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8741.259 Hz
FIDRES         0.266762 Hz
AQ            1.8743796 sec
RG                  256
DW               57.200 usec
DE                6.00 usec
TE               296.1 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.50 usec
PL1                -2.00 dB
SFO1         400.2336755 MHz

F2 - Processing parameters
SI                32768
SF           400.2300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
EXPNO                  2
PROCNO                 1
Date_           20140820
Time                5.47
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816244 sec
RG                 2050
DW               20.800 usec
DE                6.50 usec
TE               293.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.50 usec
PL1               -1.50 dB
PL1W        51.09312820 W
SFO1        100.6680954 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2               -2.00 dB
PL12              16.17 dB
PL13              17.00 dB
PL2W        15.00864029 W
PL12W        0.22873959 W
PL13W        0.18894759 W
SFO2        400.3116012 MHz
SI                32768
SF          100.6580300 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```