# Supporting Information

## Oxidative Dual C–H Thiolation of Imidazopyridines with Ethers or Alkanes Using Elemental Sulphur

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## 1. General Information

$^{1}H$ and $^{13}C$ NMR spectra were measured on a Bruker Avance-III 600 instrument (600 MHz for $^{1}H$, 151 MHz for $^{13}C$ NMR spectroscopy) using $CDCl_3$ as the solvent. Chemical shifts for $^{1}H$ and $^{13}C$ NMR were referred to internal $Me_4Si$ (0 ppm) as the standard. Mass spectra were measured on an Agilent GC-MS-5975C Plus spectrometer (EI). LCMS (ESI) analysis was measured on a AB SCIEX, API3200. HRMS (ESI) analysis was measured on a Thermo Scientific LTQ Orbitrap XL. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet.

## 2. Experimental Procedure

### (1) Typical experimental procedure for the dual C–H thiolation

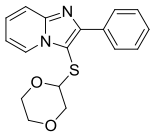
To a 15-mL tube with a Teflon cap, equipped with a magnetic stirring bar was charged with **1a** (0.4 mmol), $S_8$ (0.8 mmol), in 1,4-Dioxane (0.5 mL). The reaction mixture was stirred at 120 ℃ for 24 hours. After the reaction finished, the mixture was extracted with ethyl acetate, the combined organic layers were dried over anhydrous $Na_2SO_4$ and evaporated under vacuum. The residue was purified by flash column chromatography (petroleum ether / ethyl acetate) to afford the desired product.

### (2) Experimental procedure for the preparation of compound 38

To a 50-mL tube with a Teflon cap, equipped with a magnetic stirring bar was charged with 2-phenylimidazo[1,2-*a*]pyridine (1 mmol), $S_8$ (2 mmol), $Ag_2CO_3$ (2 mmol) in DMF (4 mL). The reaction mixture was stirred at 120 ℃ for 48 hours. After the reaction finished, the reaction mixture was extracted with ethyl acetate, the organic layer was washed with brine, dried with anhydrous $Na_2SO_4$ and evaporated under vacuum. The residue was purified by flash column chromatography (petroleum ether / ethyl acetate) to afford the desired product **38** in 60% yield.

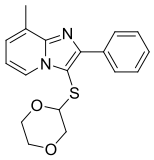
## 3. The data of products

**3-(1,4-dioxan-2-ylthio)-2-phenylimidazo[1,2-*a*]pyridine (3)**



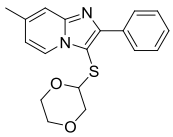
Brown oil. $^{1}H$ NMR (600 MHz, $CDCl_3$) δ 8.55 (d, *J* = 6.8 Hz, 1H), 8.15 (d, *J* = 7.3 Hz, 2H), 7.60 (d, *J* = 9.0 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.27 – 7.22 (m, 1H), 6.85 (t, *J* = 6.8 Hz, 1H), 4.74 (dd, *J* = 6.1, 2.8 Hz, 1H), 3.95 – 3.91 (m, 1H), 3.76 (dd, *J* = 11.9, 2.8 Hz, 1H), 3.55 – 3.45 (m, 4H). $^{13}C$ NMR (151 MHz, $CDCl_3$) δ 150.6, 146.8, 133.6, 128.6, 128.4, 128.3, 126.4, 125.1, 117.4, 112.7, 107.3, 84.2, 69.7, 66.2, 64.7. IR (KBr, $cm^{-1}$): 2967, 2916, 2853, 1600, 1492, 1465, 1445, 1353, 1123, 871, 777, 759. LRMS (EI, 70 eV) m/z (%): 312 (2), 226 (100), 225 (42), 181 (10), 78 (36). HRMS (ESI) for $C_{17}H_{17}N_2O_2S^+$ $(M+H)^+$: calcd 313.1005, found 313.1006.

**3-(1,4-dioxan-2-ylthio)-8-methyl-2-phenylimidazo[1,2-*a*]pyridine (4)**



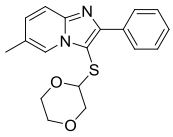
Brown solid, mp: 91.2 – 93.5 $^{o}$C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.49 (d, *J* = 6.8 Hz, 1H), 8.22 (d, *J* = 7.8 Hz, 2H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 6.8 Hz, 1H), 6.85 (t, *J* = 6.8 Hz, 1H), 4.80 (dd, *J* = 5.9, 2.7 Hz, 1H), 4.00 (dt, *J* = 11.8, 4.1 Hz, 1H), 3.82 (dd, *J* = 11.9, 2.6 Hz, 1H), 3.62 – 3.50 (m, 4H), 2.69 (s, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 150.3, 147.0, 133.8, 128.8, 128.3, 128.2, 127.4, 125.3, 122.9, 112.7, 107.6, 84.1, 69.7, 66.2, 64.5, 16.8. IR (KBr, $cm^{-1}$): 2984, 2964, 2916, 2853, 1600, 1506, 1489, 1462, 1445, 1339, 1124, 895, 862, 800, 777. LRMS (EI, 70 eV) m/z (%): 326 (1), 240 (100), 92 (25), 87 (12), 65 (10). HRMS (ESI) for $C_{18}H_{19}N_2O_2S^+$ $(M+H)^+$: calcd 327.1162, found 327.1160.

**3-(1,4-dioxan-2-ylthio)-7-methyl-2-phenylimidazo[1,2-*a*]pyridine (5)**



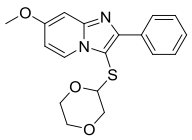
Brown solid, mp: 80.1 – 81.4 $^{o}$C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.47 (d, *J* = 7.0 Hz, 1H), 8.21 (d, *J* = 7.4 Hz, 2H), 7.46 – 7.42 (m, 3H), 7.37 (t, *J* = 7.4 Hz, 1H), 6.74 (d, *J* = 7.0 Hz, 1H), 4.77 (dd, *J* = 6.2, 2.7 Hz, 1H), 4.02 – 3.94 (m, 1H), 3.81 (dd, *J* = 11.9, 2.7 Hz, 1H), 3.63 – 3.49 (m, 4H), 2.43 (s, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 150.4, 147.1, 137.7, 133.7, 128.6, 128.3, 128.3, 124.3, 115.8, 115.3, 106.5, 84.2, 69.6, 66.2, 64.8, 21.4. IR (KBr, $cm^{-1}$): 2984, 2964, 2916, 2853, 1600, 1506, 1489, 1462, 1445, 1339, 1124, 895, 862, 800, 777. LRMS (EI, 70 eV) m/z (%): 326 (3), 240 (100), 92 (21), 87 (13), 65 (12). HRMS (ESI) for $C_{18}H_{19}N_2O_2S^+$ $(M+H)^+$: calcd 327.1162, found 327.1160.

**3-(1,4-dioxan-2-ylthio)-6-methyl-2-phenylimidazo[1,2-*a*]pyridine (6)**



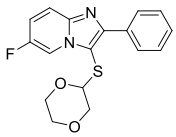
Brown solid, mp: 114.3 – 116.0 $^{o}$C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.28 (s, 1H), 8.16 – 8.10 (m, 2H), 7.47 (d, *J* = 9.0 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 9.0 Hz, 1H), 4.71 (dd, *J* = 6.0, 2.7 Hz, 1H), 3.91 (dt, *J* = 11.8, 4.1 Hz, 1H), 3.74 (dd, *J* = 11.9, 2.6 Hz, 1H), 3.55 – 3.37 (m, 4H), 2.30 (s, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 150.5, 145.8, 133.9, 129.4, 128.5, 128.3, 128.2, 122.7, 122.4, 116.8, 106.8, 84.1, 69.7, 66.2, 64.5, 18.5. IR (KBR, $cm^{-1}$): 2984, 2964, 2916, 2853, 1600, 1506, 1489, 1462, 1445, 1339, 1124, 895, 862, 800, 777. LRMS (EI, 70 eV) m/z (%): 326 (3), 240 (100), 92 (23), 87 (10), 65 (11). HRMS (ESI) for $C_{18}H_{19}N_2O_2S^+$ $(M+H)^+$: calcd 327.1162, found 327.1160.

**3-(1,4-dioxan-2-ylthio)-7-methoxy-2-phenylimidazo[1,2-*a*]pyridine (7)**



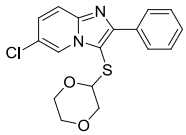
Light yellow solid, mp: 99.1 – 101.4 °C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.42 (d, *J* = 7.5 Hz, 1H), 8.20 (d, *J* = 7.3 Hz, 2H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 1H), 6.95 (d, *J* = 2.3 Hz, 1H), 6.62 (dd, *J* = 7.5, 2.4 Hz, 1H), 4.76 (dd, *J* = 6.5, 2.7 Hz, 1H), 3.99 – 3.95 (m, 1H), 3.89 (s, 3H), 3.81 (dd, *J* = 11.9, 2.7 Hz, 1H), 3.63 – 3.51 (m, 4H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 159.4, 150.1, 148.1, 133.5, 128.4, 128.3, 128.2, 125.6, 107.5, 105.8, 94.7, 84.3, 69.6, 66.2, 65.0, 55.7. IR (KBr, $cm^{-1}$): 2964, 2920, 2849, 1533, 1474, 1442, 1345, 1241, 1212, 1121, 1068, 903, 868, 824, 759, 736. LRMS (EI, 70 eV) m/z (%): 342 (2), 256 (100), 255 (23), 241 (12), 108 (23), 87 (10). HRMS (ESI) for $C_{18}H_{19}N_2O_3S^+$ $(M+H)^+$: calcd 343.1111, found 343.1111.

**3-(1,4-dioxan-2-ylthio)-6-fluoro-2-phenylimidazo[1,2-*a*]pyridine (8)**



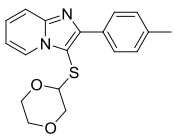
Brown solid, mp: 95.5 – 97.8 °C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.20 (s, 2H), 7.66 (s, 1H), 7.48 (s, 2H), 7.40 (s, 1H), 7.25 (s, 1H), 4.83 (s, 1H), 4.01 (s, 1H), 3.84 (d, *J* = 10.6 Hz, 1H), 3.62 (s, 2H), 3.57 (s, 2H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 153.6 (d, $J_{C-F}$ = 238.6 Hz, 1C), 151.5, 144.1, 133.1, 130.0, 128.5, 128.3, 118.5 (d, $J_{C-F}$ = 19.6 Hz, 1C), 117.8, 112.1 (d, $J_{C-F}$ = 42.3 Hz, 1C), 109.1, 84.2, 69.5, 66.2, 64.6. IR (KBr, $cm^{-1}$): 3034, 2984, 2964, 2916, 2853, 1618, 1539, 1506, 1439, 1368, 1168, 1118, 1083, 895, 862, 800, 777. LRMS (EI, 70 eV) m/z (%): 330 (2), 244 (100), 243 (31) 199 (18), 96 (31), 87 (25). HRMS (ESI) for $C_{17}H_{16}FN_2O_2S^+$ $(M+H)^+$: calcd 331.0911, found 331.0914.

**3-(1,4-dioxan-2-ylthio)-6-chloro-2-phenylimidazo[1,2-*a*]pyridine (9)**



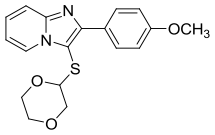
Light yellow solid, mp: 109.5 – 111.8 °C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.66 (d, *J* = 1.1 Hz, 1H), 8.21 (d, *J* = 7.6 Hz, 2H), 7.61 (d, *J* = 9.4 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.29 – 7.26 (m, 1H), 4.84 (dd, *J* = 6.0, 2.7 Hz, 1H), 4.02 (dt, *J* = 11.7, 4.0 Hz, 1H), 3.85 (dd, *J* = 11.9, 2.7 Hz, 1H), 3.64 – 3.53 (m, 4H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 151.3, 145.1, 133.2, 128.6, 128.5, 128.4, 127.7, 123.2, 121.1, 117.8, 108.2, 84.3, 69.6, 66.2, 64.6. IR (KBr, $cm^{-1}$): 2969, 2920, 2853, 1600, 1492, 1462, 1439, 1404, 1359, 1330, 1112, 1071, 900, 880, 815, 774, 700. LRMS (EI, 70 eV) m/z (%): 346 (2), 269 (100), 259 (27), 215 (13), 114 (10), 112 (29), 87 (34), 76 (11). HRMS (ESI) for $C_{17}H_{16}ClN_2O_2S^+$ $(M+H)^+$: calcd 347.0615, found 347.0615.

**3-(1,4-dioxan-2-ylthio)-2-*p*-tolylimidazo[1,2-*a*]pyridine (10)**



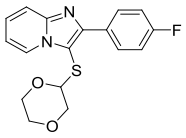
Brown oil. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.53 (d, *J* = 6.8 Hz, 1H), 8.05 (d, *J* = 8.1 Hz, 2H), 7.58 (d, *J* = 9.0 Hz, 1H), 7.23 (d, *J* = 7.2 Hz, 1H), 7.19 (s, 1H), 6.83 (t, *J* = 6.8 Hz, 1H), 4.72 (dd, *J* = 6.2, 2.8 Hz, 1H), 3.96 – 3.89 (m, 1H), 3.75 (dd, *J* = 11.9, 2.8 Hz, 1H), 3.56 – 3.43 (m, 4H), 2.33 (s, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 150.7, 146.8, 138.2, 130.8, 129.1, 128.5, 126.3, 125.1, 117.3, 112.5, 106.9, 84.2, 69.7, 66.2, 64.8, 21.4. IR (KBr, $cm^{-1}$): 2960, 2919, 2857, 1616, 1499, 1469, 1345, 1108, 1076, 903, 868, 824, 759. LRMS (EI, 70 eV) m/z (%): 326 (3), 240 (100), 87 (11), 78 (31). HRMS (ESI) for $C_{18}H_{19}N_2O_2S^+$ $(M+H)^+$: calcd 327.1162, found 327.1162.

**3-(1,4-dioxan-2-ylthio)-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyridine (11)**



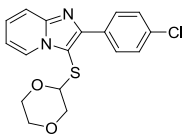
Brown oil. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.50 (d, *J* = 6.8 Hz, 1H), 8.12 (d, *J* = 8.6 Hz, 2H), 7.55 (d, *J* = 8.9 Hz, 1H), 7.22 – 7.18 (m, 1H), 6.91 (d, *J* = 8.3 Hz, 2H), 6.80 (t, *J* = 6.7 Hz, 1H), 4.74 – 4.69 (m, 1H), 3.93 – 3.89 (m, 1H), 3.78 (d, *J* = 1.0 Hz, 3H), 3.74 (d, *J* = 11.7 Hz, 1H), 3.53 – 3.43 (m, 4H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 159.8, 150.5, 146.7, 129.9, 126.3, 126.2, 125.0, 117.1, 113.8, 112.5, 106.3, 84.1, 69.7, 66.2, 64.8, 55.3. IR (KBr, $cm^{-1}$): 2976, 2967, 2854, 2831, 1610, 1465, 1357, 1345, 1248, 1177, 1124, 868, 839, 788, 759, 741. LRMS (EI, 70 eV) m/z (%): 326 (3), 240 (100), 239 (38), 92 (27), 87 (10), 65 (12). HRMS (ESI) for $C_{18}H_{19}N_2O_3S^+$ $(M+H)^+$: calcd 343.1111, found 343.1111.

**3-(1,4-dioxan-2-ylthio)-2-(4-fluorophenyl)imidazo[1,2-*a*]pyridine (12)**



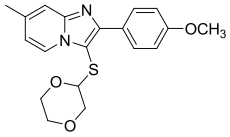
Yellow solid, mp: 83.5 – 85.6 °C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.53 (d, *J* = 6.8 Hz, 1H), 8.16 (d, *J* = 2.9 Hz, 2H), 7.59 (d, *J* = 9.0 Hz, 1H), 7.28 – 7.24 (m, 1H), 7.09 (t, *J* = 8.7 Hz, 2H), 6.87 (t, *J* = 6.6 Hz, 1H), 4.74 (dd, *J* = 6.1, 2.8 Hz, 1H), 3.95 – 3.91 (m, 1H), 3.77 (dd, *J* = 11.9, 2.8 Hz, 1H), 3.56 – 3.46 (m, 4H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 162.9 (d, $J_{C-F}$ = 249.1 Hz, 1C), 149.7, 146.7, 130.4 (d, $J_{C-F}$ = 7.6 Hz, 1C), 129.8 (d, $J_{C-F}$ = 3.2 Hz, 1C), 126.5, 125.0, 117.3, 115.2 (d, $J_{C-F}$ = 21.1 Hz, 1C), 112.7, 107.0, 84.1, 69.6, 66.2, 64.6. IR (KBr, $cm^{-1}$): 2967, 2920, 2855, 1608, 1500, 1465, 1345, 1212, 1159, 1125, 1092, 891, 871, 853, 794, 756, 733. LRMS (EI, 70 eV) m/z (%): 330 (3), 244 (100), 243 (34), 87(24), 78 (37). HRMS (ESI) for $C_{17}H_{16}FN_2O_2S^+$ $(M+H)^+$: calcd 331.0911, found 331.0911.

**3-(1,4-dioxan-2-ylthio)-2-(4-chlorophenyl)imidazo[1,2-*a*]pyridine (13)**



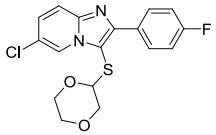
Yellow solid, mp: 103.1 – 104.3 °C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.52 (d, *J* = 6.9 Hz, 1H), 8.13 (d, *J* = 8.6 Hz, 2H), 7.58 (d, *J* = 9.0 Hz, 1H), 7.36 (d, *J* = 8.6 Hz, 2H), 7.26 – 7.23 (m, 1H), 6.85 (td, *J* = 6.8, 0.9 Hz, 1H), 4.73 (dd, *J* = 6.0, 2.8 Hz, 1H), 3.97 – 3.88 (m, 1H), 3.76 (dd, *J* = 11.9, 2.8 Hz, 1H), 3.60 – 3.46 (m, 4H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 149.5, 146.9, 134.3, 132.2, 129.8, 128.5, 126.6, 125.1, 117.5, 112.8, 107.4, 84.1, 69.7, 66.2, 64.7. IR (KBr, $cm^{-1}$): 2978, 2964, 2924, 2856, 1598, 1489, 1454, 1407, 1341, 1121, 1084, 891, 867, 833, 763, 725. LRMS (EI, 70 eV) m/z (%): 346 (2), 260 (100), 259 (18), 225 (22), 224 (15), 87 (40), 78 (58). HRMS (ESI) for $C_{17}H_{16}ClN_2O_2S^+$ $(M+H)^+$: calcd 347.0615, found 347.0615.

**3-(1,4-dioxan-2-ylthio)-2-(4-methoxyphenyl)-7-methylimidazo[1,2-*a*]pyridine (14)**



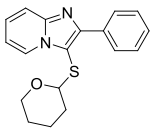
White solid, mp: 103.1 – 104.3 °C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.46 (d, *J* = 6.9 Hz, 1H), 8.19 (d, *J* = 8.6 Hz, 2H), 7.41 (s, 1H), 7.00 (d, *J* = 8.6 Hz, 2H), 6.73 (d, *J* = 6.9 Hz, 1H), 4.77 (dd, *J* = 6.2, 2.3 Hz, 1H), 4.03 – 3.97 (m, 1H), 3.87 (s, 3H), 3.83 (dd, *J* = 11.9, 2.3 Hz, 1H), 3.61 – 3.52 (m, 4H), 2.44 (s, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 159.7, 150.1, 146.9, 137.7, 129.8, 126.1, 124.2, 115.6, 115.2, 113.7, 105.5, 84.2, 69.6, 66.2, 64.9, 55.3, 21.4. IR (KBr, $cm^{-1}$): 2960, 2911, 2852, 1613, 1530, 1462, 1351, 1295, 1247, 1177, 1118, 1071, 1032, 870, 835, 788, 753. LRMS (EI, 70 eV) m/z (%): 356 (3), 270 (100), 255(12), 92 (25), 87 (8), 65 (10). HRMS (ESI) for $C_{19}H_{21}N_2O_3S^+$ $(M+H)^+$: calcd 357.1267, found 357.1268.

**3-(1,4-dioxan-2-ylthio)-6-chloro-2-(4-fluorophenyl)imidazo[1,2-*a*]pyridine (15)**



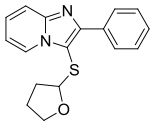
Yellow solid, mp: 147.9 – 149.6 °C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.63 (d, *J* = 0.8 Hz, 1H), 8.21 (dd, *J* = 8.4, 5.6 Hz, 2H), 7.59 (d, *J* = 9.4 Hz, 1H), 7.29 – 7.27 (m, 1H), 7.16 (t, *J* = 8.6 Hz, 2H), 4.83 (dd, *J* = 5.9, 2.7 Hz, 1H), 4.04 – 3.99 (m, 1H), 3.85 (dd, *J* = 11.9, 2.7 Hz, 1H), 3.64 – 3.54 (m, 4H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 163.0 (d, $J_{C-F}$ = 244.6 Hz, 1C), 150.5, 145.1, 130.4 (d, $J_{C-F}$ = 7.6 Hz, 1C), 129.4 (d, $J_{C-F}$ = 3.0 Hz, 1C), 127.9, 123.2, 121.2, 117.8, 115.4 (d, $J_{C-F}$ = 21.1 Hz, 1C), 107.9, 84.2, 69.6, 66.2, 64.6. IR (KBr, $cm^{-1}$): 3072, 2970, 2923, 2858, 1604, 1527, 1492, 1460, 1410, 1363, 1330, 1212, 1151, 1118, 1089, 894, 868, 800, 723. LRMS (EI, 70 eV) m/z (%): 364 (4), 278 (100), 277 (30), 233 (19), 114 (15), 112 (46), 87 (66), 76 (14). HRMS (ESI) for $C_{17}H_{15}ClFN_2O_2S^+$ $(M+H)^+$: calcd 365.0521, found 365.0516.

**2-phenyl-3-(tetrahydro-*2H*-pyran-2-ylthio)imidazo[1,2-*a*]pyridine (16)**



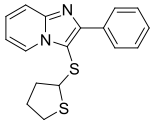
Yellow oil, $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.61 (d, *J* = 6.9 Hz, 1H), 8.28 – 8.24 (m, 2H), 7.63 (d, *J* = 9.0 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.27 – 7.23 (m, 1H), 6.85 (td, *J* = 6.8, 0.8 Hz, 1H), 4.84 (dd, *J* = 7.0, 3.4 Hz, 1H), 3.98 – 3.90 (m, 1H), 3.39 – 3.35 (m, 1H), 1.91 – 1.86 (m, 1H), 1.81 – 1.77 (m, 1H), 1.73 – 1.66 (m, 1H), 1.57 – 1.46 (m, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 150.1, 146.6, 133.9, 128.6, 128.2, 128.1, 126.1, 125.3, 117.3, 112.3, 109.1, 87.4, 66.1, 31.6, 25.2, 21.8. IR (KBr, $cm^{-1}$): 2928, 2852, 1595, 1498, 1463, 1436, 1345, 774, 753, 732, 700, 686. LRMS (EI, 70 eV) m/z (%): 310 (2), 226 (80), 225 (100), 181 (20), 78 (45). HRMS (ESI) for $C_{18}H_{19}N_2OS^+$ $(M+H)^+$: calcd 311.1218, found 311.1212.

**2-phenyl-3-(tetrahydrofuran-2-ylthio)imidazo[1,2-*a*]pyridine (17)**



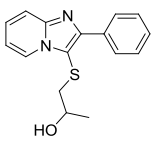
Yellow oil, $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.62 (d, *J* = 6.8 Hz, 1H), 8.26 (d, *J* = 7.3 Hz, 2H), 7.65 (d, *J* = 8.9 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.29 – 7.26 (m, 1H), 6.89 (t, *J* = 6.6 Hz, 1H), 5.37 (dd, *J* = 6.9, 3.7 Hz, 1H), 3.83 – 3.77 (m, 2H), 2.25 – 2.19 (m, 1H), 2.01 – 1.89 (m, 2H), 1.83 – 1.78 (m, 1H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 150.1, 146.6, 133.9, 128.6, 128.2, 128.2, 126.2, 124.9, 117.3, 112.5, 109.5, 89.2, 68.0, 32.5, 24.8. IR (KBr, $cm^{-1}$): 2928, 2852, 1595, 1498, 1463, 1436, 1345, 774, 753, 732, 700, 686. LRMS (EI, 70 eV) m/z (%): 296 (12), 226 (90), 225 (100), 181 (23), 87 (50). HRMS (ESI) for $C_{17}H_{17}N_2OS^+$ $(M+H)^+$: calcd 297.1062, found 297.1060.

**2-phenyl-3-(tetrahydrothiophen-2-ylthio)imidazo[1,2-*a*]pyridine (18)**



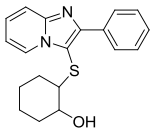
Yellow solid, mp: 106.2 – 108.5 $^{o}$C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.60 (d, *J* = 6.7 Hz, 1H), 8.31 (d, *J* = 7.6 Hz, 2H), 7.68 (d, *J* = 8.9 Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.31 (t, *J* = 7.7 Hz, 1H), 6.94 (t, *J* = 6.6 Hz, 1H), 4.55 (d, *J* = 3.1 Hz, 1H), 3.02 – 2.99 (m, 1H), 2.79 – 2.75 (m, 1H), 2.11 – 2.09 (m, 1H), 1.96 – 1.87 (m, 2H), 1.85 – 1.78 (m, 1H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 150.0, 146.3, 133.6, 128.5, 128.4, 128.4, 126.5, 124.6, 117.6, 112.9, 111.4, 56.8, 38.4, 33.3, 28.0. IR (KBr, $cm^{-1}$): 2928, 2852, 1595, 1498, 1463, 1436, 1345, 774, 753, 732, 700, 686. LRMS (EI, 70 eV) m/z (%): 312 (2), 226 (100), 225 (33), 181 (13), 87 (95), 78 (45). HRMS (ESI) for $C_{17}H_{17}N_2S_2^+$ $(M+H)^+$: calcd 313.0828, found 313.0828.

**2-(2-phenylimidazo[1,2-*a*]pyridin-3-ylthio)propan-1-ol (19)**



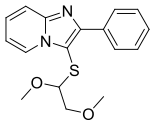
Brown oil. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.55 (d, *J* = 6.7 Hz, 1H), 8.21 (d, *J* = 7.5 Hz, 2H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.41 (t, *J* = 7.3 Hz, 1H), 7.37 – 7.29 (m, 1H), 6.97 (t, *J* = 6.7 Hz, 1H), 3.54 (m, 1H), 2.75 – 2.72 (m, 1H), 2.73 (br s, 1H), 2. 57 – 2.54 (m, 1H), 1.10 (d, *J* = 6.2 Hz, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 149.4, 146.0, 130.1, 128.9, 128.7, 128.6, 128.6, 126.9, 124.6, 117.4, 113.4, 66.0, 44.3, 21.9. IR (KBr, $cm^{-1}$): 3410, 2962, 2923, 2854, 1599, 1498, 1462, 1439, 1345, 773, 757, 730, 701. LRMS (EI, 70 eV) m/z (%): 284 (16), 226 (65), 225 (100), 181 (21), 78 (43). HRMS (ESI) for $C_{16}H_{17}N_2OS^+$ $(M+H)^+$: calcd 285.1056, found 285.1058.

**2-(2-phenylimidazo[1,2-*a*]pyridin-3-ylthio)cyclohexanol (20)**



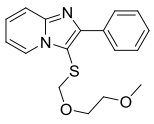
White solid, mp: 70.1 – 73.7 °C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.65 (d, *J* = 6.8 Hz, 1H), 8.23 (d, *J* = 7.3 Hz, 2H), 7.74 (d, *J* = 8.9 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.42 (t, *J* = 7.4 Hz, 1H), 7.38 – 7.31 (m, 1H), 6.97 (t, *J* = 6.7 Hz, 1H), 3.15 (m, 1H), 3.14 (br s, 1H), 2.67 – 2.53 (m, 1H), 2.02 – 1.78 (m, 2H), 1.62 – 1.49 (m, 2H), 1.21 – 1.05 (m, 4H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 151.0, 146.6, 133.6, 128.7, 128.6, 128.6, 126.4, 125.0, 117.4, 112.9, 108.2, 72.4, 58.1, 34.3, 32.5, 25.8, 24.0. IR (KBr, $cm^{-1}$): 3413, 297, 2931, 2857, 1616, 1498, 1466, 1444, 1392, 1347, 1072, 1049, 759, 694. LRMS (EI, 70 eV) m/z (%): 324 (15), 226 (100), 225 (50), 181 (13), 78 (34). HRMS (ESI) for $C_{19}H_{21}N_2OS^+$ $(M+H)^+$: calcd 325.1369, found 325.1368.

**3-(1,2-dimethoxyethylthio)-2-phenylimidazo[1,2-*a*]pyridine (21a)**



Brown oil. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.60 (d, *J* = 6.8 Hz, 1H), 8.21 (d, *J* = 7.9 Hz, 2H), 7.68 (d, *J* = 8.9 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.3 Hz, 1H), 7.34 – 7.30 (m, 1H), 6.94 (t, *J* = 6.8 Hz, 1H), 4.48 – 4.42 (m, 1H), 3.33 (s, 5H), 3.17 (s, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 151.4, 146.8, 133.8, 128.9, 128.3, 128.2, 126.2, 124.9, 117.5, 112.6, 107.1, 91.3, 74.2, 58.9, 57.6. IR (KBr, $cm^{-1}$): 2922, 2872, 2823, 1601, 1496, 1468, 1439, 1347, 1082, 838, 774, 756, 741, 694. LRMS (EI, 70 eV) m/z (%): 314 (11), 226 (100), 225(41), 181 (13), 89 (33), 78 (45), 59 (32). HRMS (ESI) for $C_{17}H_{19}N_2O_2S^+$ $(M+H)^+$: calcd 315.1162, found 315.1161.

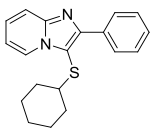
**3-(1,2-dimethoxyethylthio)-2-phenylimidazo[1,2-*a*]pyridine (21b)**



Brown oil. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.57 (d, *J* = 6.8 Hz, 1H), 8.19 (d, *J* = 7.6 Hz, 2H), 7.68 (d, *J* = 8.9 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.3 Hz, 1H), 7.32 – 7.27 (m, 1H), 6.91 (t, *J* = 6.7 Hz, 1H), 4.77 (s, 2H), 3.62 – 3.59 (m, 2H), 3.28 – 3.24 (m, 5H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 150.2, 146.6, 133.7, 128.7, 128.2, 128.2, 126.2, 124.8, 117.5, 112.7, 109.2, 78.1, 71.2, 68.6, 59.0. IR (KBr, $cm^{-1}$): 2922, 2872, 2823, 1601, 1496, 1468, 1439, 1347, 1082, 838, 774, 756, 741, 694. LRMS (EI, 70 eV) m/z (%): 314 (38), 226 (20), 225(60), 181 (21), 89 (67), 78 (65), 59

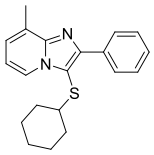
(100). HRMS (ESI) for $C_{17}H_{19}N_2O_2S^+$ $(M+H)^+$: calcd 315.1162, found 315.1161.

**3-(cyclohexylthio)-2-phenylimidazo[1,2-*a*]pyridine (22)**



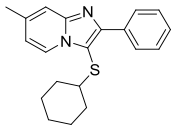
Brown oil. $^1$H NMR (600 MHz, $CDCl_3$) δ 8.46 (d, *J* = 6.8 Hz, 1H), 8.29 (d, *J* = 1.3 Hz, 1H), 8.28 (d, *J* = 0.6 Hz, 1H), 7.57 (d, *J* = 8.9 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 7.21 – 7.15 (m, 1H), 6.81 (td, *J* = 6.8, 0.9 Hz, 1H), 2.79 (tt, *J* = 10.9, 3.6 Hz, 1H), 1.69 (d, *J* = 13.0 Hz, 2H), 1.60 – 1.54 (m, 2H), 1.44 – 1.38 (m, 1H), 1.25 – 1.17 (m, 2H), 1.05 (td, *J* = 9.6, 4.5 Hz, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 149.8, 146.4, 134.1, 128.4, 128.2, 128.1, 125.8, 124.6, 117.4, 112.5, 109.8, 48.9, 33.4, 25.9, 25.4. IR (KBr, $cm^{-1}$): 2928, 2851 1601, 1492, 1466, 1442, 1345, 1263, 1228, 1171, 997, 773, 756, 739, 697. LRMS (EI, 70 eV) m/z (%): 308 (17), 226 (100), 225 (48), 181 (12), 78 (35). HRMS (ESI) for $C_{19}H_{21}N_2S^+$ $(M+H)^+$: calcd 309.1420, found 309.1420.

**3-(cyclohexylthio)-8-methyl-2-phenylimidazo[1,2-*a*]pyridine (23)**



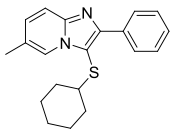
Brown solid, mp: 90.2 – 92.6 °C. $^1$H NMR (600 MHz, $CDCl_3$) δ 8.40 (d, *J* = 6.8 Hz, 1H), 8.37 – 8.32 (m, 2H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 6.8 Hz, 1H), 6.80 (t, *J* = 6.8 Hz, 1H), 2.85 (tt, *J* = 10.9, 3.7 Hz, 1H), 2.67 (s, 3H), 1.79 – 1.73 (m, 2H), 1.65 – 1.62 (m, 2H), 1.49 (d, *J* = 1.6 Hz, 1H), 1.31 – 1.24 (m, 2H), 1.14 – 1.11 (m, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 149.5, 146.7, 134.3, 128.6, 128.2, 127.9, 127.4, 124.7, 122.5, 112.5, 110.0, 48.9, 33.4, 26.0, 25.6, 16.8. IR (KBr, $cm^{-1}$): 2928, 2852, 1604, 1495, 1462, 1445, 1345, 1262, 1224, 1174, 1000, 773, 753, 736, 691. LRMS (EI, 70 eV) m/z (%): 322 (17), 240 (100), 92 (27), 65 (11). HRMS (ESI) for $C_{20}H_{23}N_2S^+$ $(M+H)^+$: calcd 323.1576, found 323.1579.

**3-(cyclohexylthio)-7-methyl-2-phenylimidazo[1,2-*a*]pyridine (24)**



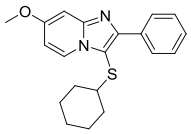
White solid, mp: 111.2 – 113.7 °C. $^1$H NMR (600 MHz, $CDCl_3$) δ 8.43 (d, *J* = 7.0 Hz, 1H), 8.36 (d, *J* = 7.5 Hz, 2H), 7.48 – 7.45 (m, 3H), 7.37 (t, *J* = 7.3 Hz, 1H), 6.76 (d, *J* = 6.9 Hz, 1H), 2.87 (tt, *J* = 10.9, 3.6 Hz, 1H), 2.45 (s, 3H), 1.78 (d, *J* = 13.2 Hz, 2H), 1.68 – 1.65 (m, 2H), 1.52 (d, *J* = 3.7 Hz, 1H), 1.32 – 1.26 (m, 2H), 1.19 – 1.14 (m, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 149.3, 146.6, 137.3, 133.9, 128.3, 128.2, 128.1, 123.8, 115.8, 115.2, 109.1, 49.0, 33.4, 26.0, 25.4, 21.4. IR (KBr, $cm^{-1}$): 2928, 2852, 1604, 1495, 1462, 1445, 1345, 1262, 1224, 1174, 773, 753, 736, 691. LRMS (EI, 70 eV) m/z (%): 322 (19), 240 (100), 92 (26), 65 (13). HRMS (ESI) for $C_{20}H_{23}N_2S^+$ $(M+H)^+$: calcd 323.1576, found 323.1577.

**3-(cyclohexylthio)-6-methyl-2-phenylimidazo[1,2-*a*]pyridine (25)**



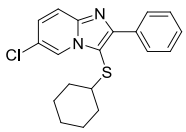
Brown solid, mp: 112.7 – 115.8 $^{o}$C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.33 (d, *J* = 7.0 Hz, 1H), 8.27 (d, *J* = 8.0 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.33 (s, 1H), 7.28 (t, *J* = 7.3 Hz, 1H), 6.65 (d, *J* = 7.0 Hz, 1H), 2.79 – 2.75 (m, 1H), 2.35 (s, 3H), 1.69 (d, *J* = 13.2 Hz, 2H), 1.58 – 1.56 (m, 2H), 1.43 (d, *J* = 3.9 Hz, 1H), 1.23 – 1.17 (m, 2H), 1.06 (t, *J* = 9.0 Hz, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 149.6, 146.8, 137.0, 134.2, 128.3, 128.2, 127.9, 123.8, 115.9, 115.1, 108.9, 49.0, 33.4, 25.9, 25.4, 21.3. IR (KBr, $cm^{-1}$): 2928, 2852, 1604, 1495, 1462, 1445, 1345, 1262, 1224, 1174, 1000, 773, 753, 736, 691. LRMS (EI, 70 eV) m/z (%): 322 (19), 240 (100), 92 (29), 65 (10). HRMS (ESI) for $C_{20}H_{23}N_2S^+$ $(M+H)^+$: calcd 323.1576, found 323.1579.

**3-(cyclohexylthio)-7-methoxy-2-phenylimidazo[1,2-*a*]pyridine (26)**



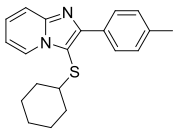
Brown solid, mp: 138.1 – 139.8 $^{o}$C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.35 (t, *J* = 7.1 Hz, 3H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 1H), 6.94 (d, *J* = 2.3 Hz, 1H), 6.61 (dd, *J* = 7.5, 2.4 Hz, 1H), 3.88 (s, 3H), 2.86 – 2.82 (m, 1H), 1.78 (d, *J* = 13.1 Hz, 2H), 1.67 – 1.64 (m, 2H), 1.51 (d, *J* = 9.9 Hz, 1H), 1.31 – 1.26 (m, 2H), 1.19 – 1.10 (m, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 158.9, 149.4, 147.8, 134.2, 128.2, 128.1, 127.9, 125.0, 108.3, 107.3, 94.8, 55.6, 49.1, 33.4, 26.0, 25.4. IR (KBr, $cm^{-1}$): 2928, 2851, 1604, 14714, 1442, 1353, 1240, 1212, 1174, 1023, 786, 773, 699. LRMS (EI, 70 eV) m/z (%): 338 (22), 256 (100), 255 (50), 240 (12), 108 (30). HRMS (ESI) for $C_{20}H_{23}N_2OS^+$ $(M+H)^+$: calcd 339.1526, found 339.1526.

**6-chloro-3-(cyclohexylthio)-2-phenylimidazo[1,2-*a*]pyridine (27)**



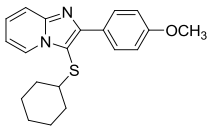
Yellow solid, mp: 107.2 – 108.9 $^{o}$C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.58 (s, 1H), 8.34 (d, *J* = 7.0 Hz, 2H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.47 (d, *J* = 6.9 Hz, 2H), 7.40 (d, *J* = 6.8 Hz, 1H), 7.28 (s, 1H), 2.90 (s, 1H), 1.77 (d, *J* = 11.5 Hz, 2H), 1.66 (s, 2H), 1.53 (s, 1H), 1.30 (d, *J* = 10.2 Hz, 2H), 1.16 (s, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 149.8, 144.2, 128.9, 128.7, 128.4, 128.4, 127.9, 122.6, 121.6, 117.6, 111.0, 49.1, 33.4, 25.9, 25.3. IR (KBr, $cm^{-1}$): 2918, 2849, 1604, 1492, 1462, 1439, 809, 773, 759, 697. LRMS (EI, 70 eV) m/z (%): 342 (15), 260 (100), 259 (33), 215 (15), 112 (29), 55 (15). HRMS (ESI) for $C_{19}H_{20}ClN_2S^+$ $(M+H)^+$: calcd 343.1030, found 343.1040.

**3-(cyclohexylthio)-2-*p*-tolylimidazo[1,2-*a*]pyridine (28)**



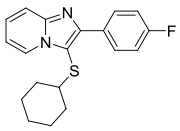
Brown solid, mp: 100.3 – 102.5 °C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.46 (d, *J* = 6.8 Hz, 1H), 8.21 (d, *J* = 8.1 Hz, 2H), 7.56 (d, *J* = 8.9 Hz, 1H), 7.20 (d, *J* = 8.5 Hz, 3H), 6.80 (t, *J* = 6.8 Hz, 1H), 2.80 (tt, *J* = 10.9, 3.6 Hz, 1H), 2.33 (s, 3H), 1.71 (d, *J* = 13.8 Hz, 2H), 1.59 – 1.57 (m, 2H), 1.44 (d, *J* = 3.0 Hz, 1H), 1.20 (d, *J* = 18.2 Hz, 2H), 1.08 – 1.05 (m, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 149.9, 146.4, 137.9, 131.2, 128.9, 128.2, 125.7, 124.5, 117.3, 112.3, 109.4, 48.9, 33.5, 26.0, 25.4, 21.4. IR (KBr, $cm^{-1}$): 2928, 2849, 1616, 1492, 1466, 1447, 1345, 824, 768, 727, 617. LRMS (EI, 70 eV) m/z (%): 322 (31), 240 (100), 239 (59), 78 (45). HRMS (ESI) for $C_{20}H_{23}N_2S^+$ $(M+H)^+$: calcd 323.1576, found 323.1578.

**3-(cyclohexylthio)-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyridine (29)**



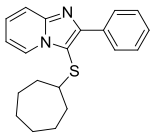
Yellow solid, mp: 84.3 – 86.2 °C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.43 (d, *J* = 6.8 Hz, 1H), 8.26 (d, *J* = 8.7 Hz, 2H), 7.53 (d, *J* = 8.9 Hz, 1H), 7.17 – 7.12 (m, 1H), 6.91 (d, *J* = 8.7 Hz, 2H), 6.77 (t, *J* = 6.8 Hz, 1H), 3.77 (s, 3H), 2.77 (tt, *J* = 10.9, 3.5 Hz, 1H), 1.69 (d, *J* = 13.2 Hz, 2H), 1.57 – 1.55 (m, 2H), 1.41 (d, *J* = 3.6 Hz, 1H), 1.23 – 1.18 (m, 2H), 1.05 (t, *J* = 8.7 Hz, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 159.6, 149.7, 146.4, 129.7, 126.4, 125.7, 124.5, 117.2, 113.6, 112.3, 108.8, 55.2, 48.9, 33.4, 26.0, 25.4. IR (KBr, $cm^{-1}$): 2931, 2846, 1609, 1466, 1438, 1347, 1248, 1174, 1038, 832, 782, 756, 730. LRMS (EI, 70 eV) m/z (%): 338 (31), 256 (100), 255 (39), 241 (18), 239 (11), 211 (15), 78 (41). HRMS (ESI) for $C_{20}H_{23}N_2OS^+$ $(M+H)^+$: calcd 339.1526, found 339.1528.

**3-(cyclohexylthio)-2-(4-fluorophenyl)imidazo[1,2-*a*]pyridine (30)**



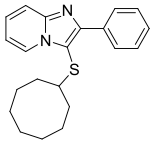
Brown oil. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.46 (d, *J* = 6.8 Hz, 1H), 8.28 (dd, *J* = 8.6, 5.7 Hz, 2H), 7.56 (d, *J* = 8.9 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 2H), 7.08 (t, *J* = 8.7 Hz, 2H), 6.84 (t, *J* = 6.8 Hz, 1H), 2.78 (tt, *J* = 10.9, 3.5 Hz, 1H), 1.87 (s, 1H), 1.69 (d, *J* = 13.1 Hz, 2H), 1.59 – 1.57 (m, 2H), 1.44 (d, *J* = 4.1 Hz, 1H), 1.23 – 1.18 (m, 2H), 1.11 – 1.03 (m, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 162.8 (d, $J_{C-F}$ = 247.6 Hz, 1C), 149.0, 146.4, 130.3, 130.2 (d, $J_{C-F}$ = 9.1 Hz, 1C), 126.0, 124.6, 117.4, 115.1 (d, $J_{C-F}$ = 21.1 Hz, 1C), 112.6, 109.5, 48.9, 33.4, 25.9, 25.4. IR (KBr, $cm^{-1}$): 2928, 2851, 1603, 1530, 1464, 1343, 1223, 1156, 841, 759, 741. LRMS (EI, 70 eV) m/z (%): 326 (16), 244 (100), 243 (41), 78 (35), 55 (10). HRMS (ESI) for $C_{19}H_{20}FN_2S^+$ $(M+H)^+$: calcd 327.1326, found 327.1330.

**3-(cycloheptylthio)-2-phenylimidazo[1,2-*a*]pyridine (31)**



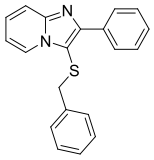
Brown oil. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.44 (d, *J* = 6.8 Hz, 1H), 8.32 – 8.27 (m, 2H), 7.57 (d, *J* = 9.0 Hz, 1H), 7.39 (t, *J* = 7.7 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 7.21 – 7.17 (m, 1H), 6.82 (t, *J* = 6.8 Hz, 1H), 3.02 (tt, *J* = 9.1, 4.5 Hz, 1H), 1.77 – 1.71 (m, 2H), 1.56 – 1.53 (m, 2H), 1.45 – 1.37 (m, 6H), 1.21 – 1.16 (m, 2H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 149.7, 146.4, 134.0, 128.4, 128.3, 128.1, 125.9, 124.5, 117.5, 112.5, 110.8, 50.1, 34.5, 28.3, 25.3. IR (KBr, cm-1): 2926, 2849, 1601, 1486, 1466, 1442, 1342, 1227, 777, 759, 736, 694. LRMS (EI, 70 eV) m/z (%): 322 (12), 226 (100), 225 (43), 181 (11), 78 (29), 55 (12). HRMS (ESI) for $C_{20}H_{23}N_2S^+$ $(M+H)^+$: calcd 323.1576, found 323.1583.

**3-(cyclooctylthio)-2-phenylimidazo[1,2-*a*]pyridine (32)**



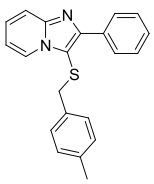
Brown oil. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.45 (d, *J* = 6.8 Hz, 1H), 8.28 – 8.27 (m), 7.58 (d, *J* = 8.9 Hz, 1H), 7.40 – 7.38 (m, 2H), 7.33 – 7.28 (m, 1H), 7.24 – 7.20 (m, 1H), 6.84 (td, *J* = 6.8, 1.0 Hz, 1H), 3.10 – 2.97 (m, 1H), 1.68 – 1.63 (m, 2H), 1.58 – 1.50 (m, 4H), 1.43 – 1.33 (m, 6H), 1.27 – 1.22 (m, 2H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 149.8, 146.4, 134.0, 128.4, 128.3, 128.1, 125.8, 124.5, 117.5, 112.5, 110.8, 49.8, 31.2, 27.2, 25.4, 24.8. IR (KBr, cm-1): 2926, 2849, 1601, 1486, 1466, 1442, 1342, 1227, 777, 759, 736, 694. LRMS (EI, 70 eV) m/z (%): 336 (7), 226 (100), 225 (35), 181 (10), 78 (25) 69 (11). HRMS (ESI) for $C_{21}H_{25}N_2S^+$ $(M+H)^+$: calcd 337.1733, found 337.1741.

**3-(benzylthio)-2-phenylimidazo[1,2-*a*]pyridine[1] (33)**



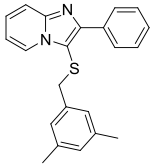
Brown oil. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.6 Hz, 2H), 8.08 (d, *J* = 6.8 Hz, 1H), 7.62 (d, *J* = 8.9 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.3 Hz, 1H), 7.23 – 7.18 (m, 1H), 7.12 – 7.04 (m, 3H), 6.92 (d, *J* = 7.1 Hz, 2H), 6.68 (t, *J* = 6.7 Hz, 1H), 3.82 (s, 2H). LRMS (EI, 70 eV) m/z (%): 316 (24), 225 (100), 181 (16), 91 (12), 78 (39). HRMS (ESI) for $C_{20}H_{17}N_2S^+$ $(M+H)^+$: calcd 317.1107, found 317.1114.

**3-(4-methylbenzylthio)-2-phenylimidazo[1,2-*a*]pyridine (34)**



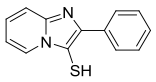
Brown oil. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.21 (d, *J* = 7.8 Hz, 2H), 8.10 (d, *J* = 6.8 Hz, 1H), 7.59 (d, *J* = 8.9 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.36 (t, *J* = 7.3 Hz, 1H), 7.22 – 7.16 (m, 1H), 6.84 (d, *J* = 7.7 Hz, 2H), 6.78 (d, *J* = 7.7 Hz, 2H), 6.67 (t, *J* = 6.8 Hz, 1H), 3.76 (s, 2H), 2.20 (s, 3H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 150.1, 146.4, 137.1, 133.9, 133.7, 129.1, 128.6, 128.3, 128.2, 128.2, 125.9, 124.3, 117.2, 112.2, 109.6, 40.3, 21.1. IR (KBr, cm-1): 3022, 2920, 1604, 1512, 1465, 1442, 1345, 1345, 1266, 1229, 997, 819, 775, 756, 736, 691. LRMS (EI, 70 eV) m/z (%): 330 (37), 225 (100), 181 (18), 105 (77), 78 (51). HRMS (ESI) for $C_{21}H_{19}N_2S^+$ $(M+H)^+$: calcd 331.1263, found 331.1269.

**3-(3,5-dimethylbenzylthio)-2-phenylimidazo[1,2-*a*]pyridine (35)**



Brown oil. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.30 – 8.25 (m, 2H), 8.10 (d, *J* = 6.8 Hz, 1H), 7.63 (d, *J* = 8.9 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.25 – 7.19 (m, 1H), 6.75 – 6.67 (m, 2H), 6.51 (s, 2H), 3.75 (s, 2H), 2.10 (s, 6H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 150.0, 146.3, 138.0, 136.8, 133.7, 128.8, 128.3, 128.3, 128.2, 126.5, 126.0, 124.3, 11 7.1, 112.1, 109.7, 40.7, 21.0. IR (KBr, cm-1): 3022, 2920, 1604, 1512, 1465, 1442, 1345, 1345, 1266, 1229, 997, 819, 775, 756, 736, 691. LRMS (EI, 70 eV) m/z (%): 34 4 (32), 225 (100), 181 (17), 119 (53), 78 (43). HRMS (ESI) for $C_{22}H_{21}N_2S^+$ $(M+H)^+$: calcd 345.1420, found 345.1427.

**2-phenylimidazo[1,2-*a*]pyridine-3-thiol (38)**

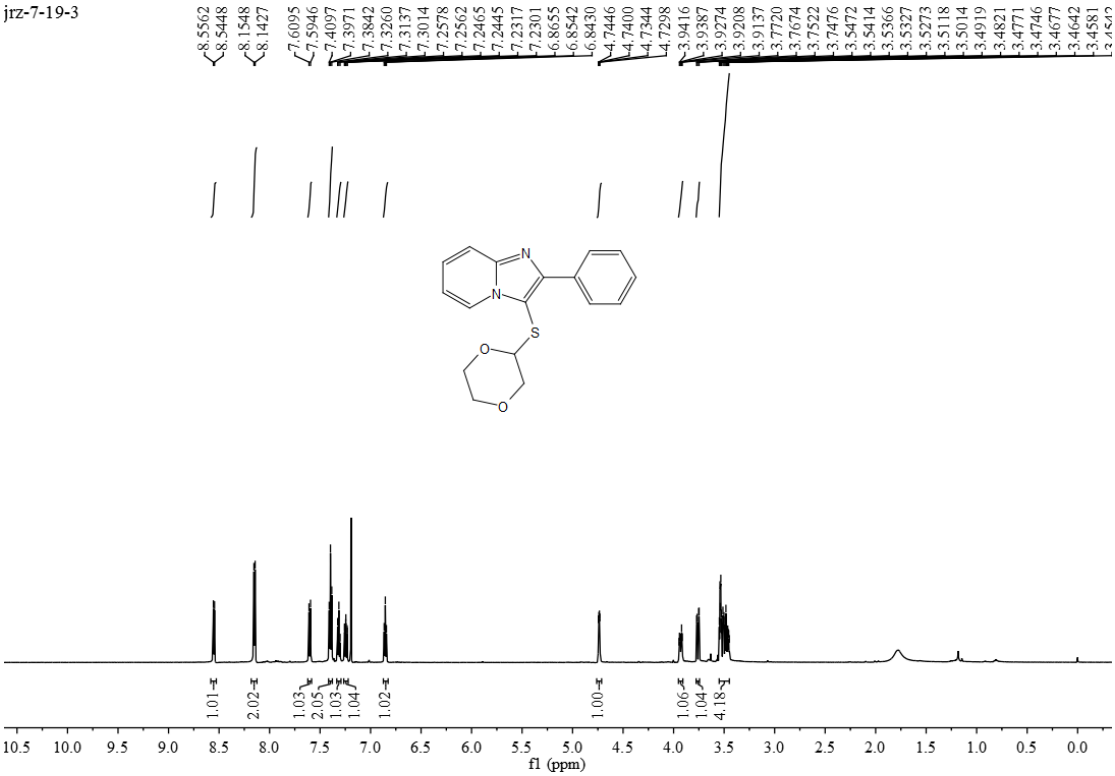


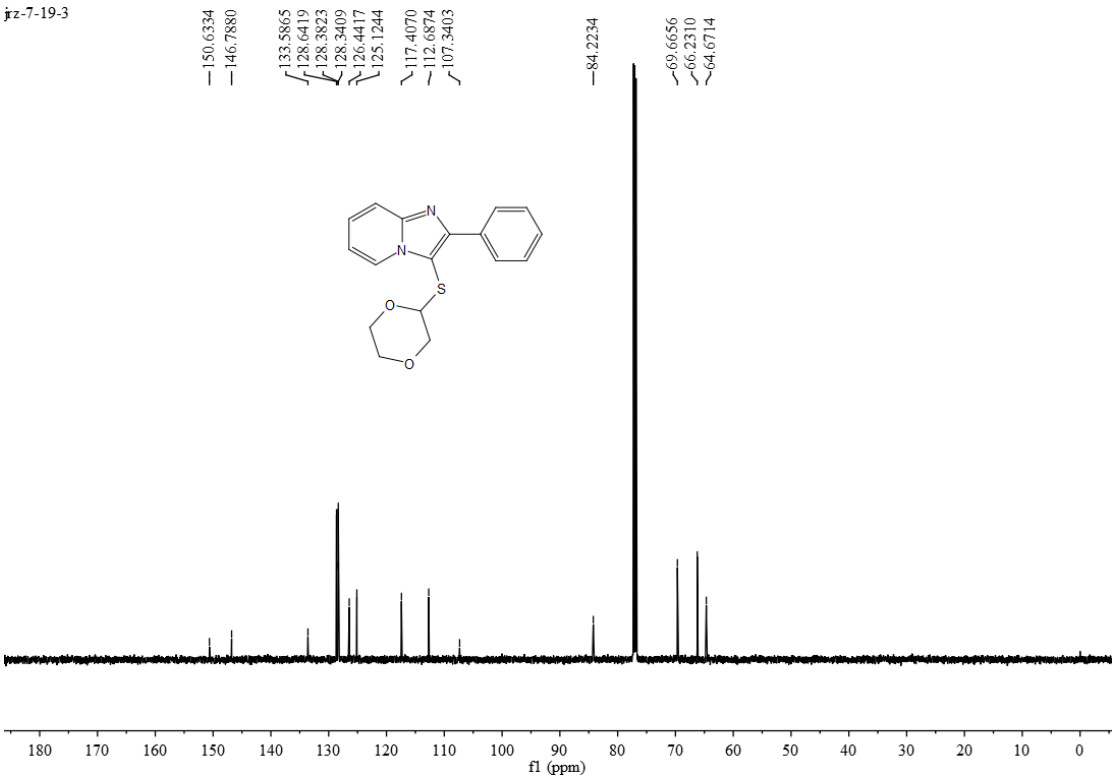
Light yellow solid, mp: 243.5 – 246.8 °C. $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.11 (d, *J* = 7.4 Hz, 2H), 7.65 – 7.46 (m, 5H), 7.22 – 7.03 (m, 1H), 6.34 – 6.32 (m, 1H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 150.9, 146.5, 133.8, 129.5, 128.9, 128.6, 126.3, 125.3, 117.4, 112.5, 107.4. IR (KBr, $cm^{-1}$): 2361, 2342, 1493, 1459, 1437, 1340, 1262, 1236, 766, 694. LRMS (EI, 70 eV) m/z (%): 226 (100), 225 (70), 181 (17), 78 (43). HRMS (ESI) for $C_{13}H_{11}N_2S^+$ $(M+H)^+$: calcd 227.0643, found 227.0641.

**References:**

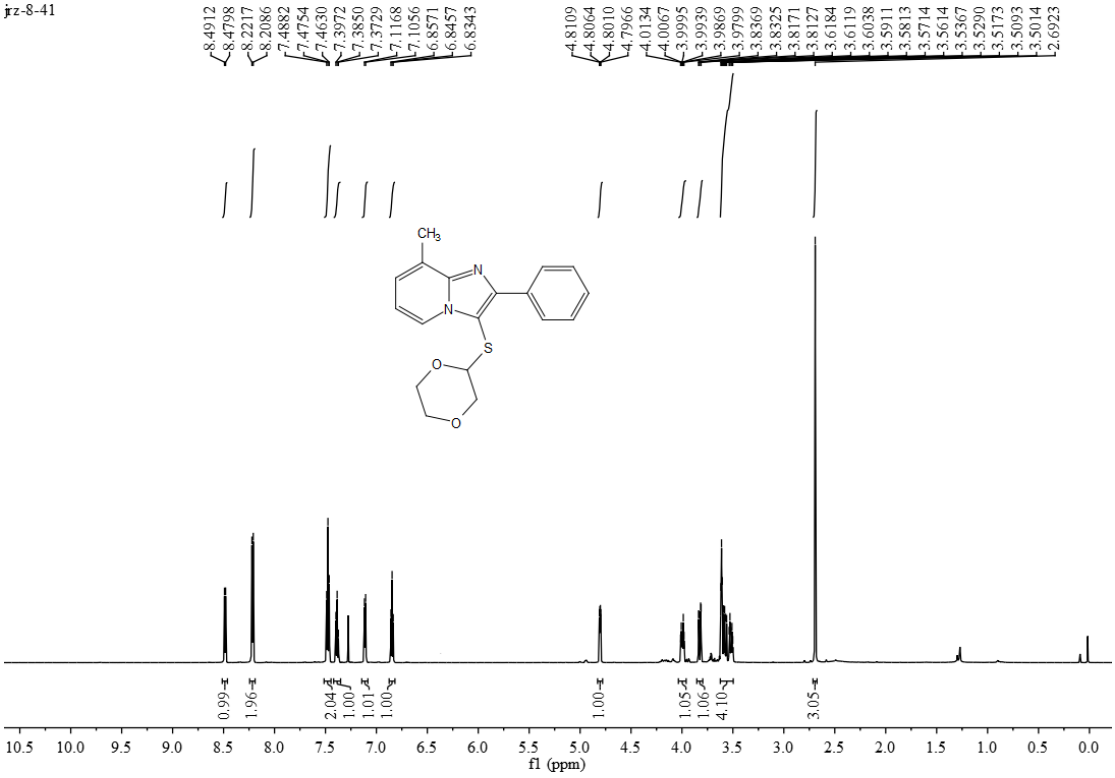
1. Y. Ding, P. Xie, W. Zhu, B. Xu, W. Zhao and A. Zhou, ***RSC Adv.***, 2016, **6**, 81932.

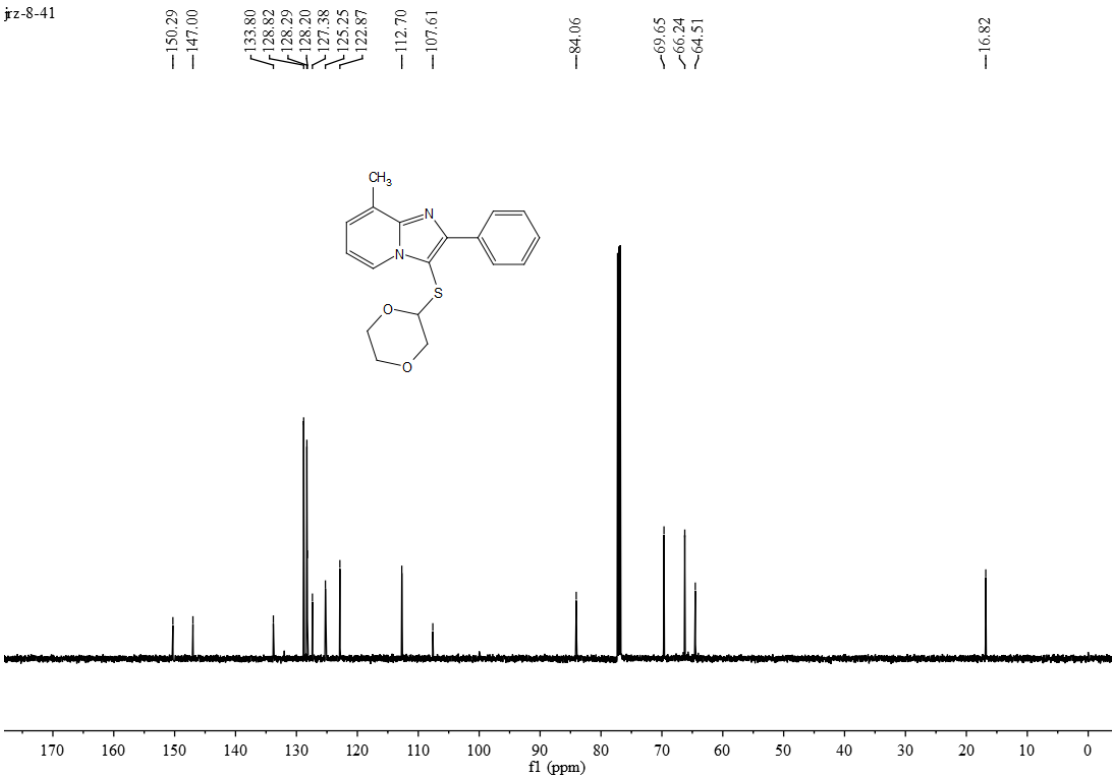
**3-(1,4-dioxan-2-ylthio)-2-phenylimidazo[1,2-*a*]pyridine (3)**



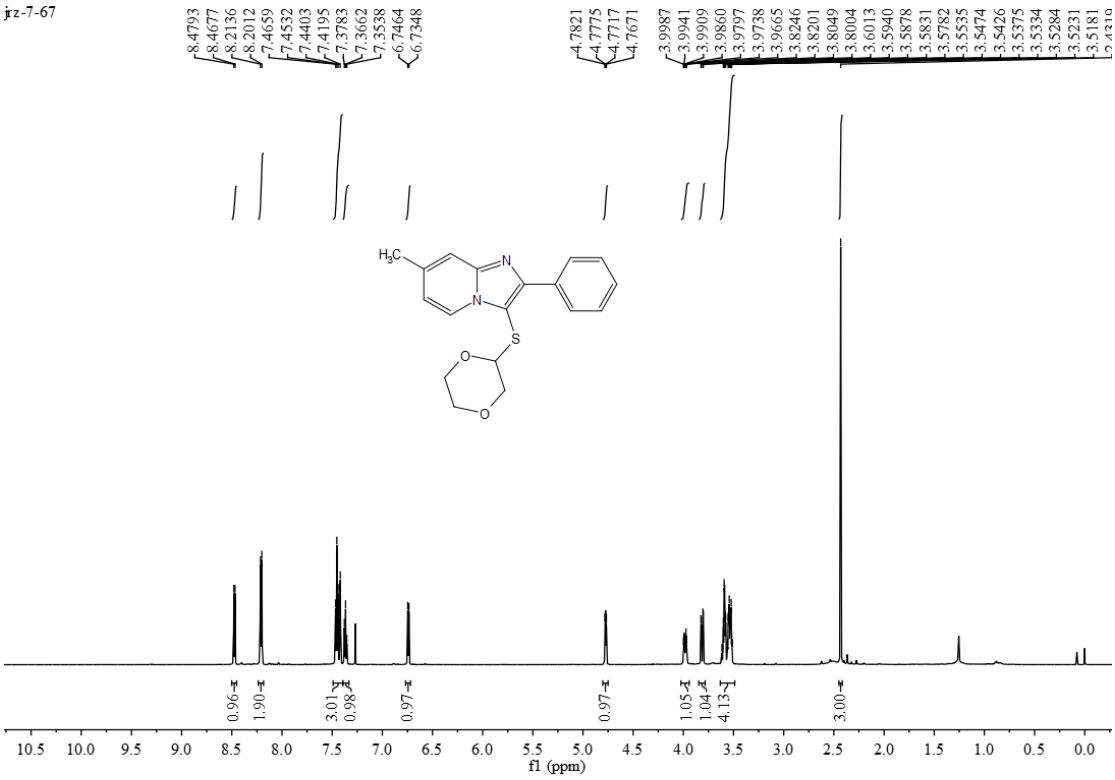



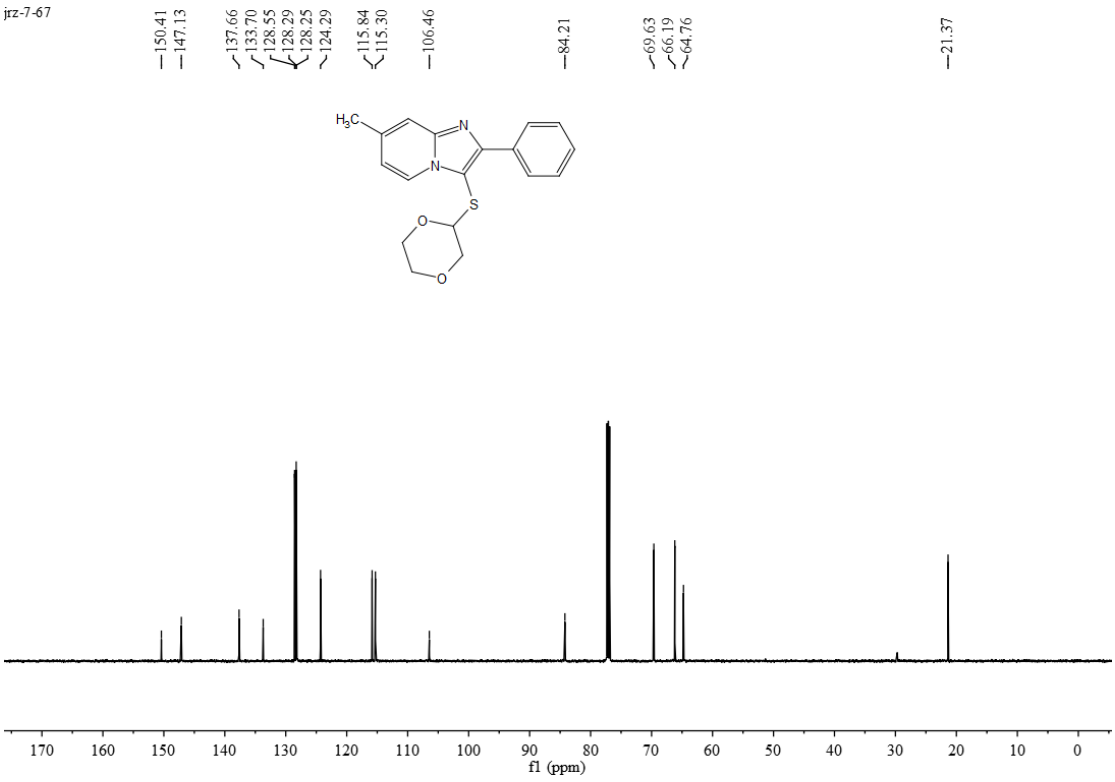
**3-(1,4-dioxan-2-ylthio)-8-methyl-2-phenylimidazo[1,2-*a*]pyridine (4)**



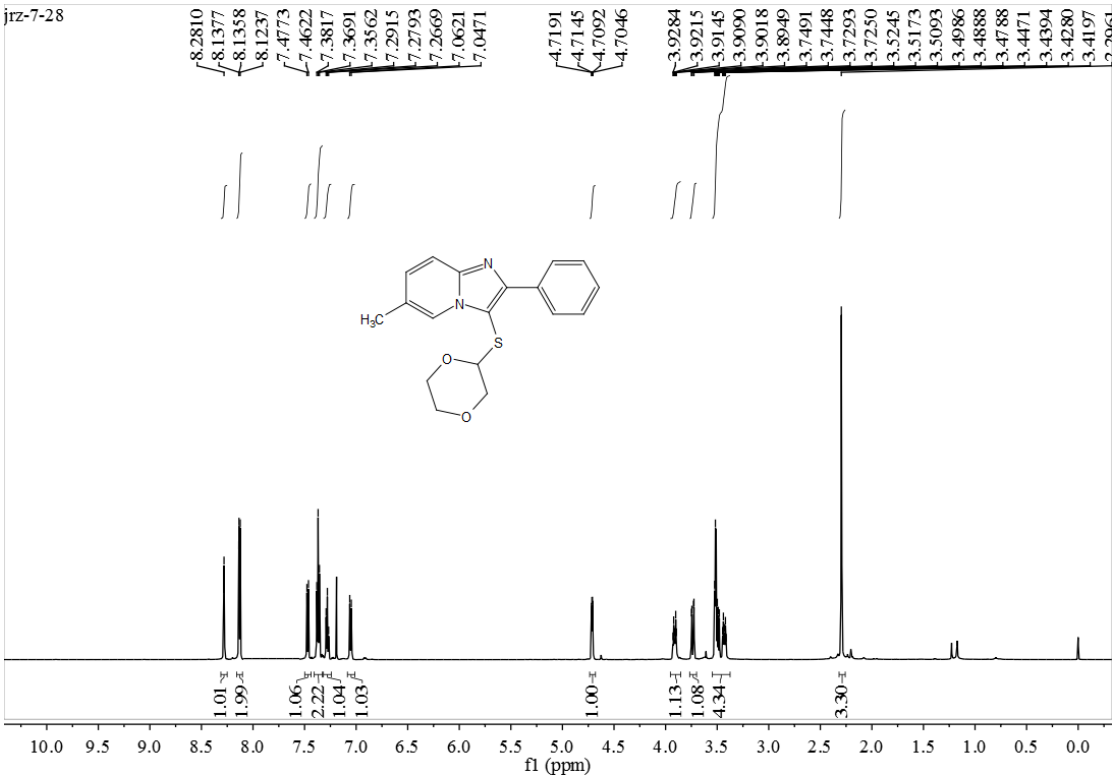



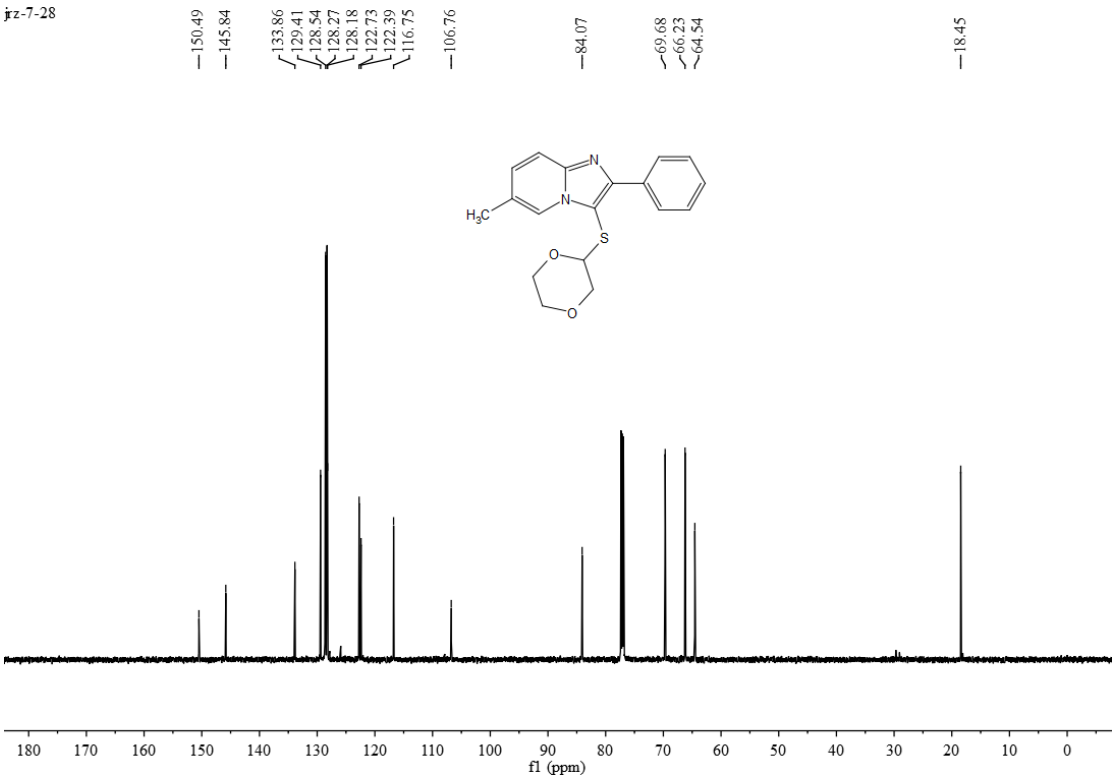
**3-(1,4-dioxan-2-ylthio)-7-methyl-2-phenylimidazo[1,2-*a*]pyridine (5)**



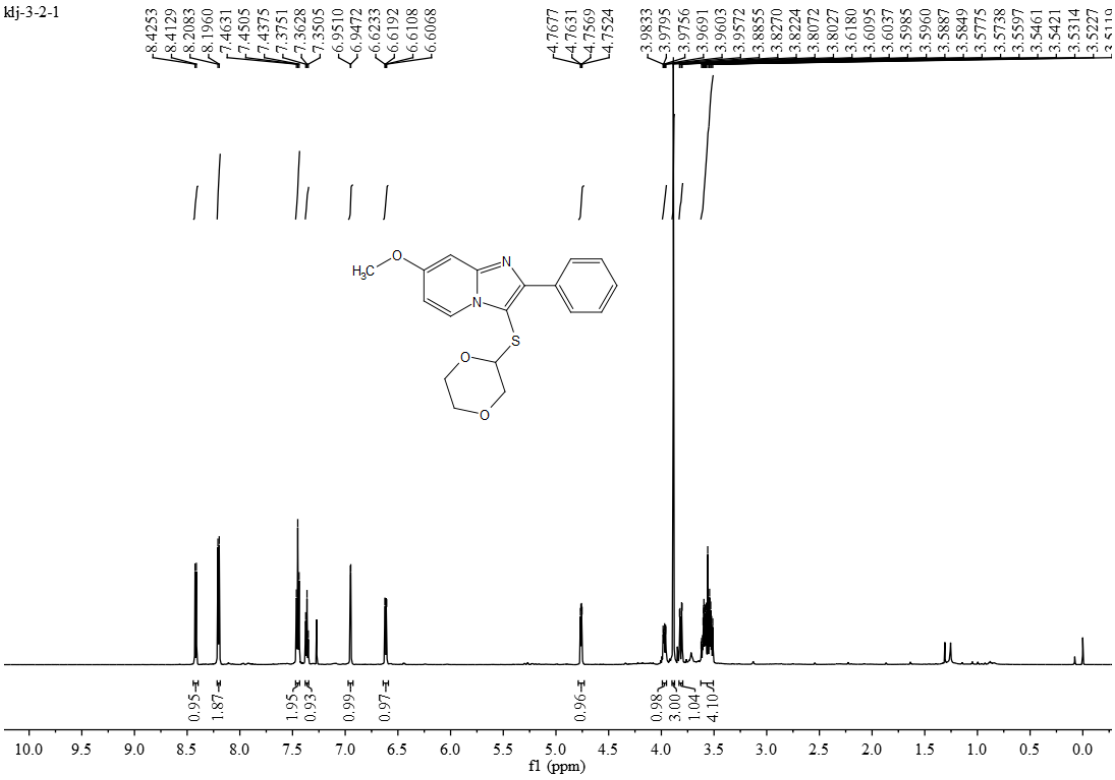



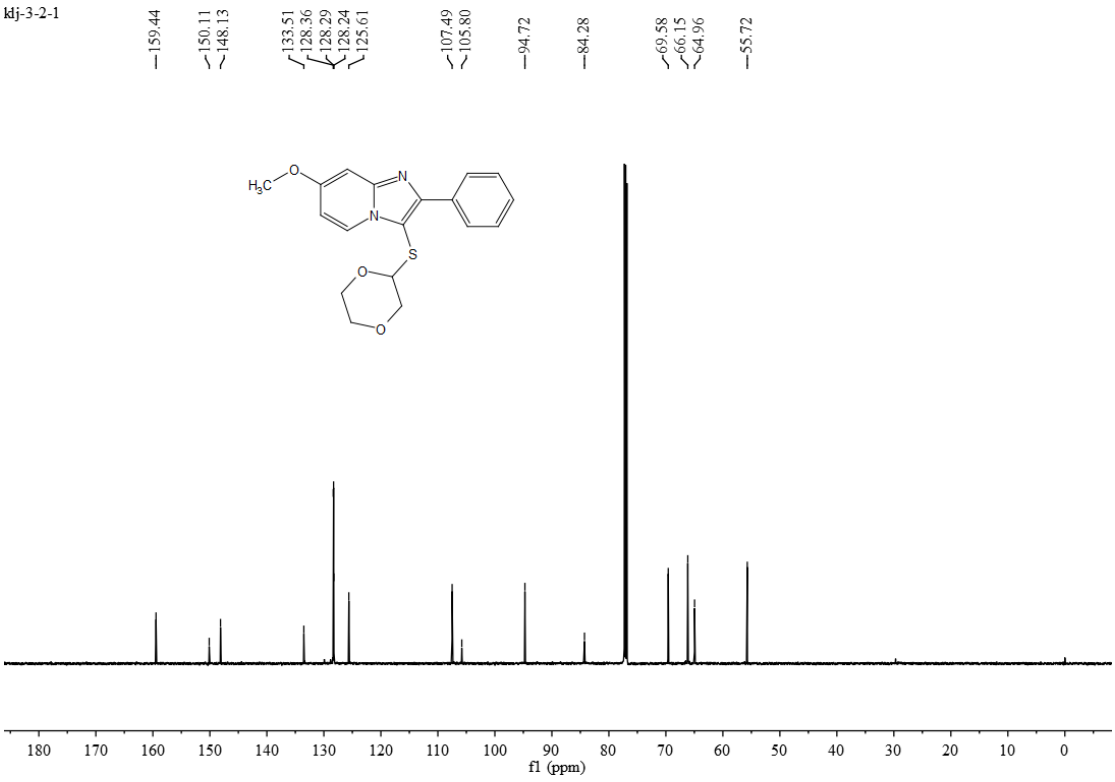
**3-(1,4-dioxan-2-ylthio)-6-methyl-2-phenylimidazo[1,2-*a*]pyridine (6)**



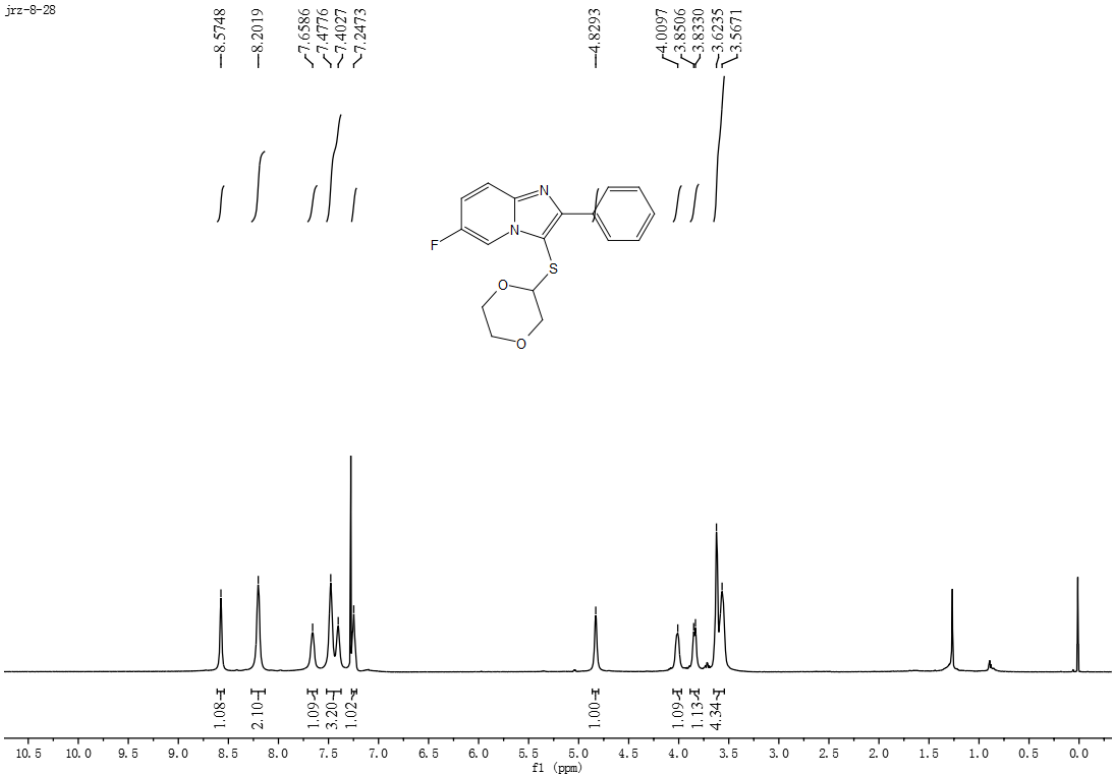



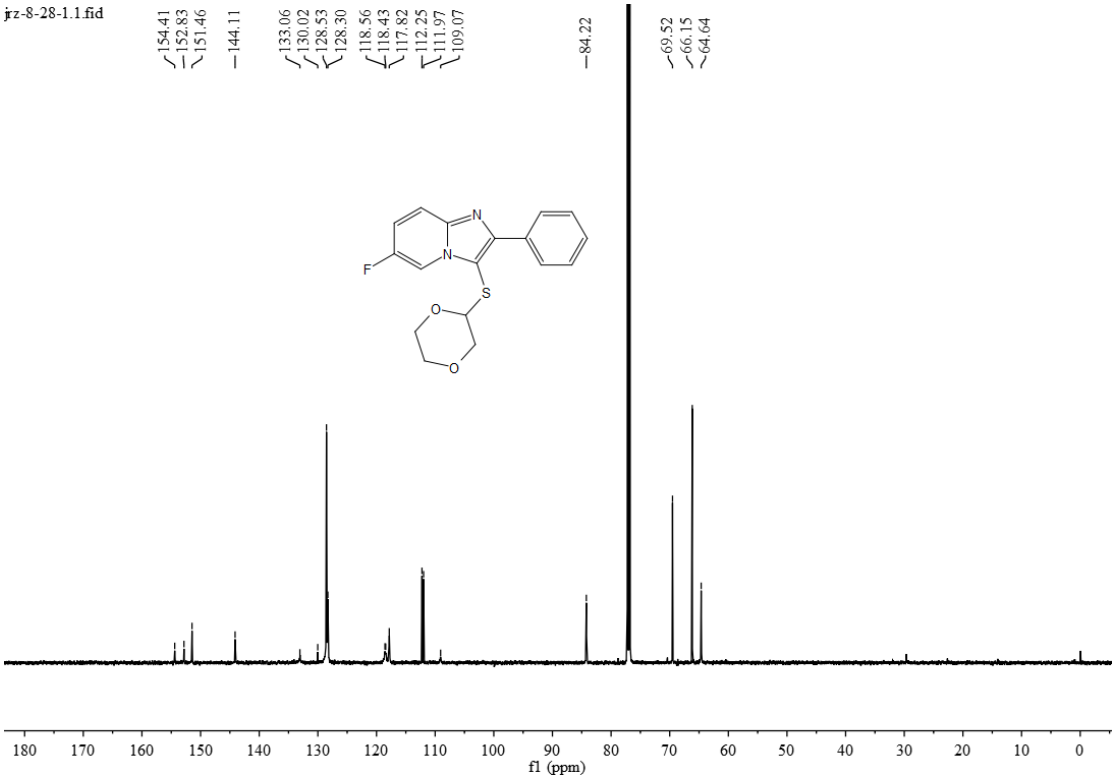
**3-(1,4-dioxan-2-ylthio)-7-methoxy-2-phenylimidazo[1,2-*a*]pyridine (7)**



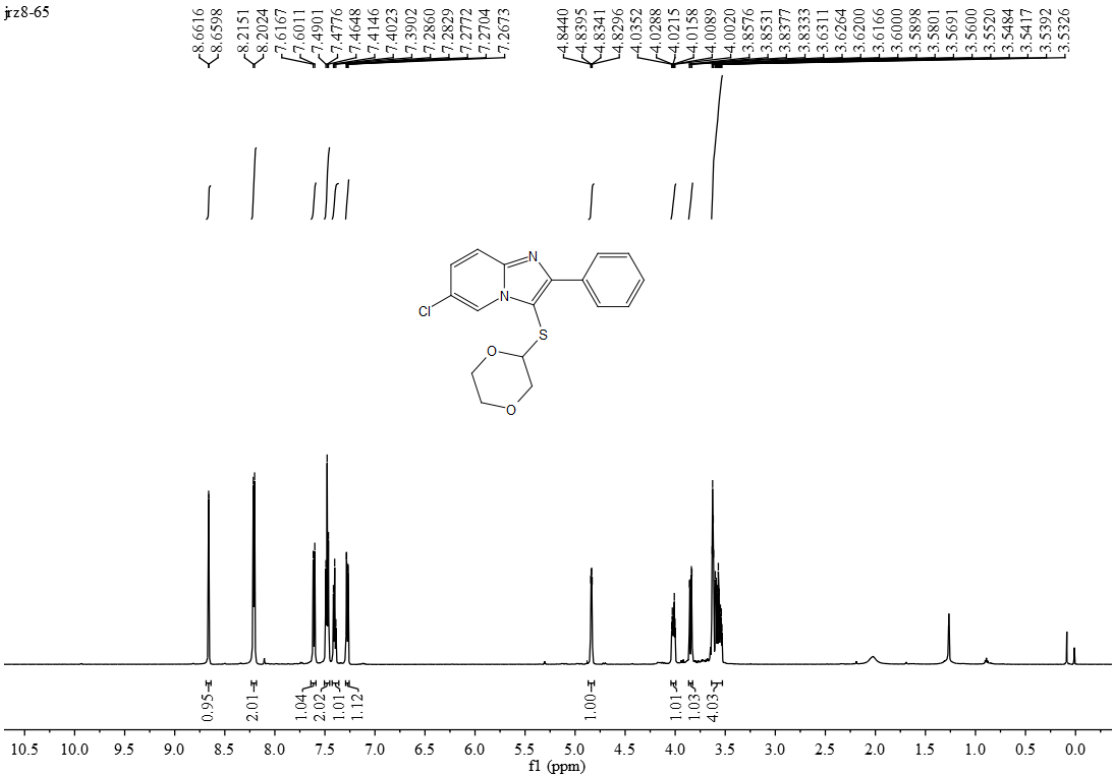



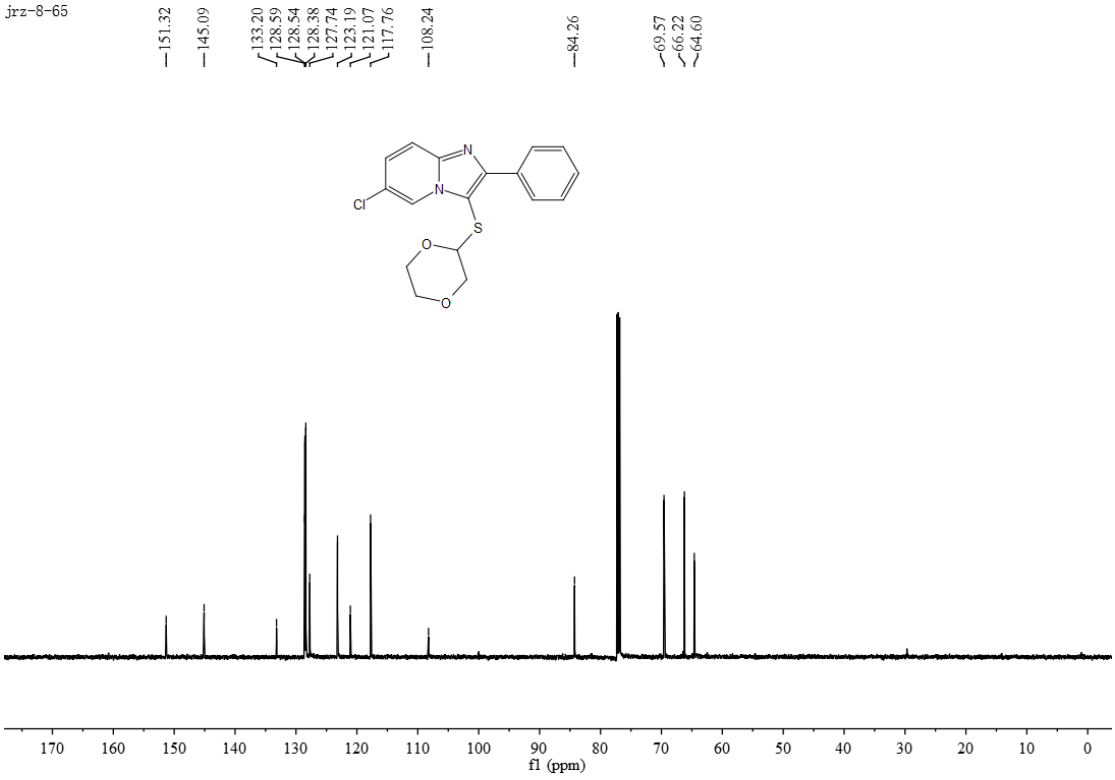
**3-(1,4-dioxan-2-ylthio)-6-fluoro-2-phenylimidazo[1,2-*a*]pyridine (8)**



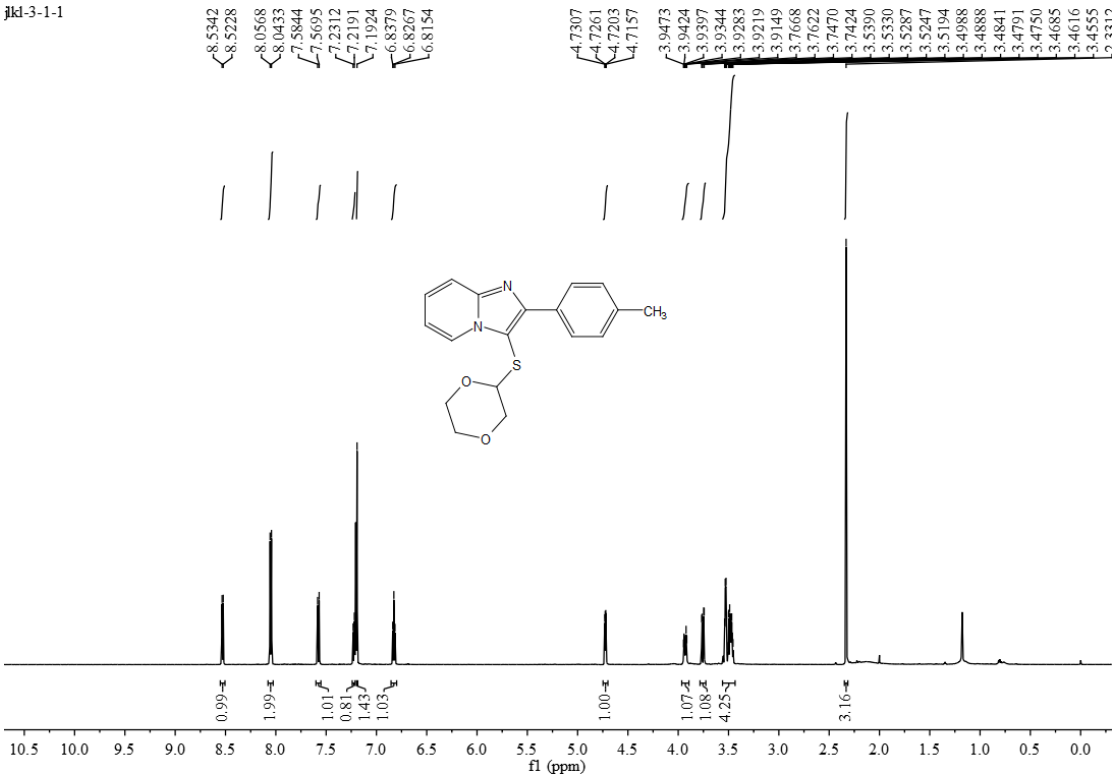



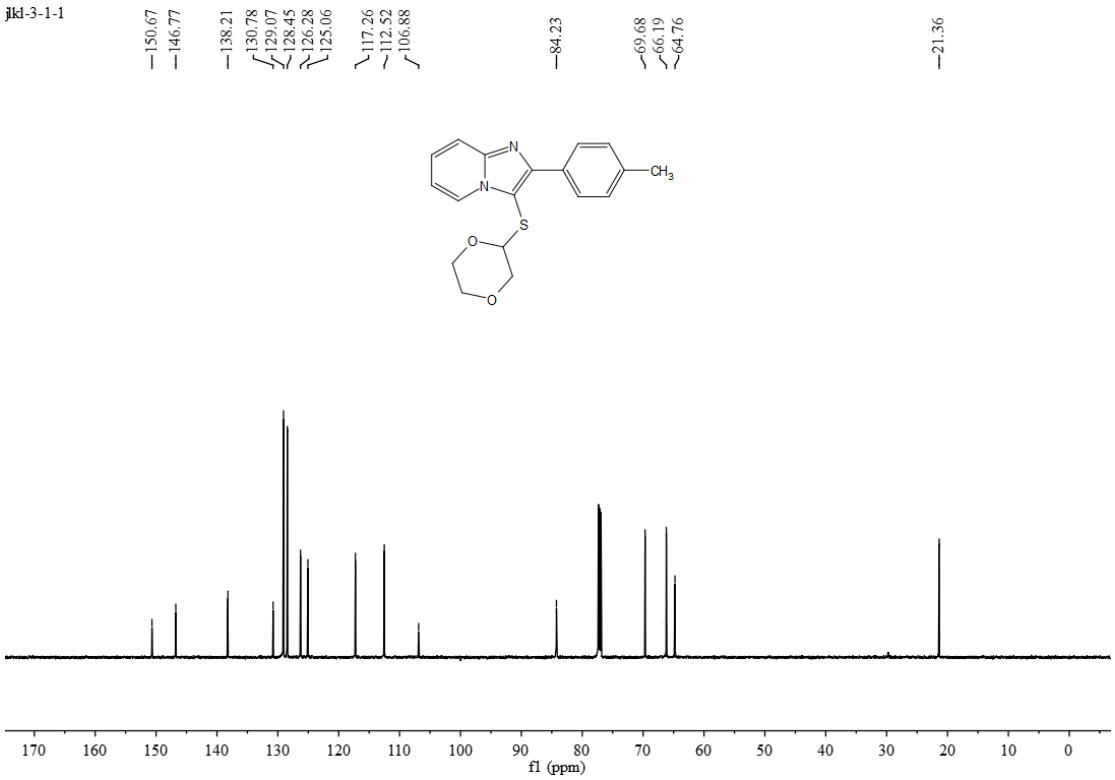
**3-(1,4-dioxan-2-ylthio)-6-chloro-2-phenylimidazo[1,2-*a*]pyridine (9)**



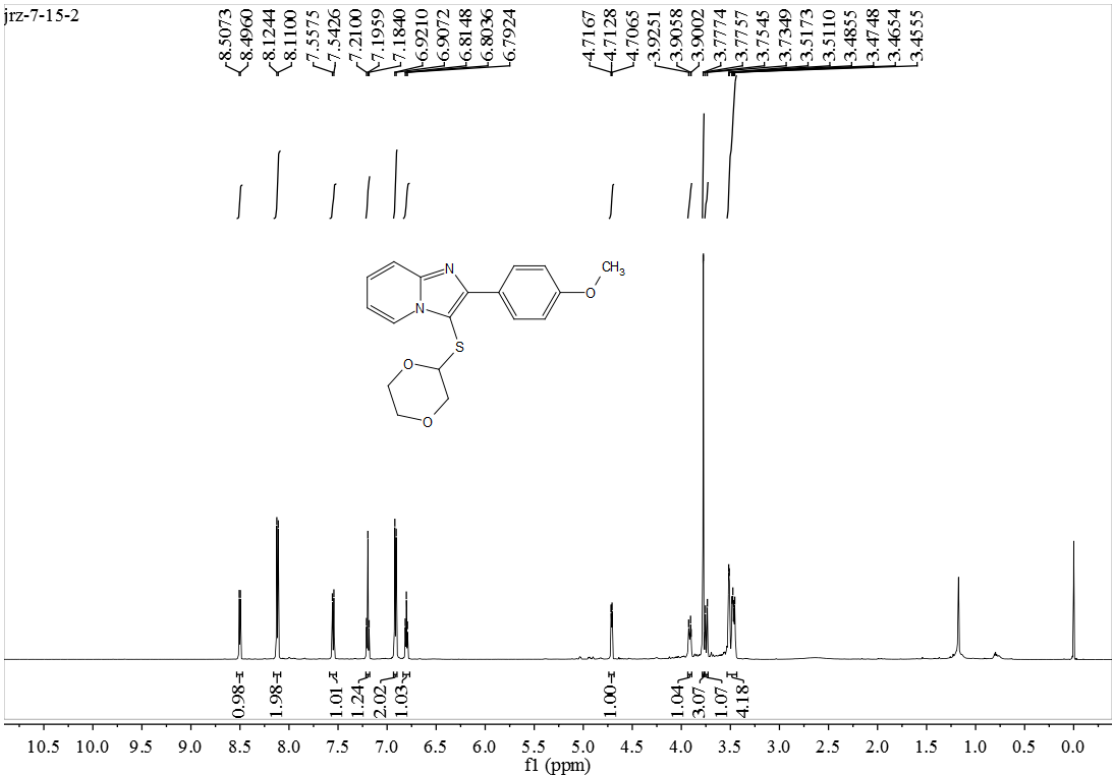



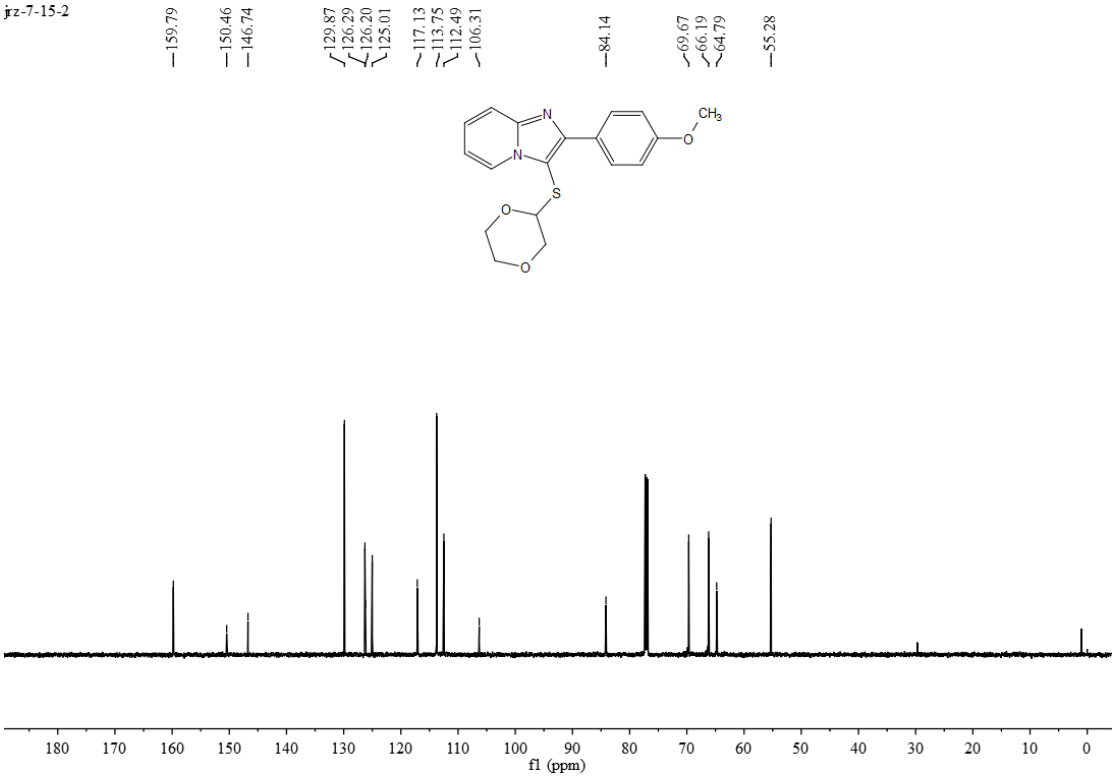
**3-(1,4-dioxan-2-ylthio)-2-p-tolylimidazo[1,2-*a*]pyridine (10)**



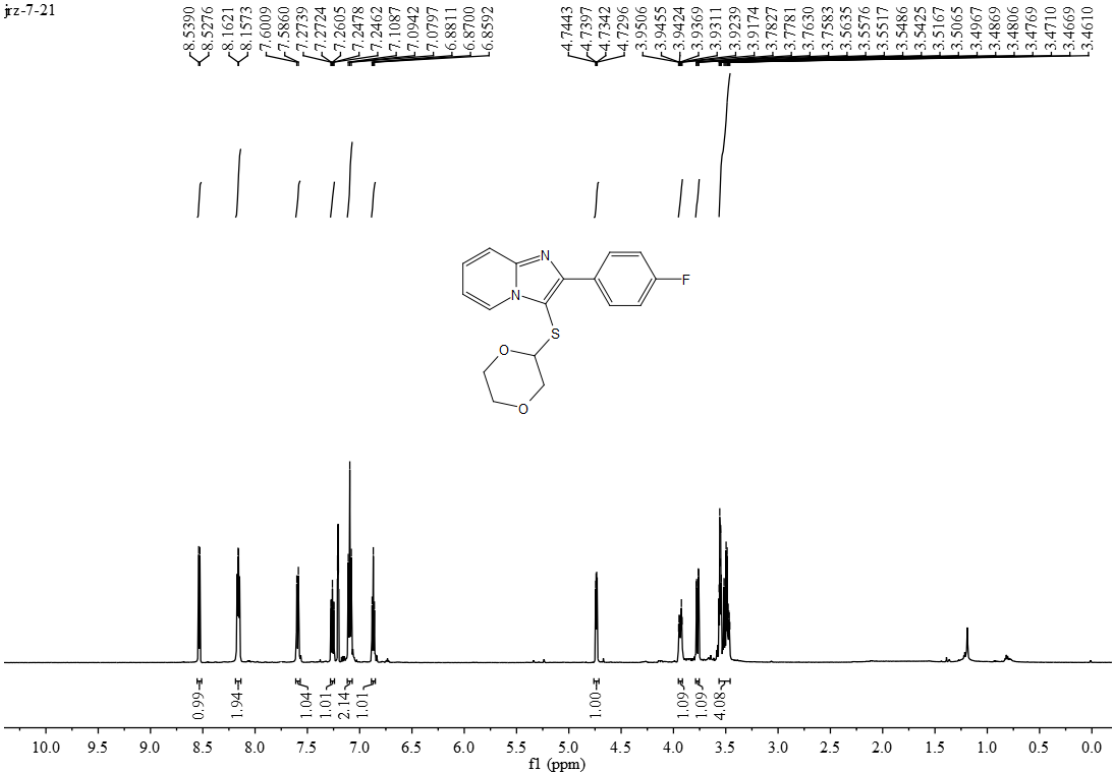



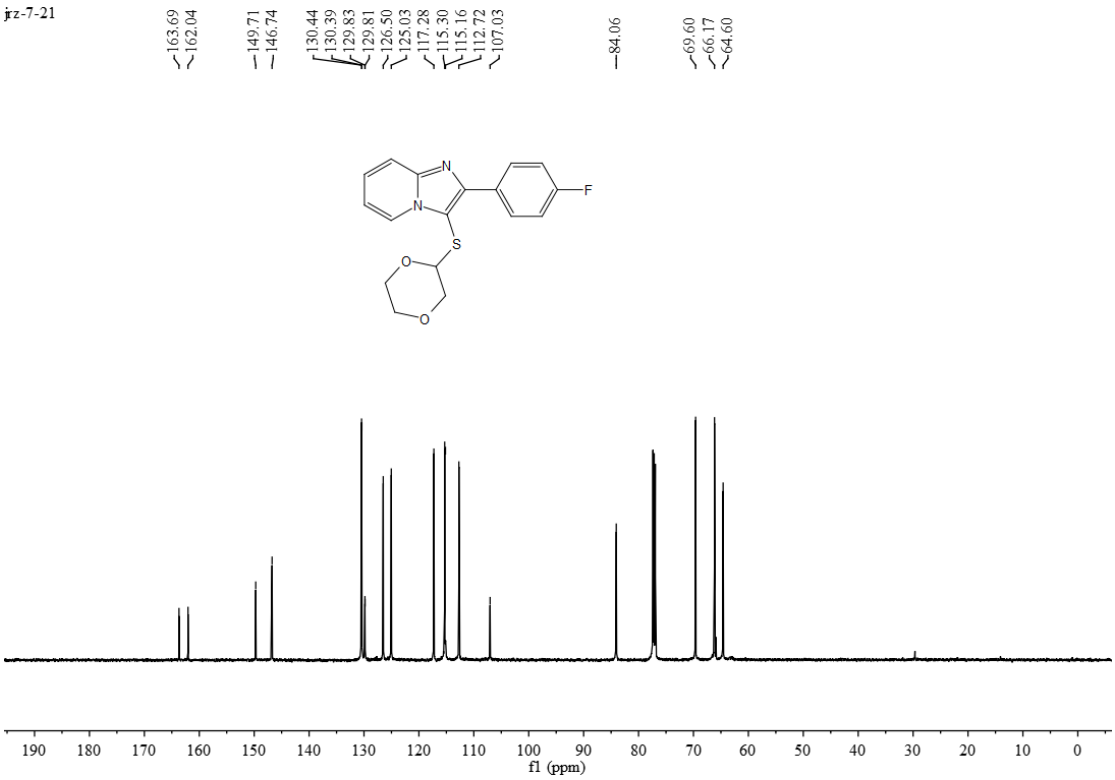
**3-(1,4-dioxan-2-ylthio)-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyridine (11)**



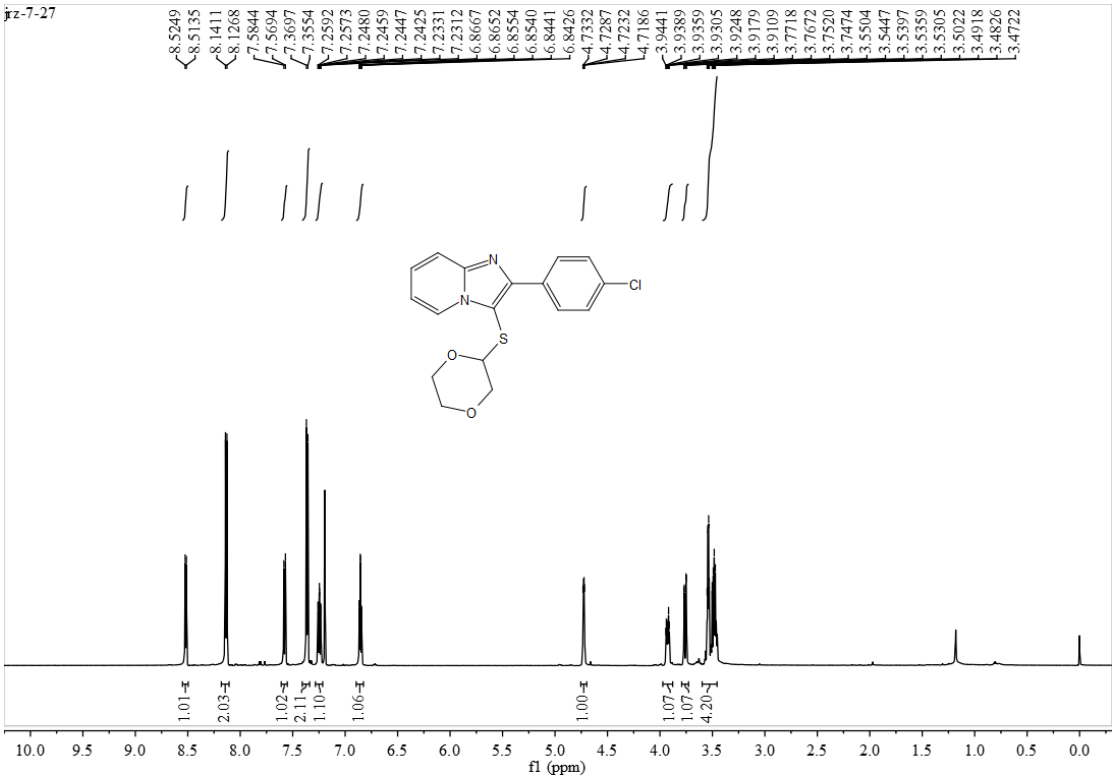



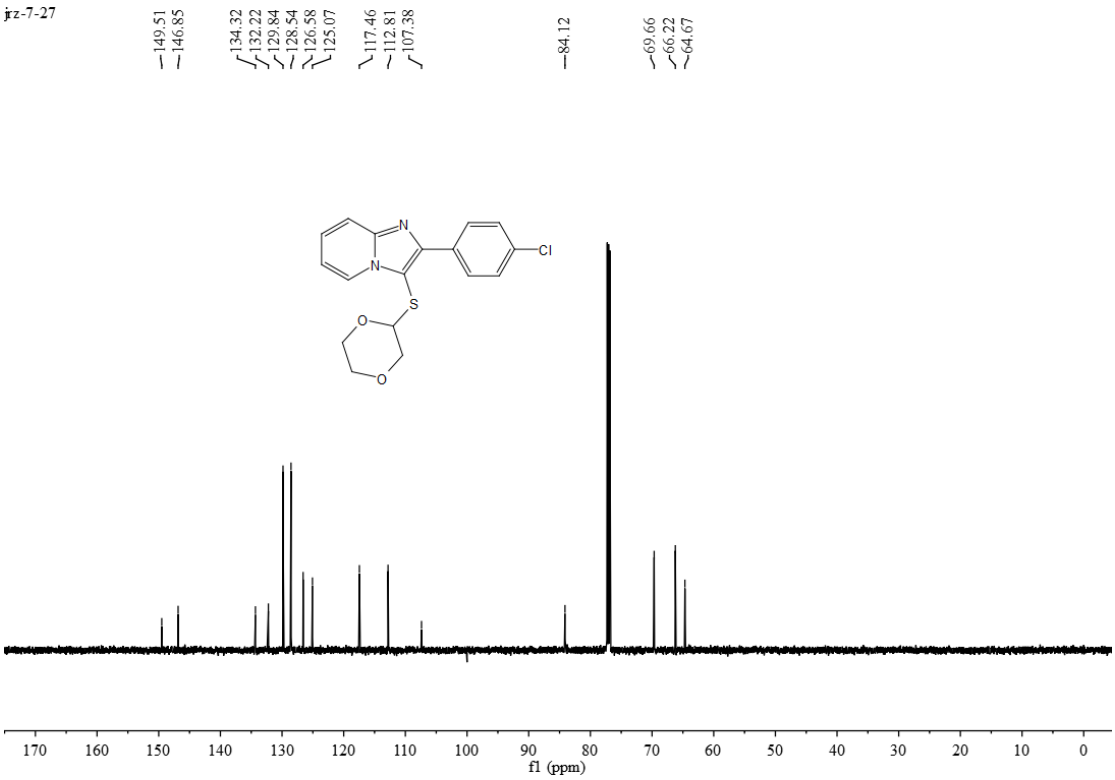
**3-(1,4-dioxan-2-ylthio)-2-(4-fluorophenyl)imidazo[1,2-*a*]pyridine (12)**



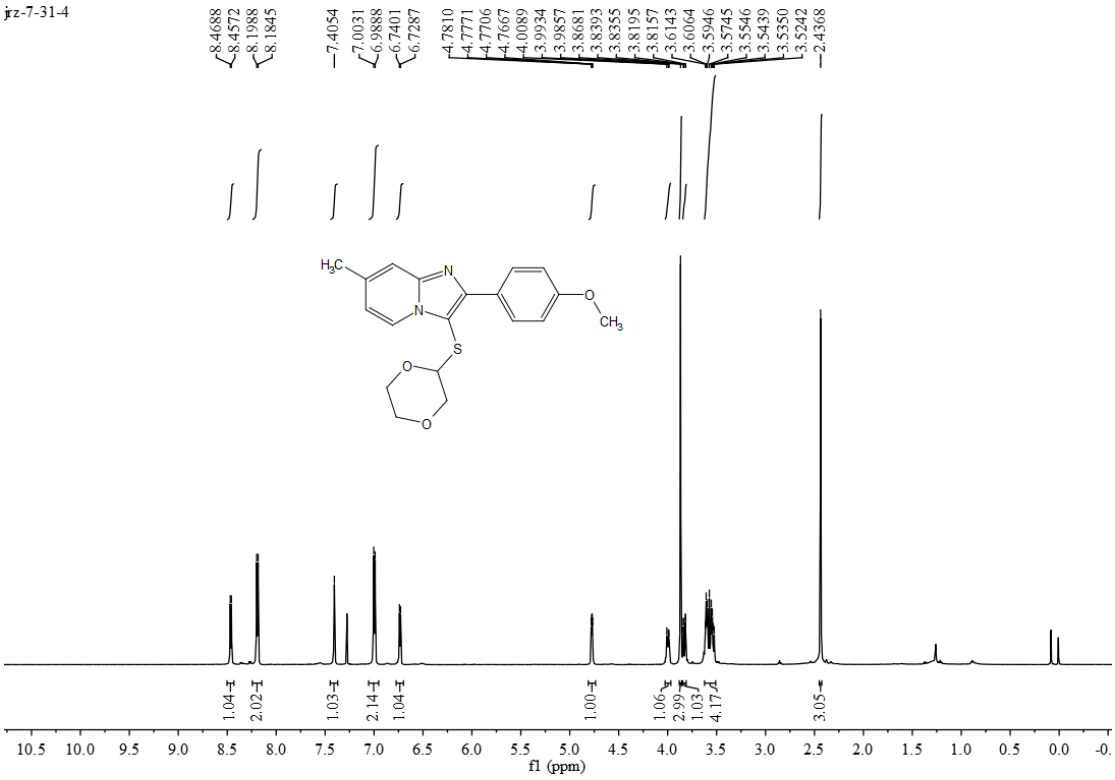



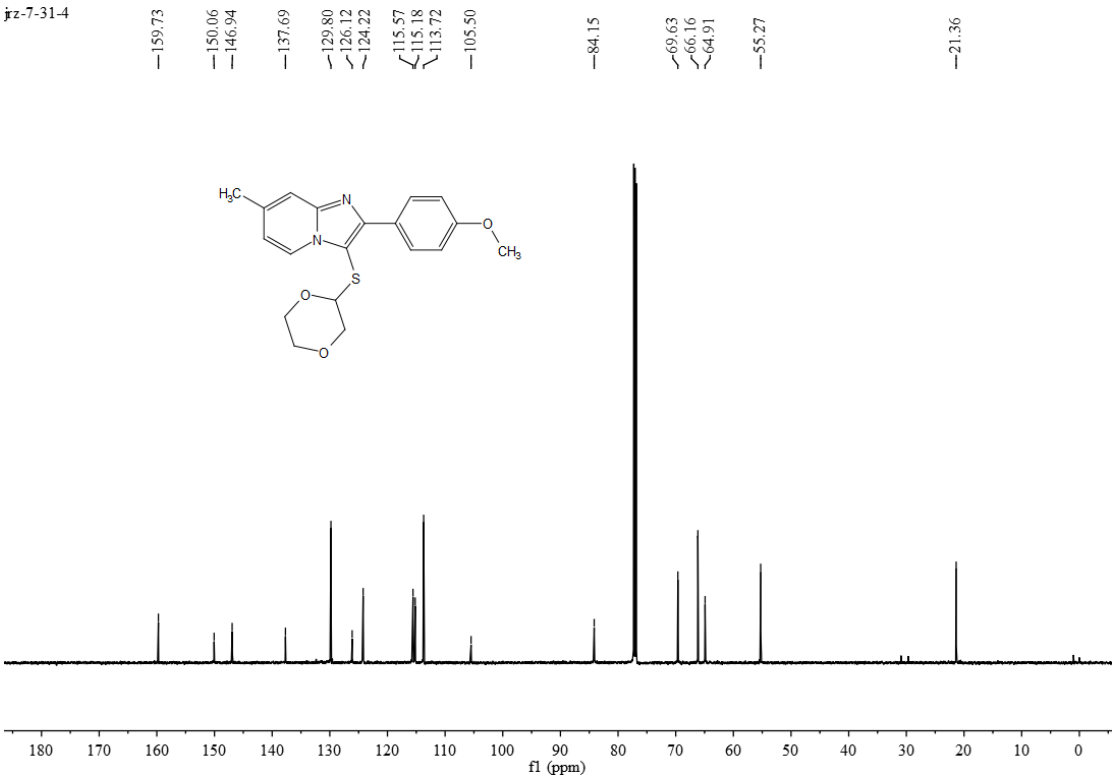
**3-(1,4-dioxan-2-ylthio)-2-(4-chlorophenyl)imidazo[1,2-*a*]pyridine (13)**



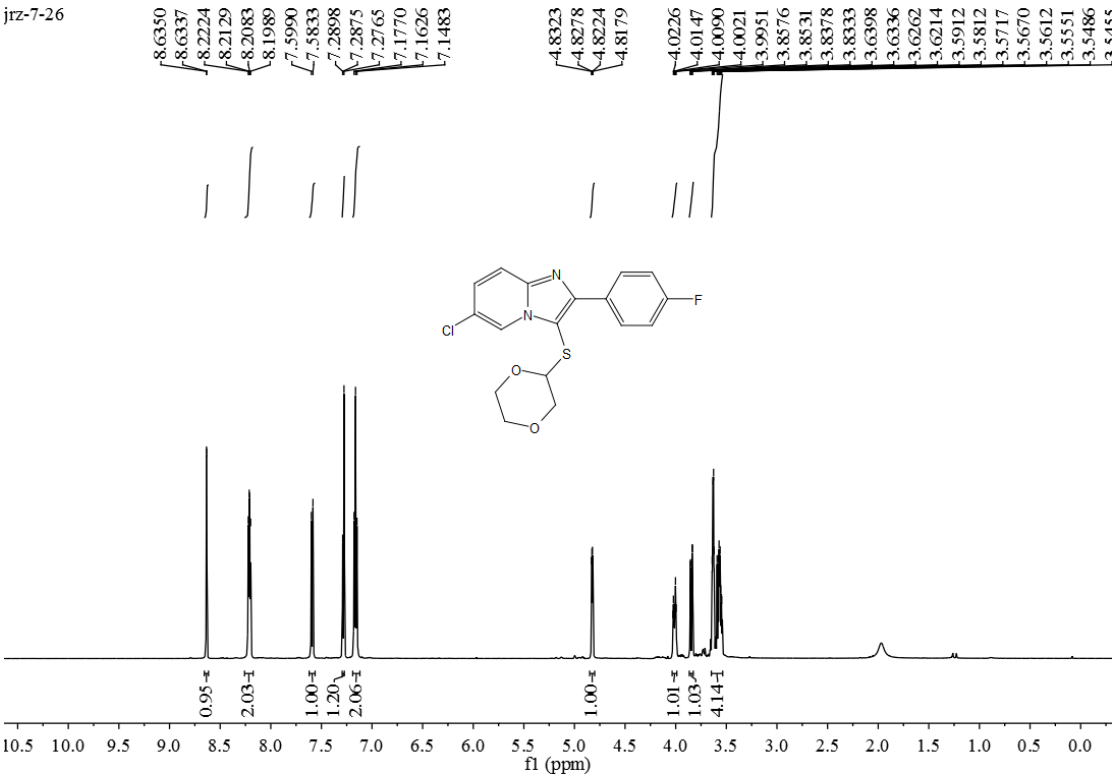



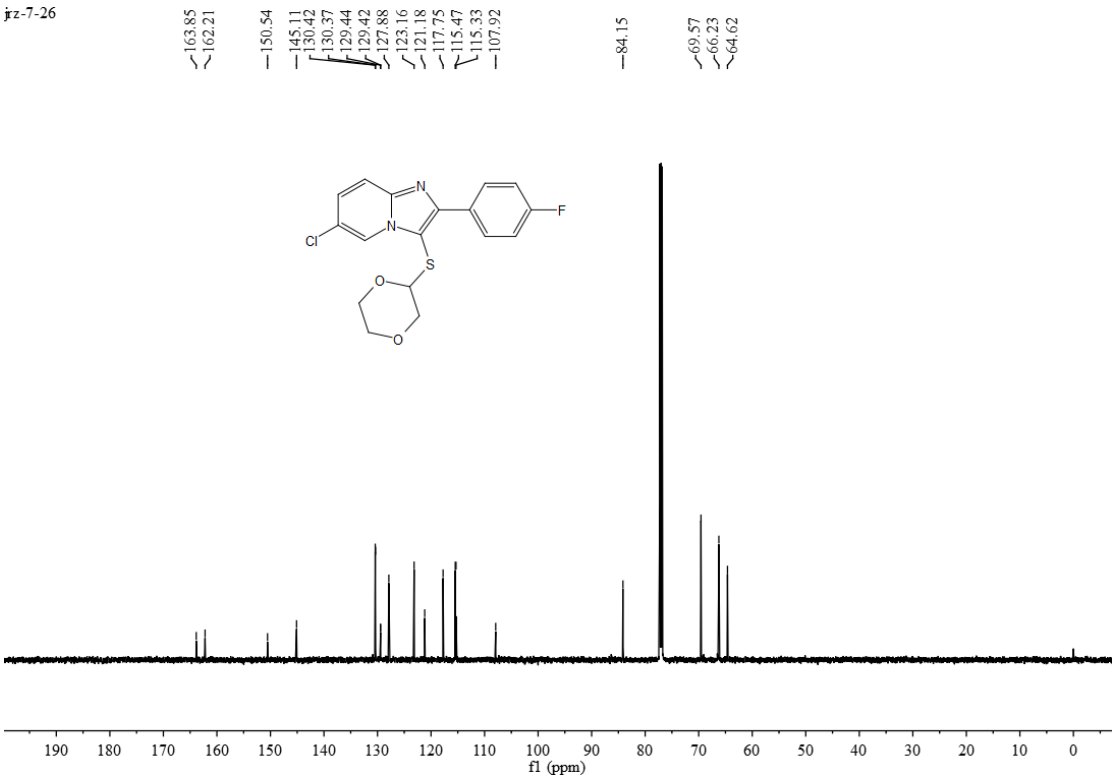
**3-(1,4-dioxan-2-ylthio)-2-(4-methoxyphenyl)-7-methylimidazo[1,2-*a*]pyridine (14)**



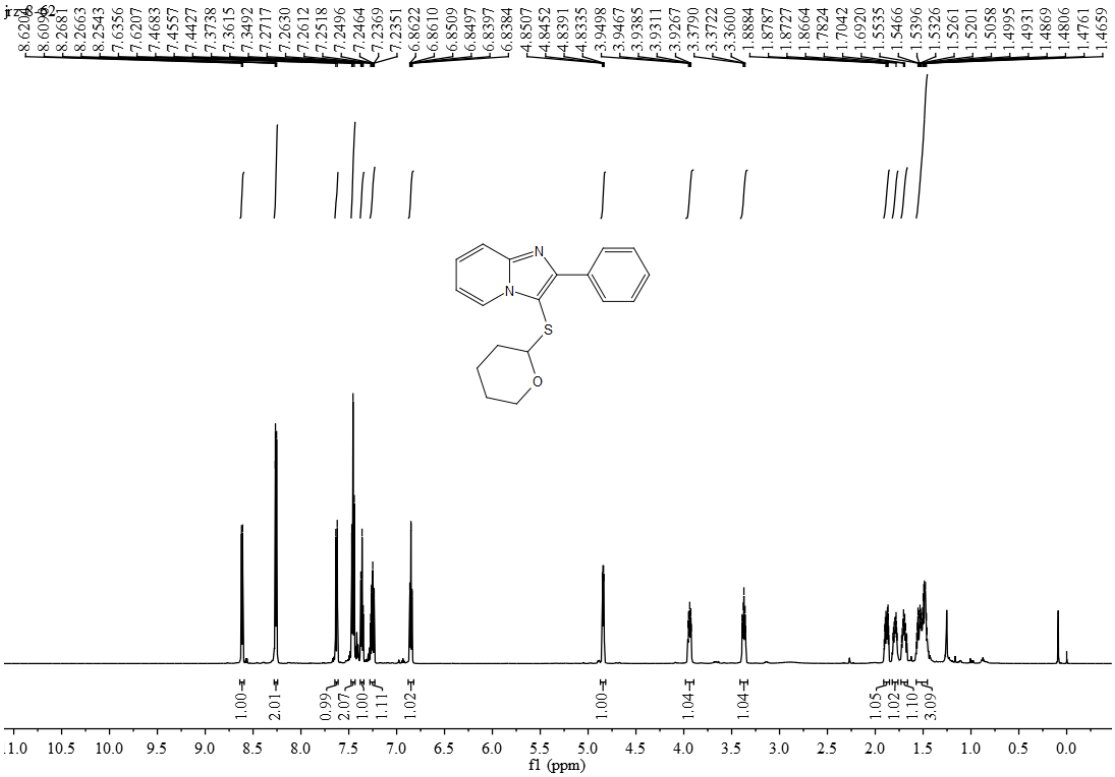



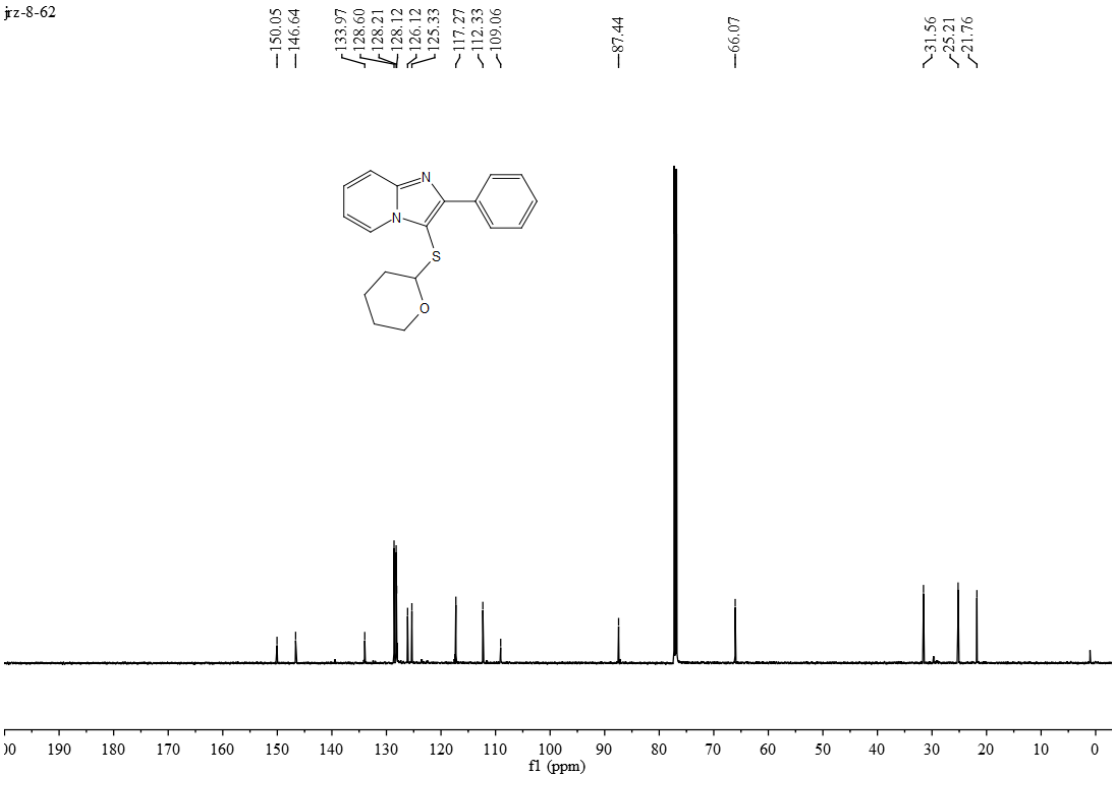
**3-(1,4-dioxan-2-ylthio)-6-chloro-2-(4-fluorophenyl)imidazo[1,2-*a*]pyridine (15)**



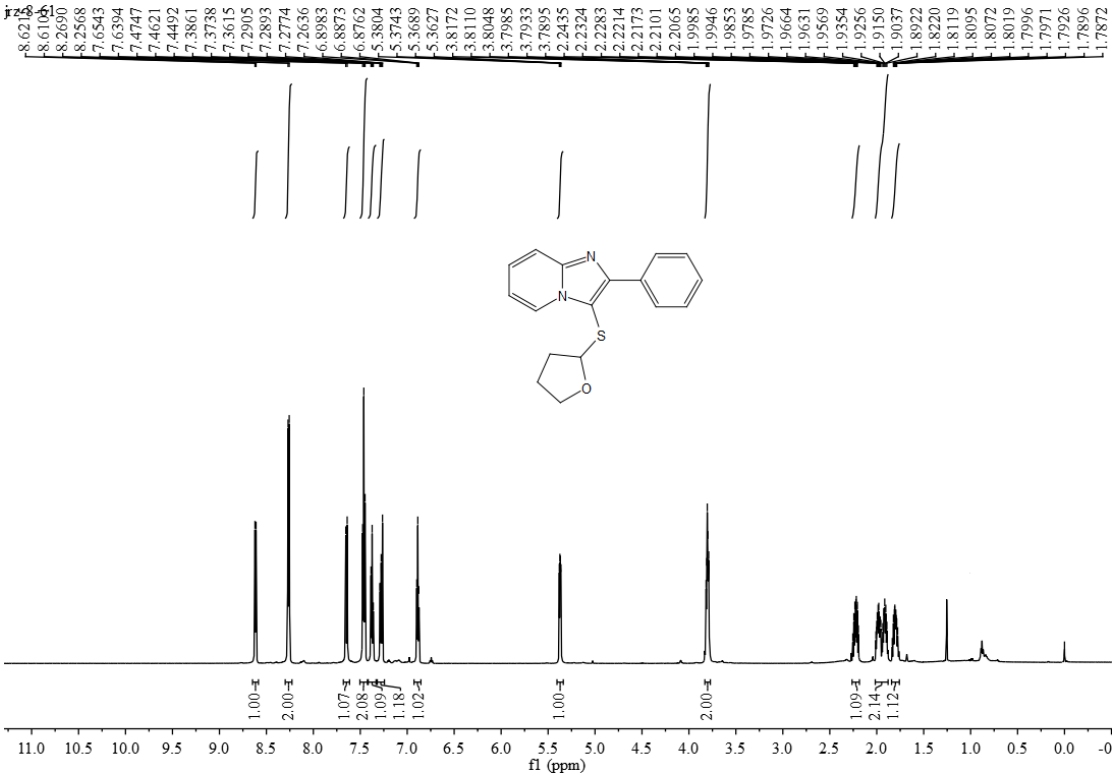



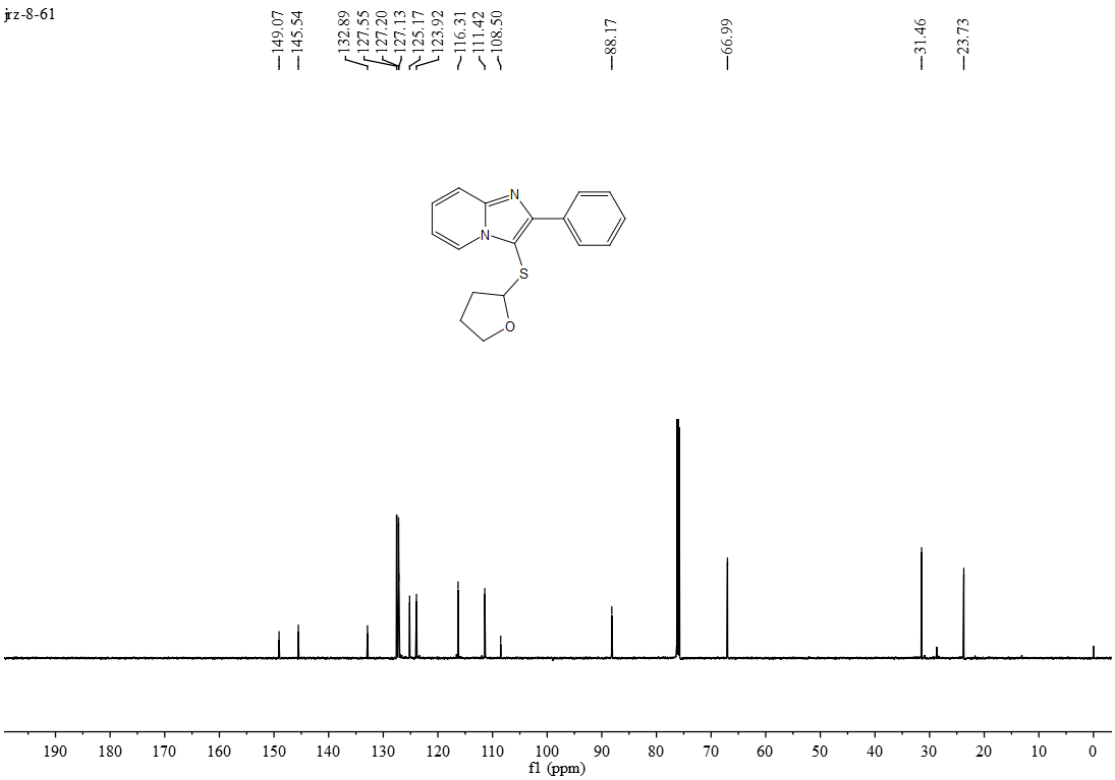
**2-phenyl-3-(tetrahydro-2H-pyran-2-ylthio)imidazo[1,2-*a*]pyridine (16)**



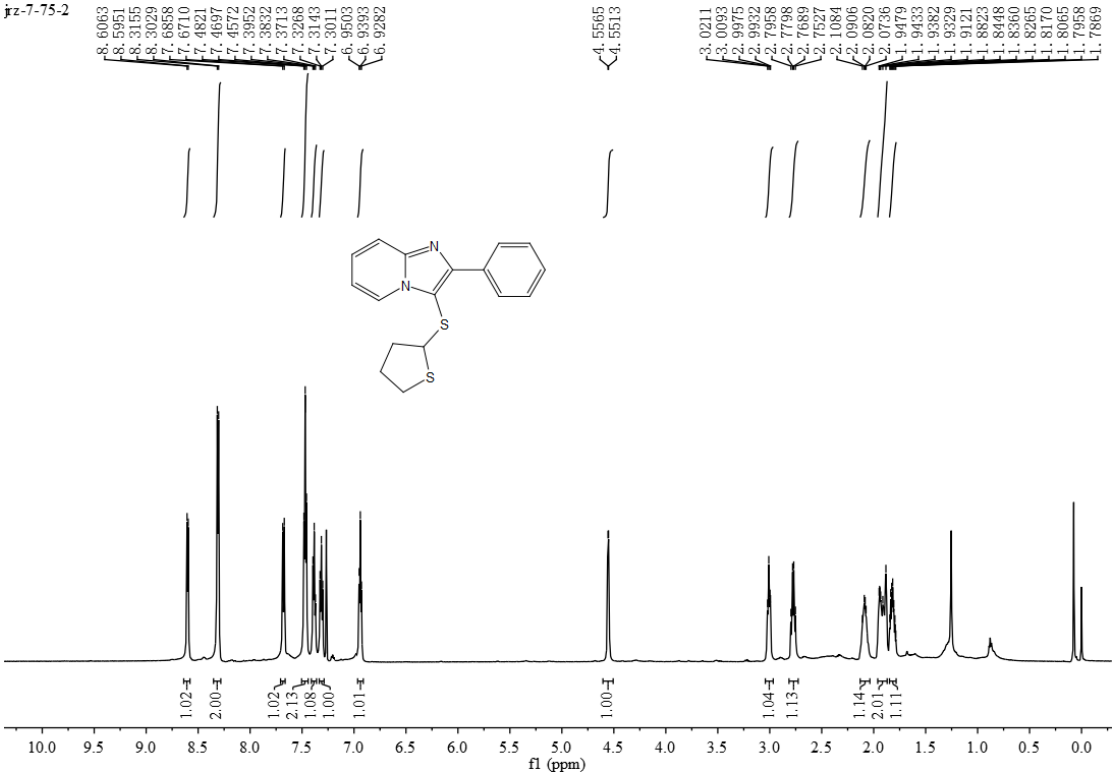



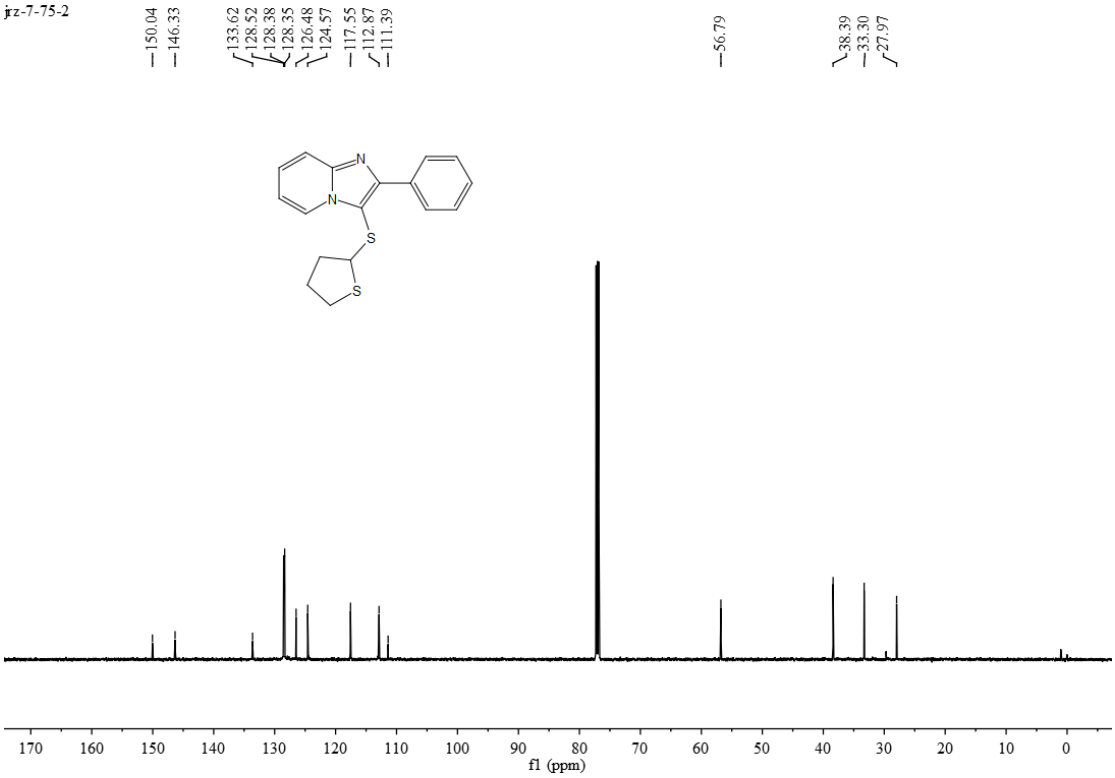
**2-phenyl-3-(tetrahydrofuran-2-ylthio)imidazo[1,2-*a*]pyridine (17)**



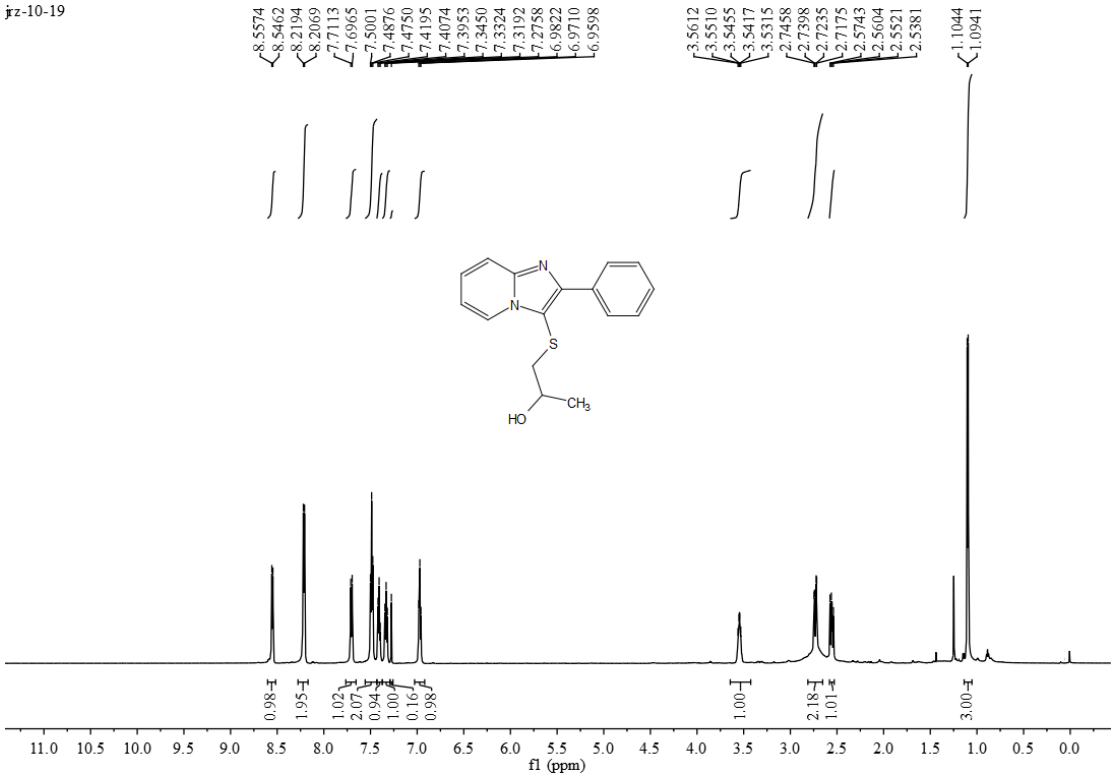



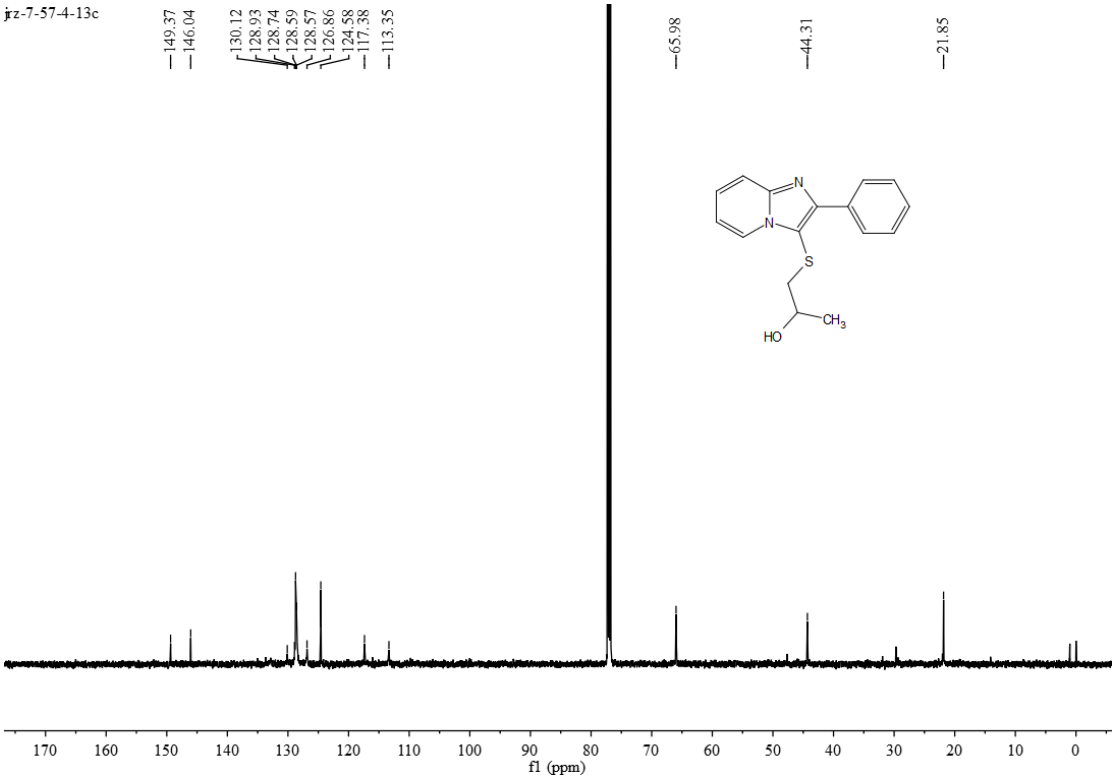
**2-phenyl-3-(tetrahydrothiophen-2-ylthio)imidazo[1,2-*a*]pyridine (18)**



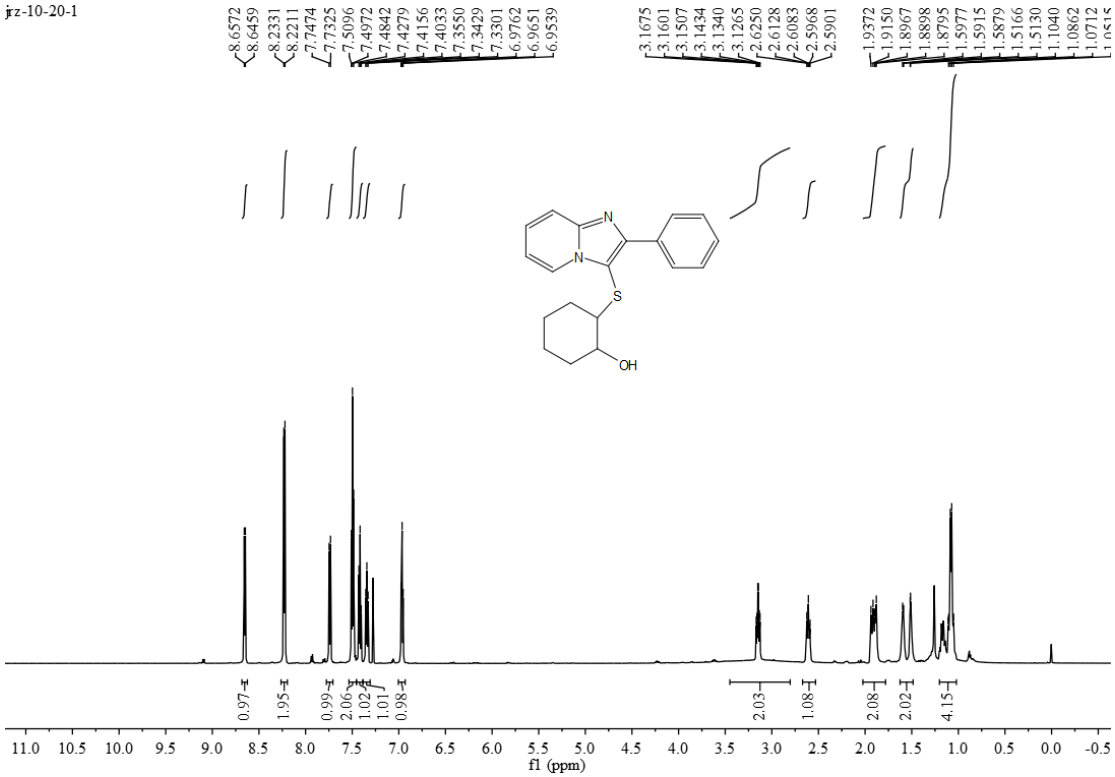



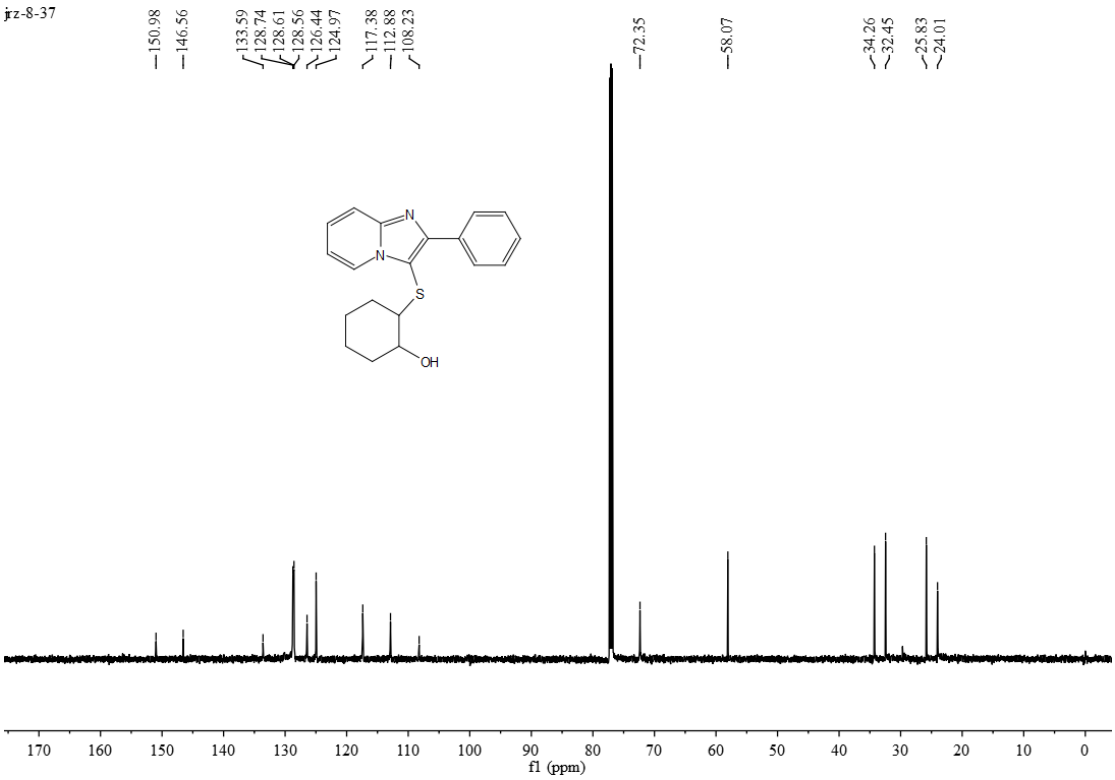
**2-(2-phenylimidazo[1,2-*a*]pyridin-3-ylthio)propan-1-ol (19)**



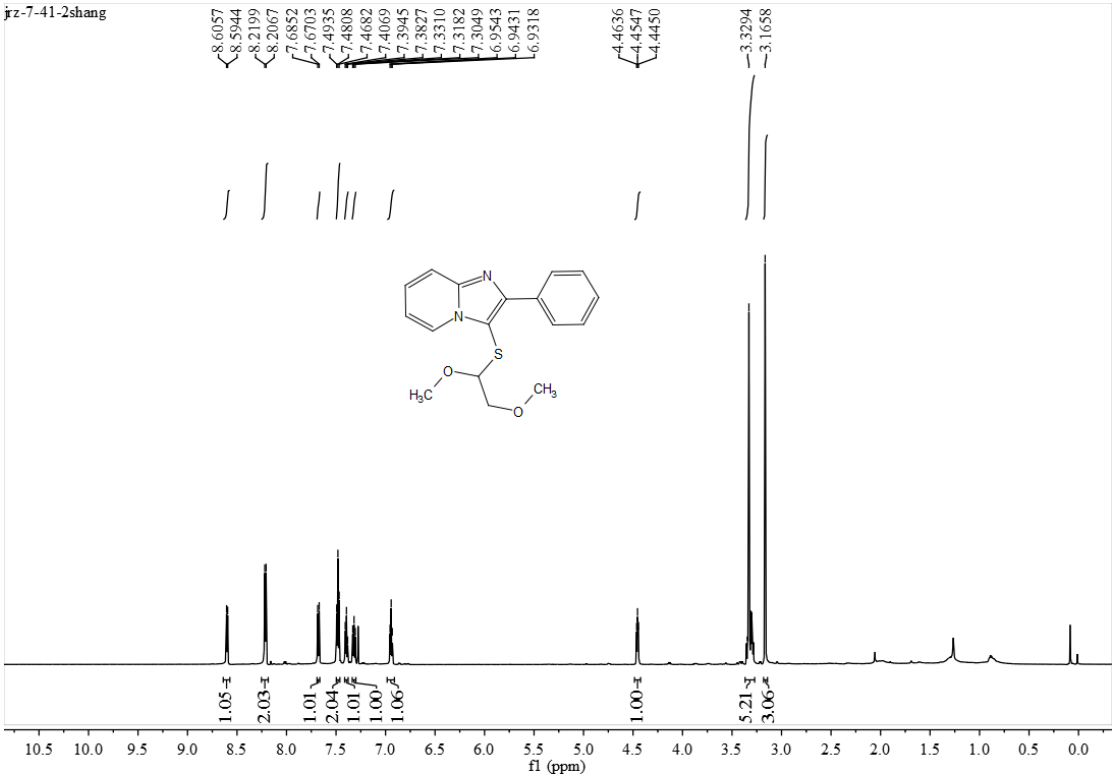



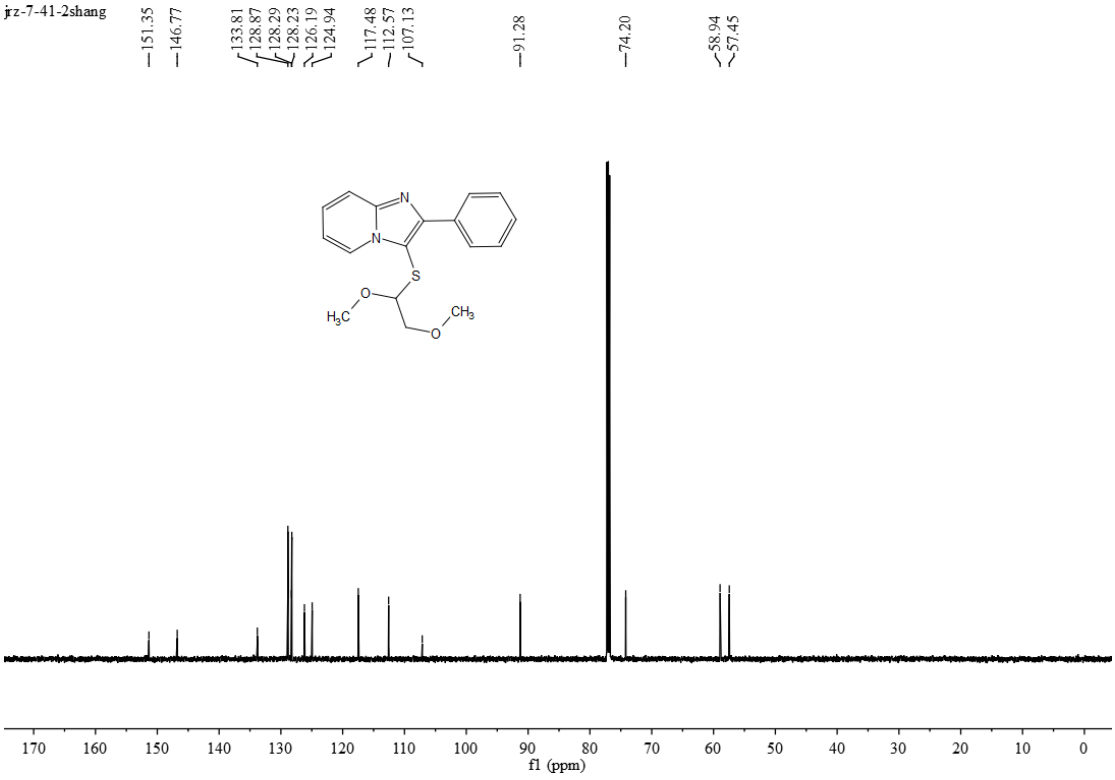
**2-(2-phenylimidazo[1,2-*a*]pyridin-3-ylthio)cyclohexanol (20)**



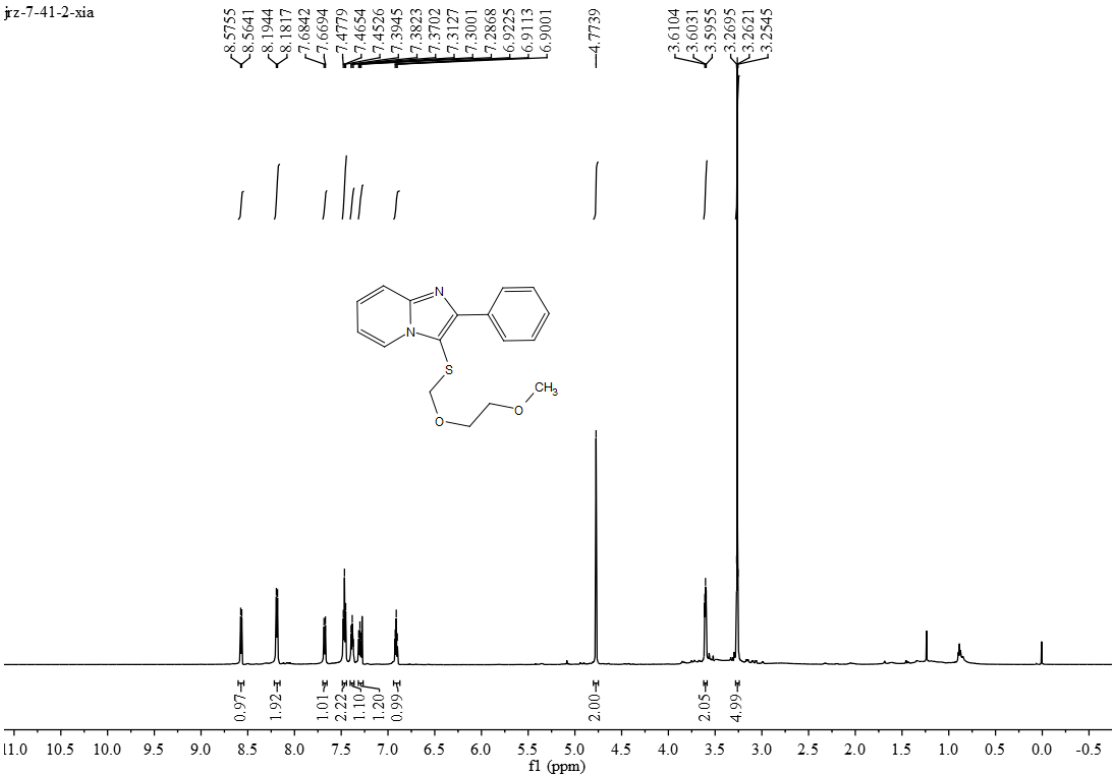



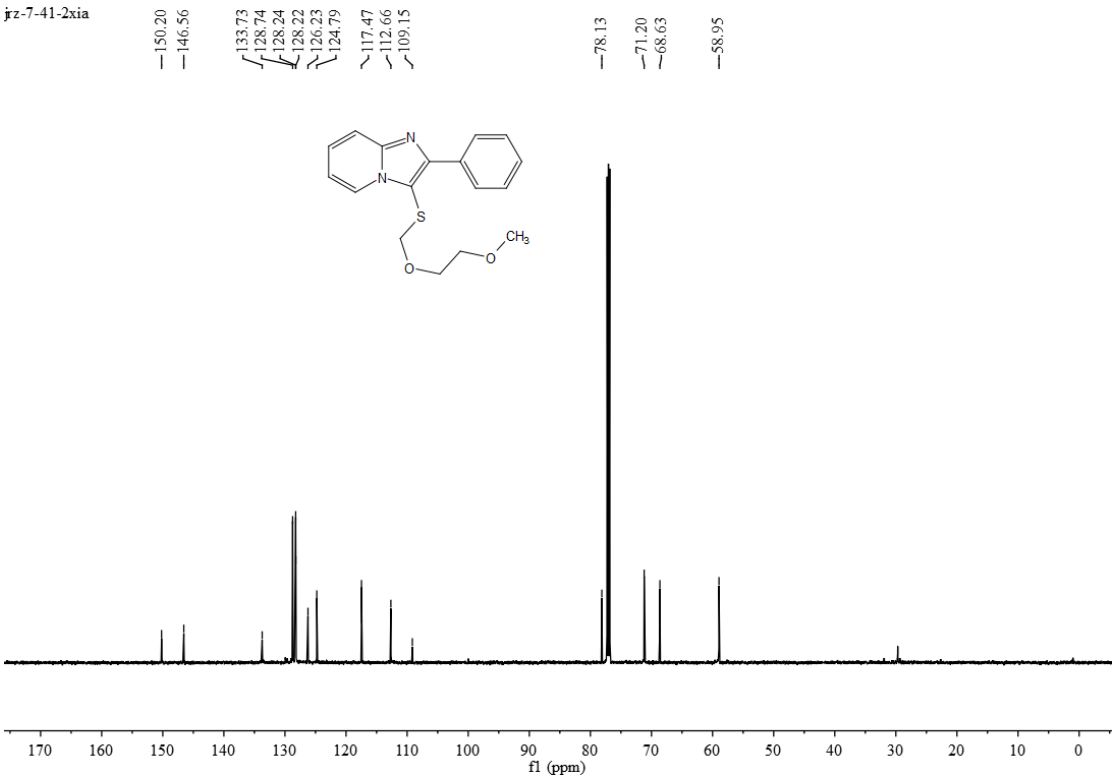
**3-(1,2-dimethoxyethylthio)-2-phenylimidazo[1,2-*a*]pyridine (21a)**



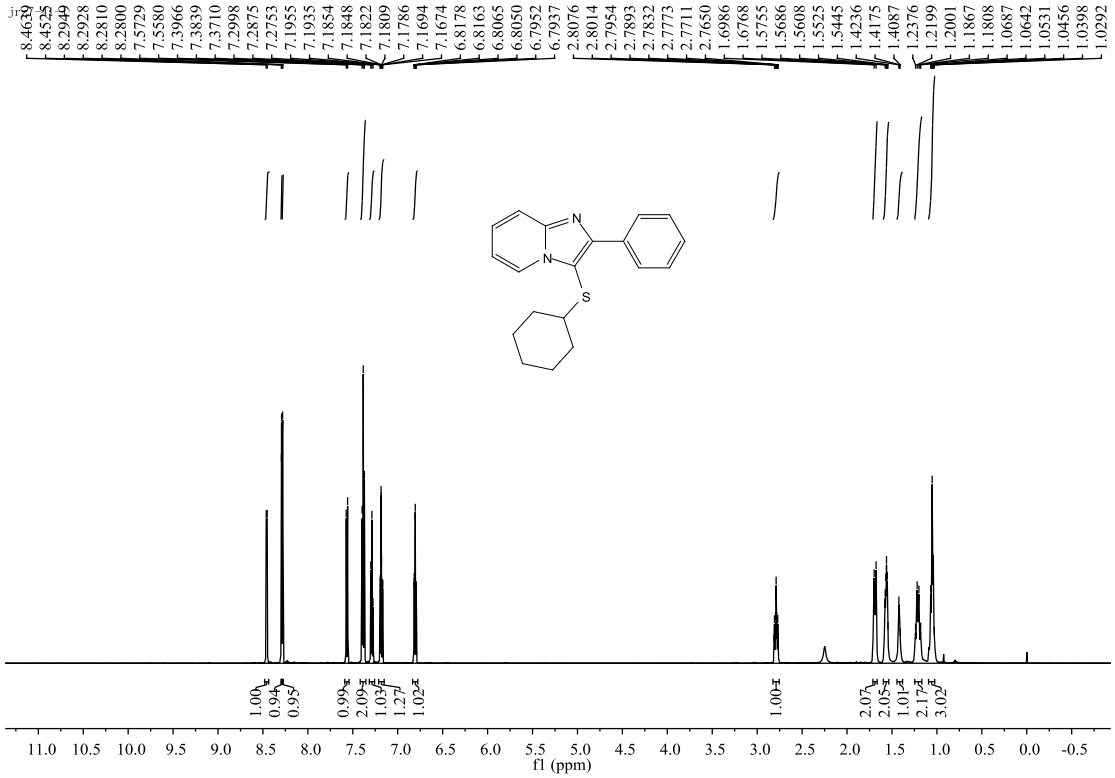



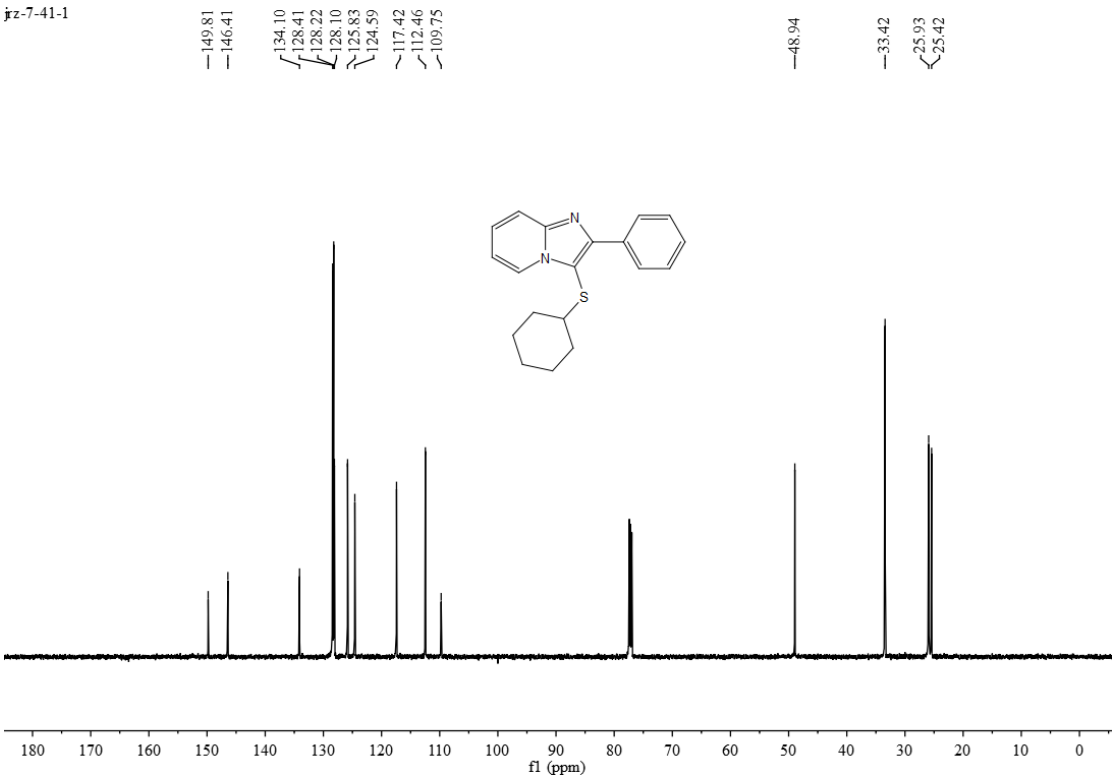
**3-(1,2-dimethoxyethylthio)-2-phenylimidazo[1,2-*a*]pyridine (21b)**



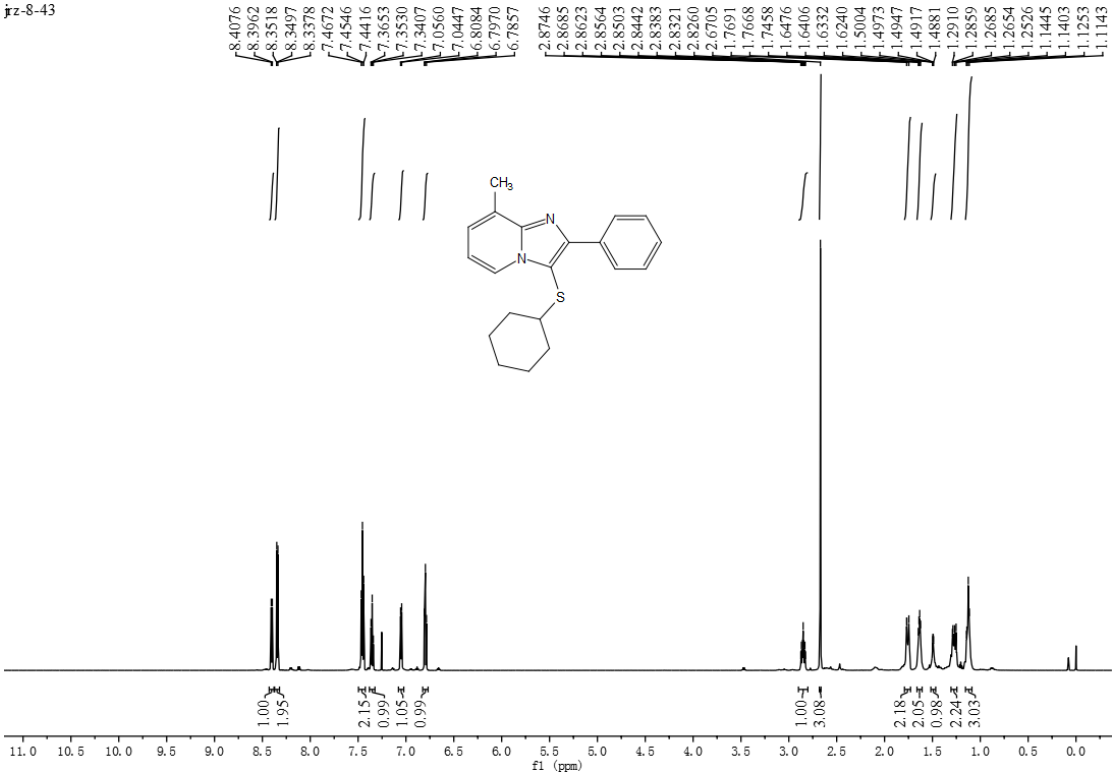



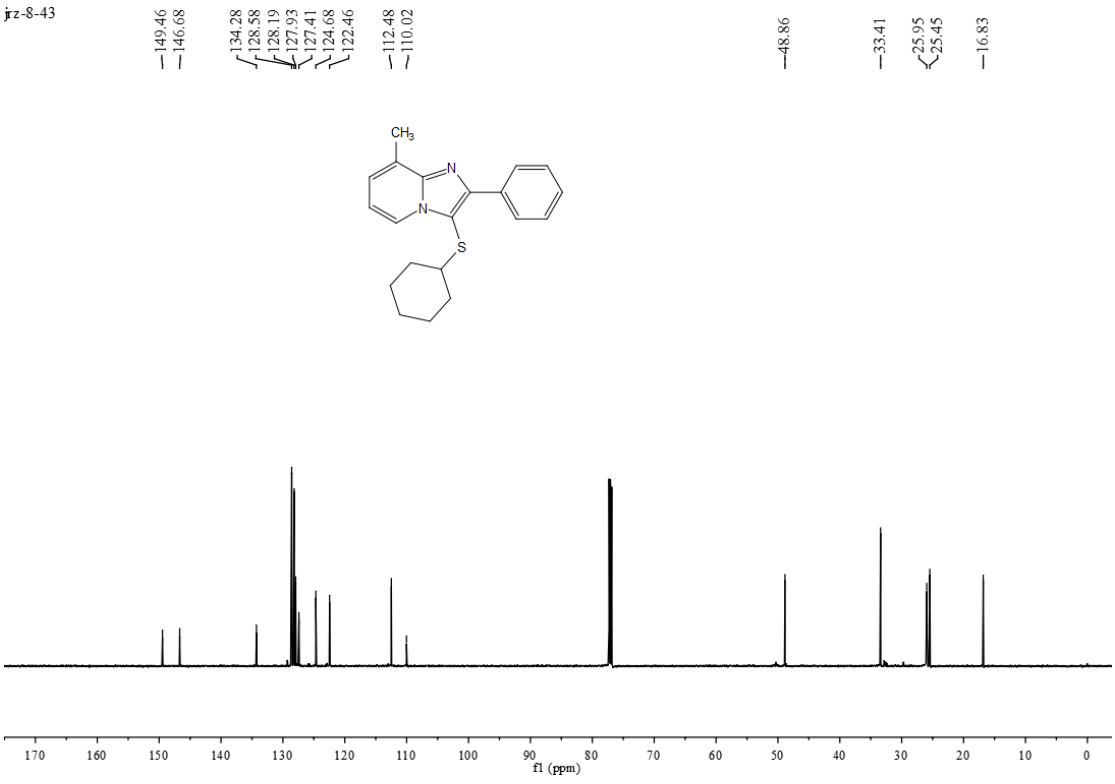
**3-(cyclohexylthio)-2-phenylimidazo[1,2-*a*]pyridine (22)**



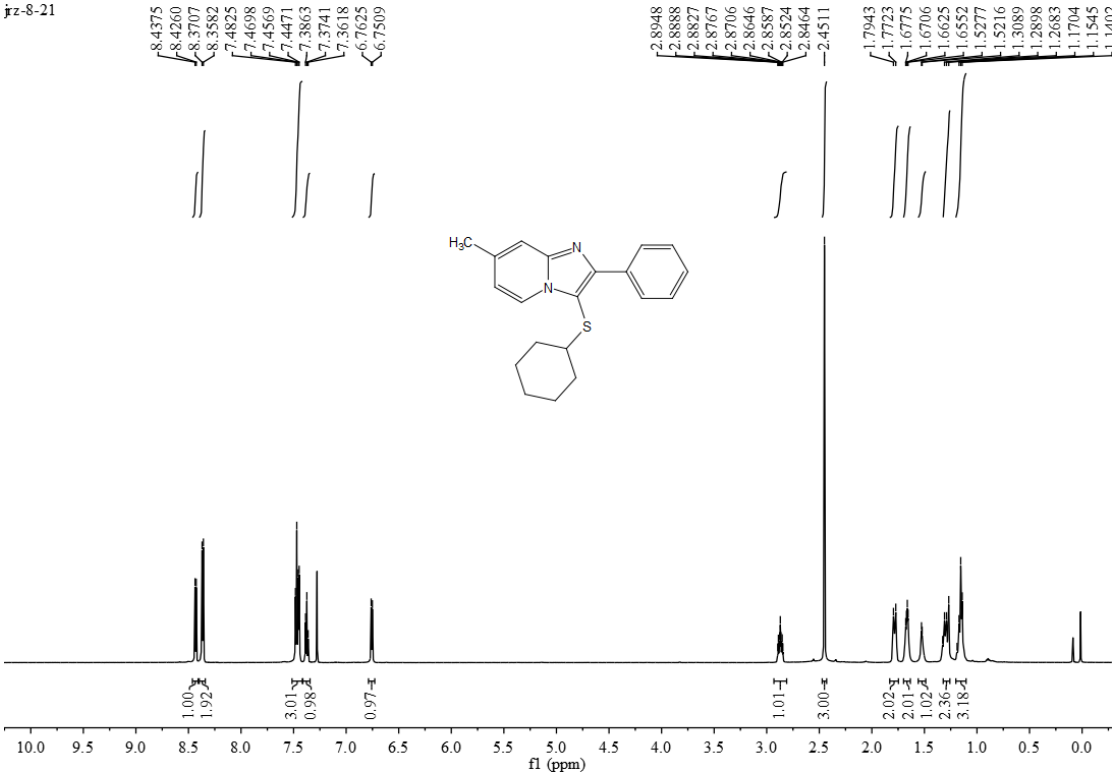



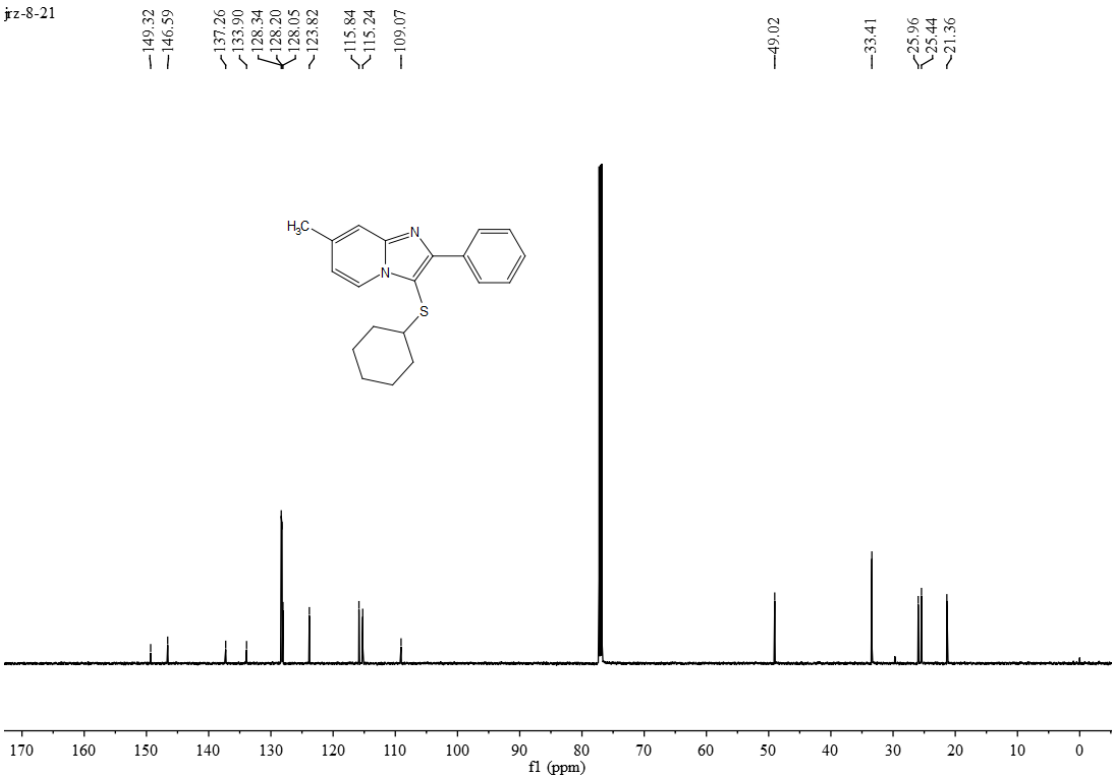
**3-(cyclohexylthio)-8-methyl-2-phenylimidazo[1,2-*a*]pyridine (23)**



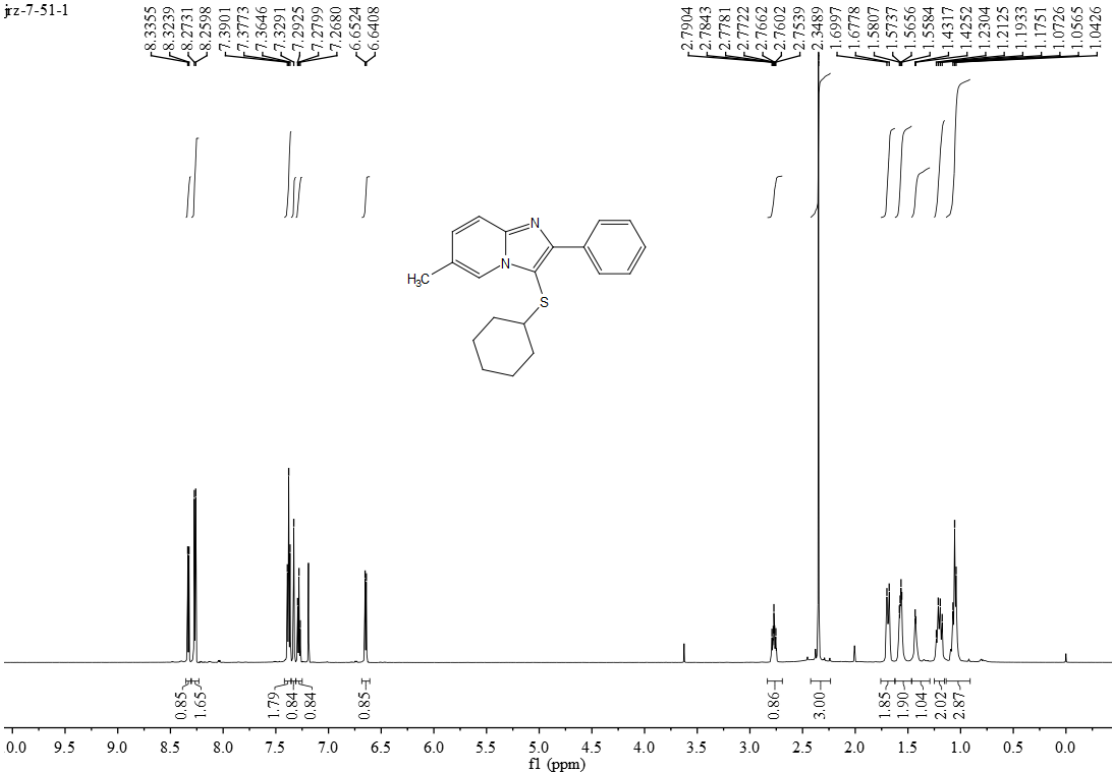



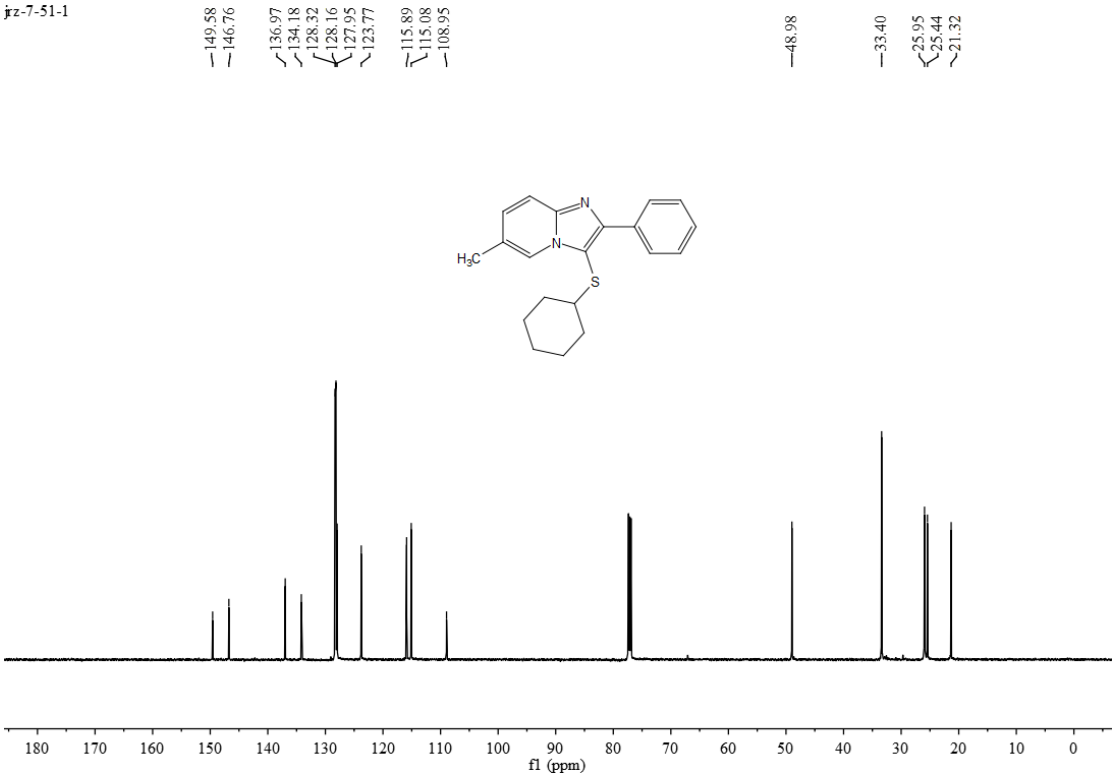
**3-(cyclohexylthio)-7-methyl-2-phenylimidazo[1,2-*a*]pyridine (24)**



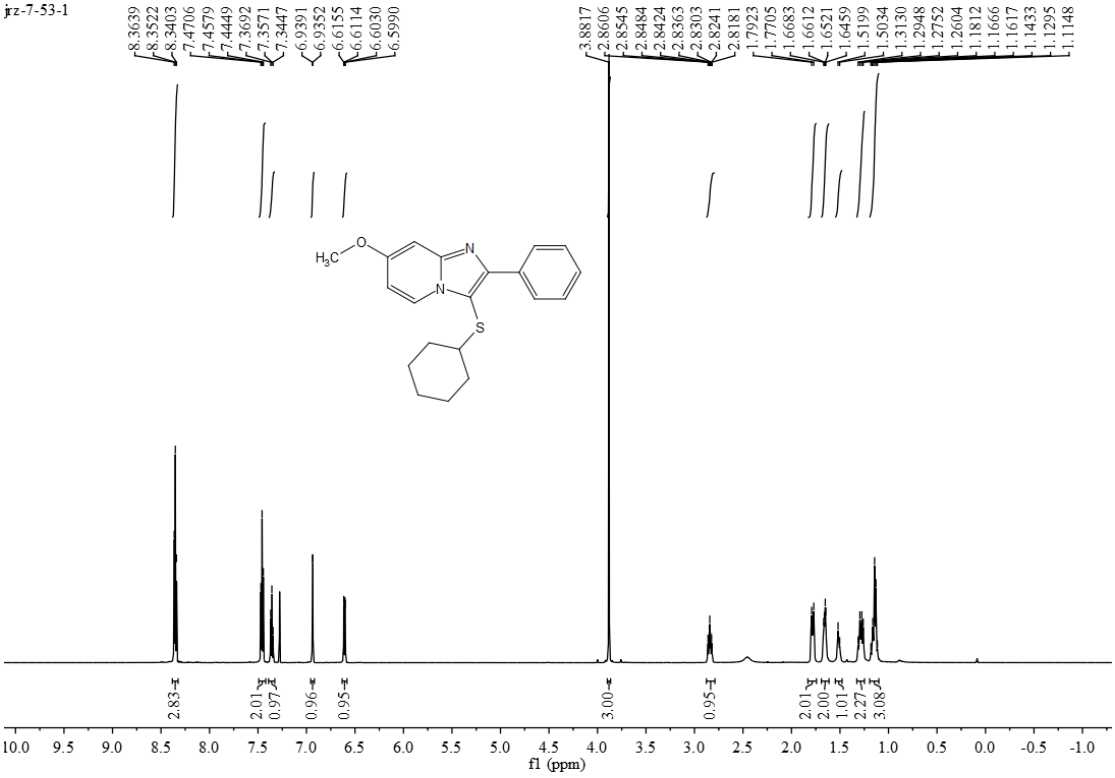



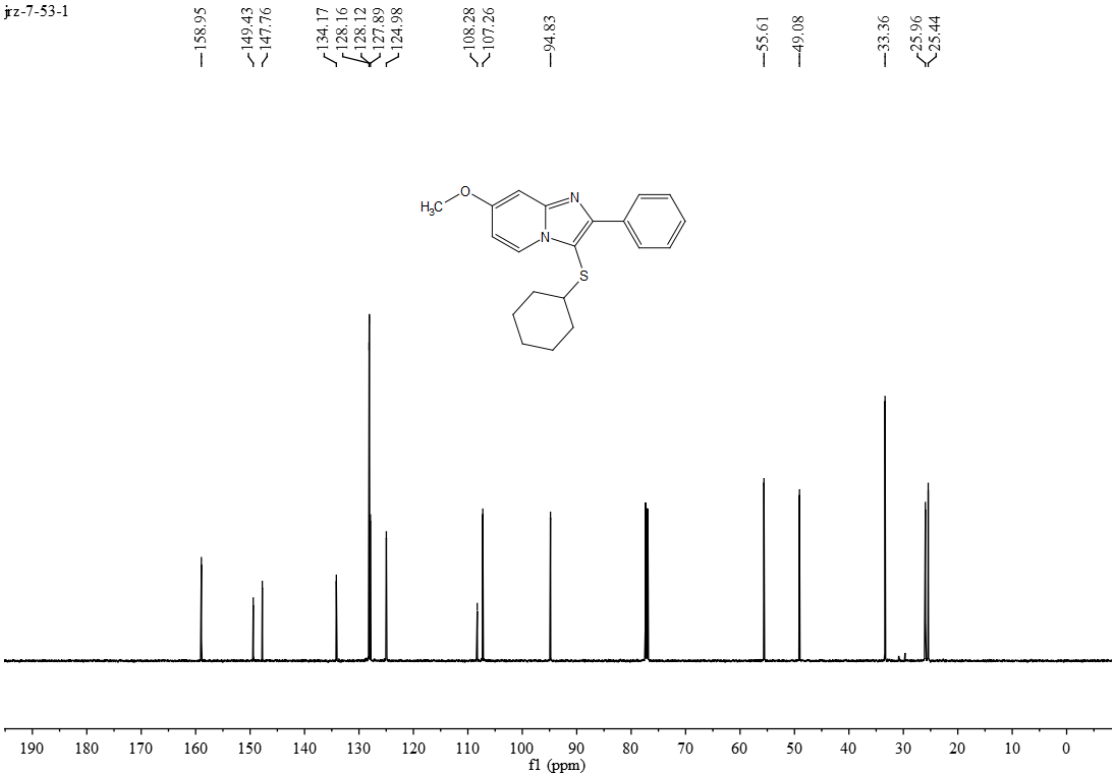
**3-(cyclohexylthio)-6-methyl-2-phenylimidazo[1,2-*a*]pyridine (25)**



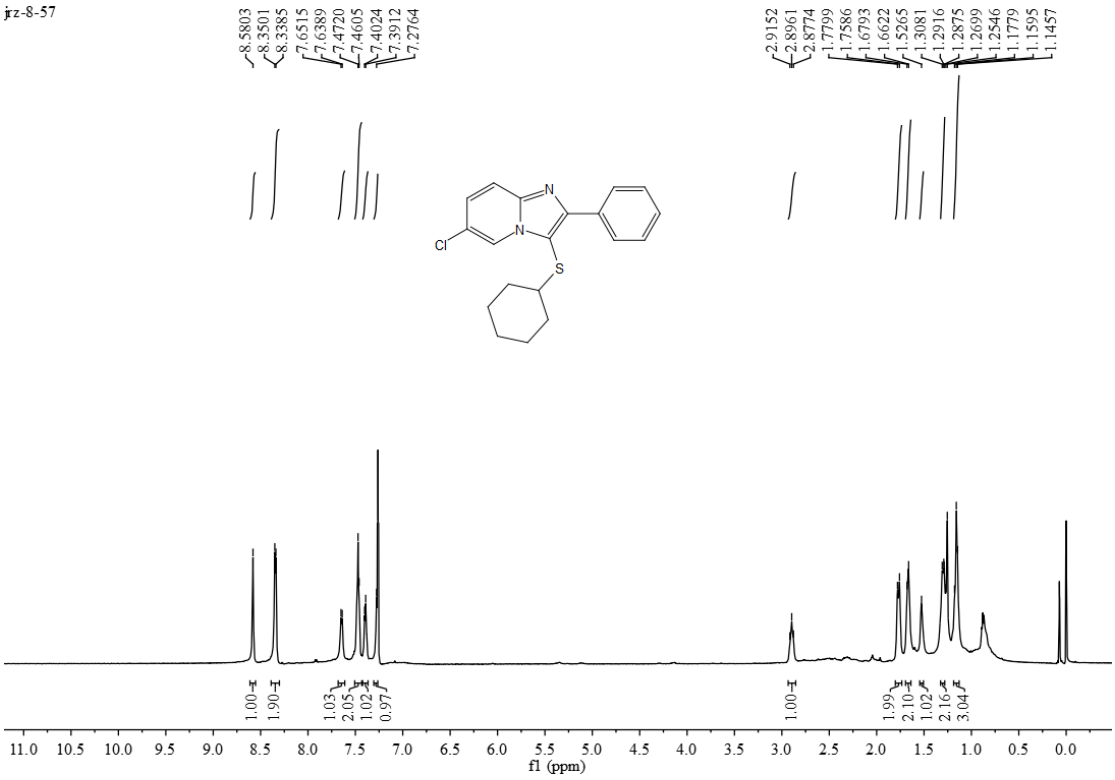



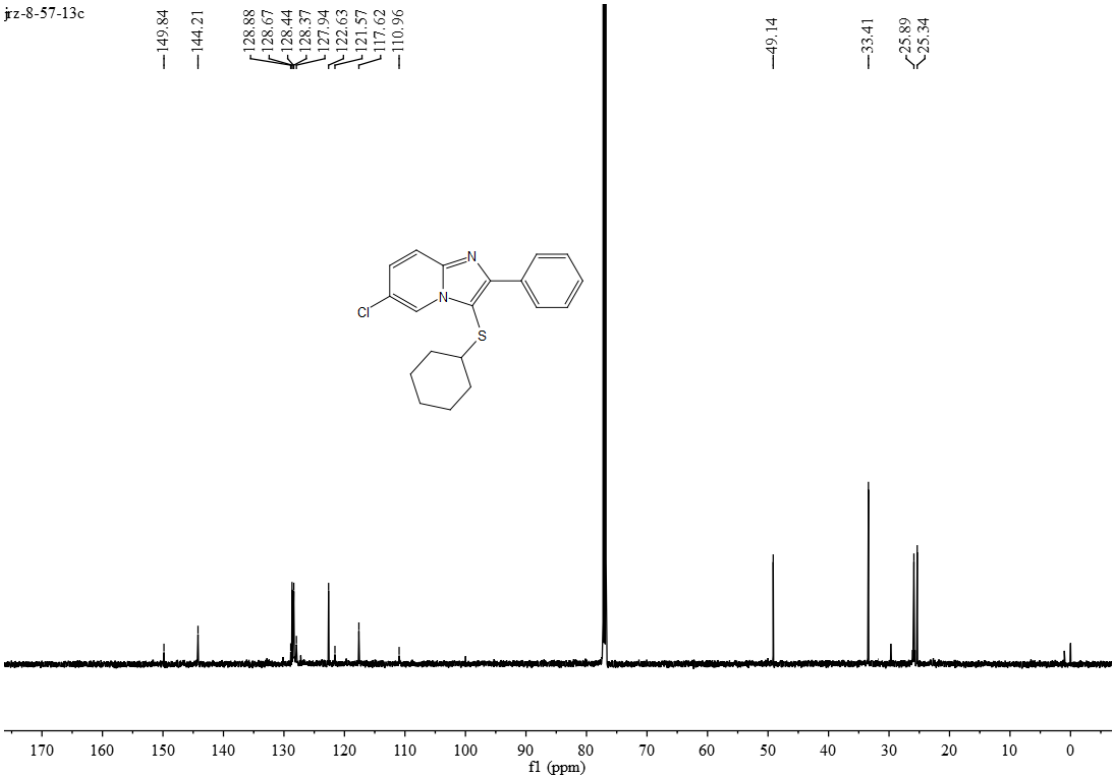
**3-(cyclohexylthio)-7-methoxy-2-phenylimidazo[1,2-*a*]pyridine (26)**



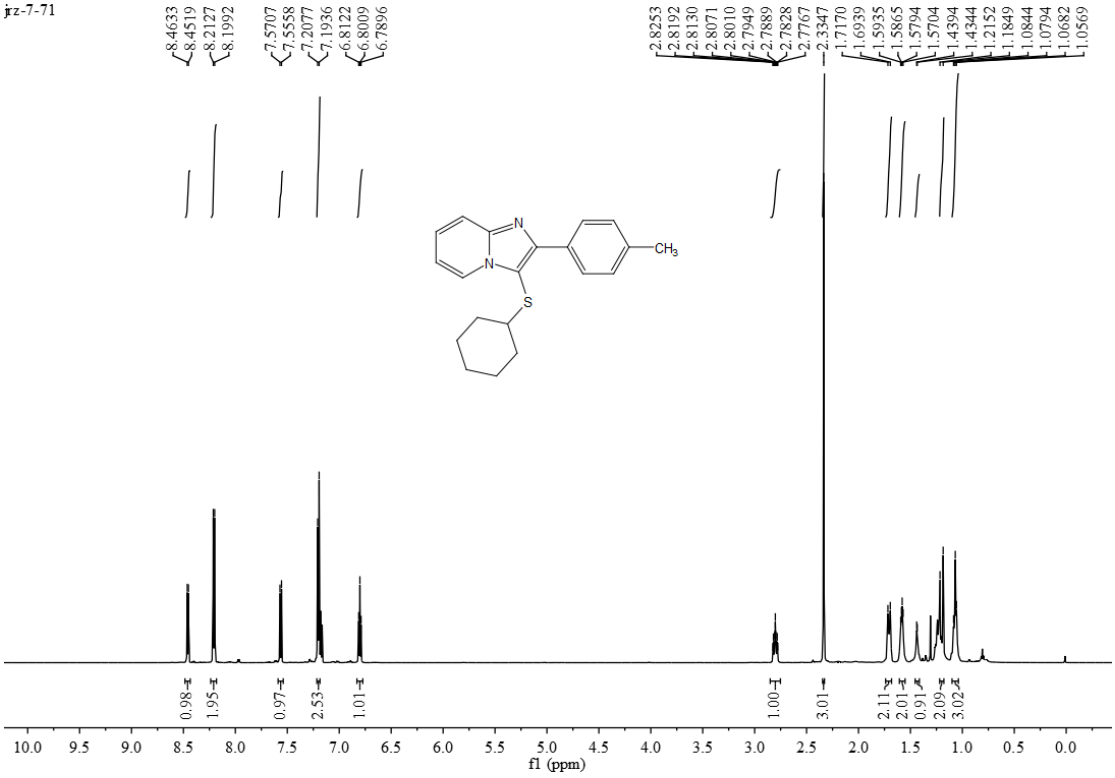



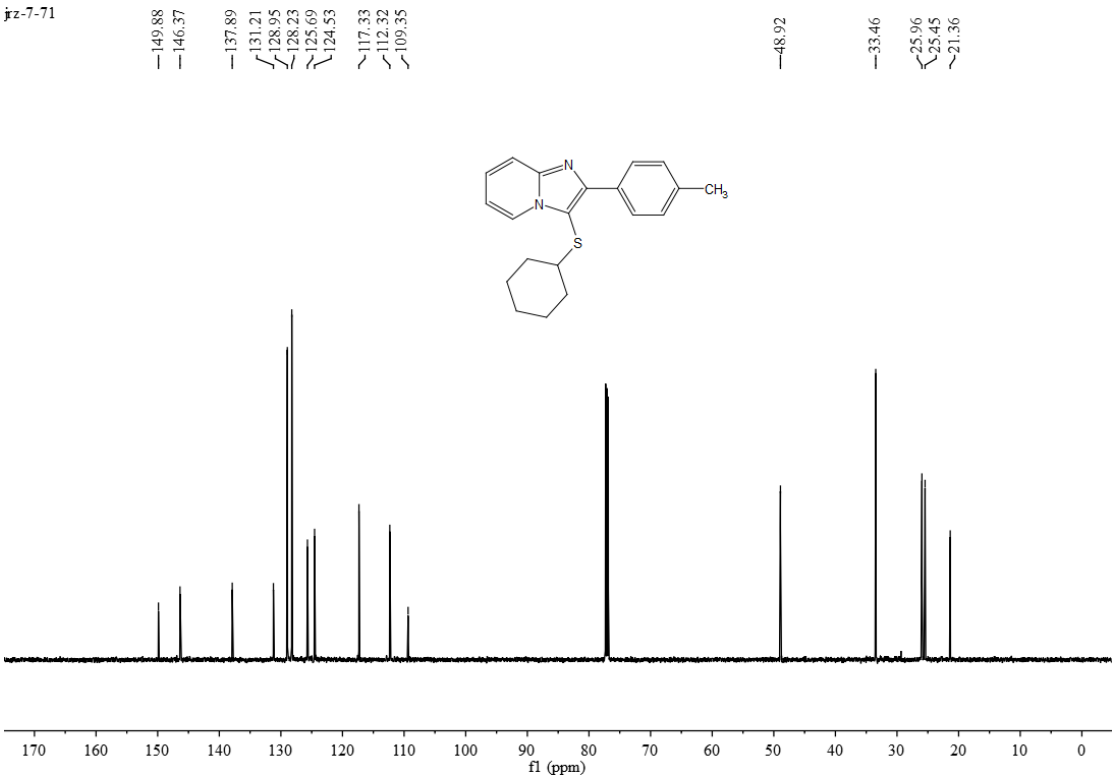
**6-chloro-3-(cyclohexylthio)-2-phenylimidazo[1,2-*a*]pyridine (27)**



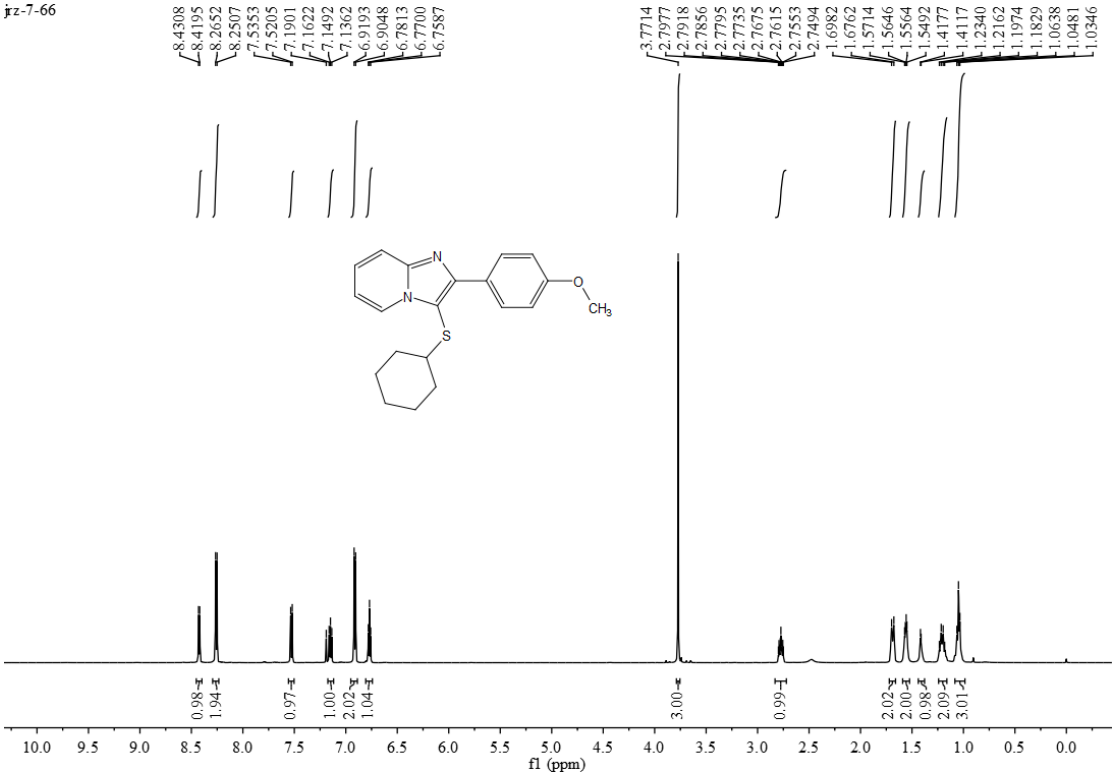



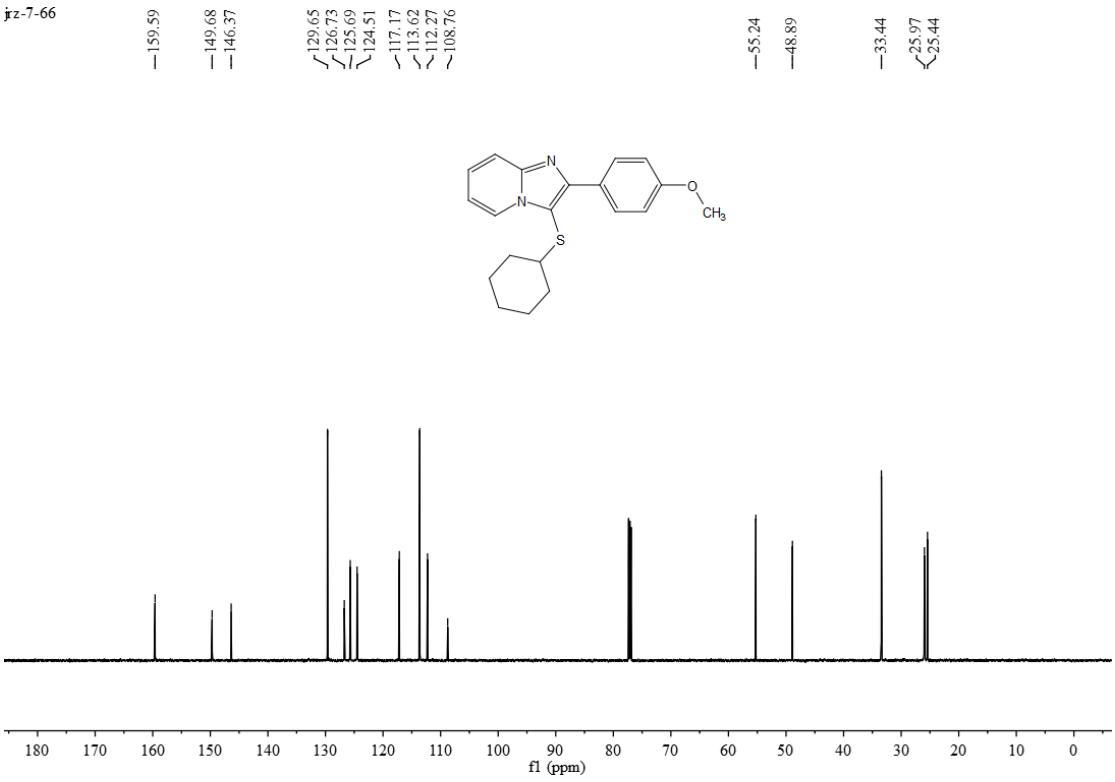
**3-(cyclohexylthio)-2-*p*-tolylimidazo[1,2-*a*]pyridine (28)**



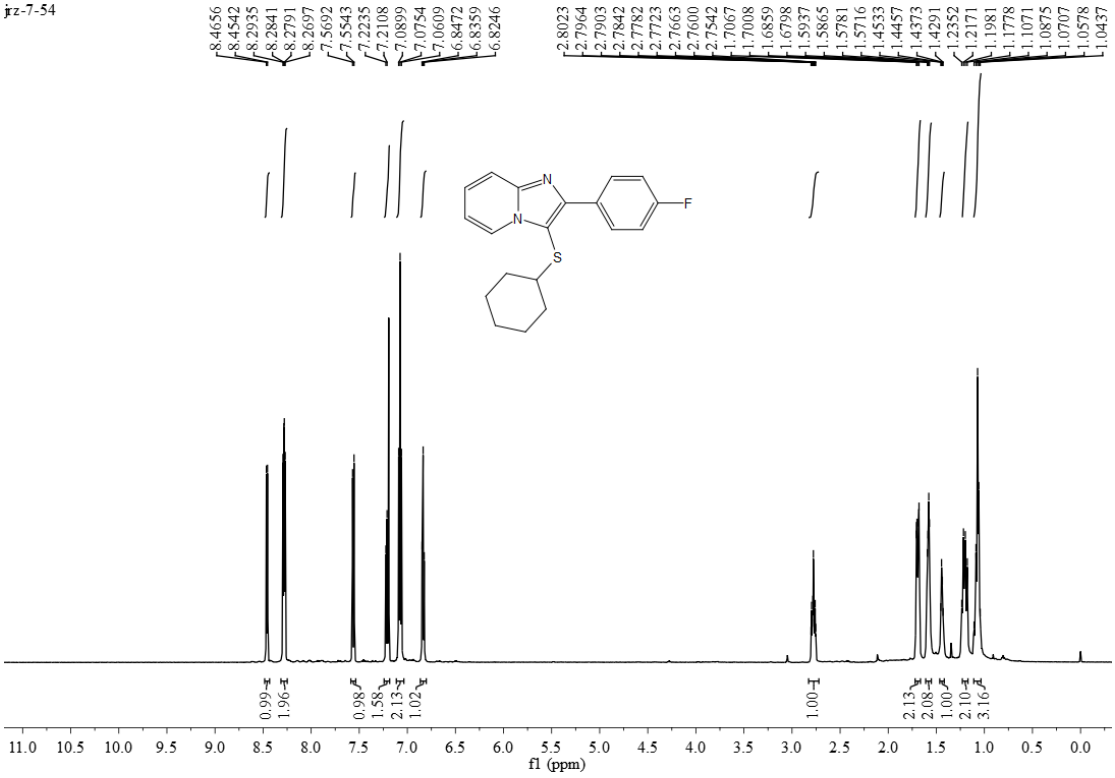



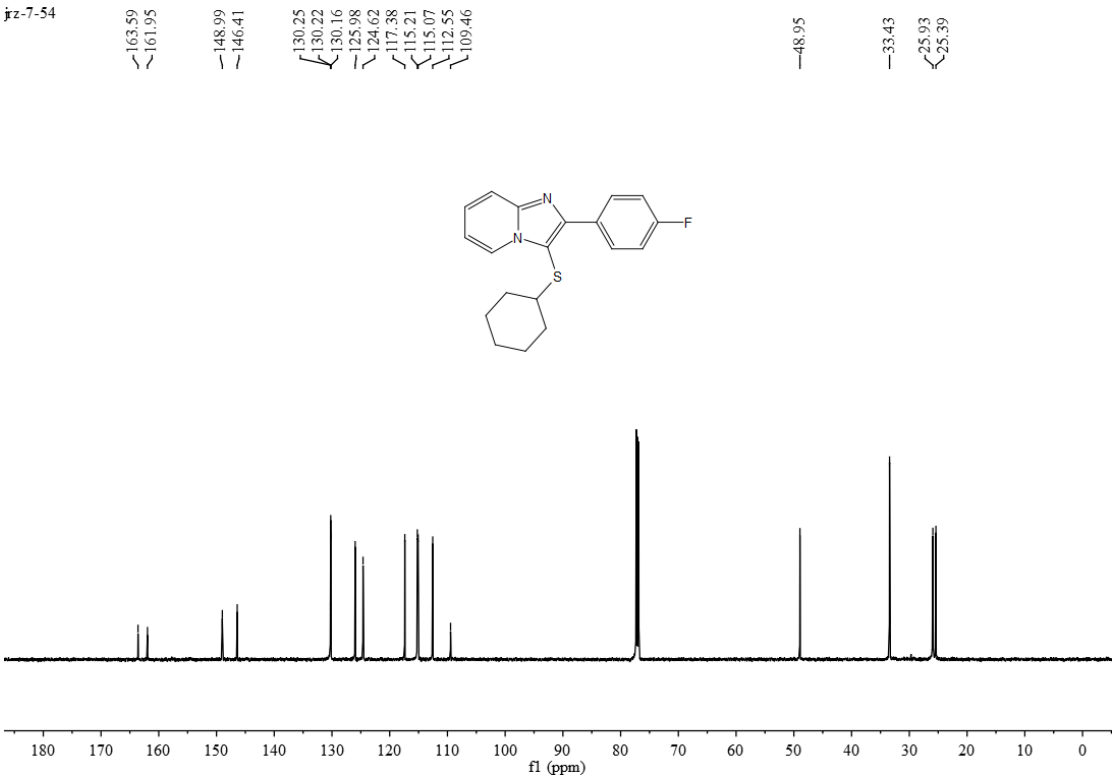
**3-(cyclohexylthio)-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyridine (29)**



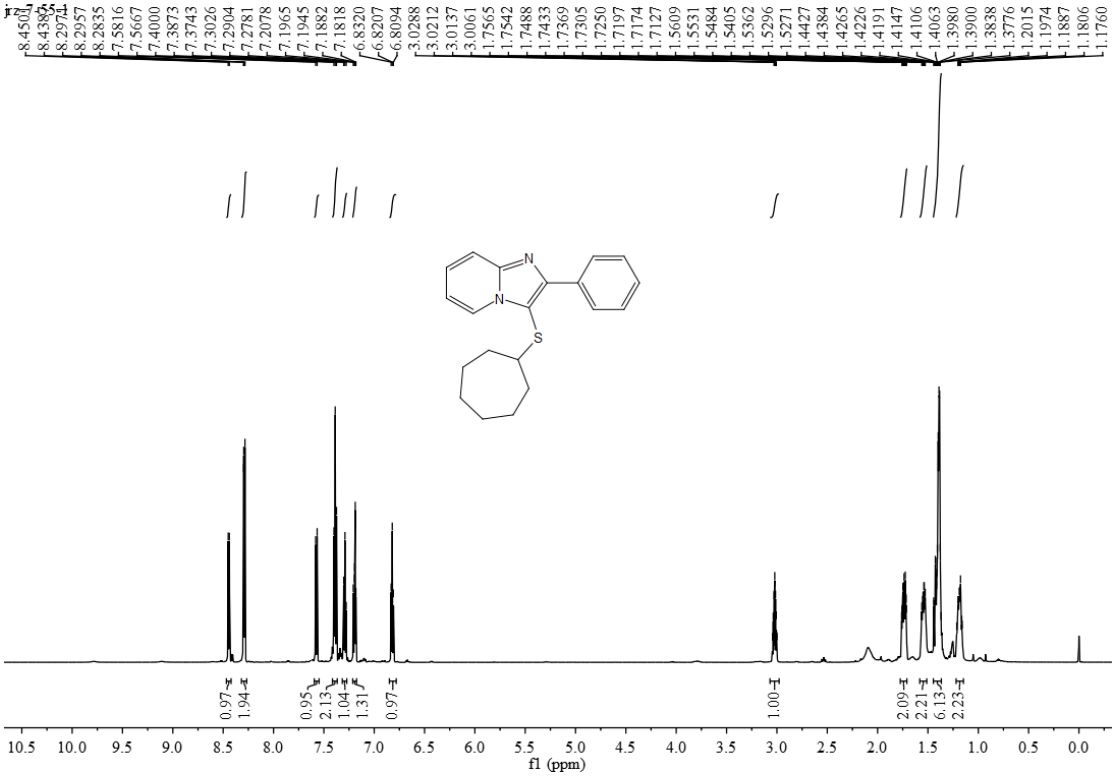



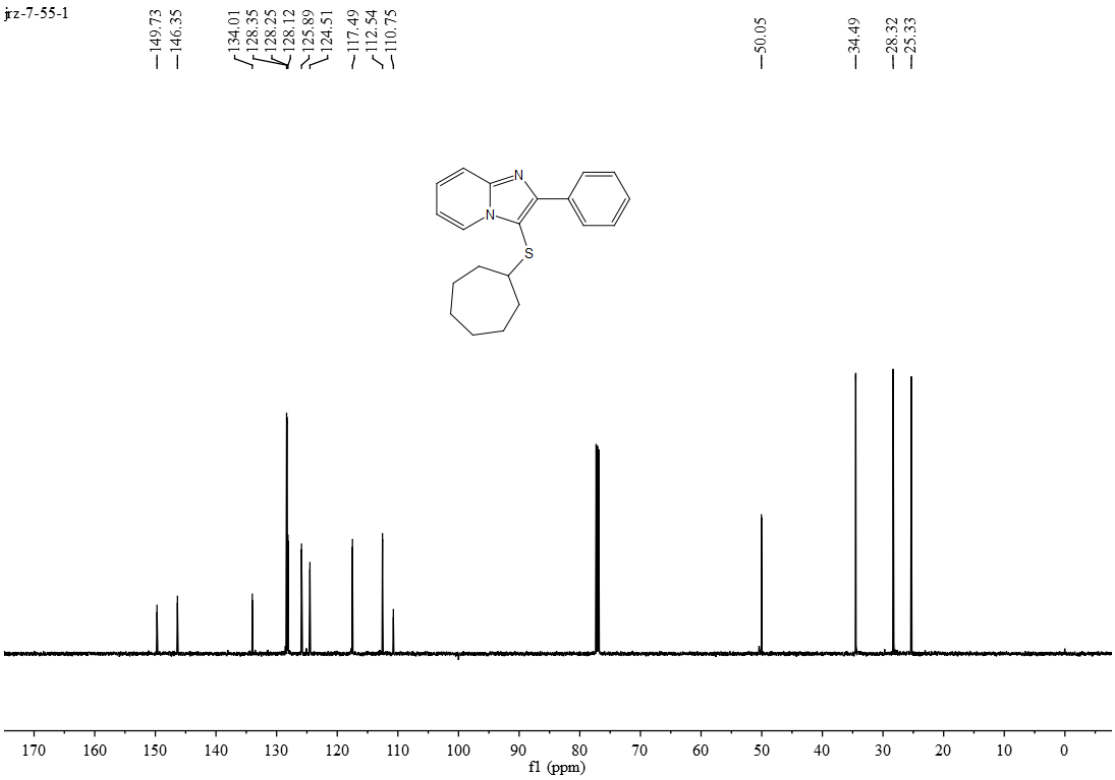
**3-(cyclohexylthio)-2-(4-fluorophenyl)imidazo[1,2-*a*]pyridine (30)**



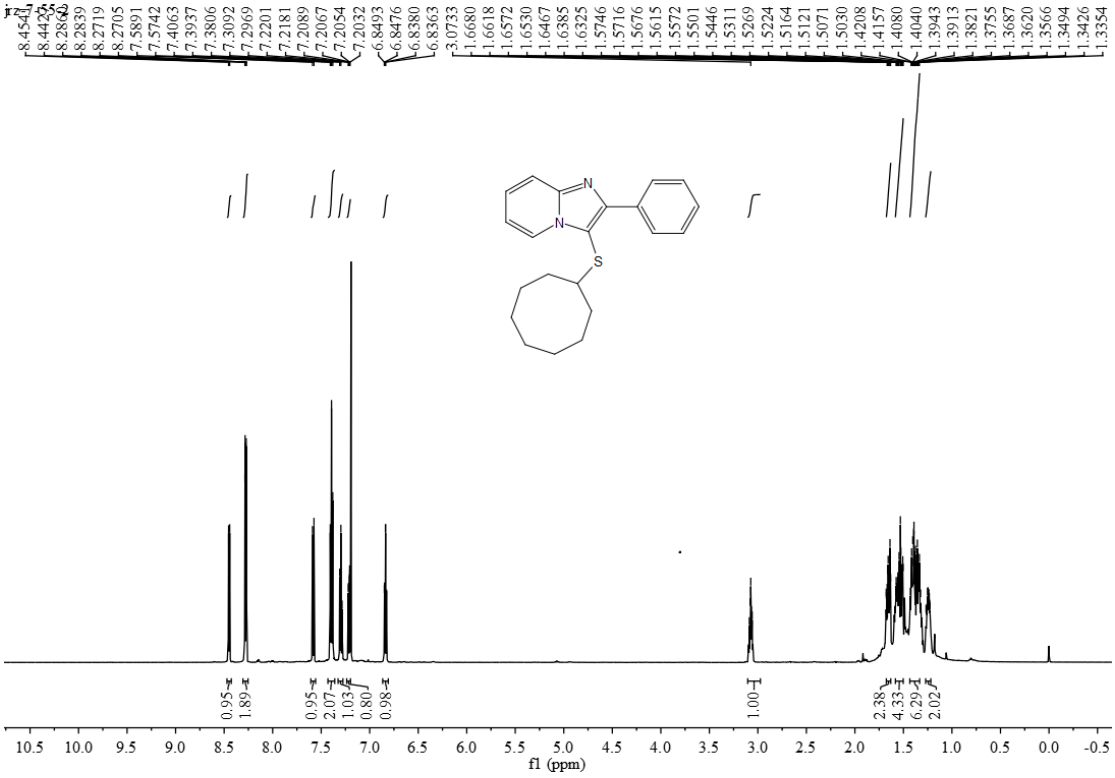



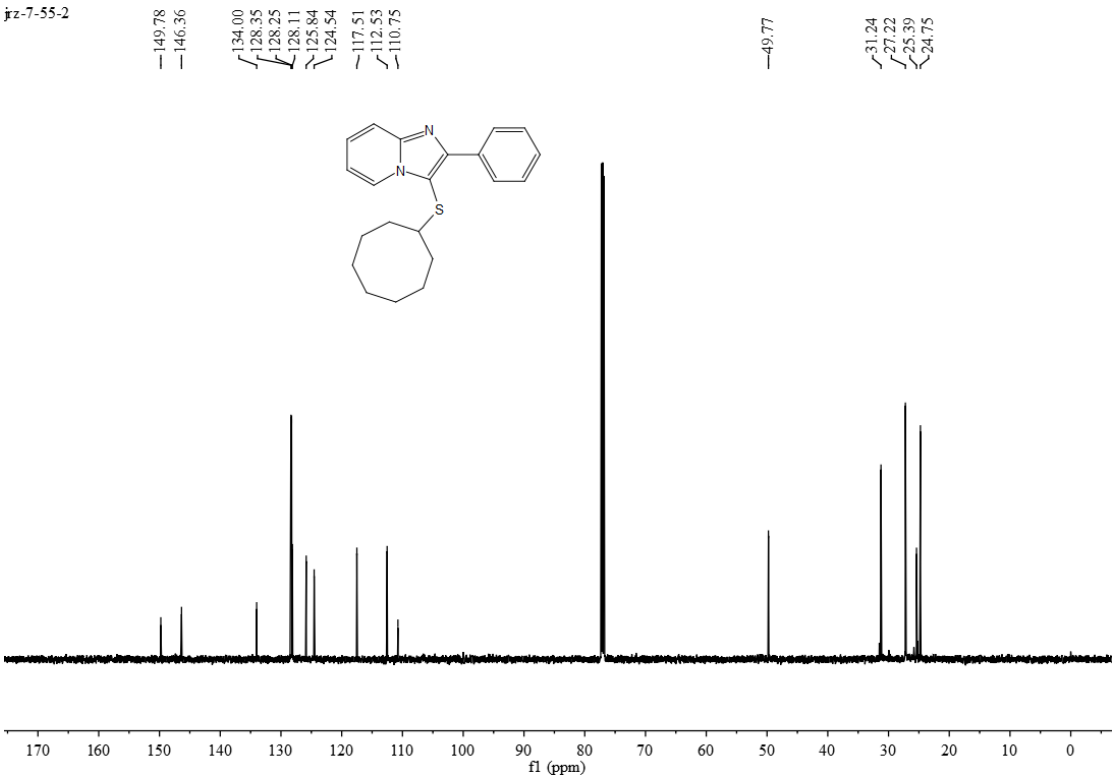
**3-(cycloheptylthio)-2-phenylimidazo[1,2-*a*]pyridine (31)**



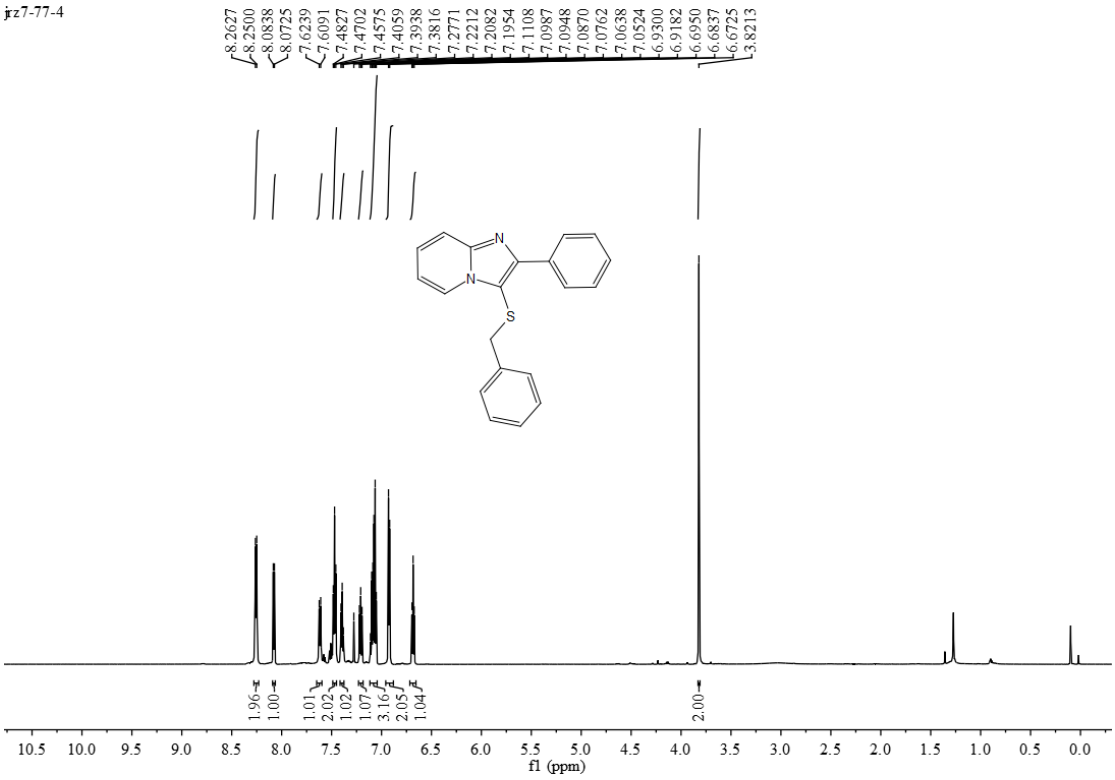



**3-(cyclooctylthio)-2-phenylimidazo[1,2-*a*]pyridine (32)**

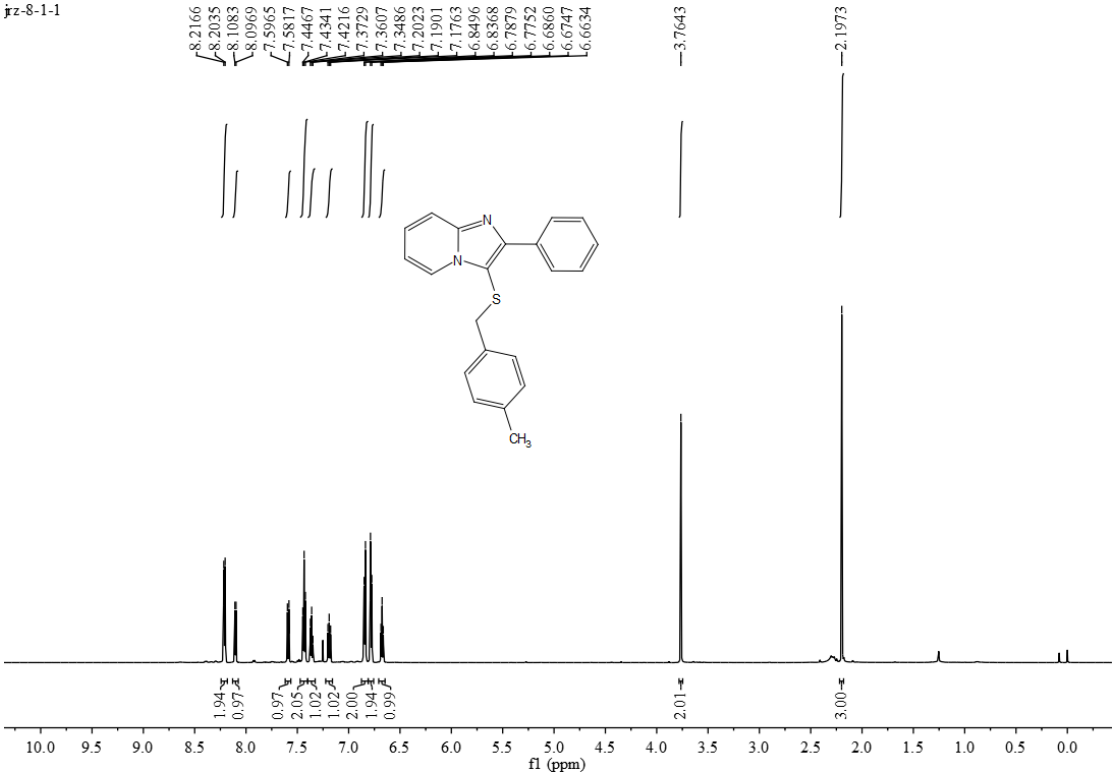


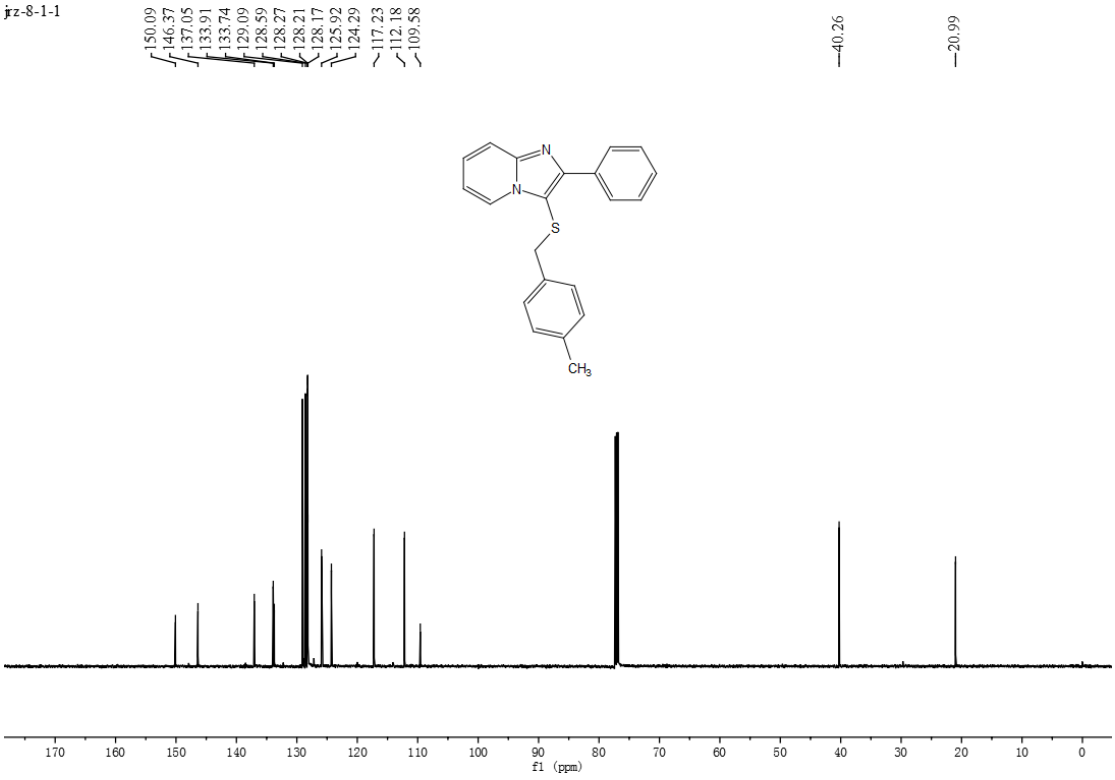



**3-(benzylthio)-2-phenylimidazo[1,2-*a*]pyridine (33)**

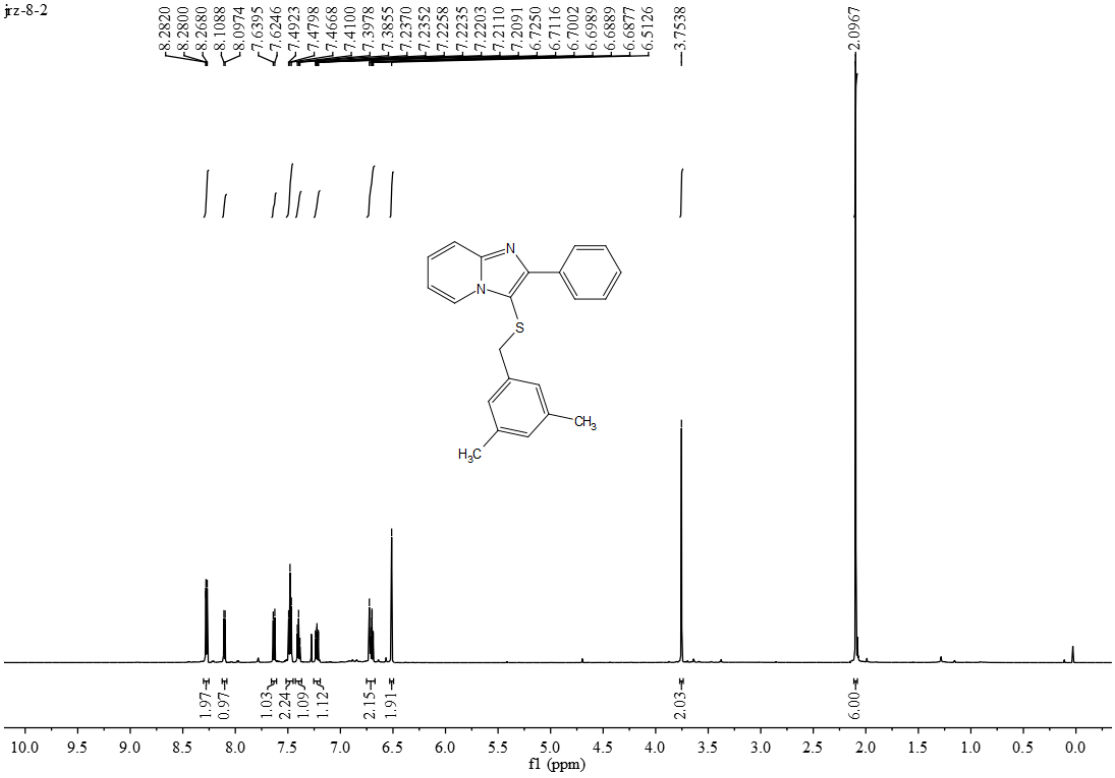


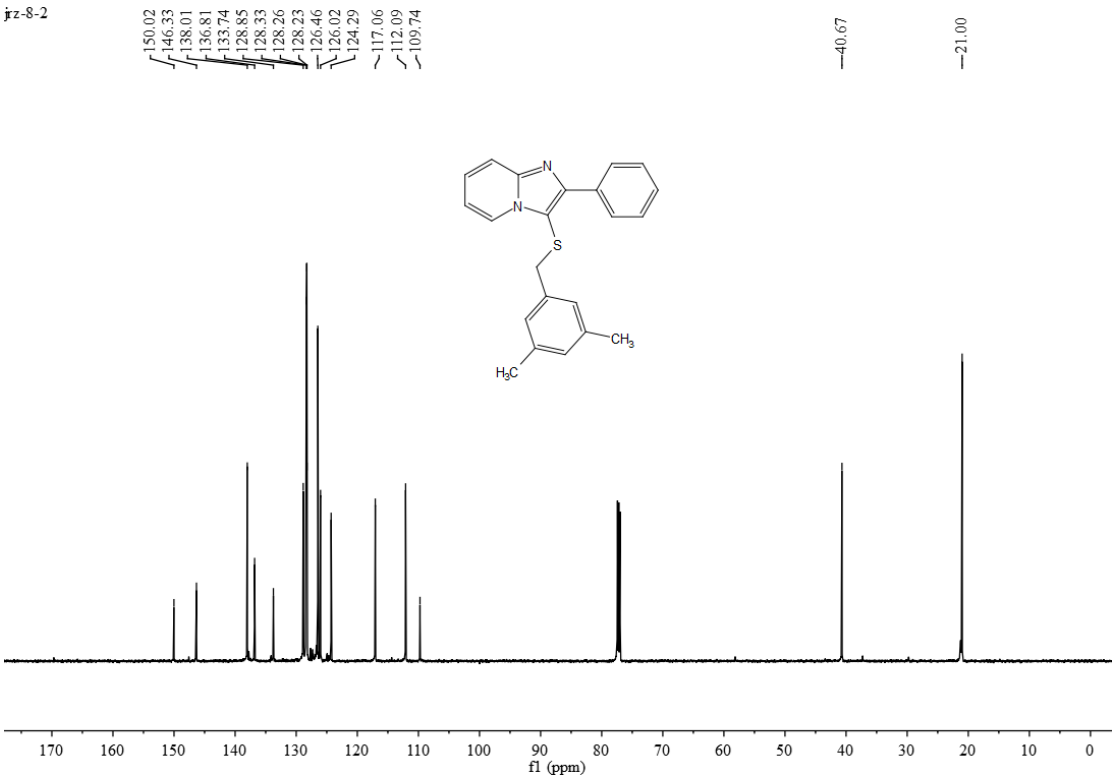
**3-(4-methylbenzylthio)-2-phenylimidazo[1,2-*a*]pyridine (34)**



**3-(3,5-dimethylbenzylthio)-2-phenylimidazo[1,2-*a*]pyridine (35)**



## 2-phenylimidazo[1,2-*a*]pyridine-3-thiol (38)