

Supplementary Information for

**Pd(0)-catalyzed Domino C-N Coupling/Hydroamination/C-H
Arylation Reactions: Efficient Synthesis and Photophysical
Properties of Azaindolo[1,2-*f*]phenanthridines**

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General information

All chemicals used are commercially available and were used without further purification. Column chromatography was performed using Merck Silicagel 60 (0.043-0.06 mm).

NMR data were recorded on a Bruker AC 250, Bruker ARX 300, Bruker ARX 500 spectrometers.

Gas chromatography-mass analysis was carried out on an AgilentHP-5890 instrument with an Agilent HP-5973 Mass Selective Detector (EI) and HP-5 capillary column using helium carrier gas. ESI HR-MS measurements were performed on an Agilent 1969A TOF mass-spectrometer. For High Resolution MS (HRMS), a Finnigan MAT95 XP was used. Only the measurements with an average deviation from the theoretical mass of $\pm 2\text{mDa}$ were accounted as correct.

Infrared Spectra were recorded on a Nicolet 550 FT – IR spectrometer with ATR sampling technique.

Absorption spectra were measured with the UV/Vis-spectrophotometer Specord 50 from Analytik Jena and the fluorescence spectra using the spectrofluorometer Fluoromax-4 of Horiba Scientific.

Experimentals

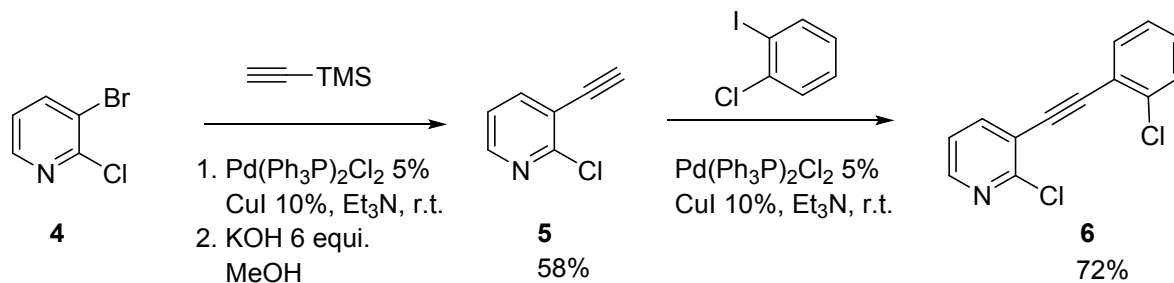
Synthesis of 3-bromo-2-(phenylethynyl)pyridine **3**:

3-bromo-2-(alkynyl)pyridines **3** were synthesized by selective Sonogashira reaction of 2,3-dibromopyridine and various terminal alkynes. Similarly, alkyne **6** was prepared from 3-bromo-2-chloropyridine **4** via three steps. Starting from **4**, alkynylation took place at position 3 because bromide is more favored than chloride in Sonogashira coupling.^{1,2,3}

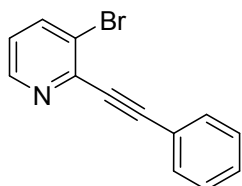
¹ Hirano, K.; Inaba, Y.; Watanabe, T.; Oishi, S.; Fujii, N.; Ohno, H. *Adv. Synth. Catal.* **2010**, *352*, 368–372.

² Jančařík, A.; Rybáček, J.; Cocq, K.; Vacek Chocholoušová, J.; Vacek, J.; Pohl, R.; Bednářová, L.; Fiedler, P.; Císařová, I.; Stará, I. G.; Starý, I. *Angew. Chem. Int. Ed. Engl.* **2013**, *52*, 9970–9975.

³ Peixoto, D.; Begouin, A.; Queiroz, M.-J. R. P. *Tetrahedron* **2012**, *68*, 7082–7094.



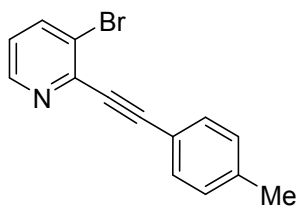
3-bromo-2-(phenylethynyl)pyridines 3a:



^1H NMR (300 MHz, CDCl_3): δ = 8.55 (dd, J = 4.7 Hz, J = 1.5 Hz, 1H), 7.92 (dd, J = 8.1 Hz, J = 1.5 Hz, 1H), 7.67 – 7.63 (m, 2H), 7.41 – 7.36 (m, 3H), 7.11 (dd, J = 8.1 Hz, $3J$ = 4.7 Hz, 1H).

^{13}C NMR (75 MHz, CDCl_3): δ = 148.4, 143.8, 139.9, 132.3 (2C), 129.5, 128.6 (2C), 123.9, 123.7, 122.1, 94.2, 87.6.

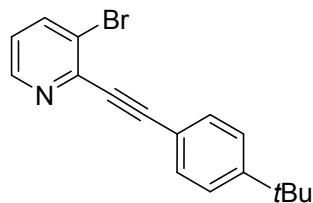
3-bromo-2-(*p*-tolylethynyl)pyridine 3b:



^1H NMR (300 MHz, CDCl_3): δ = 8.53 (dd, J = 4.7 Hz, J = 1.5 Hz, 1H), 7.91 (dd, J = 8.1 Hz, $4J$ = 1.5 Hz, 1H), 7.57 - 7.52 (m, 2H), 7.21 - 7.16 (m, 2H), 7.10 (dd, J = 8.1 Hz, J = 4.7 Hz, 1H), 2.38 (s, 3H).

^{13}C NMR (75 MHz, CDCl_3): δ = 148.3, 143.9, 139.9, 139.9, 132.2 (2C), 129.3 (2C), 123.8, 123.5, 118.9, 94.8, 87.1, 21.8.

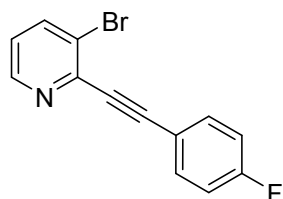
3-bromo-2-((4-(*tert*-butyl)phenyl)ethynyl)pyridine 3c:



¹H NMR (250 MHz, CDCl₃): δ = 8.54 (dd, J = 4.7 Hz, J = 1.4 Hz, 1H), 7.92 (dd, J = 8.1 Hz, J = 1.5 Hz, 1H), 7.62 - 7.56 (m, 2H), 7.43 - 7.37 (m, 2H), 7.11 (dd, J = 8.1 Hz, J = 4.7 Hz, 1H), 1.33 (s, 9H).

¹³C NMR (63 MHz, CDCl₃): δ = 153.0, 148.3, 144.0, 140.0, 132.1 (2C), 125.6 (2C), 123.9, 123.5, 119.0, 94.7, 87.1, 35.1, 31.3.

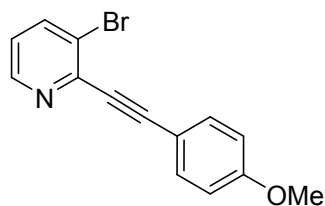
3-bromo-2-((4-fluorophenyl)ethynyl)pyridine 3d:



¹H NMR (250 MHz, CDCl₃): δ = 8.54 (dd, J = 4.7 Hz, J = 1.5 Hz, 1H), 7.92 (dd, J = 8.2 Hz, J = 1.5 Hz, 1H), 7.67 - 7.59 (m, 2H), 7.12 (dd, J = 8.2 Hz, J = 4.7 Hz, 1H), 7.11 - 7.02 (m, 2H).

¹³C NMR (63 MHz, CDCl₃): δ = 163.3 (d, J = 251.4 Hz), 148.39, 143.7, 140.0, 134.4 (d, J = 8.6 Hz), 123.9, 123.7, 118.2 (d, J = 3.6 Hz), 115.9 (d, J = 22.2 Hz), 93.2, 87.3.

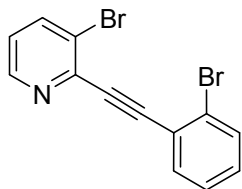
3-bromo-2-((4-methoxyphenyl)ethynyl)pyridine 3e:



¹H NMR (300 MHz, CDCl₃): δ = 8.52 (dd, J = 4.7 Hz, J = 1.4 Hz, 1H), 7.91 (dd, J = 8.1 Hz, J = 1.5 Hz, 1H), 7.62 - 7.55 (m, 2H), 7.09 (dd, J = 8.1 Hz, J = 4.7 Hz, 1H), 6.93 - 6.86 (m, 2H), 3.83 (s, 3H).

¹³C NMR (75 MHz, CDCl₃): δ = 160.7, 148.2, 144.1, 139.9, 133.9 (2C), 123.7, 123.3, 114.3 (2C), 114.1, 94.9, 86.7, 55.5.

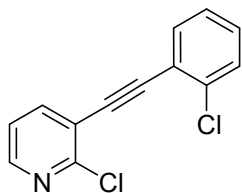
3-bromo-2-((2-bromophenyl)ethynyl)pyridine **3f**:



¹H NMR (250 MHz, CDCl₃) δ = 8.58 (dd, J = 4.7, 1.5 Hz, 1H), 7.94 (dd, J = 8.2, 1.5 Hz, 1H), 7.75 – 7.59 (m, 2H), 7.40 – 7.19 (m, 2H), 7.15 (dd, J = 8.2, 4.7 Hz, 1H).

¹³C NMR (63 MHz, CDCl₃) δ = 148.5, 143.6, 140.1, 134.4, 132.8, 130.6, 127.2, 126.0, 124.4, 124.2, 123.9, 92.1, 91.5.

2-chloro-3-((2-chlorophenyl)ethynyl)pyridine



¹H NMR (250 MHz, CDCl₃) δ = 8.39 (dd, J = 4.8, 1.9 Hz, 1H), 7.93 (dd, J = 7.7, 1.9 Hz, 1H), 7.69 – 7.58 (m, 1H), 7.54 – 7.44 (m, 1H), 7.41 – 7.22 (m, 3H).

¹³C NMR (63 MHz, CDCl₃) δ = 152.5, 148.7, 141.6, 136.4, 133.7, 130.3, 129.6, 126.7, 122.4, 122.0, 120.4, 93.6, 89.2.

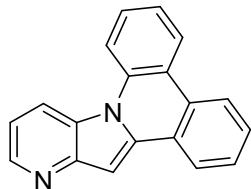
MS (EI, 70 eV): $m/z(\%)$ = 247 (M^+ , 100), 212 (37), 177 (52), 160 (5), 150 (22), 124 (13), 111 (4), 99 (10), 75 (18), 62 (6), 51 (3), 39 (2).

General procedure for synthesis of azaindolo[1,2-*f*]phenanthridines:

3-bromo-2-(phenylethynyl)pyridine **3** (0.3 mmol), 2-bromoaniline **7** (1.1 equiv., 0.33 mmol), Pd(Ph₃P)₄ (10 mol%, 0.03 mmol), Xantphos (10 mol%, 0.03 mmol), and Cs₂CO₃ (3 equiv., 0.9 mmol) were placed in a dried pressure tube equipped with a septum. Then dried and degassed DMF (4 mL) was added under argon. The reaction was back-filled with argon three times and the septum was replaced with a Teflon cap. The reaction mixture was allowed to stir at 120 °C for 24 h. Then the reaction mixture was cooled to room temperature and was filtered through a

pad of Celite. The filtrate was dried under reduced pressure, and the product **3** was obtained after flash chromatography on a silica gel column with ethyl acetate.

Pyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine **8aa**



Yellowish solid, 86%. M.p.: 144 - 145 °C.

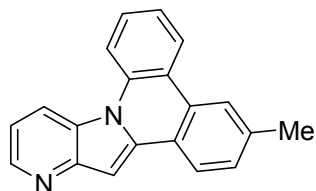
¹H NMR (300 MHz, CDCl₃) δ = 8.62 (dd, *J* = 4.6, 1.0 Hz, 1H), 8.50 (d, *J* = 8.6 Hz, 1H), 8.35 – 8.17 (m, 2H), 8.17 – 7.90 (m, 2H), 7.53 – 7.43 (m, 3H), 7.39 – 7.09 (m, 3H).

¹³C NMR (63 MHz, CDCl₃) δ = 147.6, 144.9, 138.3, 135.2, 129.0, 128.9, 128.5, 127.0, 126.9, 125.2, 124.9, 124.3, 123.7, 122.4, 121.9, 121.3, 116.2, 116.0, 96.8.

IR (ATR, cm⁻¹): = 3123 (w), 3099 (w), 3062 (w), 3034 (w), 1887 (w), 1598 (m), 1580 (w), 1556 (s), 1503 (w), 1488 (w), 1479 (m), 1453 (m), 1440 (s), 1414 (s), 1401 (w), 1378 (m), 1356 (m), 1325 (w), 1311 (w), 1303 (w), 1279 (m), 1236 (m), 1186 (m), 1138 (w), 1127 (w), 1110 (w), 1073 (w), 1051 (w), 1042 (w), 973 (w), 954 (w), 943 (w), 923 (w), 908 (w), 877 (w), 862 (w), 833 (w), 805 (w), 774 (w), 745 (s), 731 (w), 708 (m), 666 (w), 640 (w), 617 (m), 608 (w), 584 (w), 574 (w), 556 (w), 537 (w).

MS (EI, 70 eV): *m/z*(%) = 268 (M⁺, 100), 240 (7), 214 (3), 134 (10), 120 (13), 106 (5). **HRMS (EI):** Calculated for C₁₉H₁₂N₂ (M⁺): 268.09950, found: 268.09952.

3-methylpyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine **8ba**



Yellowish solid, 61%. M.p.: 162 - 164 °C.

¹H NMR (300 MHz, CDCl₃) δ = 8.72 – 8.54 (m, 1H), 8.50 – 8.36 (m, 1H), 8.19 (dd, *J* = 10.5, 5.7 Hz, 2H), 7.95 – 7.78 (m, 2H), 7.54 – 7.36 (m, 1H), 7.34 – 7.09 (m, 4H), 2.45 (s, 3H).

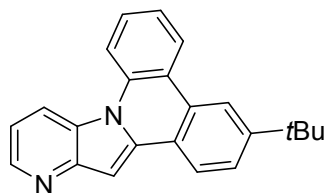
^{13}C NMR (75 MHz, CDCl_3) δ = 147.9, 144.8, 138.8, 138.5, 135.3, 129.7, 128.8, 126.8, 124.8, 124.1, 123.5, 122.6, 122.5, 121.9, 121.0, 115.9, 115.8, 96.1, 22.0. (one signal of C tertiary could not be detected).

IR(ATR, cm^{-1}): = 3120 (w), 3093 (w), 3061 (w), 3032 (w), 2917 (w), 2851 (w), 1914 (w), 1883 (w), 1613 (w), 1598 (m), 1575 (w), 1557 (m), 1550 (w), 1493 (w), 1481 (w), 1444 (s), 1414 (s), 1375 (m), 1349 (m), 1306 (m), 1283 (m), 1238 (m), 1208 (w), 1189 (m), 1164 (w), 1149 (w), 1127 (w), 1115 (w), 1079 (m), 1039 (m), 956 (m), 943 (w), 923 (m), 913 (w), 903 (w), 873 (m), 834 (w), 810 (s), 772 (m), 755 (s), 734 (s), 714 (w), 660 (w), 651 (w), 623 (m), 610 (m), 578 (s), 545 (w), 532 (s).

MS (EI, 70 eV): m/z (%) = 282 (M^+ , 100), 266 (4), 140 (10), 128 (2), 126 (5).

HR-MS (EI): calculated for $\text{C}_{20}\text{H}_{14}\text{N}_2$ (M^+): 282.11515, found: 282.11477.

3-(*tert*-butyl)pyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine 8ca



Yellowish solid, 69%. M.p.: 176 – 178 °C.

^1H NMR (300 MHz, CDCl_3) δ = 8.63 (d, J = 4.1 Hz, 1H), 8.53 (d, J = 8.6 Hz, 1H), 8.41 – 8.29 (m, 2H), 8.24 (d, J = 1.7 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.64 – 7.48 (m, 2H), 7.42 – 7.32 (m, 2H), 7.22 (dd, J = 8.5, 4.6 Hz, 1H), 1.47 (s, 9H).

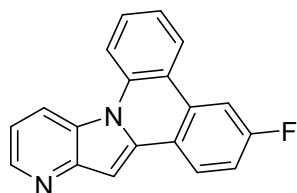
^{13}C NMR (75 MHz, CDCl_3) δ = 152.1, 148.0, 144.9, 138.5, 135.5, 128.9, 127.0, 126.6, 126.5, 124.9, 124.2, 123.6, 122.8, 122.4, 121.1, 118.7, 116.1, 116.0, 96.3, 35.4, 31.4 (3C).

IR (ATR, cm^{-1}): = 3060 (w), 3025 (w), 2947 (m), 2902 (w), 2860 (w), 1931 (w), 1884 (w), 1732 (w), 1615 (w), 1598 (m), 1578 (w), 1557 (m), 1504 (w), 1494 (m), 1479 (w), 1463 (w), 1443 (s), 1413 (s), 1392 (w), 1357 (w), 1348 (m), 1303 (w), 1275 (m), 1265 (m), 1242 (w), 1205 (w), 1187 (m), 1162 (w), 28 1151 (w), 1127 (w), 1115 (w), 1097 (w), 1070 (w), 1053 (w), 1039 (w), 1021 (w), 970 (w), 956 (m), 925 (w), 913 (w), 875 (m), 832 (w), 813 (m), 788 (s), 769 (m), 756 (s), 738 (s), 710 (w), 657 (w), 648 (w), 623 (s), 608 (w), 584 (m), 542 (s).

MS (EI, 70 eV): $m/z(\%) = 324 (M^+, 100), 309 (98), 294 (28), 290 (4), 281 (12), 268 (15), 240 (4), 154 (4), 146 (4), 140 (24), 132 (6), 126 (4), 41 (3), 39 (3).$

HR-MS (EI): calculated for $C_{23}H_{20}N_2 (M^+)$: 324.16210, found: 324.16196.

3-fluoropyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine 8da



Yellowish solid, 88%. M.p.: 213 - 215 °C.

1H NMR (300 MHz, $CDCl_3$) $\delta = 8.61$ (d, $J = 3.6$ Hz, 1H), 8.41 (d, $J = 8.6$ Hz, 1H), $8.23 - 8.11$ (m, 1H), 8.02 (dd, $J = 8.1, 1.3$ Hz, 1H), 7.95 (dd, $J = 8.8, 5.7$ Hz, 1H), 7.66 (dd, $J = 10.6, 2.5$ Hz, 1H), $7.55 - 7.45$ (m, 1H), $7.32 - 7.23$ (m, 2H), $7.23 - 7.08$ (m, 3H).

^{19}F NMR (63 MHz, $CDCl_3$) $\delta = 110.77$ Hz.

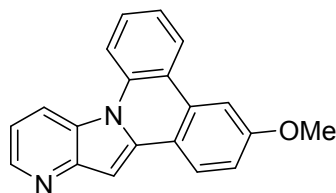
^{13}C NMR (63 MHz, $CDCl_3$) $\delta = 163.1$ (d, $J = 248.2$ Hz), 147.7, 145.1, 137.5, 135.5, 129.7, 129.1 (d, $J = 8.4$ Hz), 127.2 (d, $J = 8.9$ Hz), 126.8, 124.4, 123.7, 121.5 (d, $J = 2.5$ Hz), 121.1, 121.1, 116.5 (d, $J = 23.2$ Hz), 116.2, 116.0, 108.5 (d, $J = 23.4$ Hz), 96.5 (d, $J = 1.3$ Hz).

IR (ATR, cm^{-1}): = 3059 (w), 3035 (w), 1616 (m), 1603 (m), 1580 (w), 1558 (m), 1551 (m), 1489 (m), 1443 (s), 1416 (s), 1379 (w), 1349 (m), 1331 (w), 1304 (w), 1272 (m), 1245 (w), 1236 (w), 1180 (s), 1135 (w), 1128 (w), 1106 (w), 1072 (w), 1054 (w), 1032 (w), 957 (m), 933 (w), 915 (w), 892 (m), 854 (w), 819 (w), 810 (m), 784 (w), 763 (s), 755 (m), 733 (s), 706 (w), 652 (m), 631 (m), 621 (m), 606 (w), 599 (m), 583 (w), 545 (w), 533 (m).

MS (EI, 70 eV): $m/z(\%) = 286 (M^+, 100), 258 (7), 232 (3), 195 (2), 143 (10), 129 (11), 115 (3).$

HR-MS (EI): calculated for $C_{19}H_{11}N_2F_1 (M^+)$: 286.09008, found: 286.08980.

3-methoxypyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine 8ea



Yellowish solid, 85%. M.p.: 200 – 201 °C.

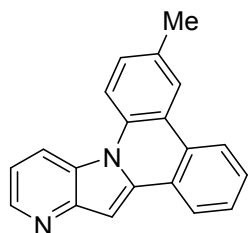
¹H NMR (300 MHz, CDCl₃) δ = 8.49 (d, *J* = 4.2 Hz, 1H), 8.31 (d, *J* = 8.5 Hz, 1H), 8.08 (d, *J* = 8.1 Hz, 1H), 7.98 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.79 (d, *J* = 8.8 Hz, 1H), 7.44 – 7.29 (m, 2H), 7.22 – 7.12 (m, 1H), 7.07 (dd, *J* = 8.5, 4.6 Hz, 1H), 7.02 (s, 1H), 6.90 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.79 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ = 160.2, 148.0, 144.7, 138.6, 135.5, 129.1, 128.5, 126.8, 126.6, 124.2, 123.5, 121.7, 120.9, 118.6, 116.3, 116.0, 115.6, 105.6, 95.2, 55.5.

IR (ATR, cm⁻¹): = 3089 (w), 3032 (w), 2999 (w), 2958 (w), 2930 (w), 2908 (w), 2831 (w), 1609 (s), 1601 (s), 1550 (s), 1493 (s), 1450 (s), 1438 (w), 1428 (w), 1414 (s), 1379 (w), 1347 (m), 1334 (w), 1303 (w), 1278 (s), 1244 (w), 1219 (s), 1190 (m), 1181 (w), 1141 (w), 1130 (w), 1111 (w), 1079 (w), 1073 (w), 1056 (w), 1041 (w), 1033 (w), 1021 (m), 980 (w), 971 (w), 956 (m), 912 (w), 905 (w), 883 (w), 872 (w), 865 (w), 830 (m), 823 (w), 813 (s), 785 (w), 766 (s), 753 (s), 736 (s), 705 (w), 656 (m), 634 (m), 623 (m), 607 (s), 584 (m), 555 (m), 539 (m).

MS (EI, 70 eV): *m/z*(%) = 298 (M⁺, 100), 283 (20), 255 (63), 227 (7), 149 (9), 127 (4), 113 (5), 99 (3). **HR-MS (EI):** calculated for C₂₀H₁₄N₂O₁ (M⁺): 298.11006, found: 298.10998.

6-methylpyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine 8ab



Yellow solid, 64%. M.p.: 184 – 186 °C.

¹H NMR (300 MHz, CDCl₃) δ = 8.60 (s, 1H), 8.39 (d, *J* = 8.5 Hz, 1H), 8.13 – 7.95 (m, 3H), 7.91 (s, 1H), 7.54 – 7.35 (m, 2H), 7.30 (s, 1H), 7.19 (d, *J* = 7.0 Hz, 2H), 2.39 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ = 147.2, 144.4, 139.9, 138.3, 133.14 133.0, 129.8, 128.8, 128.3, 127.0, 125.0, 125.0, 124.4, 122.4, 121.7, 121.3, 116.0, 115.7, 96.2, 21.2.

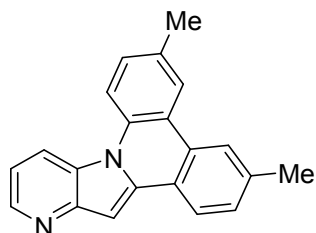
IR (ATR, cm⁻¹): = 3124 (w), 3069 (w), 3036 (w), 2954 (w), 2916 (m), 2850 (m), 2746 (w), 1942 (w), 1900 (w), 1877 (w), 1860 (w), 1823 (w), 1795 (w), 1600 (m), 1577 (w), 1569 (m), 1553 (s), 1524 (w), 1496 (m), 1450 (s), 1416 (s), 1387 (w), 1372 (w), 1354 (m), 1324 (w), 1310 (w), 1300

(w), 1279 (m), 1236 (w), 1193 (w), 1182 (m), 1165 (w), 1145 (w), 1124 (m), 1116 (m), 1066 (w), 1042 (w), 999 (w), 972 (w), 955 (m), 937 (w), 910 (m), 883 (w), 866 (m), 853 (m), 828 (w), 801 (m), 790 (s), 772 (m), 748 (s), 730 (w), 720 (w), 710 (w), 694 (w), 660 (w), 643 (m), 620 (w), 576 (s), 540 (m).

MS (EI, 70 eV): $m/z(\%) = 282 (M^+, 100), 266 (4), 252 (3), 140 (16), 126 (5), 113 (2), 100 (2)$.

HRMS (EI): calculated for $C_{20}H_{14}N_2 (M^+)$: 282.11515, found: 282.11484.

3,6-dimethylpyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 8bb



Yellowish solid, 72%. M.p.: 208 – 210 °C.

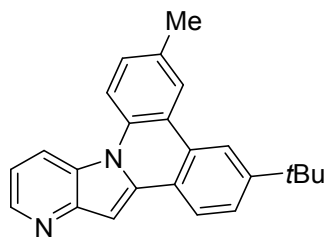
1H NMR (300 MHz, $CDCl_3$) $\delta = 8.59$ (s, 1H), 8.36 (d, $J = 8.5$ Hz, 1H), 7.98 (d, $J = 8.5$ Hz, 1H), 7.88 (d, $J = 8.3$ Hz, 2H), 7.79 (s, 1H), 7.35 – 6.87 (m, 4H), 2.45 (s, 3H), 2.38 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) $\delta = 147.71, 144.59, 138.65, 138.40, 133.12, 132.85, 129.55, 129.47, 126.82, 126.71, 124.81, 124.23, 122.63, 122.41, 121.65$ (2C), 120.88, 115.63, 95.65, 22.00, 21.15.

IR (ATR, cm^{-1}): = 3154 (w), 3115 (w), 3097 (w), 3056 (w), 3025 (w), 3004 (w), 2952 (w), 2917 (m), 2851 (w), 1920 (w), 1898 (w), 1854 (w), 1613 (w), 1601 (m), 1569 (w), 1549 (s), 1491 (m), 1481 (w), 1434 (w), 1416 (s), 1373 (w), 1352 (w), 1300 (w), 1281 (m), 1262 (w), 1237 (m), 1205 (w), 1192 (m), 1152 (w), 1121 (w), 1099 (w), 1069 (w), 1041 (m), 957 (m), 929 (w), 906 (w), 877 (m), 867 (w), 817 (w), 806 (s), 784 (s), 754 (s), 741 (w), 716 (w), 694 (w), 660 (m), 629 (w), 622 (w), 590 (m), 578 (m), 560 (w), 533 (s).

MS (EI, 70 eV): $m/z(\%) = 296 (M^+, 100), 279 (11), 266 (2), 148 (6), 147 (3), 146 (3), 140 (7), 126 (2)$. **HR-MS (EI):** calculated for $C_{21}H_{16}N_2 ([M+1]^+)$: 297.13862, found: 297.13882.

3-(*tert*-butyl)-6-methylpyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 8cb



Yellow solid, 32%; M.p. 197 - 199 °C.

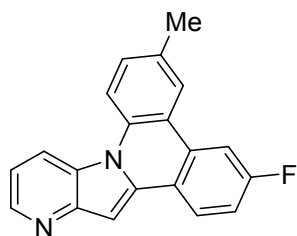
¹H NMR (300 MHz, CDCl₃): δ = 8.67 – 8.56 (m, 1H), 8.49 (d, J = 8.5 Hz, 1H), 8.23 – 8.07 (m, 4H), 7.63 – 7.57 (m, 1H), 7.36 – 7.29 (m, 2H), 7.20 (dd, J = 8.5 Hz, J = 4.5 Hz, 1H), 2.51 (s, 3H), 1.48 (s, 9H).

¹³C NMR (75 MHz, CDCl₃): δ = 152.0, 147.9, 144.8, 138.4, 133.4, 133.1, 129.8, 126.7, 126.3, 125.0, 124.3, 122.9, 122.3, 121.0, 118.6, 116.0, 115.8, 96.0, 35.4, 31.5, 21.3 (3C) (one signal of C tertiary could not be detected).

IR (ATR, cm⁻¹): = 3033 (w), 2956 (m), 2914 (w), 2864 (w), 1615 (w), 1600 (w), 1569 (w), 1556 (m), 1548 (m), 1489 (w), 1482 (w), 1460 (w), 1444 (w), 1427 (w), 1414 (s), 1391 (w), 1379 (w), 1357 (m), 1353 (m), 1301 (w), 1280 (m), 1263 (m), 1240 (w), 1202 (w), 1187 (w), 1159 (w), 1131 (w), 1121 (w), 1067 (w), 1045 (w), 958 (m), 941 (w), 925 (w), 904 (w), 880 (m), 865 (w), 830 (m), 811 (w), 786 (s), 774 (s), 757 (s), 736 (w), 722 (m), 666 (w), 656 (w), 634 (w), 620 (w), 611 (w), 578 (m), 552 (s), 533 (w).

MS (EI, 70 eV): $m/z(\%)$ = 338 (M⁺, 100), 323 (85), 308 (29), 295 (9), 282 (11), 266 (3), 161 (7), 153 (4), 152 (3), 147 (23), 140 (8), 139 (5), 133 (4), 41 (5), 39 (4). **HR-MS (EI):** calculated for C₂₄H₂₂N₂ (M⁺): 338.17775, found: 338.17773.

3-fluoro-6-methylpyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine 8db



Yellow solid, 79%. M.p.: 233 – 235 °C.

¹H NMR (300 MHz, CDCl₃) δ = 8.68 (s, 1H), 8.45 (d, *J* = 8.5 Hz, 1H), 8.11 – 8.01 (m, 2H), 7.84 (s, 1H), 7.76 – 7.69 (m, 1H), 7.35 – 7.22 (m, 3H), 7.19 (dd, *J* = 8.4 Hz, *J* = 2.3 Hz, 1H), 2.48 (s, 3H).

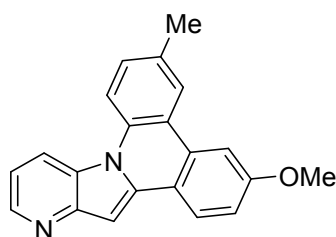
¹⁹F NMR (63 MHz, CDCl₃) δ = 110.92.

¹³C NMR (63 MHz, CDCl₃) δ = 163.1 (d, *J* = 247.9 Hz), 147.5, 144.9, 137.5, 133.3, 133.3, 130.5, 129.1 (d, *J* = 8.4 Hz), 127.2 (d, *J* = 8.9 Hz), 124.6, 121.6 (d, *J* = 2.4 Hz), 121.0, 120.9 (d, *J* = 3.0 Hz), 116.4 (d, *J* = 23.2 Hz), 116.0, 115.8, 108.5 (d, *J* = 23.4 Hz), 96.1, 21.2. (Signal of one C tertiary could not be detected).

IR (ATR, cm⁻¹): = 3033 (w), 2956 (m), 2914 (w), 2864 (w), 1615 (w), 1600 (w), 1569 (w), 1556 (m), 1548 (m), 1489 (w), 1482 (w), 1460 (w), 1444 (w), 1427 (w), 1414 (s), 1391 (w), 1379 (w), 1357 (m), 1353 (m), 1301 (w), 1280 (m), 1263 (m), 1240 (w), 1202 (w), 1187 (w), 1159 (w), 1131 (w), 1121 (w), 1067 (w), 1045 (w), 958 (m), 941 (w), 925 (w), 904 (w), 880 (m), 865 (w), 830 (m), 811 (w), 786 (s), 774 (s), 757 (s), 736 (w), 722 (m), 666 (w), 656 (w), 634 (w), 620 (w), 611 (w), 578 (m), 552 (s), 533 (w).

MS (EI, 70 eV): *m/z*(%) = 338 (M⁺, 100), 323 (85), 308 (29), 295 (9), 282 (11), 266 (3), 161 (7), 153 (4), 147 (23), 140 (8), 139 (5), 133 (4), 41 (5), 39 (4). **HR-MS (EI):** calculated for C₂₄H₂₂N₂ (M⁺): 338.17775, found: 338.17773.

3-methoxy-6-methylpyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine 8eb



Yellow solid, 37%, M.p.: 183 – 185 °C.

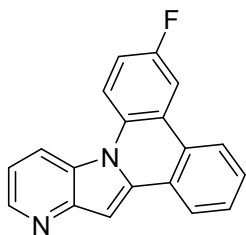
¹H NMR (300 MHz, CDCl₃) δ = 8.57 (s, 1H), 8.47 (d, *J* = 8.5 Hz, 1H), 8.12 (d, *J* = 8.5 Hz, 1H), 7.99 (d, *J* = 8.8 Hz, 1H), 7.93 (s, 1H), 7.53 (d, *J* = 2.4 Hz, 1H), 7.31 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.24 – 7.13 (m, 2H), 7.07 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.95 (s, 3H), 2.46 (s, 3H).

^{13}C NMR (63 MHz, CDCl_3) δ = 160.5, 147.2, 143.7, 139.1, 133.3, 130.2, 128.8, 127.0, 126.9, 124.5, 121.7, 121.4, 118.6, 116.4, 115.9, 115.4, 105.8, 94.5, 55.7, 21.3. (one signal of C tertiary could not be detected).

IR (ATR, cm^{-1}): = 3094 (w), 3029 (w), 3005 (w), 2916 (w), 2839 (w), 2054 (m), 1722 (w), 1610 (s), 1572 (w), 1546 (s), 1493 (s), 1467 (w), 1452 (w), 1432 (w), 1418 (s), 1378 (w), 1353 (w), 1333 (w), 1300 (w), 1282 (s), 1243 (w), 1223 (s), 1194 (m), 1188 (m), 1152 (w), 1125 (w), 1074 (w), 1028 (s), 959 (m), 936 (w), 906 (w), 860 (w), 833 (m), 819 (m), 803 (w), 782 (s), 773 (m), 751 (s), 710 (w), 682 (w), 668 (w), 633 (m), 621 (w), 587 (w), 579 (w), 545 (s).

MS (EI, 70 eV): $m/z(\%)$ = 312 (M^+ , 100), 297 (16), 269 (53), 253 (4), 239 (2), 156 (10), 134 (7), 121 (3), 120 (3), 107 (2). HR-MS (EI): calculated for $\text{C}_{21}\text{H}_{16}\text{N}_2\text{O}_1$ (M^+): 312.12571, found: 312.12596.

6-fluoropyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine 8ac (10e)



Yellow solid, 41%. M.p.: 220 – 221 °C.

^1H NMR (300 MHz, CDCl_3) δ = 8.65 (d, J = 4.0 Hz, 1H), 8.44 (d, J = 8.6 Hz, 1H), 8.23 (dd, J = 9.2, 4.8 Hz, 1H), 8.16 – 8.07 (m, 1H), 8.07 – 8.00 (m, 1H), 7.90 (dd, J = 10.0, 2.8 Hz, 1H), 7.60 – 7.47 (m, 2H), 7.36 (s, 1H), 7.28 – 7.16 (m, 2H).

^{19}F NMR (282 MHz, CDCl_3) δ -118.20.

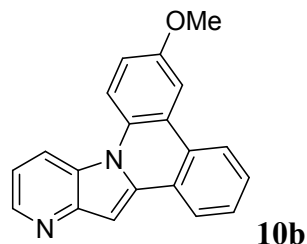
^{13}C NMR (75 MHz, CDCl_3) δ = 159.0 (d, J = 243.3 Hz), 147.7, 145.3, 137.9, 131.8 (d, J = 2.1 Hz), 129.3, 129.0, 126.8, 126.2 (d, J = 2.5 Hz), 125.6, 125.1, 124.0 (d, J = 7.7 Hz), 122.7, 120.7, 117.5 (d, J = 8.1 Hz), 116.5, 116.1 (d, J = 23.2 Hz), 110.6 (d, J = 23.9 Hz), 97.1.

IR (ATR, cm^{-1}): = 3131.1 (w), 3056.8 (w), 3031.7 (w), 2920.8 (w), 2850.5 (w), 1942.2 (w), 1889.7 (w), 1573.4 (m), 1557.6 (s), 1496.3 (m), 1452.2 (m), 1420.5 (s), 1280.2 (m), 1243.7 (m), 1201.1 (m), 1174.1 (m), 1137.7 (m), 1108.0 (w), 1168.8 (m), 957.1 (m), 909.6 (m), 856.1 (m), 806.8 (m), 782.8 (m), 746.5 (s), 577.9 (m).

MS (EI, 70 eV): $m/z(\%) = 286 (M^+, 100), 258 (7), 232 (5), 208 (2), 195 (3), 168 (3), 143 (6), 128 (3), 99 (2), 87 (2), 75 (2), 62 (5), 51 (3), 39 (3).$

HR-MS (EI): calculated for $C_{19}H_{11}N_2F_1 (M^+)$: 286.09008, found: 286.09014

6-methoxypyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 10b



Yellowish solid, 51%. M.p.: 156 – 157 °C.

1H NMR (300 MHz, $CDCl_3$) $\delta = 8.61$ (d, $J = 4.0$ Hz, 1H), 8.41 (d, $J = 8.6$ Hz, 1H), 8.13 (d, $J = 9.2$ Hz, 1H), 8.10 – 8.00 (m, 2H), 7.64 (d, $J = 2.8$ Hz, 1H), 7.53 – 7.39 (m, 2H), 7.32 (s, 1H), 7.19 (dd, $J = 8.6, 4.6$ Hz, 1H), 7.03 (dd, $J = 9.1, 2.9$ Hz, 1H), 3.89 (s, 3H).

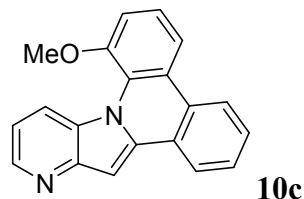
^{13}C NMR (63 MHz, $CDCl_3$) $\delta = 155.7, 147.4, 144.7, 137.9, 129.7, 128.8, 128.6, 126.8, 126.7, 125.4, 125.1, 123.3, 122.5, 120.84, 117.1, 116.3, 115.3, 108.4, 96.3, 55.7.$

IR (ATR, cm^{-1}): = 3133.5 (w), 3055.6 (w), 2919.6 (w), 2849.1 (w), 1957.7 (w), 1925.7 (w), 1900.2 (w), 1726.6 (w), 1616.8 (m), 1606.1 (m), 1569.7 (m), 1552.5 (s), 1500.3 (m), 1453.4 (m), 1419.4 (s), 1350.4 (m), 1218.9 (m), 1185.5 (m), 1138.4 (m), 1018.3 (m), 956.6 (m), 850.5 (m), 789.6 (m), 755.3 (s), 694.9 (m), 583.2 (m).

MS (EI, 70 eV): $m/z(\%) = 298 (M^+, 100), 283 (37), 255 (70), 227 (11), 200 (5), 174 (4), 149 (8), 127 (7), 114 (11), 100 (5), 87 (7), 75 (4), 63 (4), 51 (4), 39 (6).$

HR-MS (EI): calculated for $C_{20}H_{14}N_2O_1 (M^+)$: 298.11006, found: 298.10977.

8-methoxypyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 10c



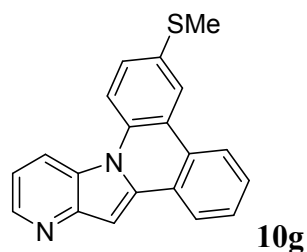
¹H NMR (300 MHz, CDCl₃) δ = 8.59 (dd, *J* = 4.5, 0.9 Hz, 1H), 8.25 – 8.12 (m, 2H), 8.10 – 8.03 (m, 1H), 7.94 (dd, *J* = 8.1, 0.9 Hz, 1H), 7.65 – 7.45 (m, 3H), 7.39 (t, *J* = 8.1 Hz, 1H), 7.22 – 7.07 (m, 2H), 3.90 (s, 3H).

¹³C NMR (63 MHz, CDCl₃) δ = 149.5, 146.9, 144.4, 139.1, 129.9, 128.9, 128.8, 127.3, 125.9, 125.4, 124.9, 124.7 (2C), 124.1, 123.1, 116.4, 115.0, 112.1, 97.6, 55.9.

MS (EI, 70 eV): *m/z*(%) = 298 (M⁺, 100), 283 (83), 253 (13), 227 (7), 201 (4), 175 (2), 142 (10), 127 (6), 114 (7), 100 (7).

HRMS (EI): calculated for C₂₀H₁₄N₂O₁ (M⁺): 298.11006, found: 298.11014.

6-(methylthio)pyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine 10g



Yellow solid, 81%. M.p.: 172 – 173 °C.

¹H NMR (300 MHz, CDCl₃) δ = 8.61 (s, 1H), 8.42 (d, *J* = 8.5 Hz, 1H), 8.17 – 7.97 (m, 4H), 7.57 – 7.42 (m, 2H), 7.35 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.31 (s, 1H), 7.22 (dd, *J* = 8.5, 4.6 Hz, 1H), 2.57 (s, 3H).

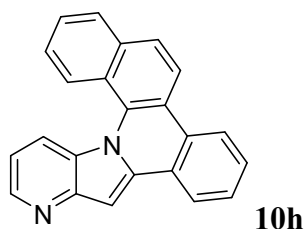
¹³C NMR (75 MHz, CDCl₃) δ = 147.2, 144.6, 138.2, 133.5, 133.0, 129.0, 128.8, 127.9, 126.4, 125.2, 125.1, 122.8, 122.6, 122.4, 121.3, 116.5, 116.2, 96.7, 16.8. (one signal of C-tertiary could not be detected).

IR (ATR, cm⁻¹): = 3031.8 (w), 3001.0 (w), 2958.0 (w), 2917.4 (w), 2849.2 (w), 1597.0 (w), 1646.3 (m), 1488.3 (w), 1449.2 (m), 1413.4 (s), 1354.0 (m), 1278.7 (m), 1189.0 (m), 1115.3 (w), 955.0 (m), 855.7 (w), 789.8 (s), 750.4 (s), 580.6 (m).

MS (EI, 70 eV): *m/z*(%) = 314 (M⁺, 100), 299 (52), 266 (9), 255 (28), 227 (4), 157 (13), 127 (6), 113 (3), 100 (2).

HRMS (EI): calculated for C₂₀H₁₄N₂S₁ (M⁺): 314.08722, found: 314.08694.

Benzo[*c*]pyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine 10h



Yellow solid, 42%. M.p.: 231 – 232 °C.

¹H NMR (300 MHz, CDCl₃) δ = 8.64 (d, *J* = 4.0 Hz, 1H), 8.34 – 8.11 (m, 4H), 7.96 – 7.84 (m, 2H), 7.79 (d, *J* = 8.7 Hz, 1H), 7.60 – 7.47 (m, 3H), 7.45 (d, *J* = 0.6 Hz, 1H), 7.43 – 7.34 (m, 1H), 7.03 (dd, *J* = 8.5, 4.5 Hz, 1H).

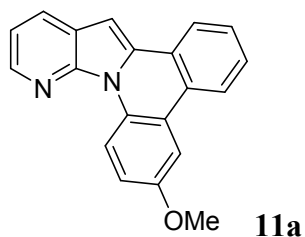
¹³C NMR (63 MHz, CDCl₃) δ = 147.6, 145.4, 139.8, 134.1, 129.9, 129.2, 129.0, 128.7, 128.3, 127.6, 127.2, 125.9, 125.2, 124.7, 124.6, 124.3, 123.7, 123.0, 122.1, 121.0, 120.5, 114.0, 97.7.

IR (ATR, cm⁻¹): = 3096.6 (w), 2958.7 (w), 2850.5 (w), 1954.5 (w), 1915.3 (w), 1808.3, 1713.7 (w), 1621.8 (w), 1576.9 (m), 1543.0 (m), 1416.8 (s), 1389.4 (m), 1274.8 (m), 1029.8 (m), 807 (m), 752.5 (s), 611.2 (m), 566.6 (m).

MS (EI, 70 eV): *m/z*(%) = 318 (M⁺, 100), 291 (12), 237 (2), 159 (41), 144 (23), 131 (9), 105 (2), 87 (1).

HRMS (EI): calculated for C₂₃H₁₄N₂ (M⁺): 318.11515, found: 318.11507.

6-methoxypyrido[3',2':4,5]pyrrolo[1,2-*f*]phenanthridine 11a



Yellowish solid, 34%. M.p.: 186 – 187 °C.

¹H NMR (300 MHz, CDCl₃) δ = 10.15 (d, *J* = 9.3 Hz, 1H), 8.50 (dd, *J* = 4.6, 1.6 Hz, 1H), 8.24 – 7.97 (m, 3H), 7.72 (d, *J* = 2.8 Hz, 1H), 7.57 – 7.39 (m, 2H), 7.34 – 7.16 (m, 2H), 7.08 (s, 1H), 3.95 (s, 3H).

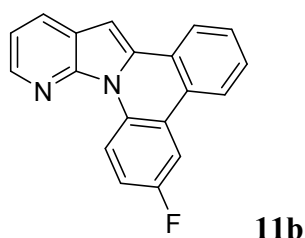
¹³C NMR (63 MHz, CDCl₃) δ = 155.8, 146.9, 141.8, 134.6, 129.9, 128.4, 128.3, 128.2, 127.4, 125.8, 124.3, 122.8, 122.7, 122.1, 120.4, 117.5, 115.5, 107.5, 92.4, 55.7.

IR (ATR, cm⁻¹): = 3104.4 (w), 2997.7 (w), 2930.7 (w), 2830.5 (w), 2089.0 (w), 1892.9 (w), 1713.5 (w), 1620.3 (w), 1563.3 (m), 1543.8 (s), 1499.5 (m), 1453.9 (m), 1407.9 (m), 1327 (m), 1293.2 (m), 1215.2 (m), 1075.3 (m), 1042.8 (m), 1016.0 (m), 945.9 (w), 855.2 (m), 792.4 (m), 758.9 (m), 729.0 (m), 607.9 (m), 566.3 (m).

MS (EI, 70 eV): m/z(%) = 298 (M⁺, 100), 283 (34), 255 (61), 227 (7), 201 (3), 175 (2), 149 (15), 127 (16), 113 (4), 100 (5).

HRMS (EI): calculated for C₂₀H₁₄N₂O₁ (M⁺): 298.11066, found: 298.11047

6-fluoropyrido[3',2':4,5]pyrrolo[1,2-f]phenanthridine **11b**



Yellowish solid, 51%. M.p.: 201 – 202 °C.

¹H NMR (300 MHz, CDCl₃) δ = 10.26 (dd, *J* = 9.3, 5.5 Hz, 1H), 8.50 (dd, *J* = 4.5, 1.3 Hz, 1H), 8.25 – 8.03 (m, 3H), 7.91 (dd, *J* = 10.3, 2.7 Hz, 1H), 7.52 (dd, *J* = 6.0, 3.3 Hz, 2H), 7.41 – 7.26 (m, 2H), 7.11 (s, 1H).

¹⁹F NMR (282 MHz, CDCl₃) δ = -118.48.

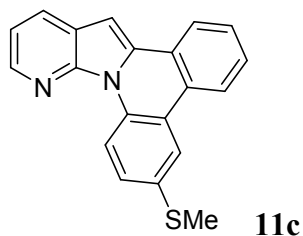
¹³C NMR (63 MHz, CDCl₃) δ = 159.3 (d, *J* = 242.1 Hz), 142.1, 134.6, 131.9, 130.4, 128.9, 128.7, 128.4, 126.8 (d, *J* = 1.9 Hz), 125.8, 124.3, 123.4 (d, *J* = 7.6 Hz), 122.9, 122.2, 121.0 (d, *J* = 7.8 Hz), 117.9, 116.4 (d, *J* = 22.4 Hz), 109.3 (d, *J* = 24.0 Hz), 93.0.

IR (ATR, cm⁻¹): = 3122.0 (w), 3054.0 (w), 1920.0 (w), 1884.2 (w), 1798.7 (w), 1661.0 (w), 1620.4 (w), 1567.0 (m), 1497.6 (m), 1454.6 (m), 1409.4 (m), 1329.7 (m), 1267.7 (m), 1174.5 (m), 1141.0 (m), 892.5 (m), 824.2 (m), 752.8 (m), 724.4 (m), 662.7 (w), 593.9 (m), 566.3 (m).

MS (EI, 70 eV): m/z(%) = 286 (M⁺, 100), 258 (10), 232 (3), 143 (17), 129 (4), 115 (3).

HRMS (EI): calculated for C₁₉H₁₁N₂F₁ (M⁺): 286.09008, found: 286.08990.

6-(methylthio)pyrido[3',2':4,5]pyrrolo[1,2-f]phenanthridine **11c**



Yellow solid, 36%. M.p.: 168 – 169 °C.

¹H NMR (300 MHz, CDCl₃) δ = 10.14 (d, J = 8.9 Hz, 1H), 8.49 (dd, J = 4.6, 1.7 Hz, 1H), 8.27 – 8.11 (m, 2H), 8.10 – 7.99 (m, 2H), 7.57 – 7.41 (m, 3H), 7.26 (dd, J = 7.9, 4.7 Hz, 1H), 7.06 (s, 1H), 2.61 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ = 147.1, 142.0, 134.7, 133.4, 132.9, 128.5 (2C), 128.4, 128.2, 127.0, 125.7, 124.2, 122.7, 122.3, 122.2, 122.0, 119.8, 117.7, 93.0, 17.2.

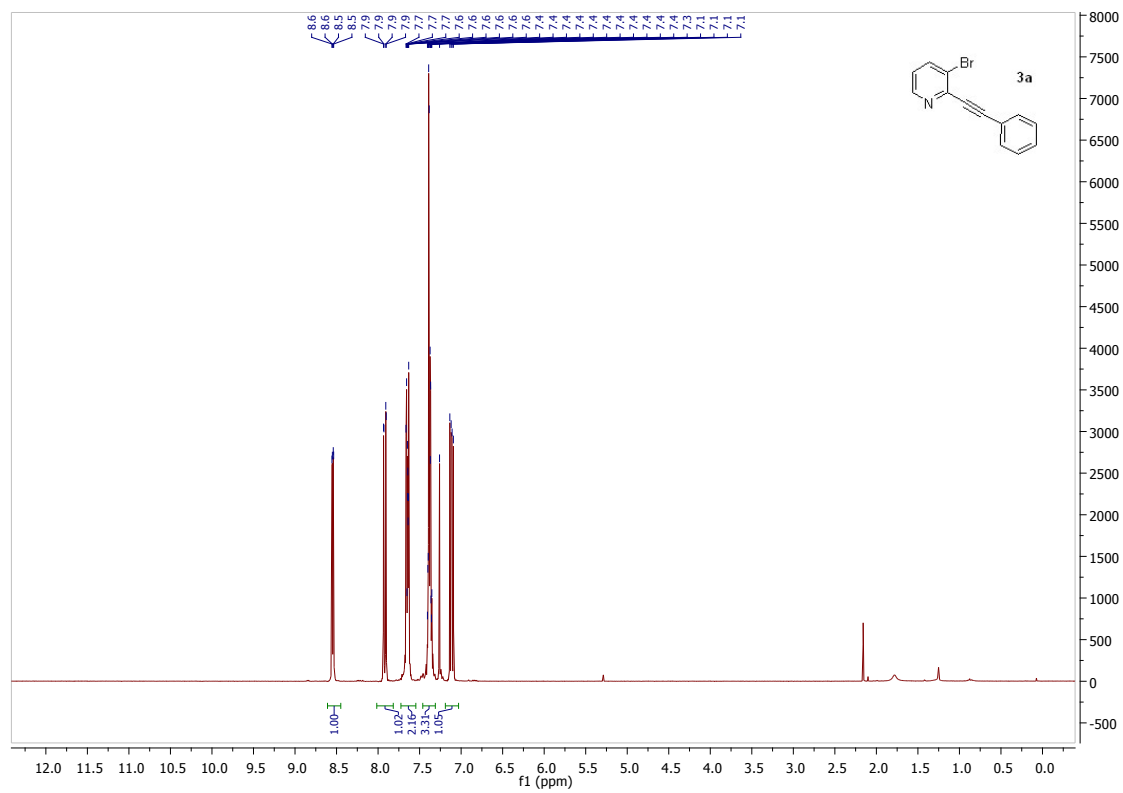
IR (ATR, cm⁻¹): = 3107.2 (w), 3037.2 (w), 2918.0 (w), 2849.6 (w), 2731.2 (w), 2520.1 (8w), 2387.1 (w), 2116.4 (w), 1959.0 (w), 1916.1 (w), 1724.9 (w), 1595.9 (m), 1541.6 (m), 1453.3 (s), 1405.6 (s), 1323.5 (m), 1103.3 (m), 955.8 (m), 818.2 (m), 793.9 (s), 758.7 (s), 730.2 (s), 646.5 (m), 585.3 (m).

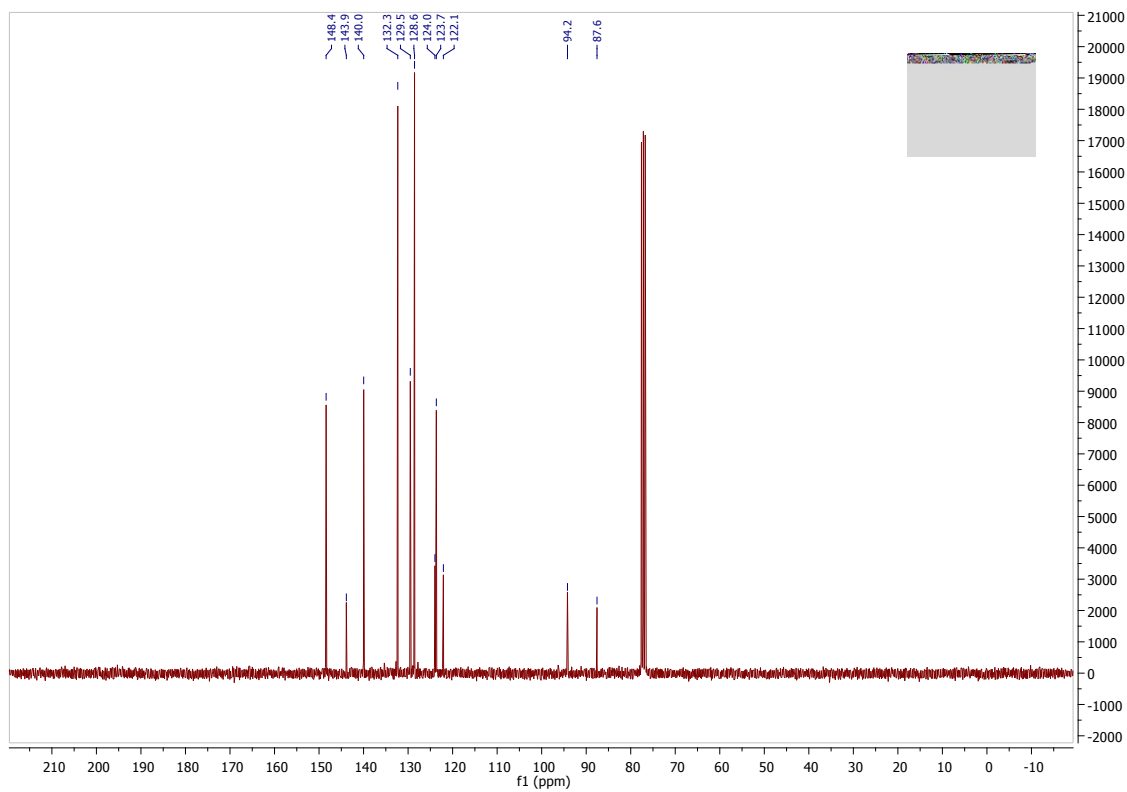
MS (EI, 70 eV): m/z (%) = 314 (M⁺, 100), 299 (59), 266 (7), 255 (29), 227 (3), 201 (1), 157 (14), 133 (5), 113 (2).

HRMS (EI): calculated for C₂₀H₁₄N₂S₁ (M⁺): 314.08722, found: 314.08645.

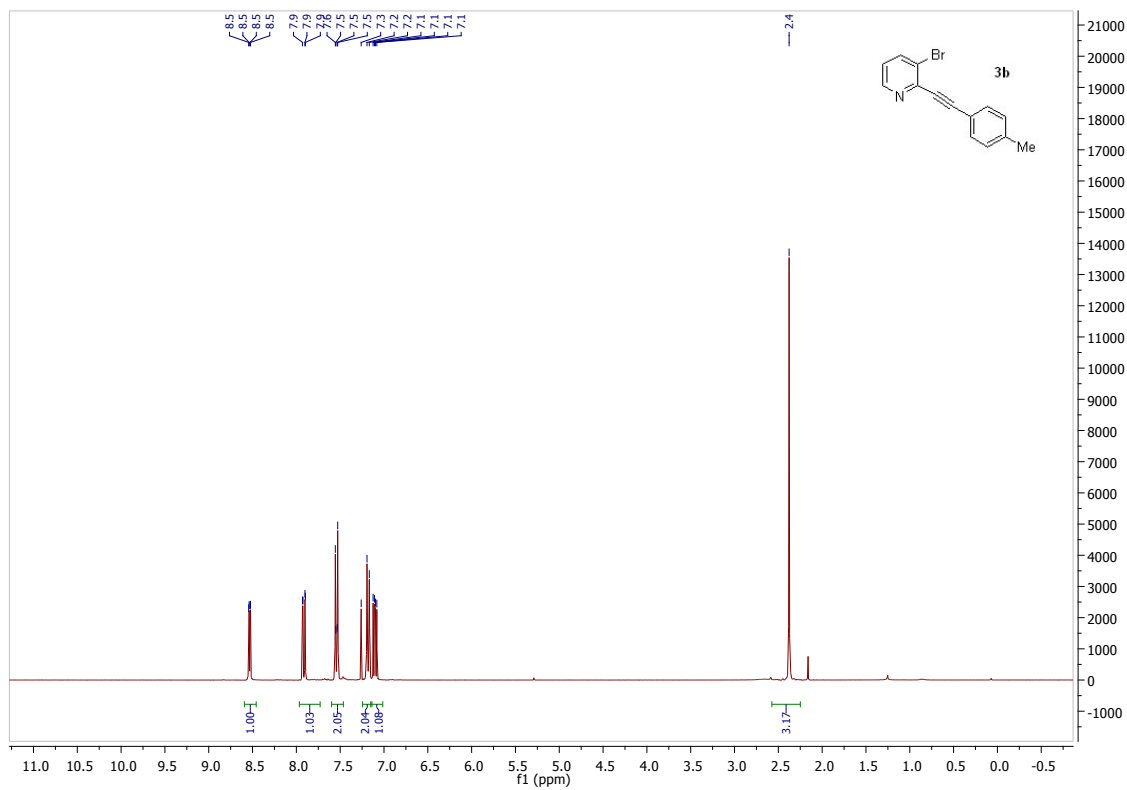
NMR spectra

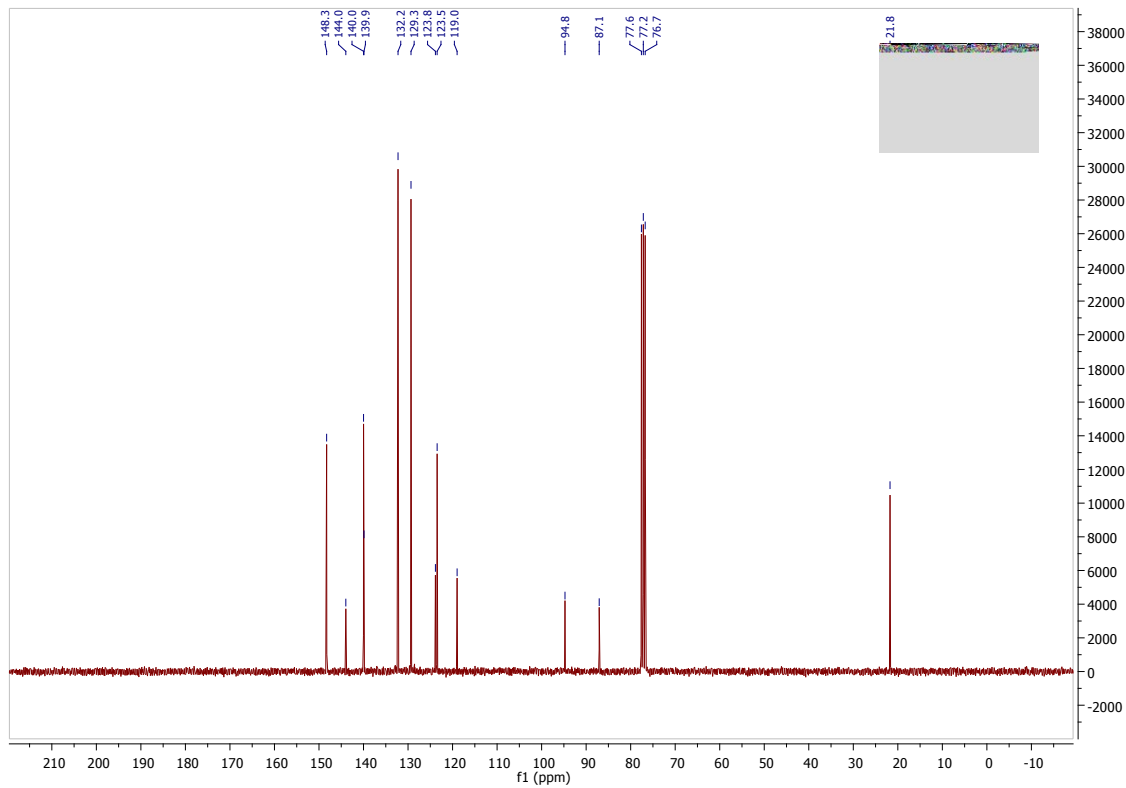
3-bromo-2-(phenylethynyl)pyridines 3a:



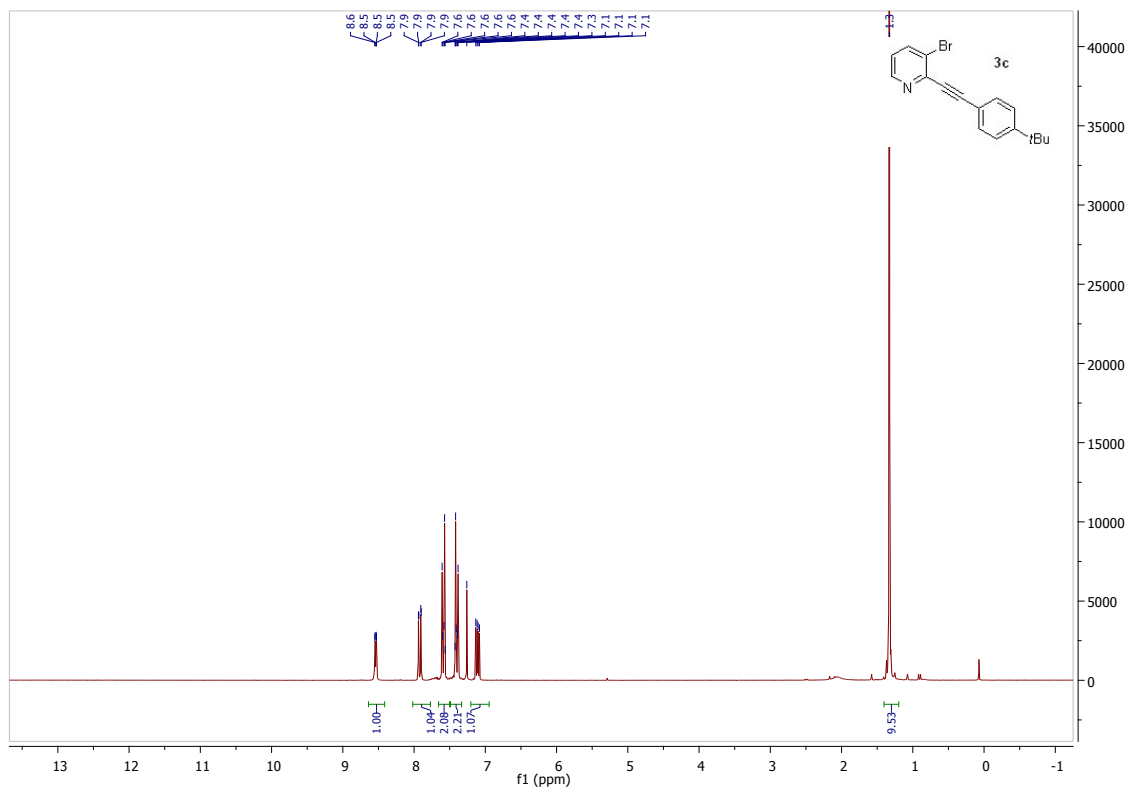


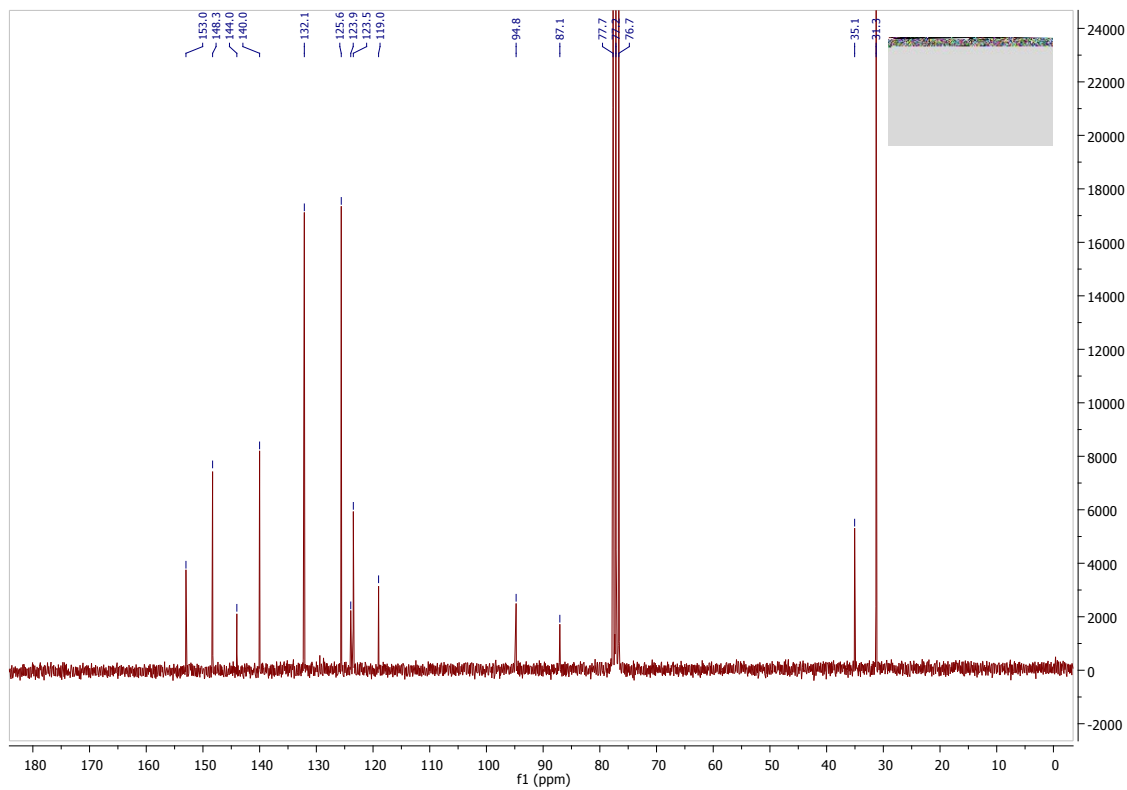
3-bromo-2-(*p*-tolylethynyl)pyridine 3b:



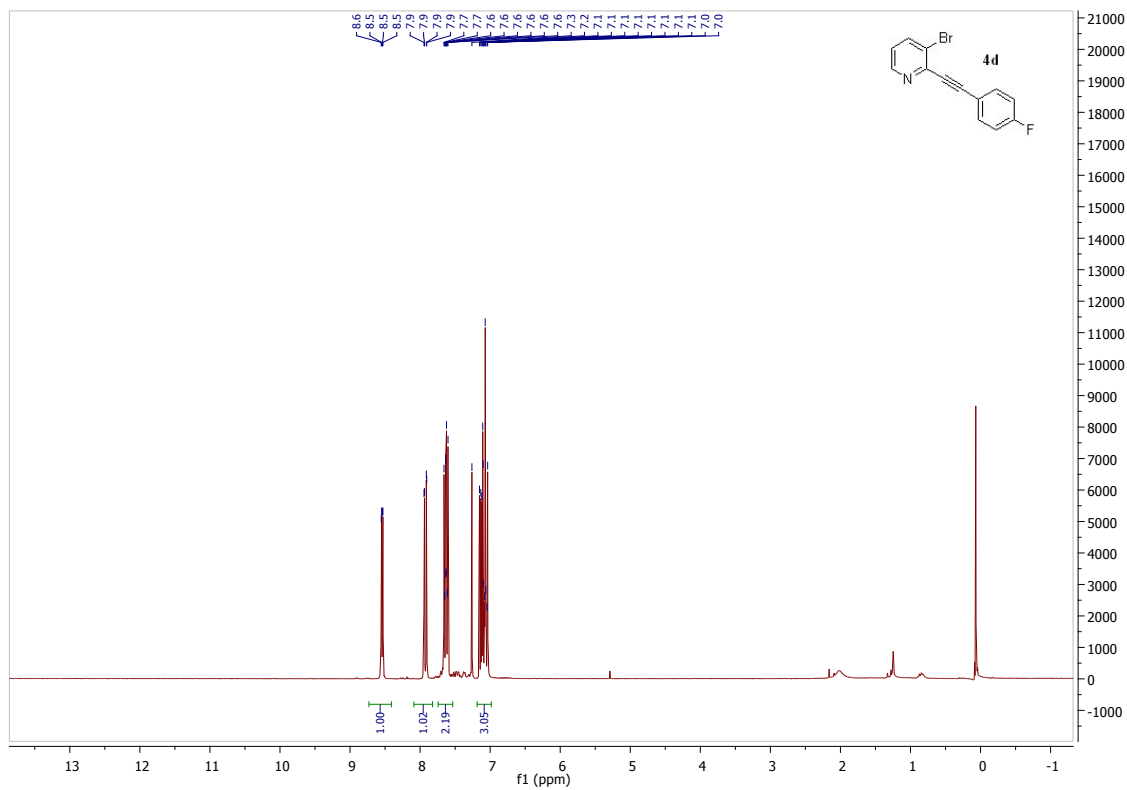


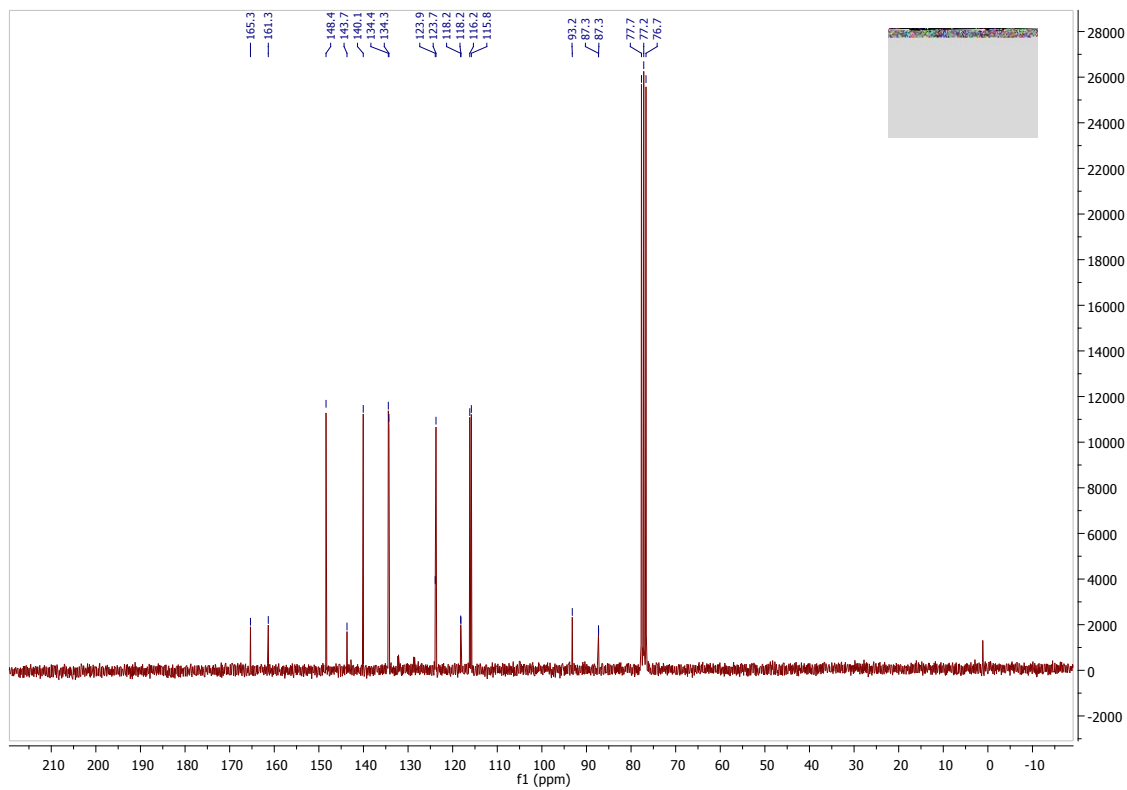
3-bromo-2-((4-*tert*-butyl)phenyl)ethynyl)pyridine 3c:



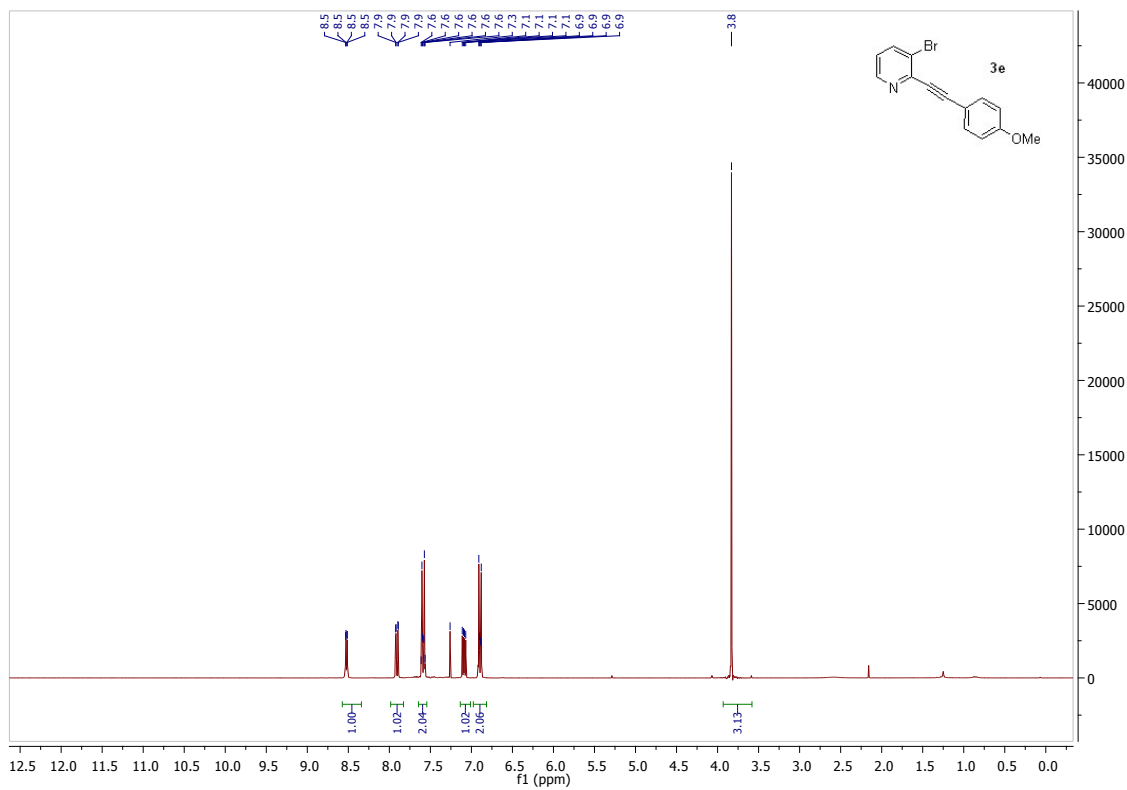


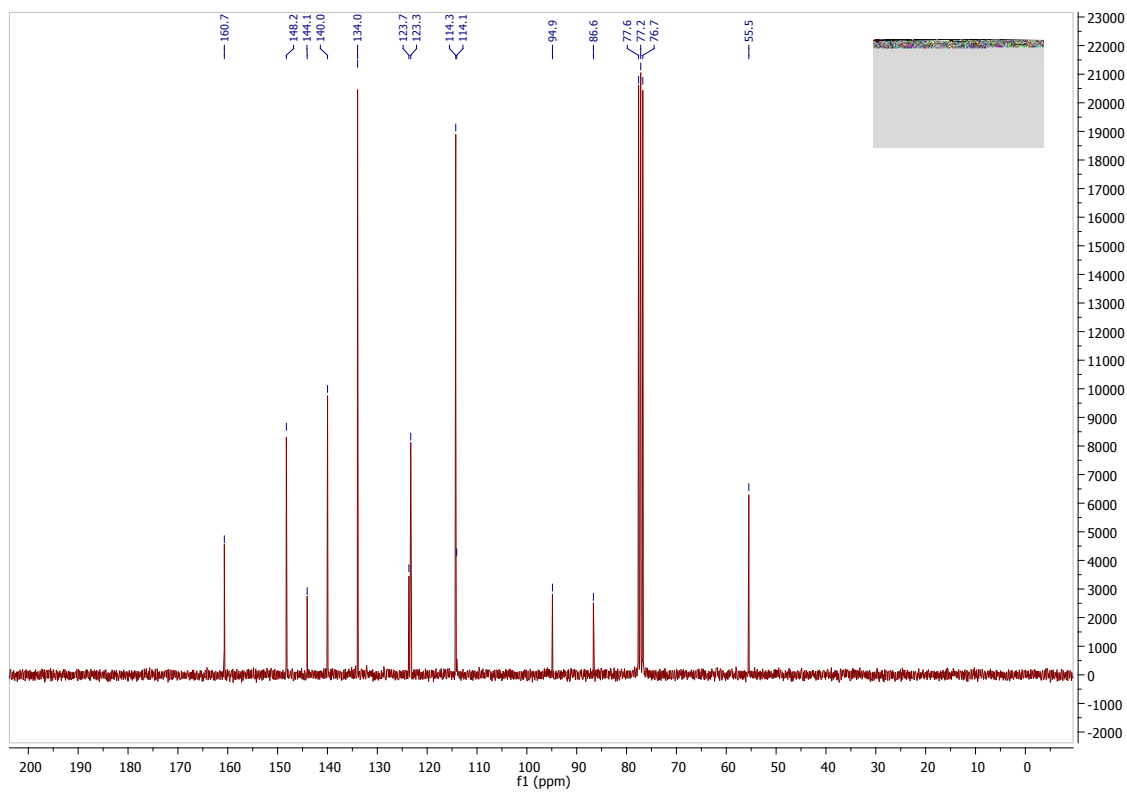
3-bromo-2-((4-fluorophenyl)ethynyl)pyridine 3d:



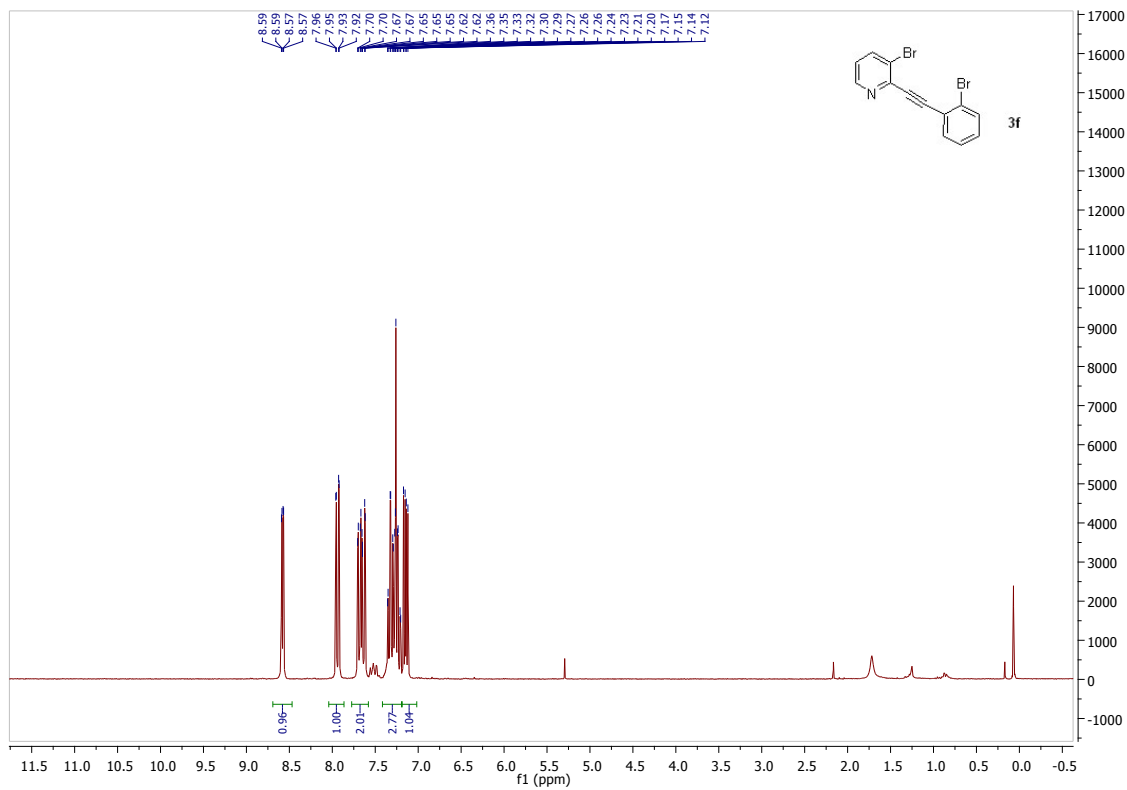


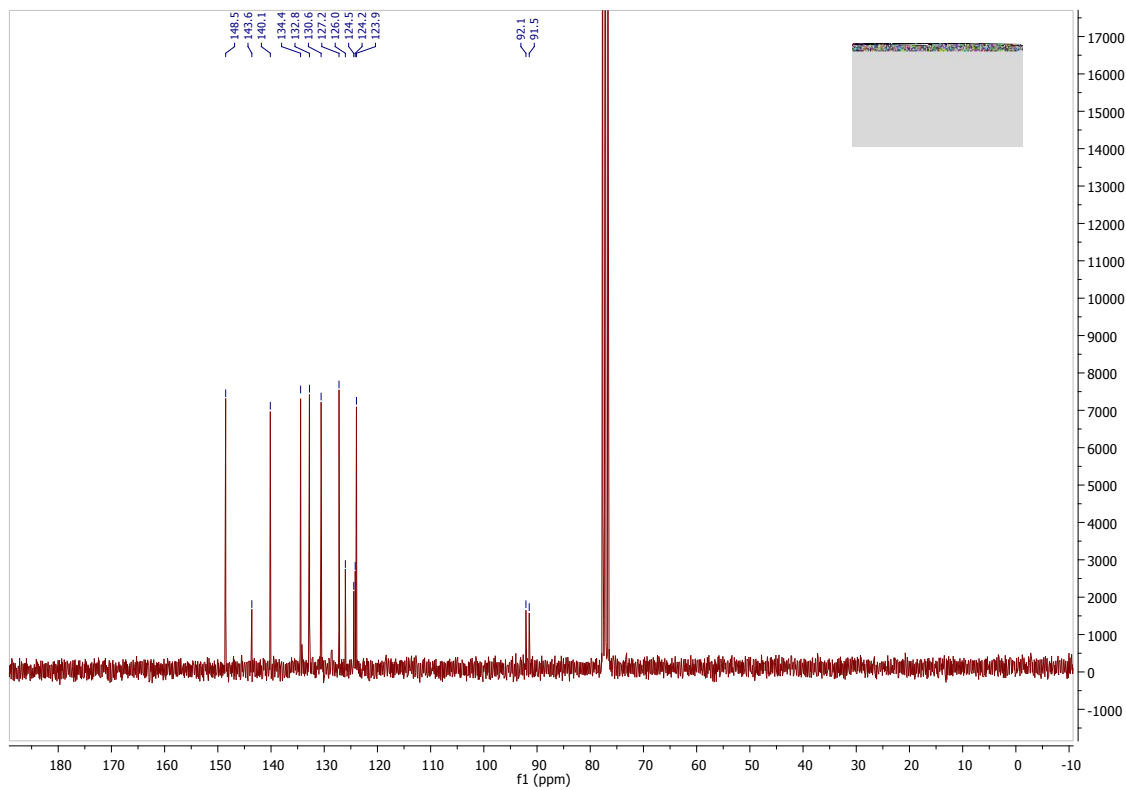
3-bromo-2-((4-methoxyphenyl)ethynyl)pyridine 3e:



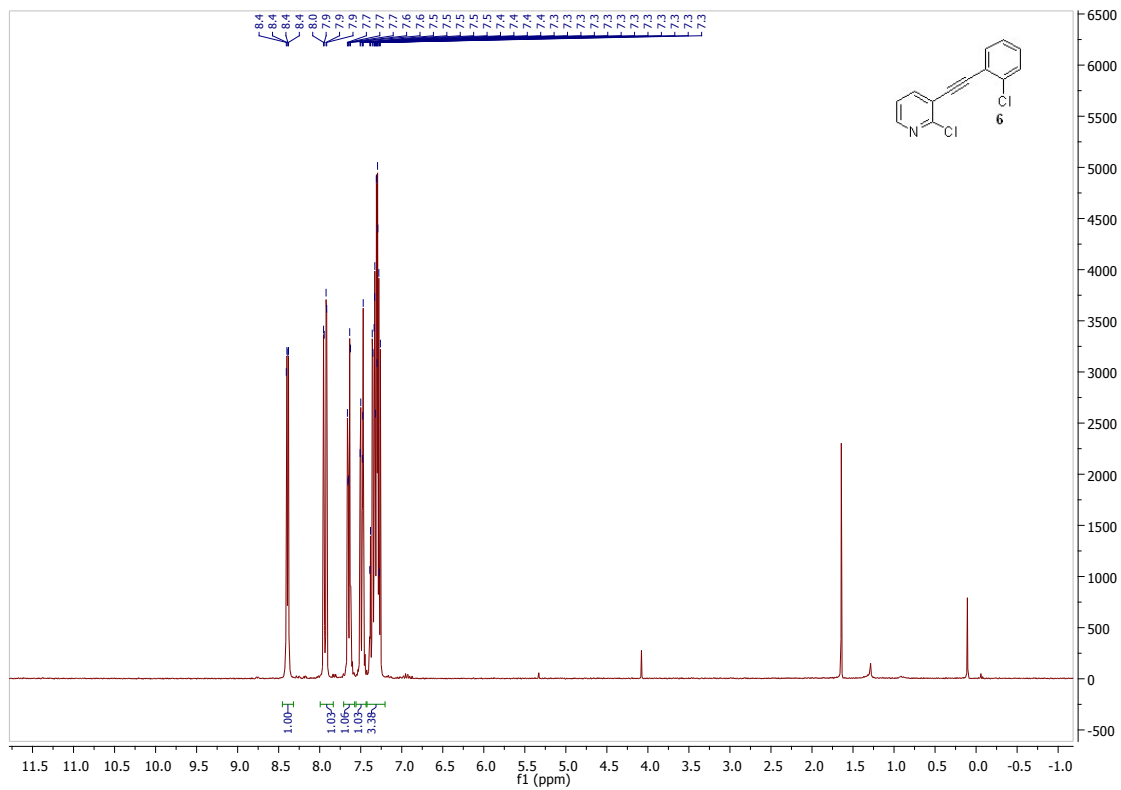


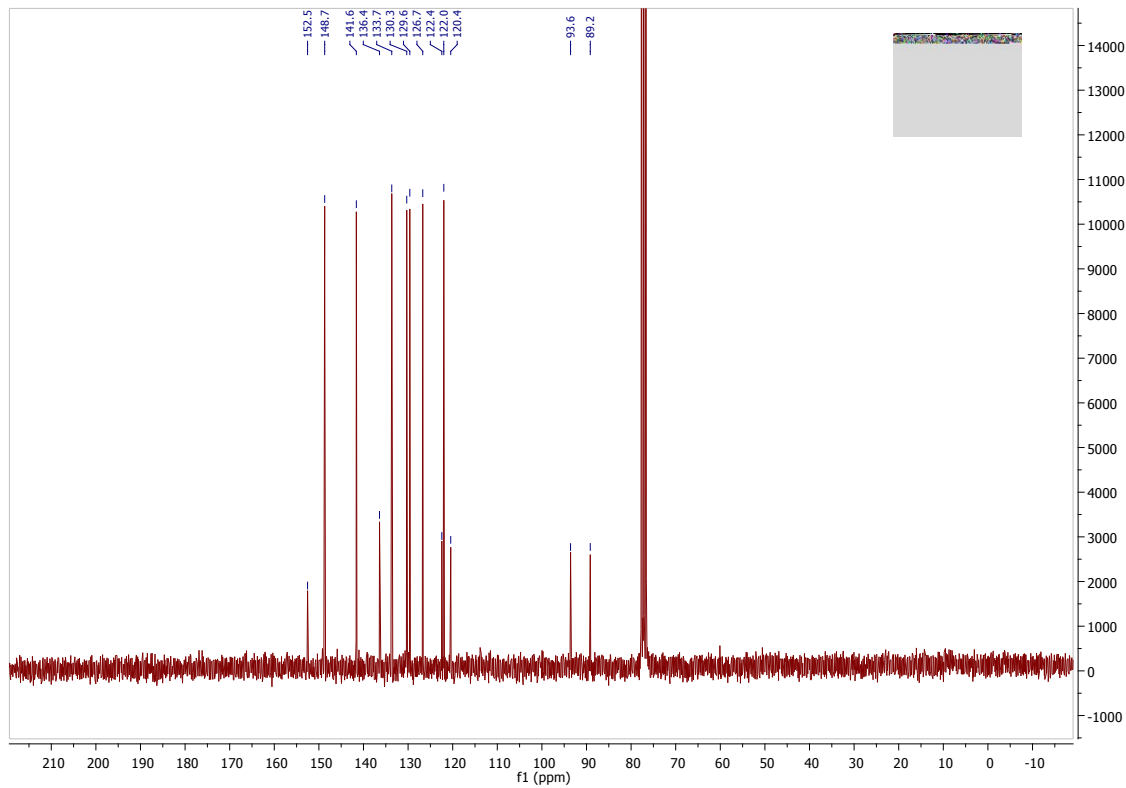
3-bromo-2-((2-bromophenyl)ethynyl)pyridine 3f:



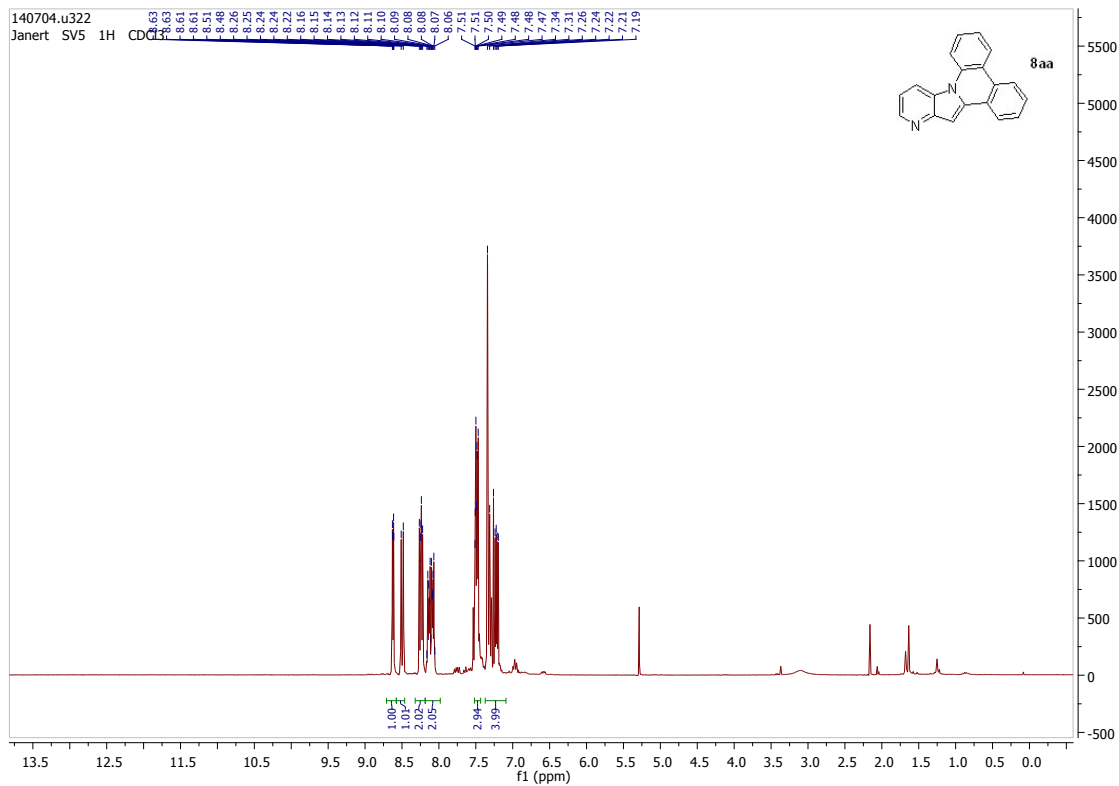


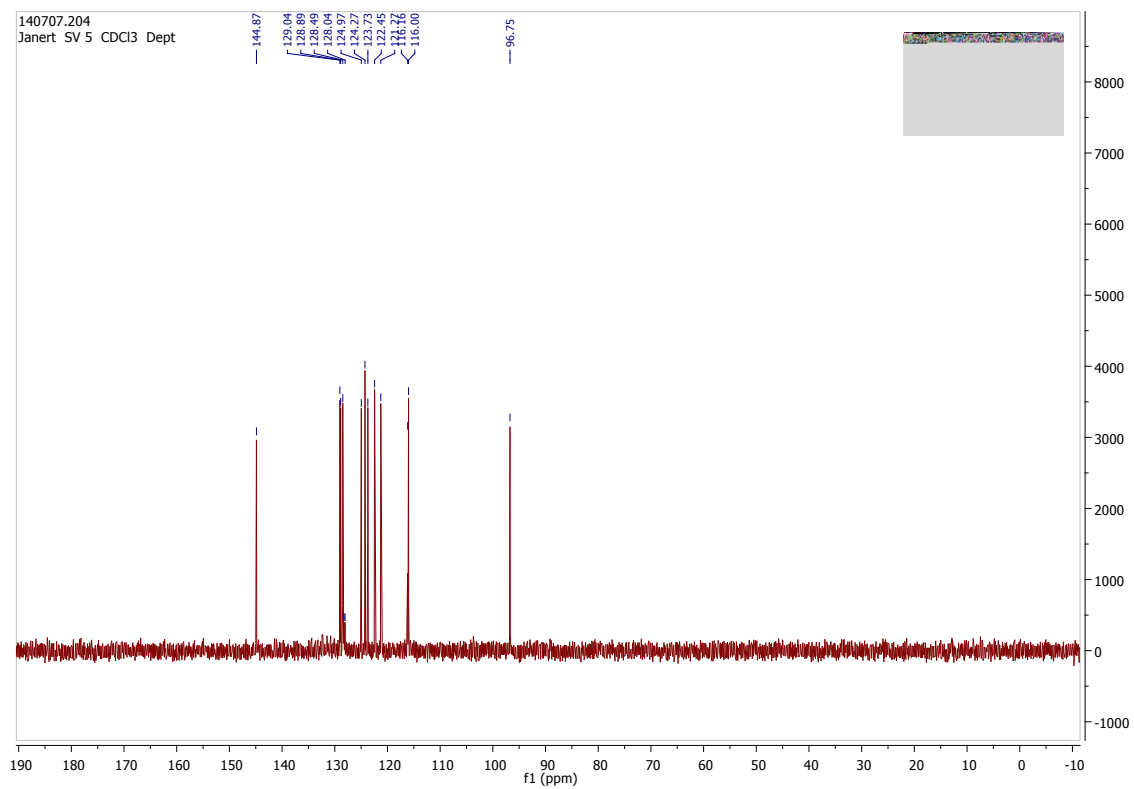
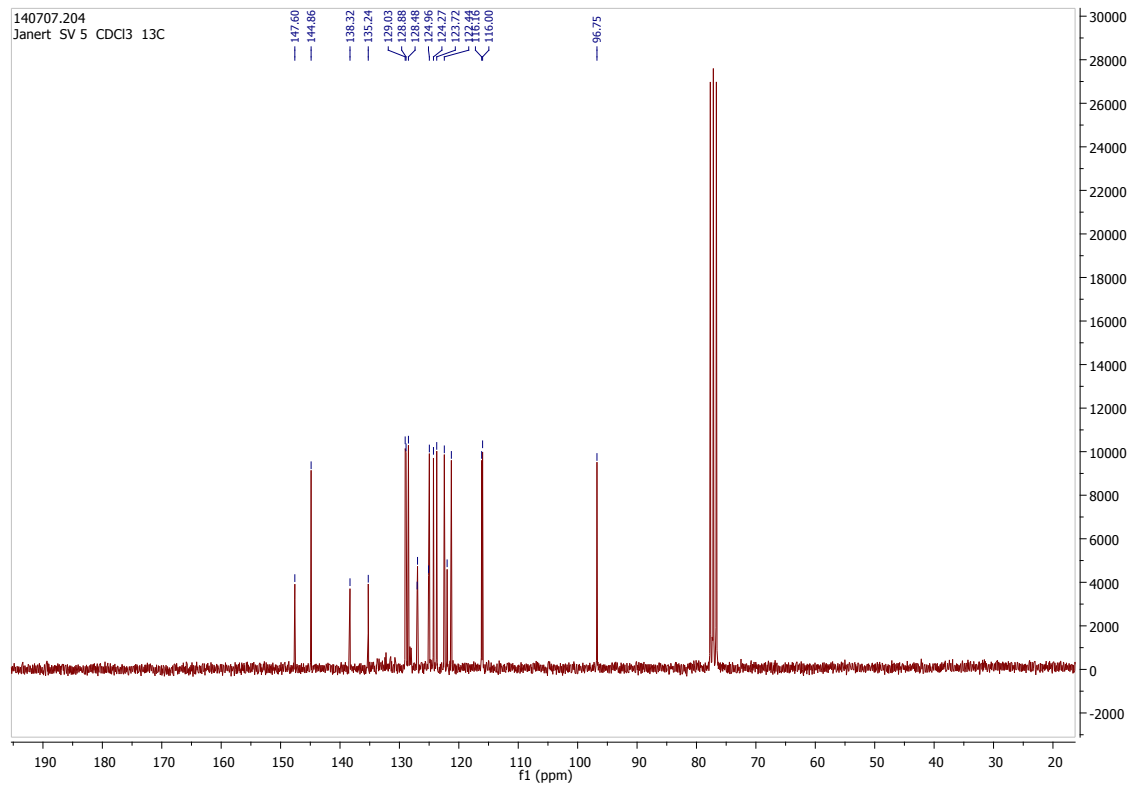
2-chloro-3-((2-chlorophenyl)ethynyl)pyridine 6



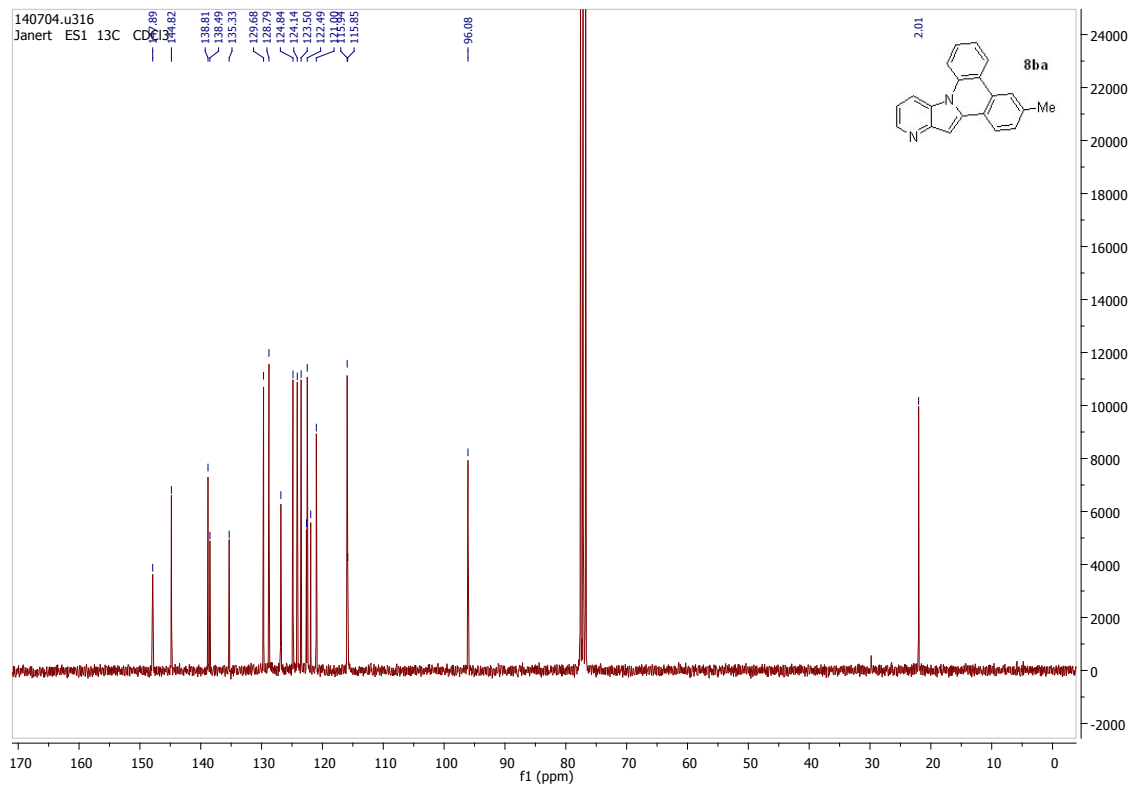
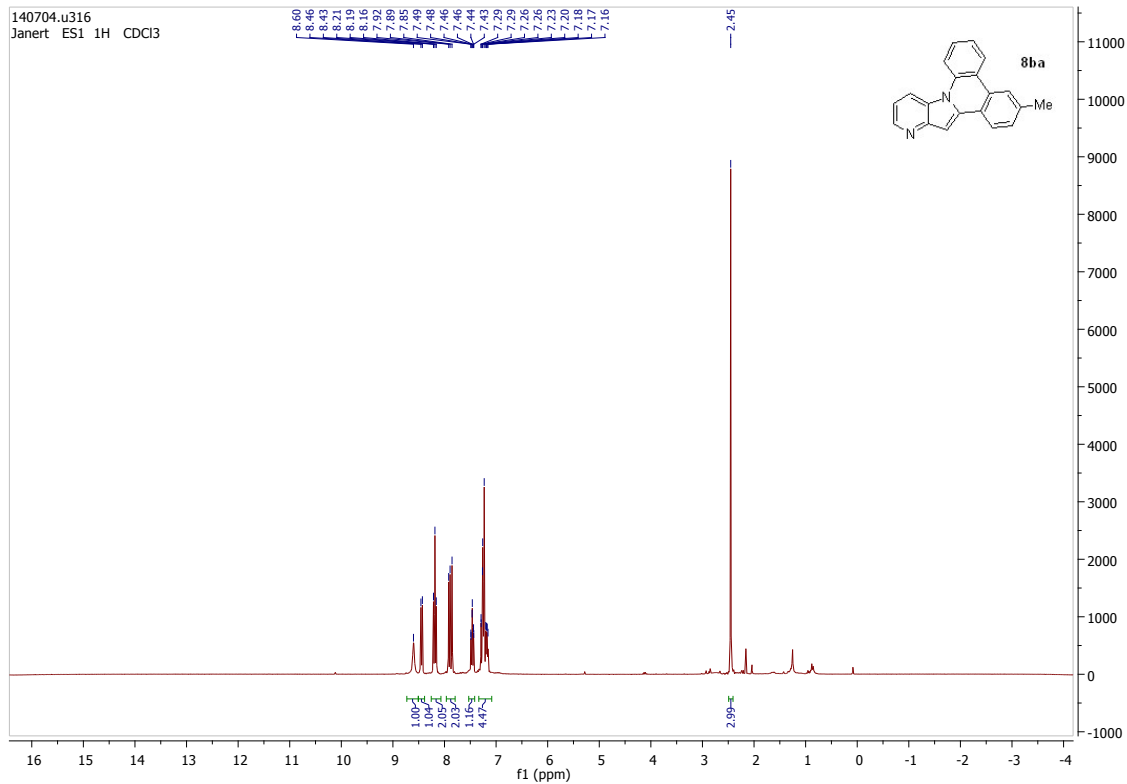


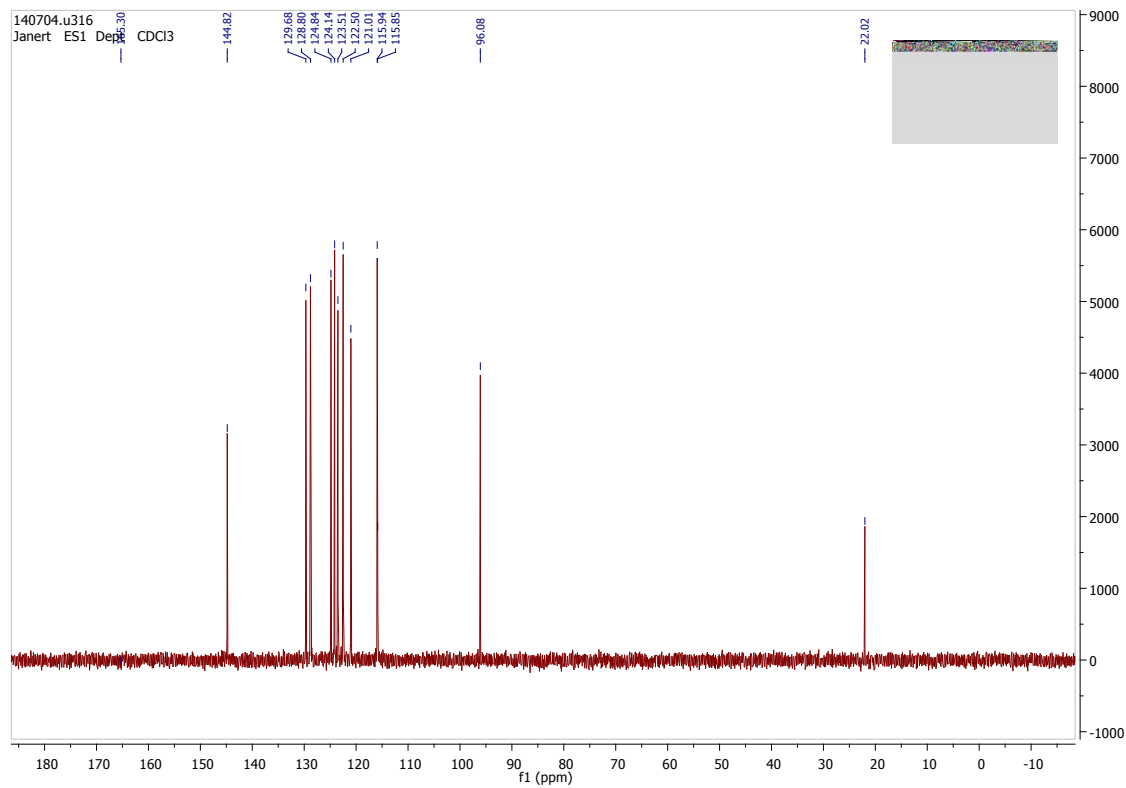
Pyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 8aa



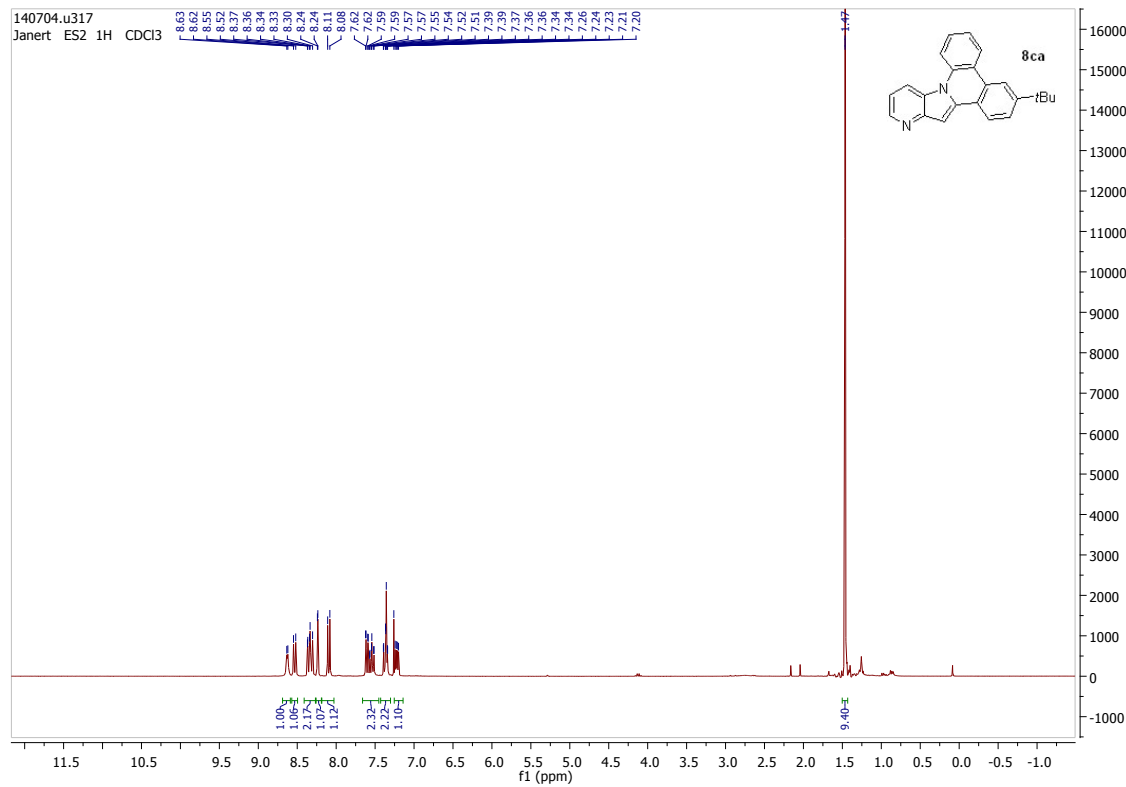


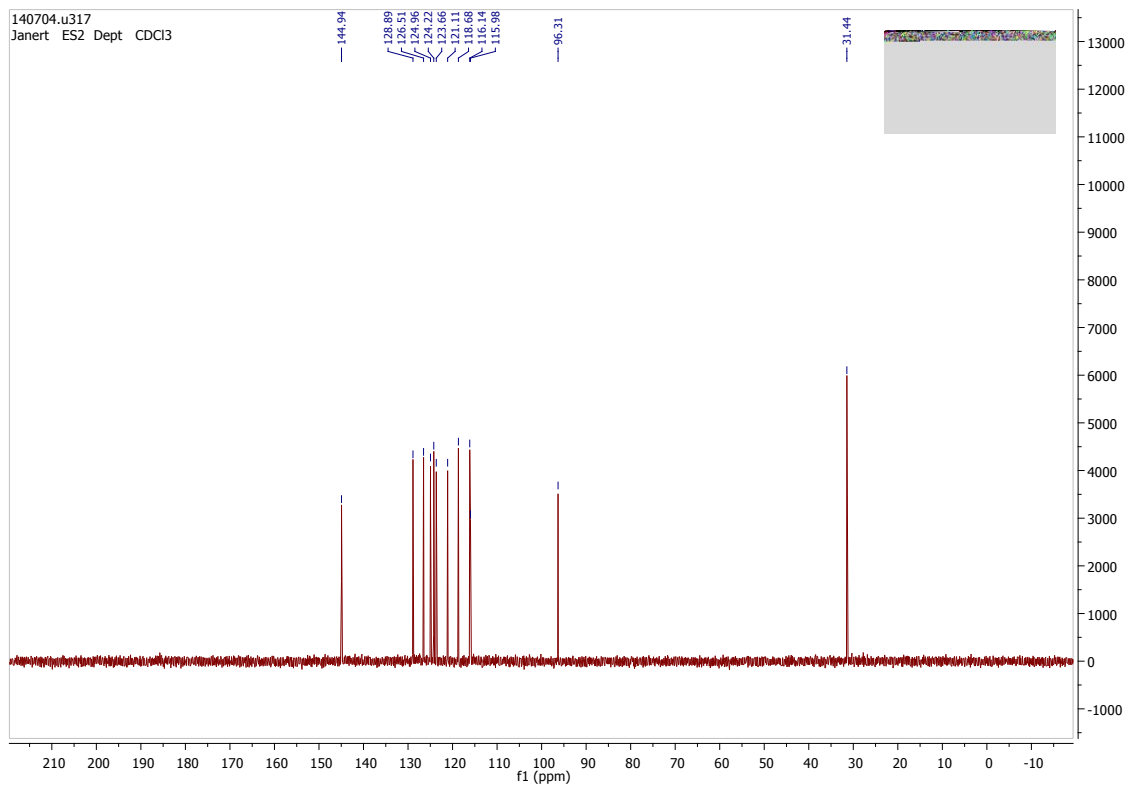
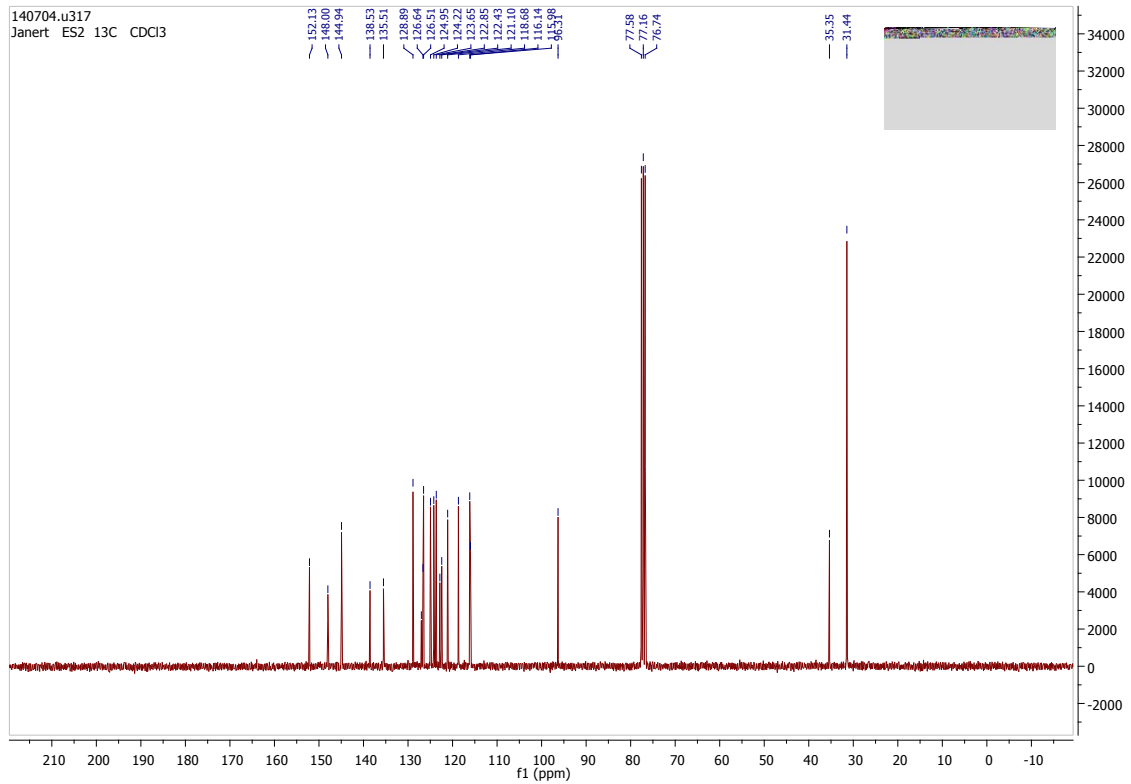
3-methylpyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine ba



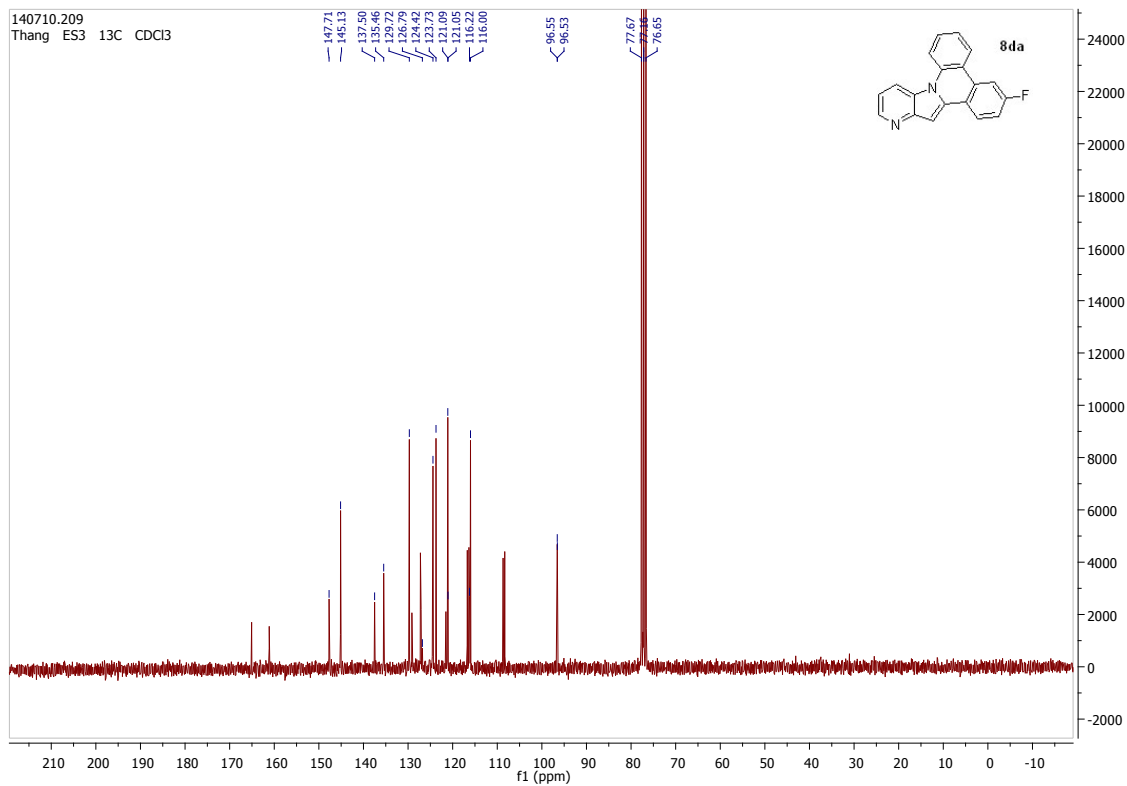
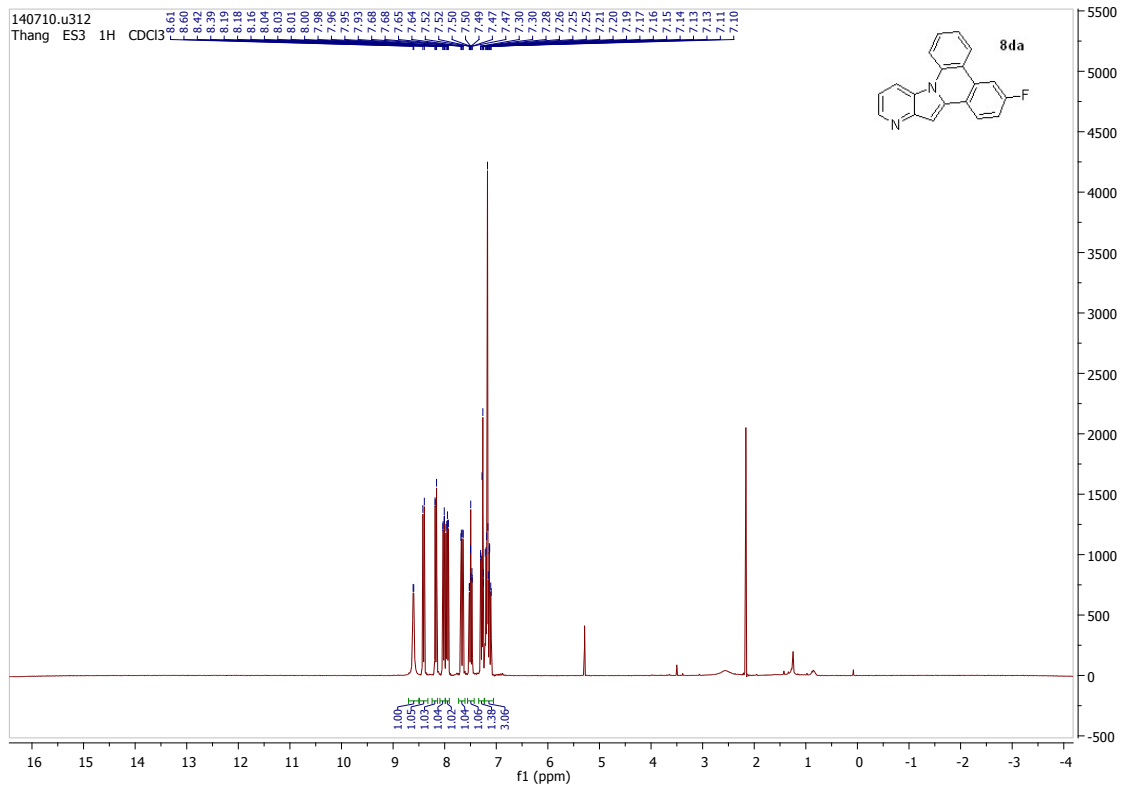


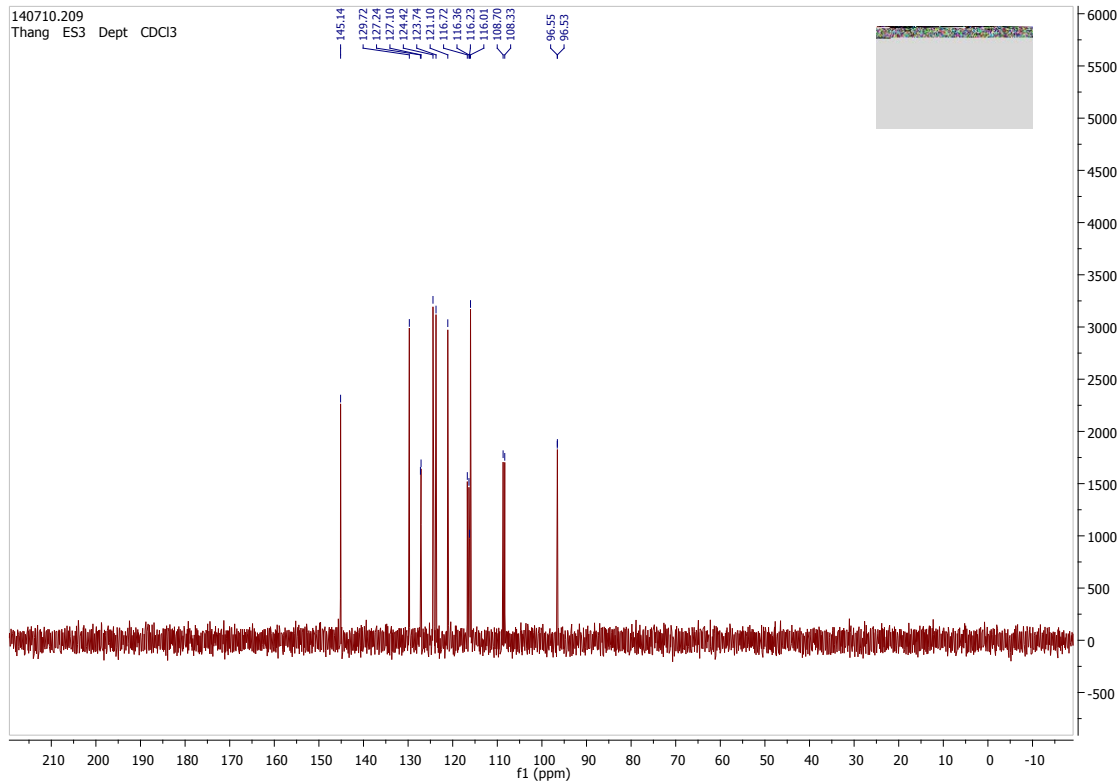
3-(*tert*-butyl)pyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine 8ca



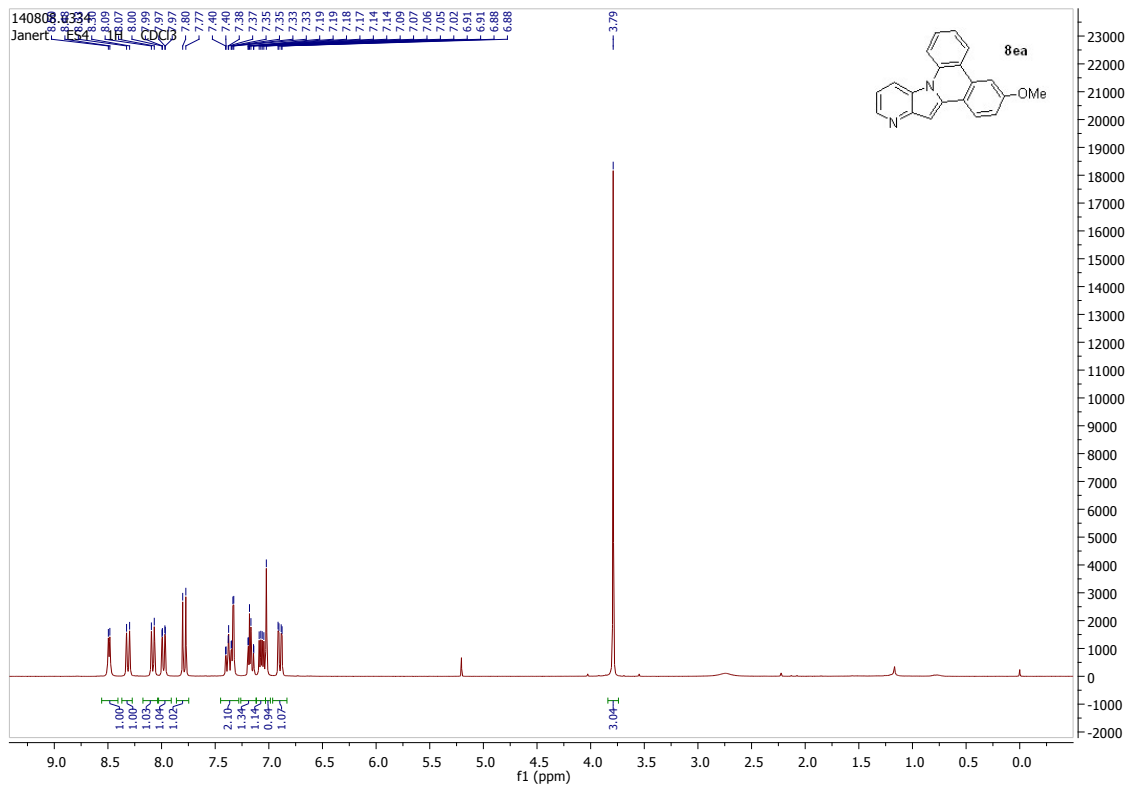


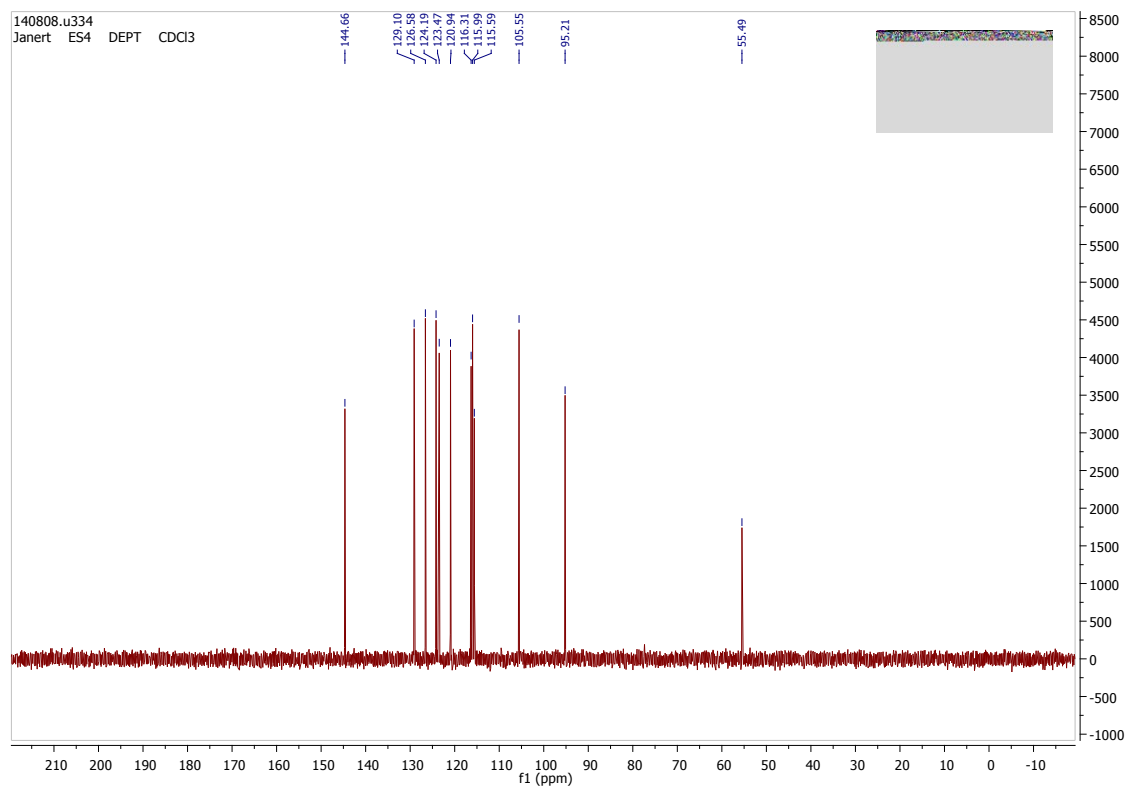
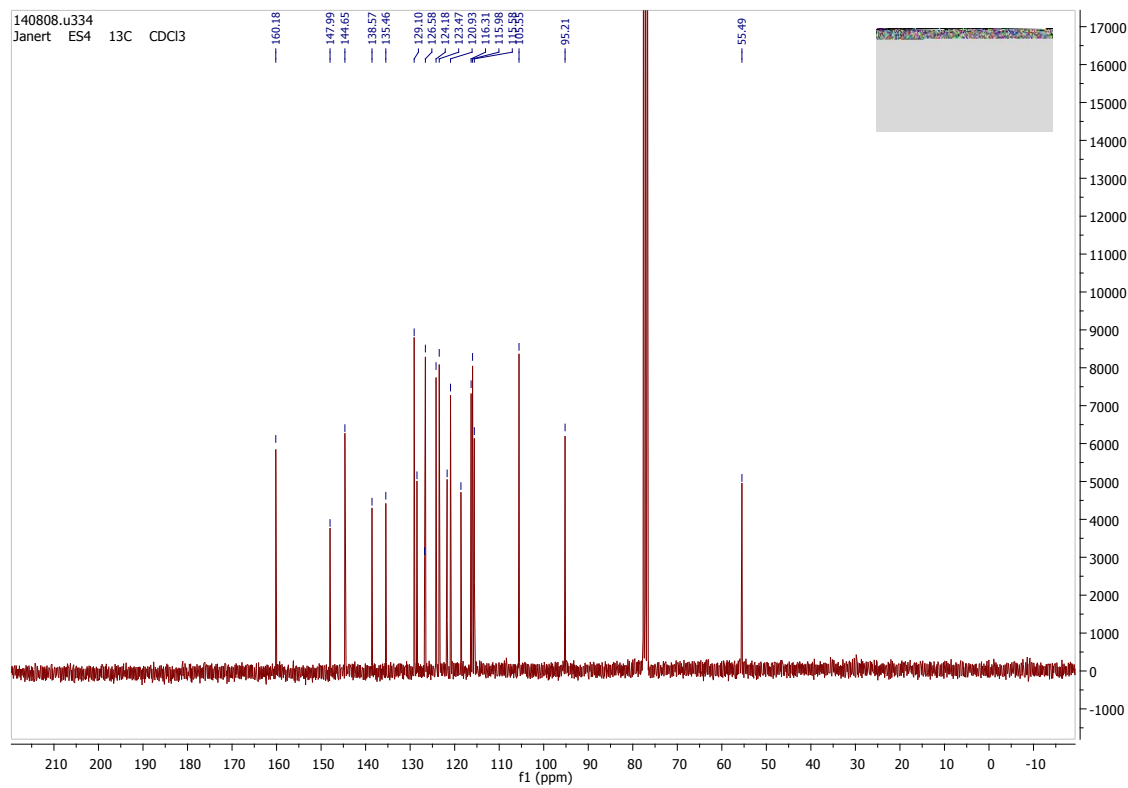
3-fluoropyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 8da



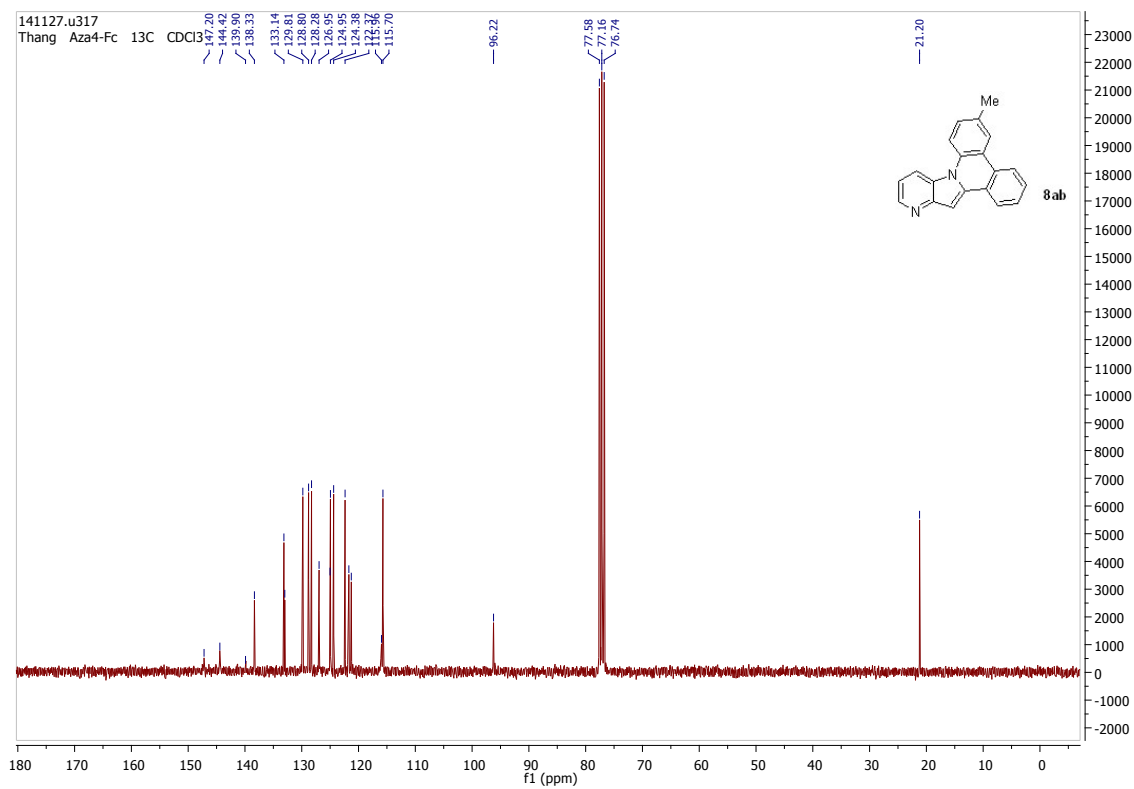
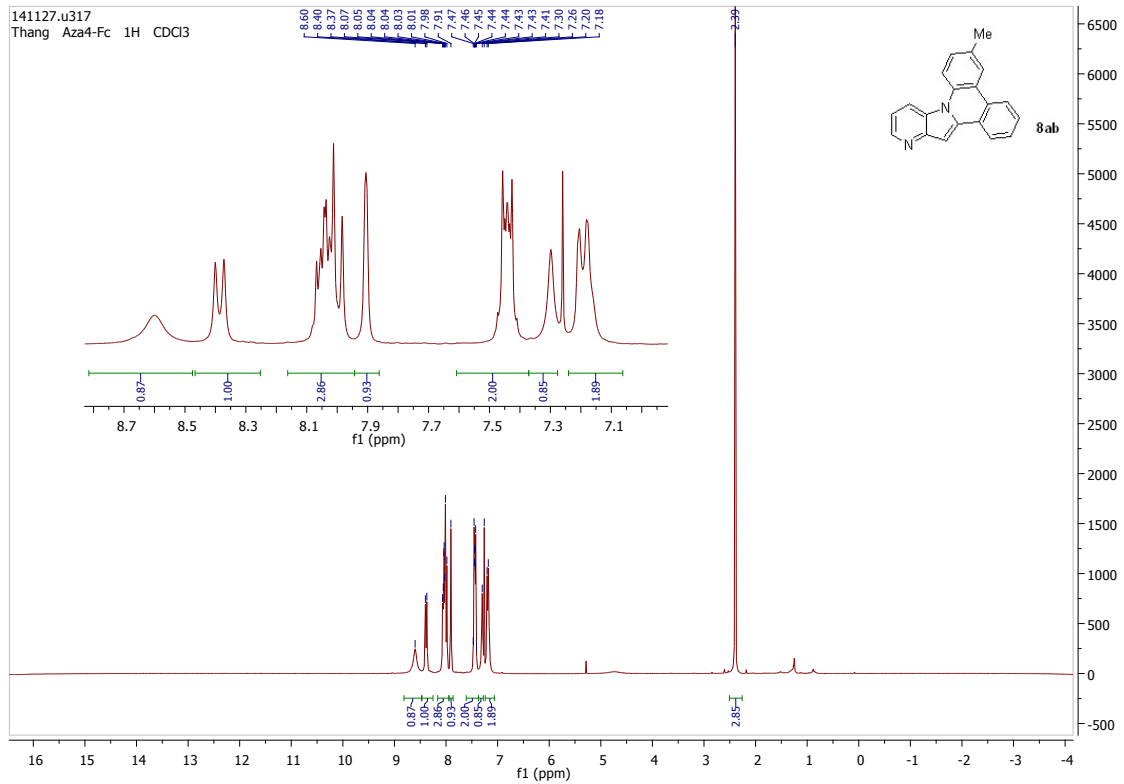


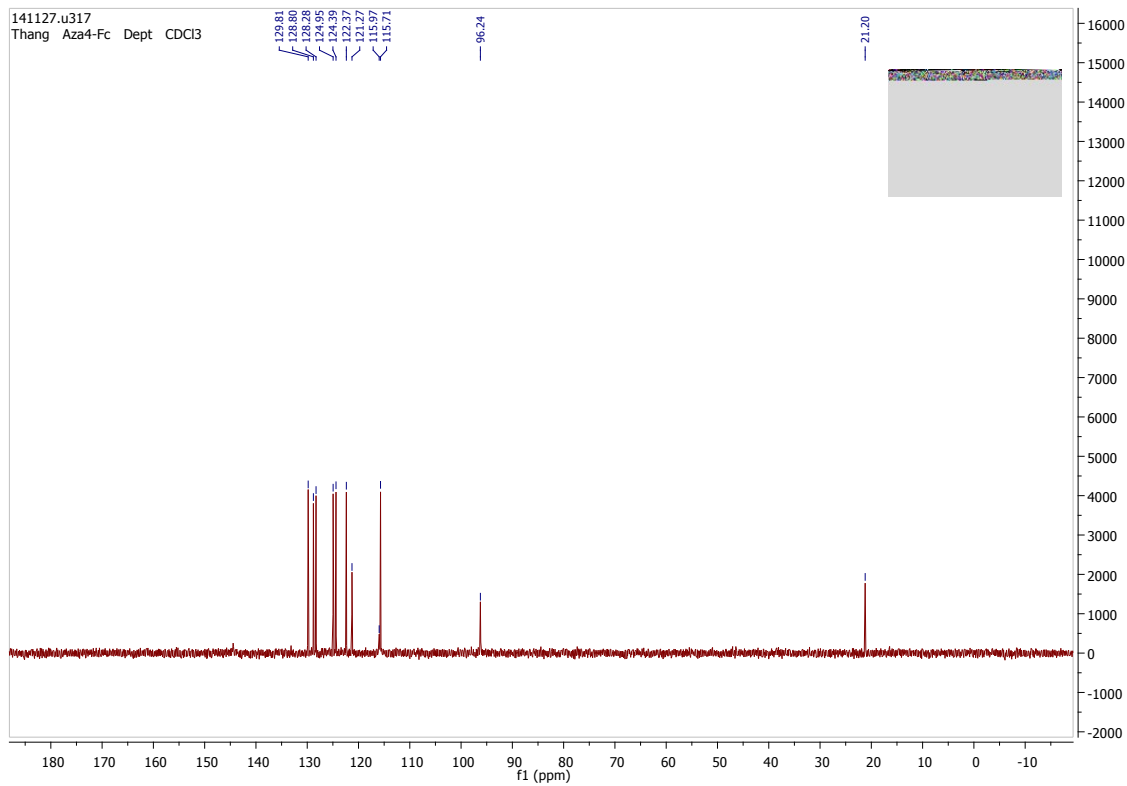
3-methoxypyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine ea



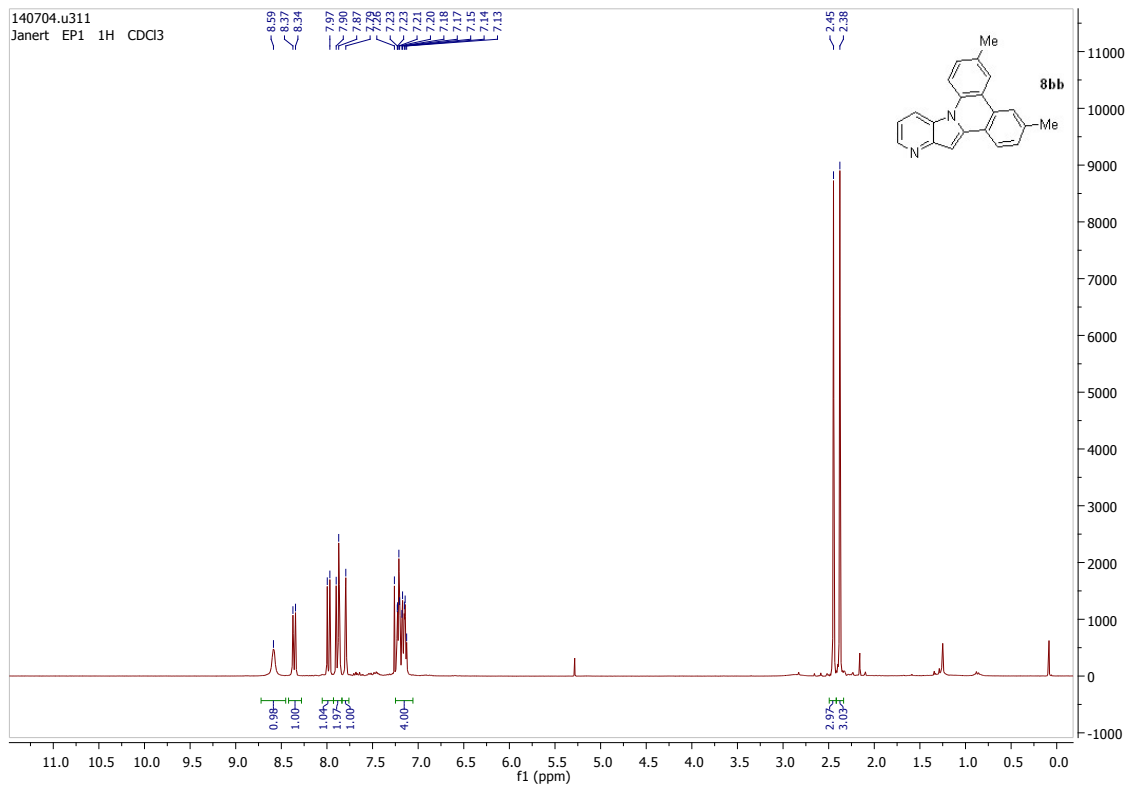


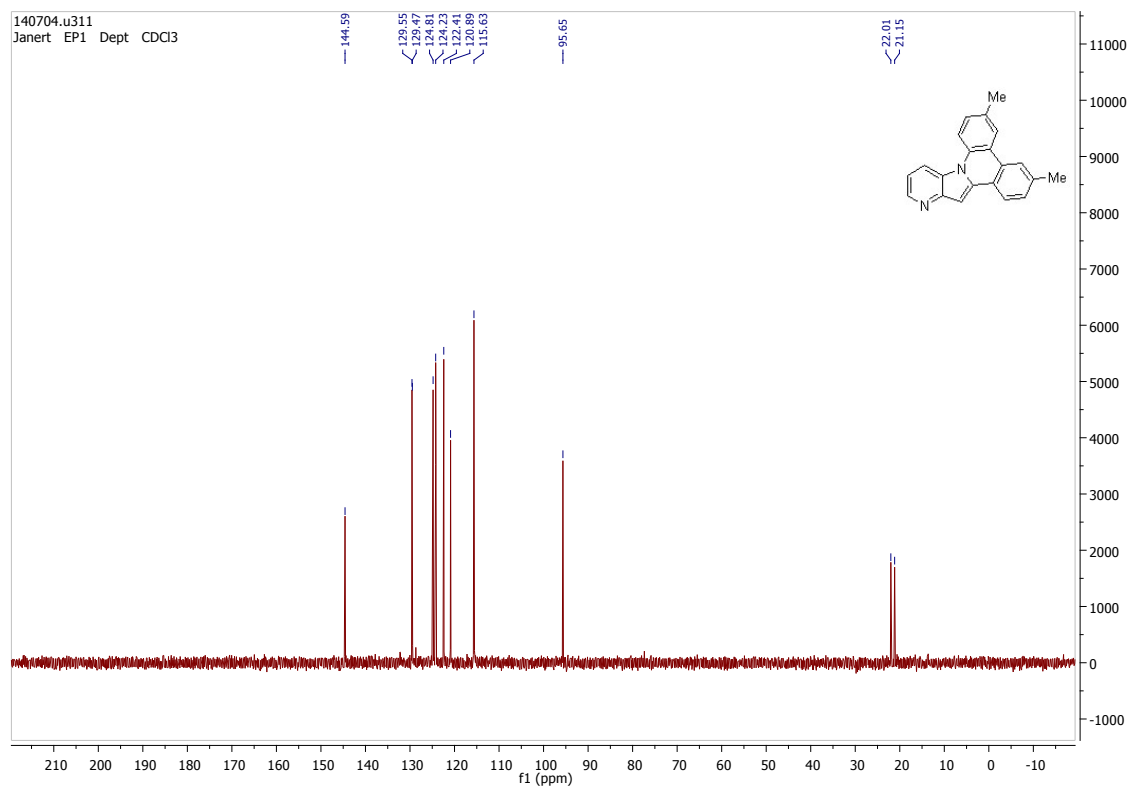
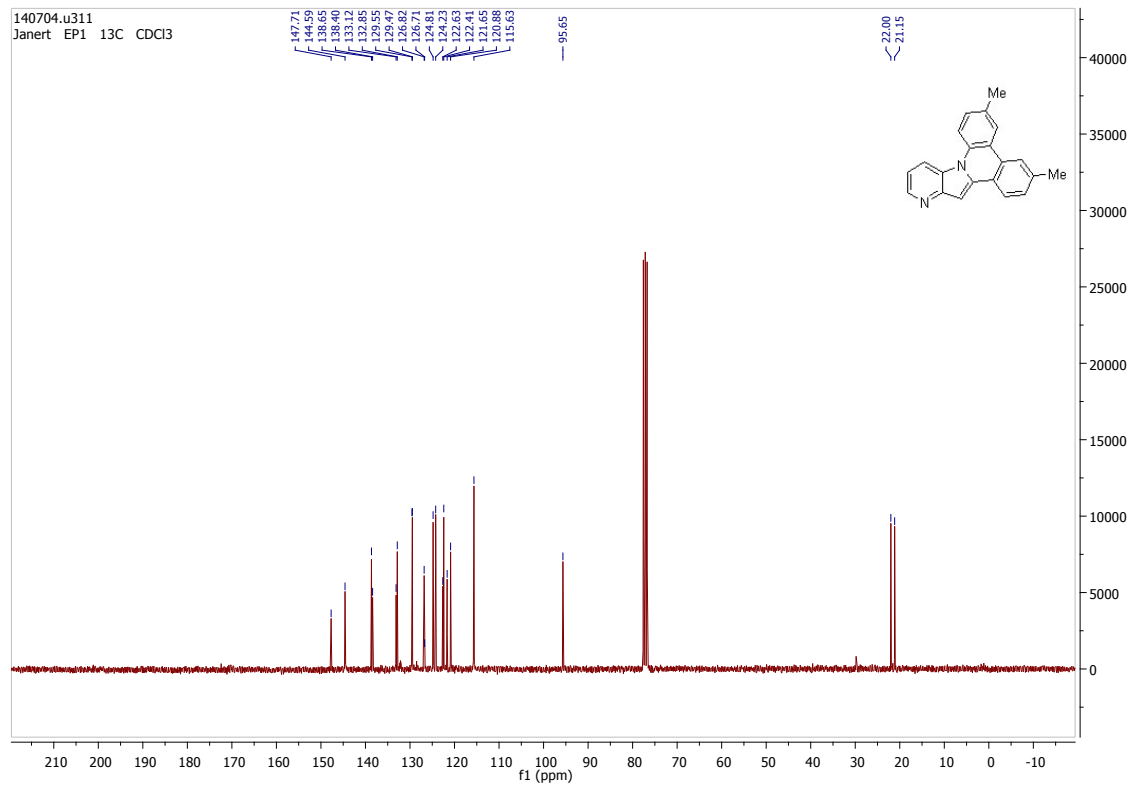
6-methylpyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 8ab





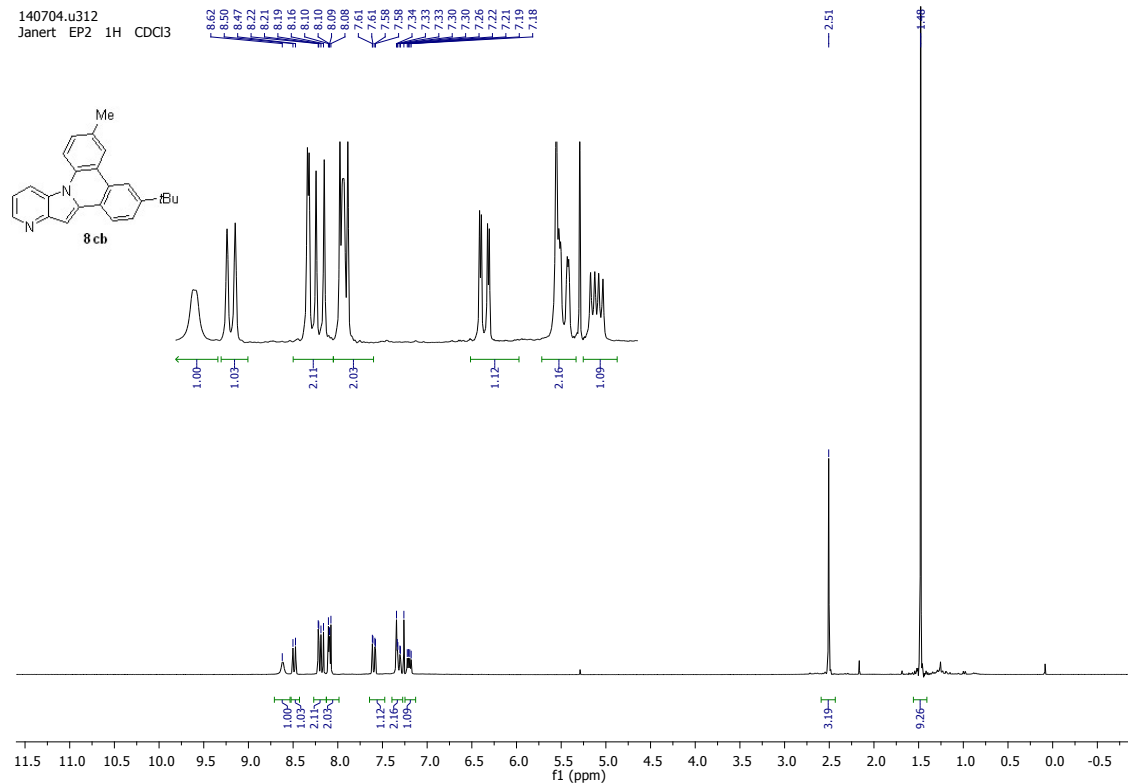
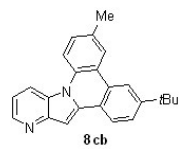
3,6-dimethylpyrido[2,3':4,5]pyrrolo[1,2-f]phenanthridine **8bb**



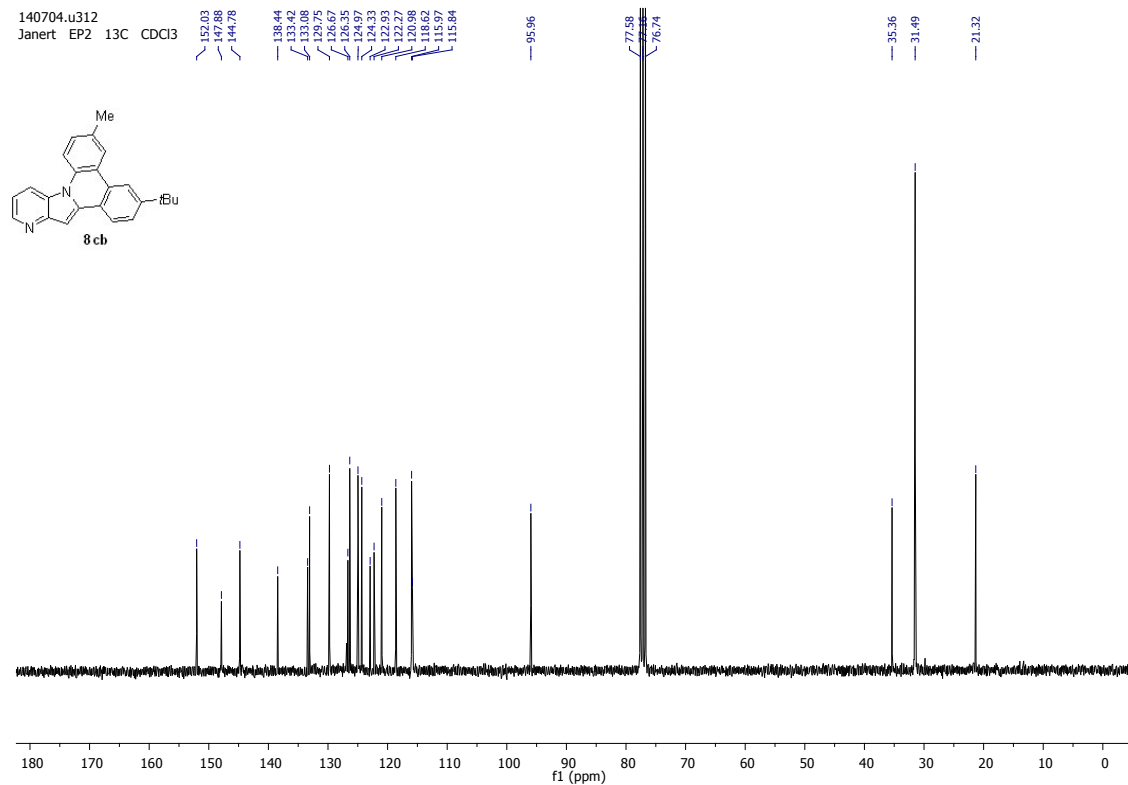
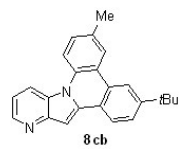


3-(tert-butyl)-6-methylpyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 8cb

140704.u312
Janert EP2 1H CDCl3



140704.u312
Janert EP2 13C CDCl3



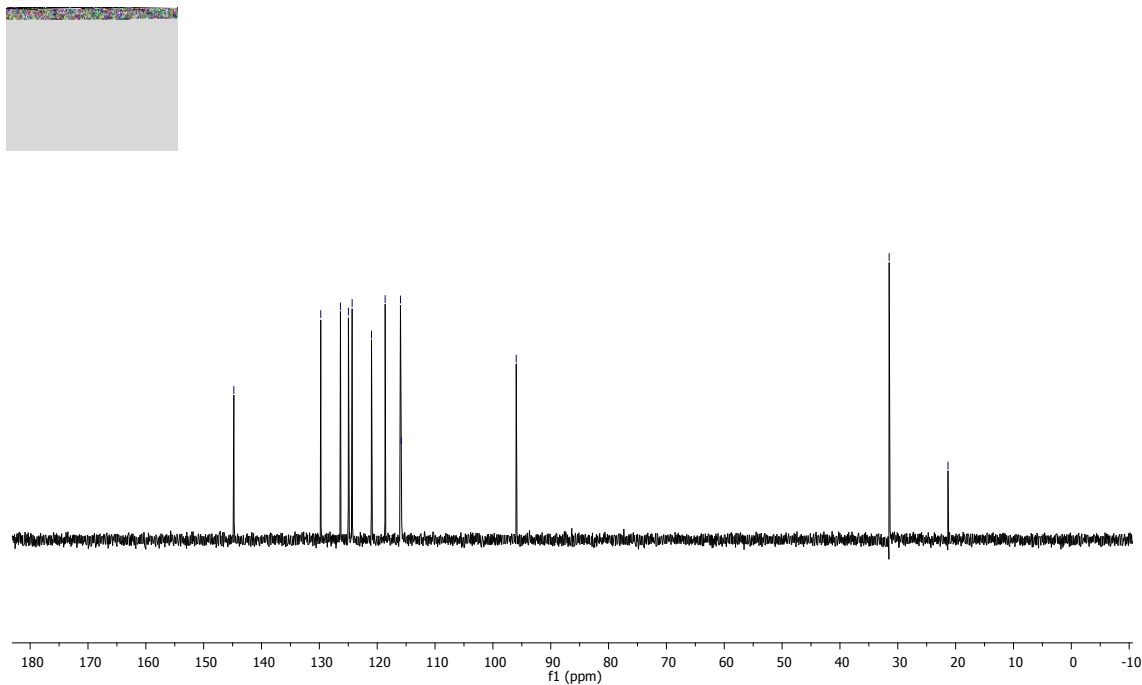
140704.u312
Janert EP2 Dept CDCl3

144.79
128.76
126.35
124.98
120.99
118.62
115.84

95.97

31.49

21.32

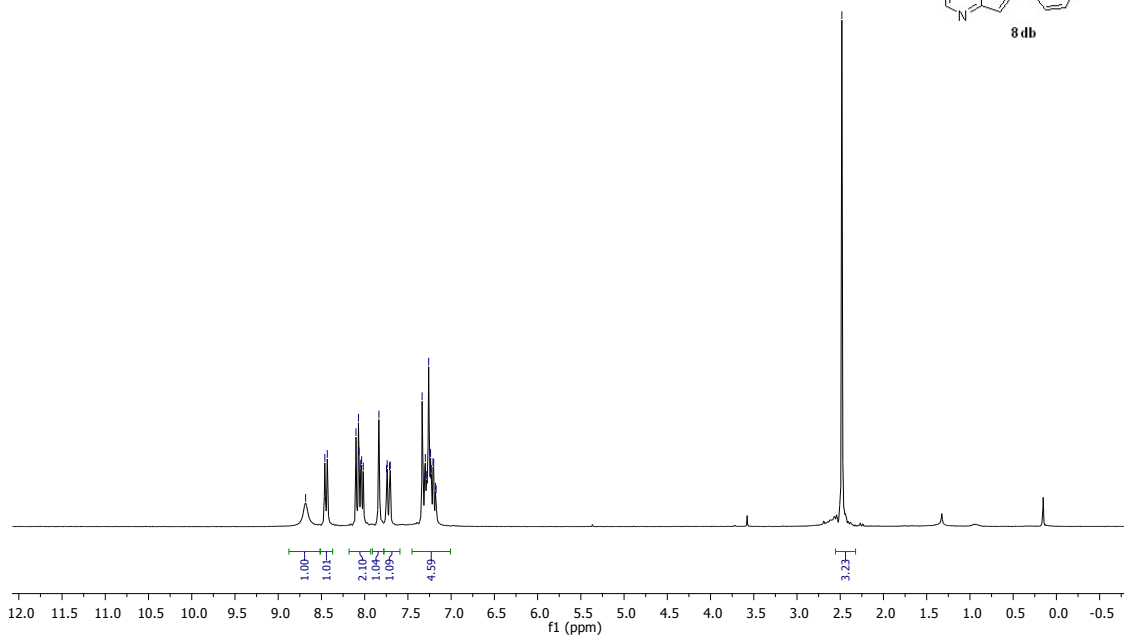
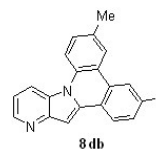


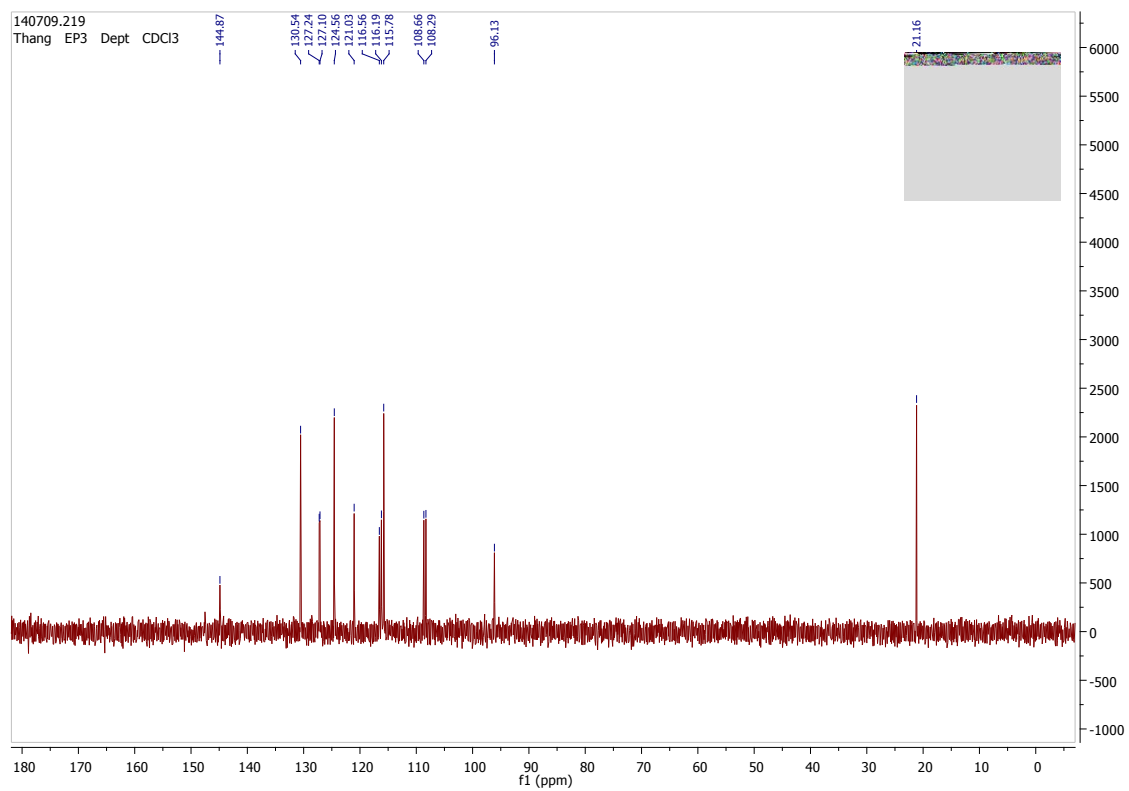
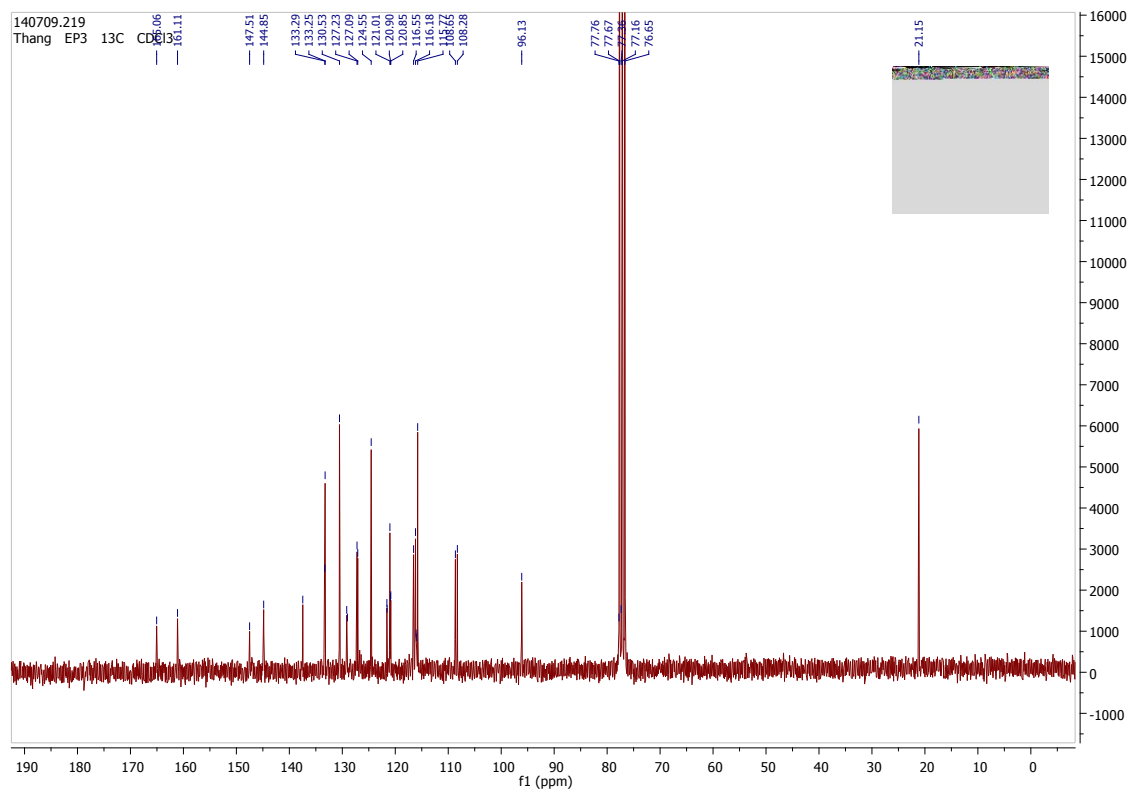
3-fluoro-6-methylpyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 8db

140709.u324
Thang EP3 1H CDCl3

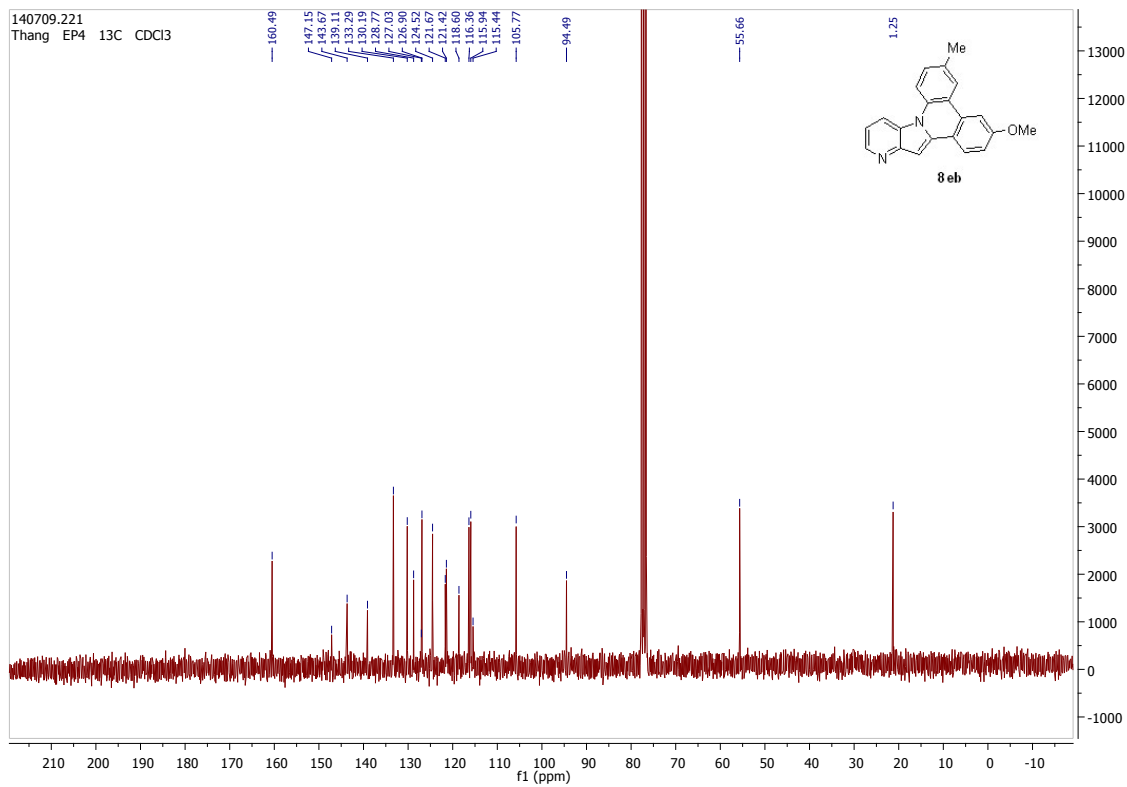
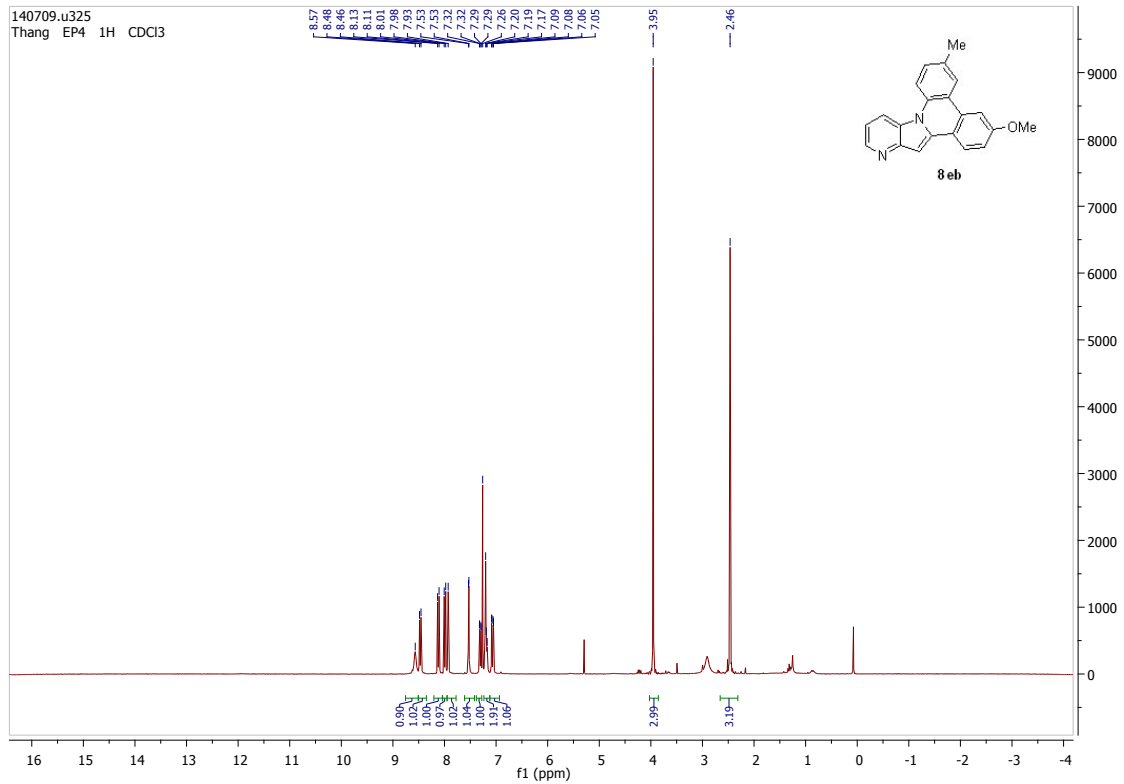
8.68
8.46
8.43
8.10
8.07
8.04
7.94
7.30
7.28
7.26
7.24
7.23
7.21
7.20
7.18
7.17

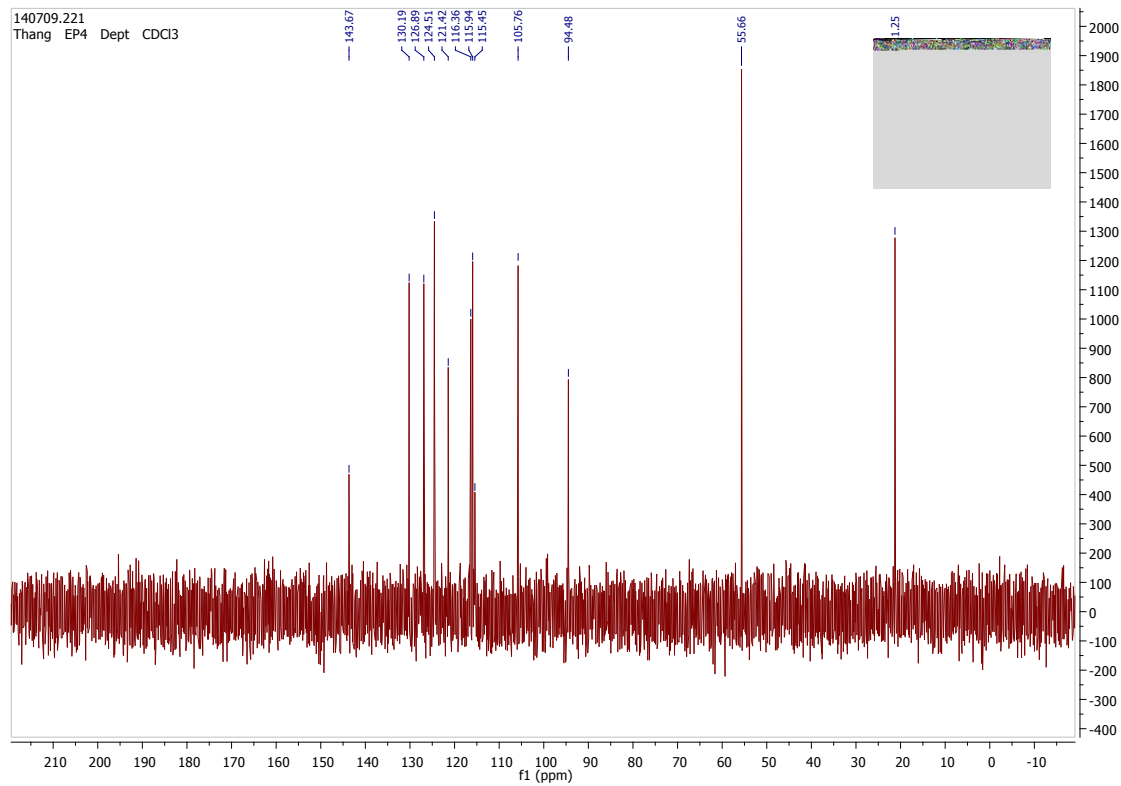
2.48



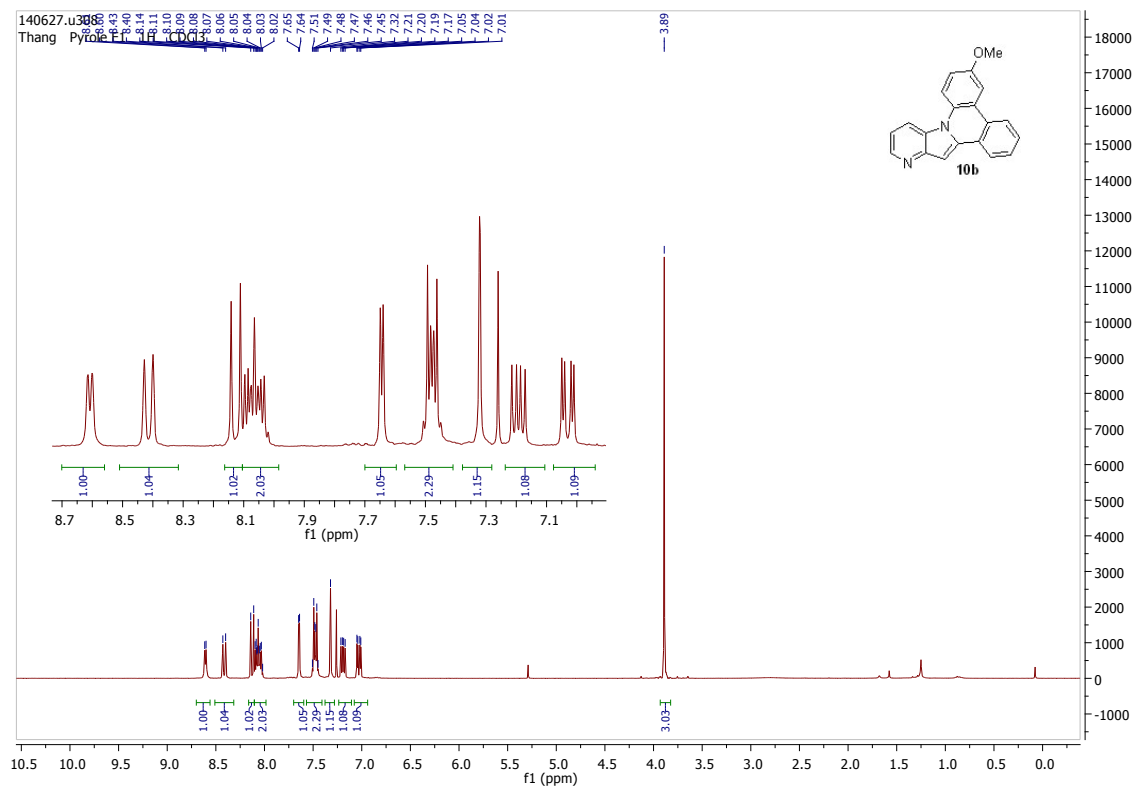


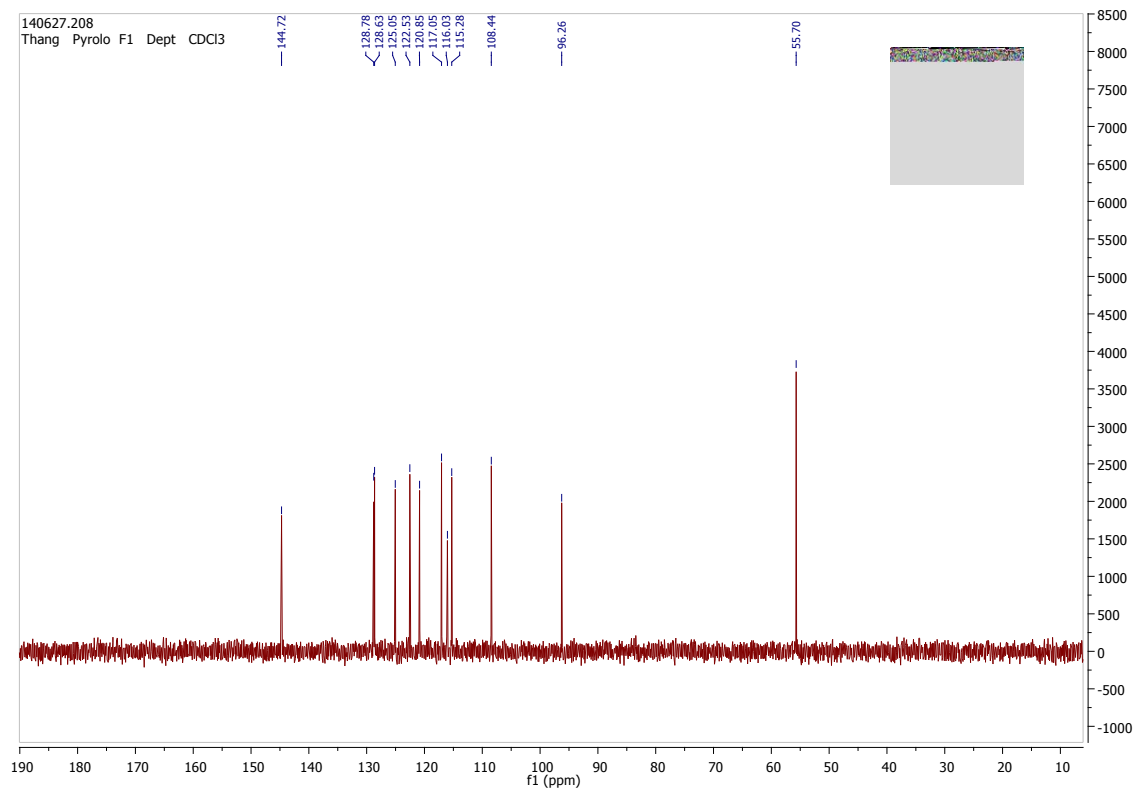
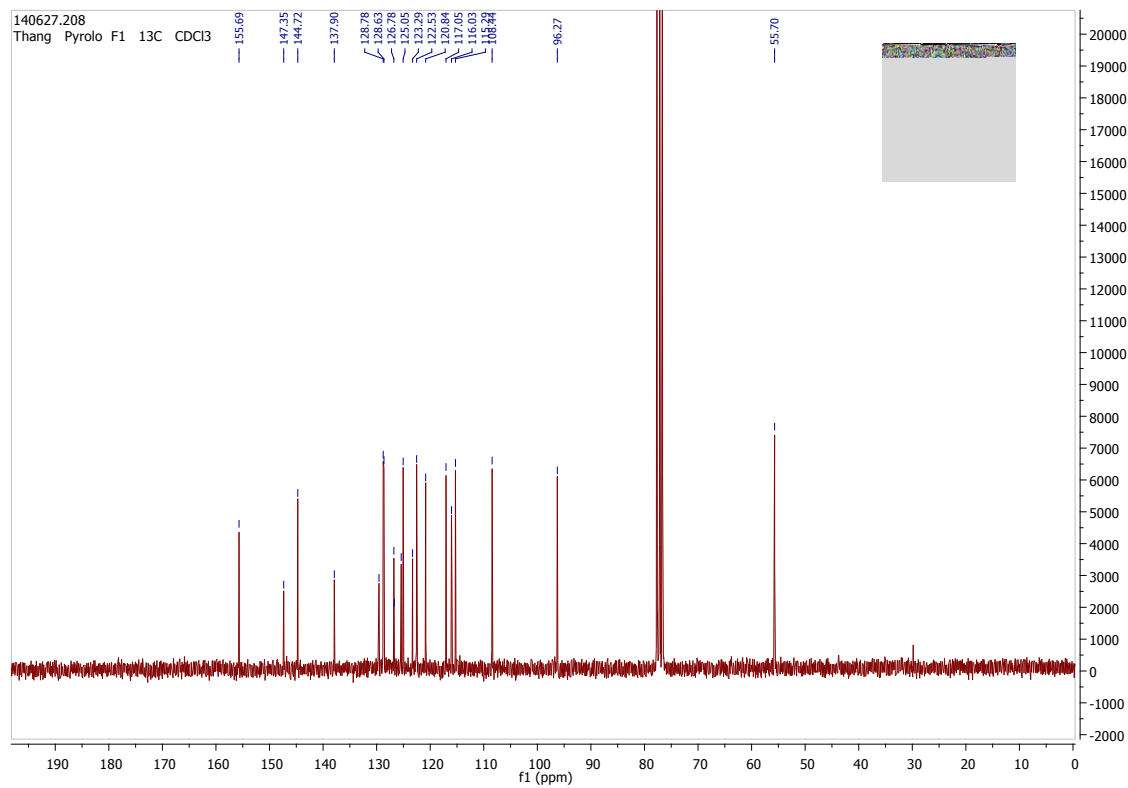
3-methoxy-6-methylpyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 8b



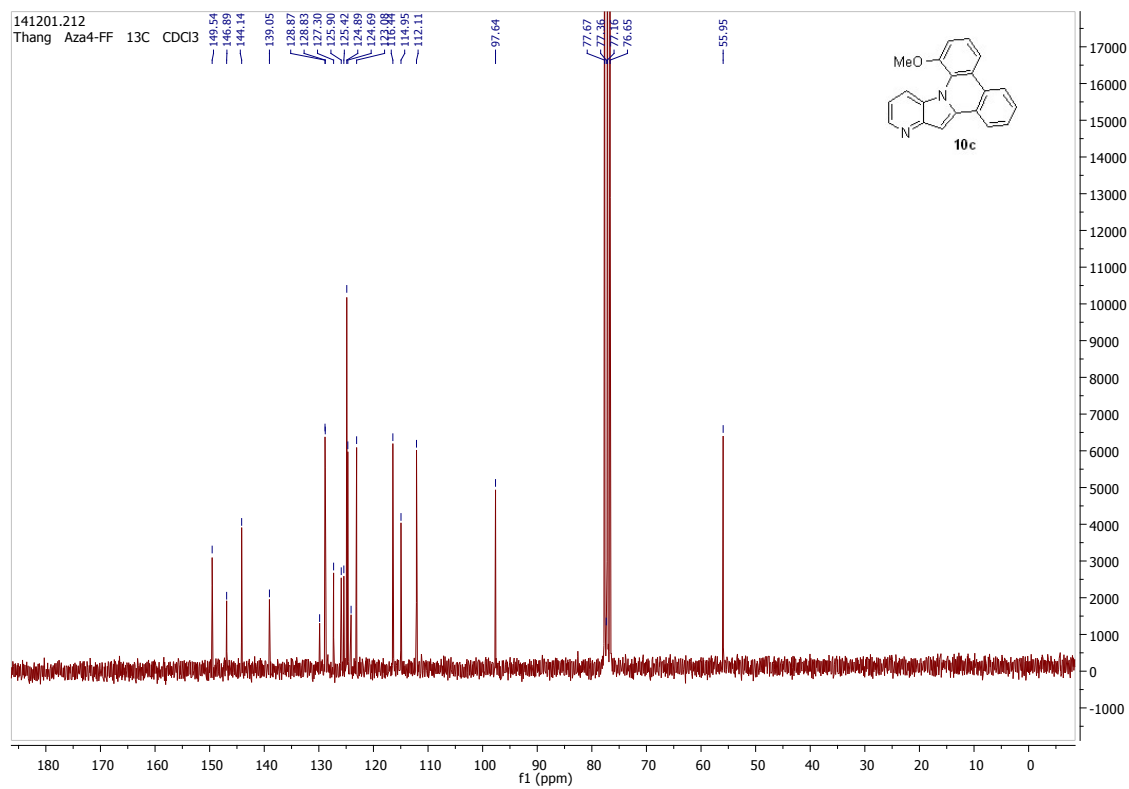
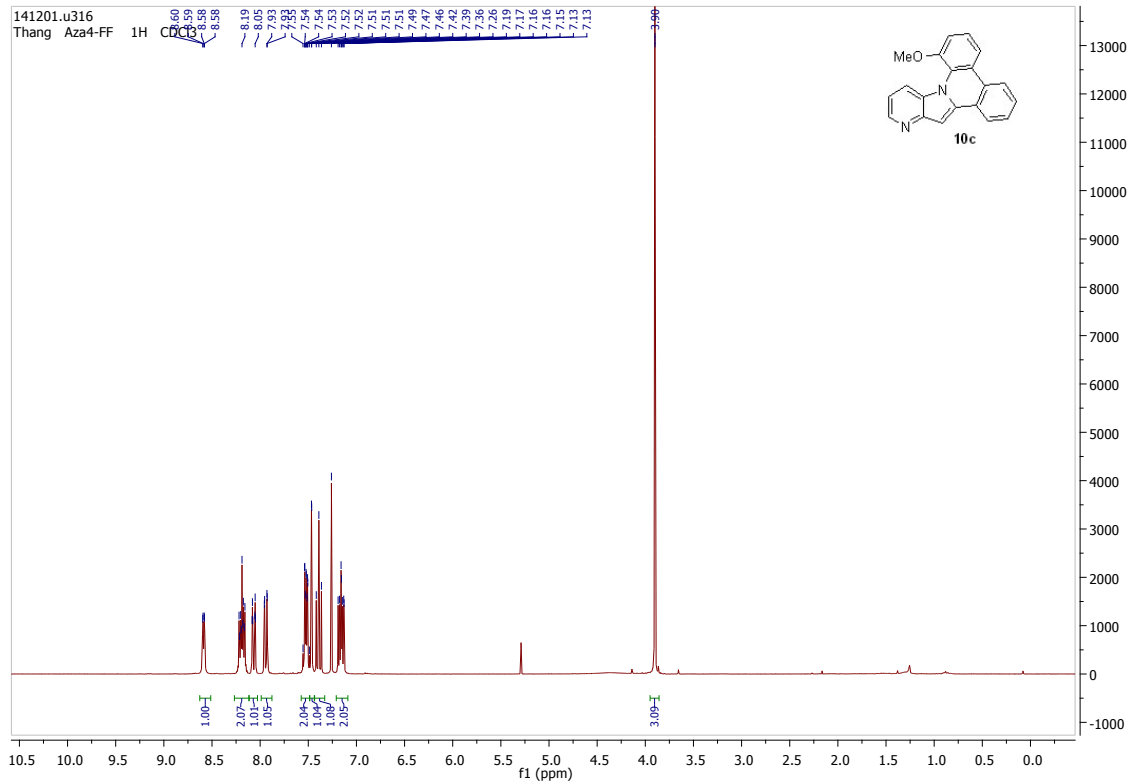


6-methoxypyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 10b

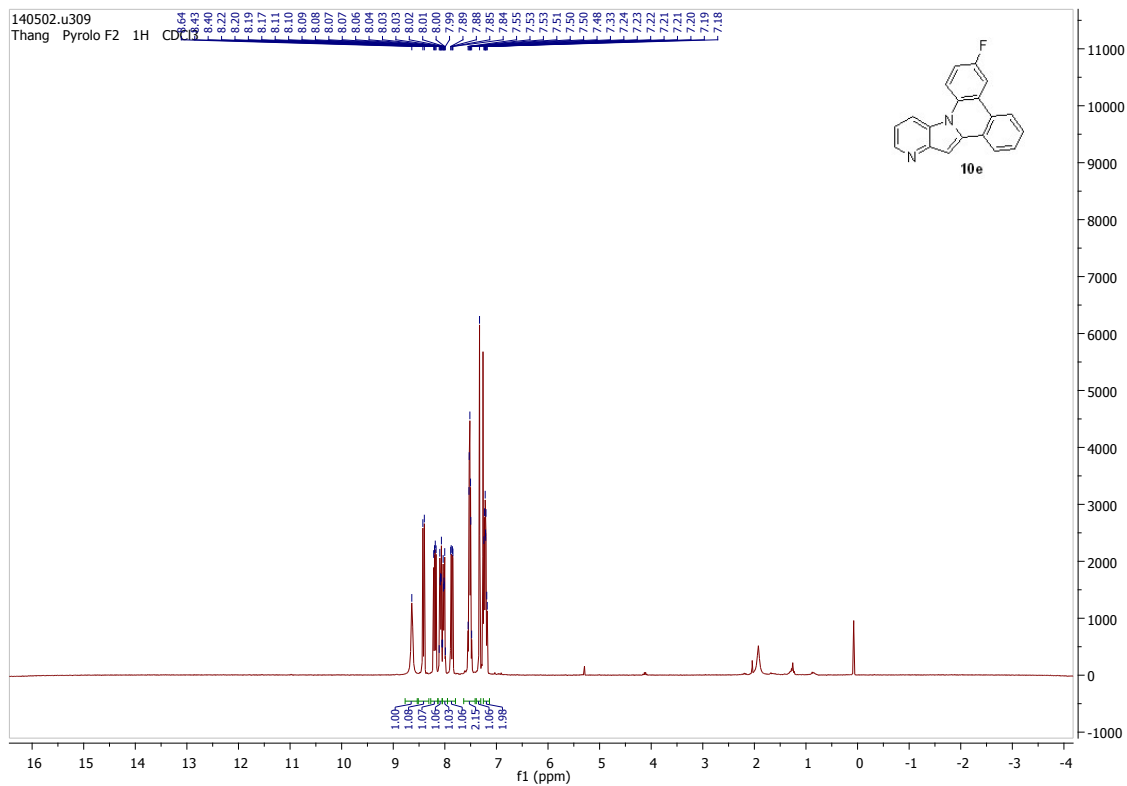
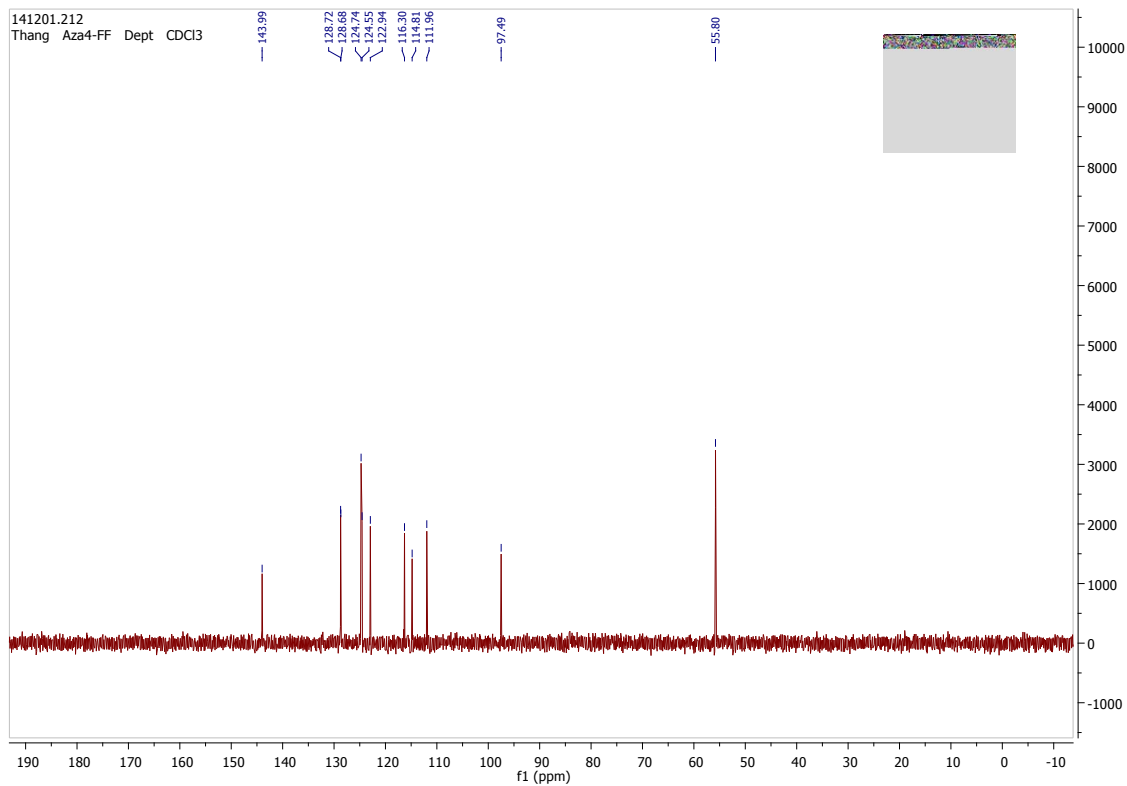


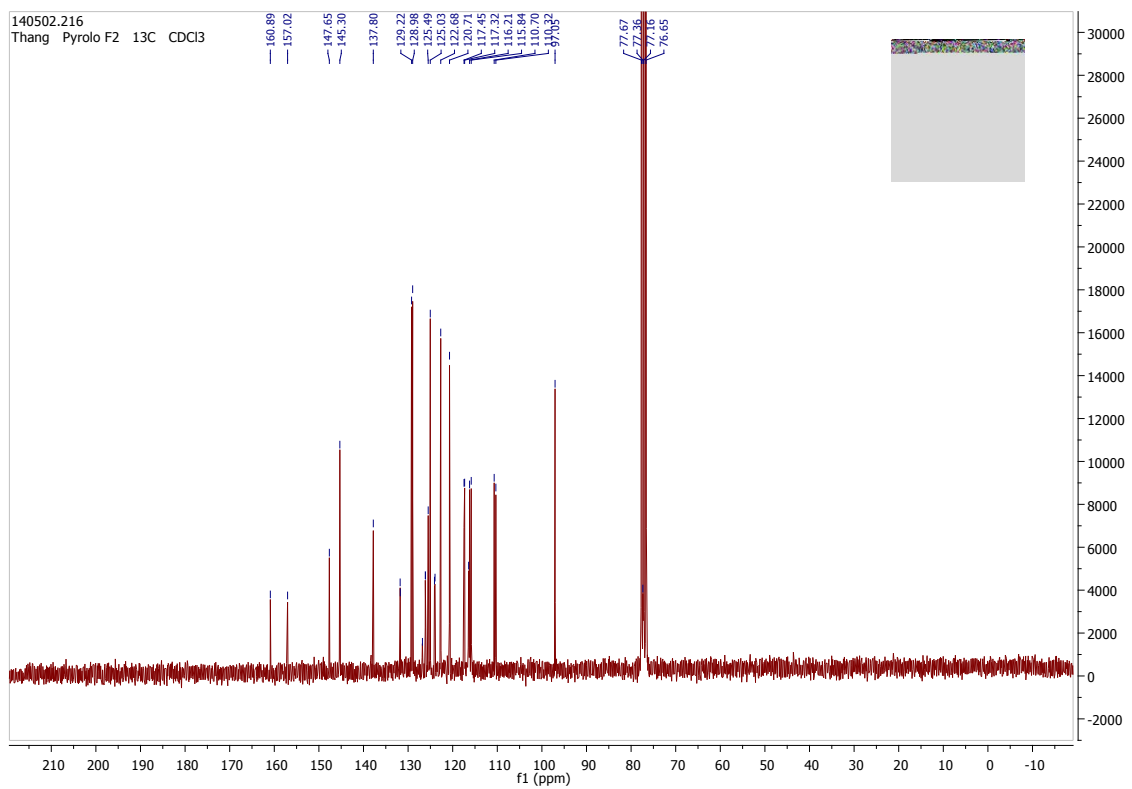
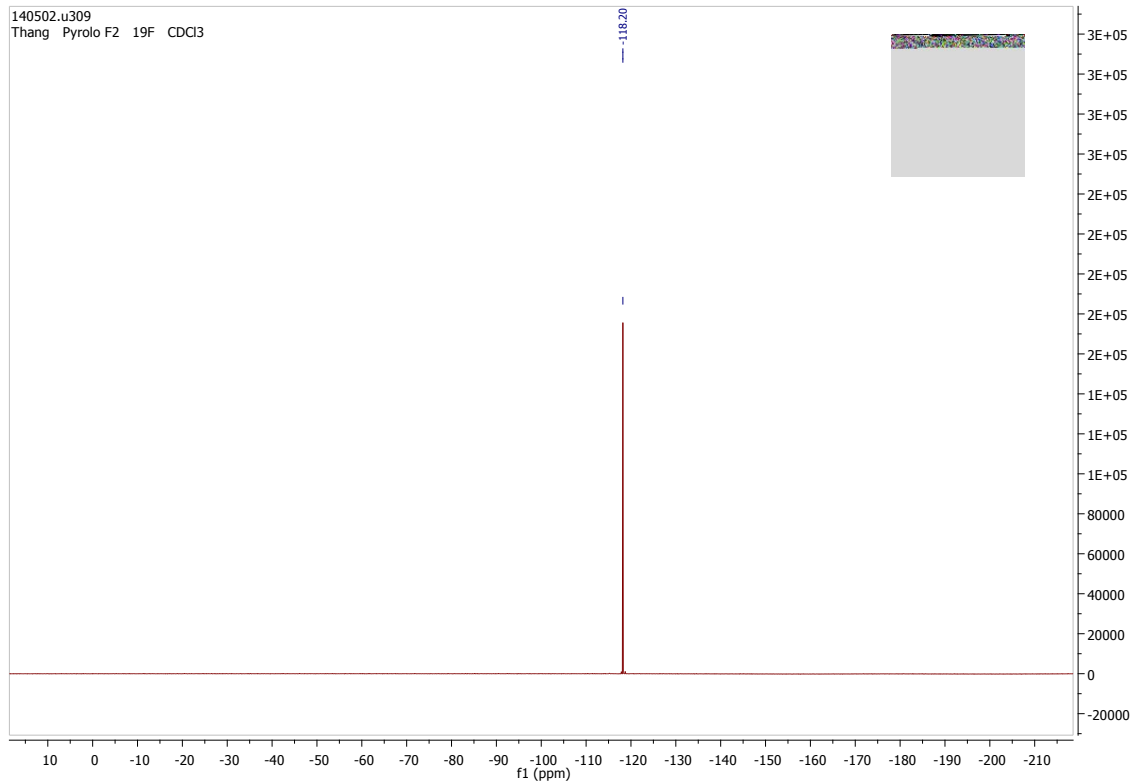


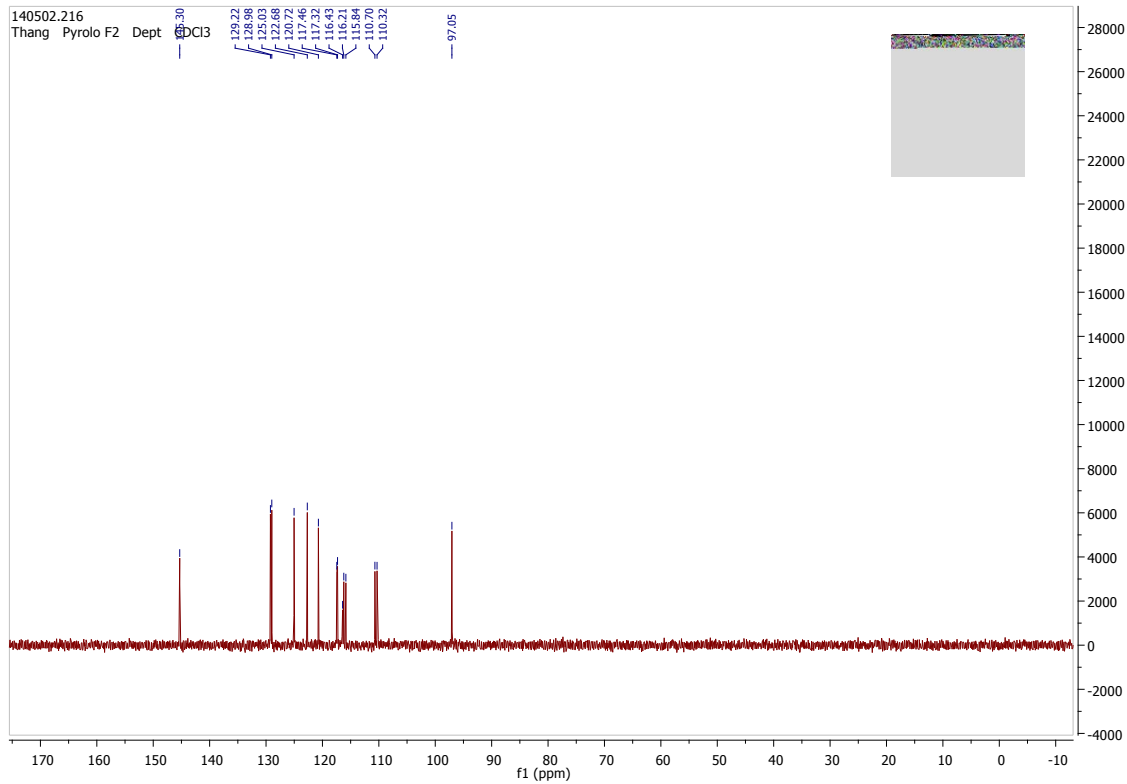
8-methoxypyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 10c



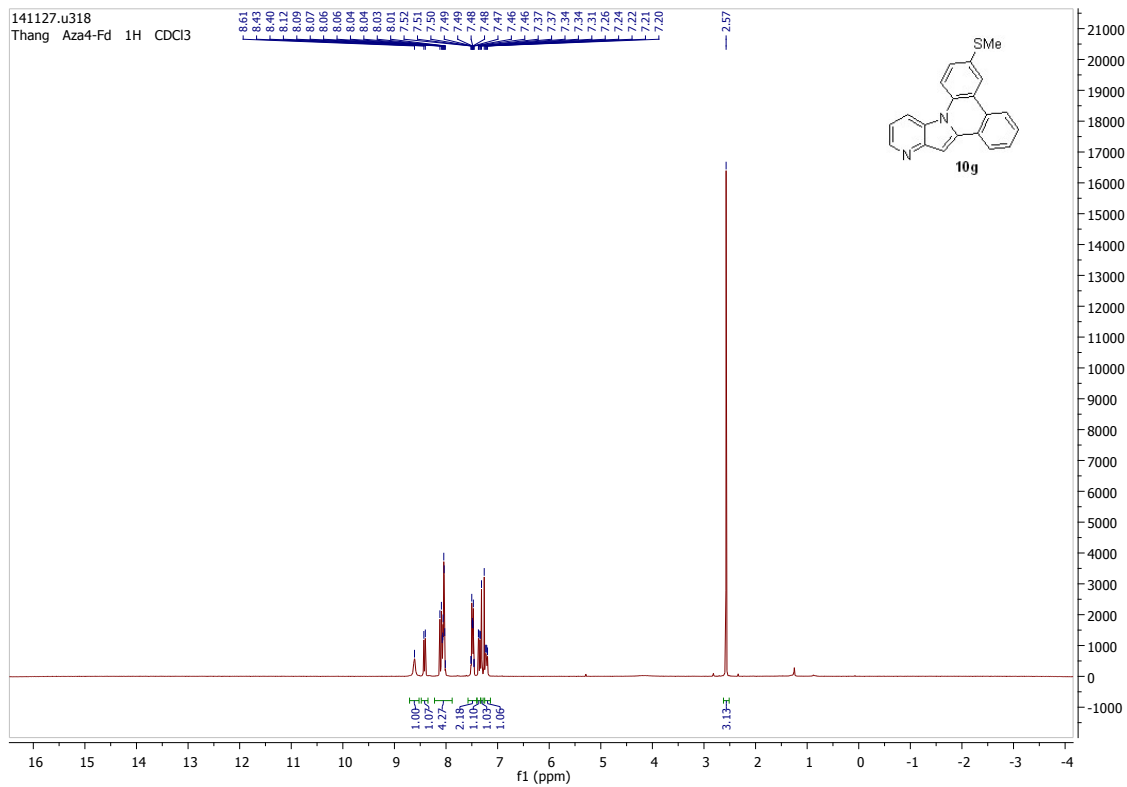
6-fluoropyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 8ac

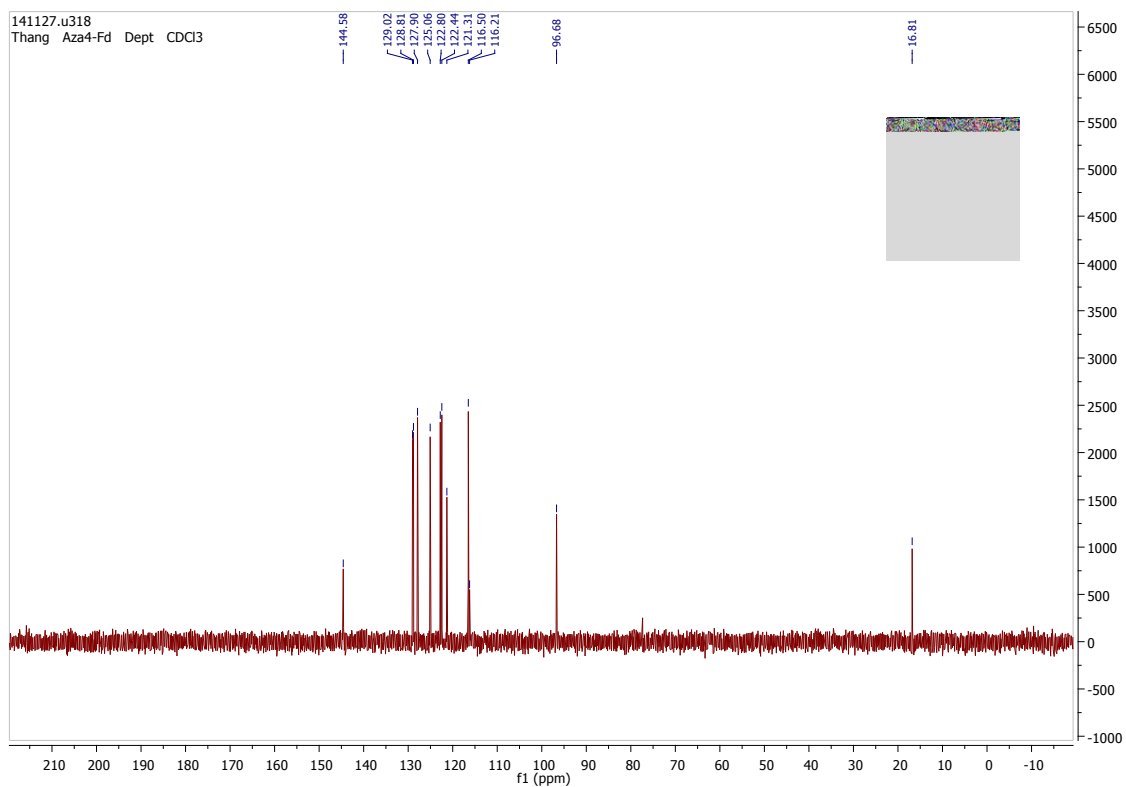
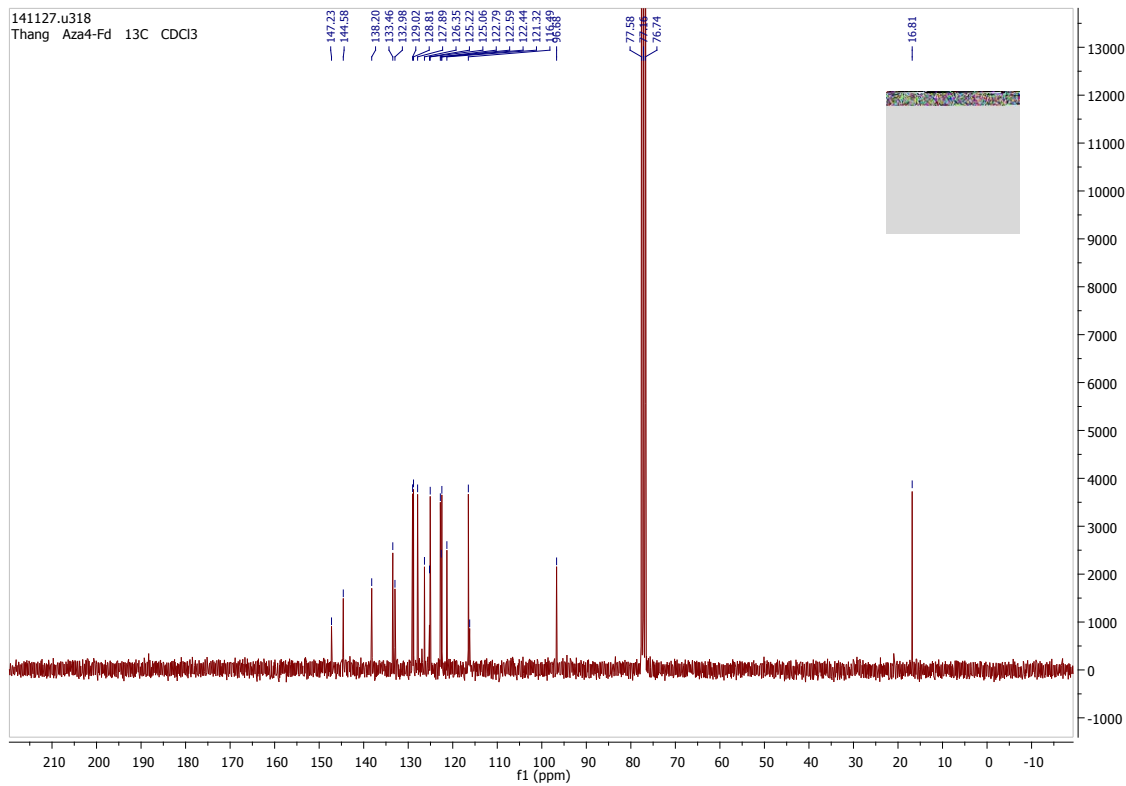




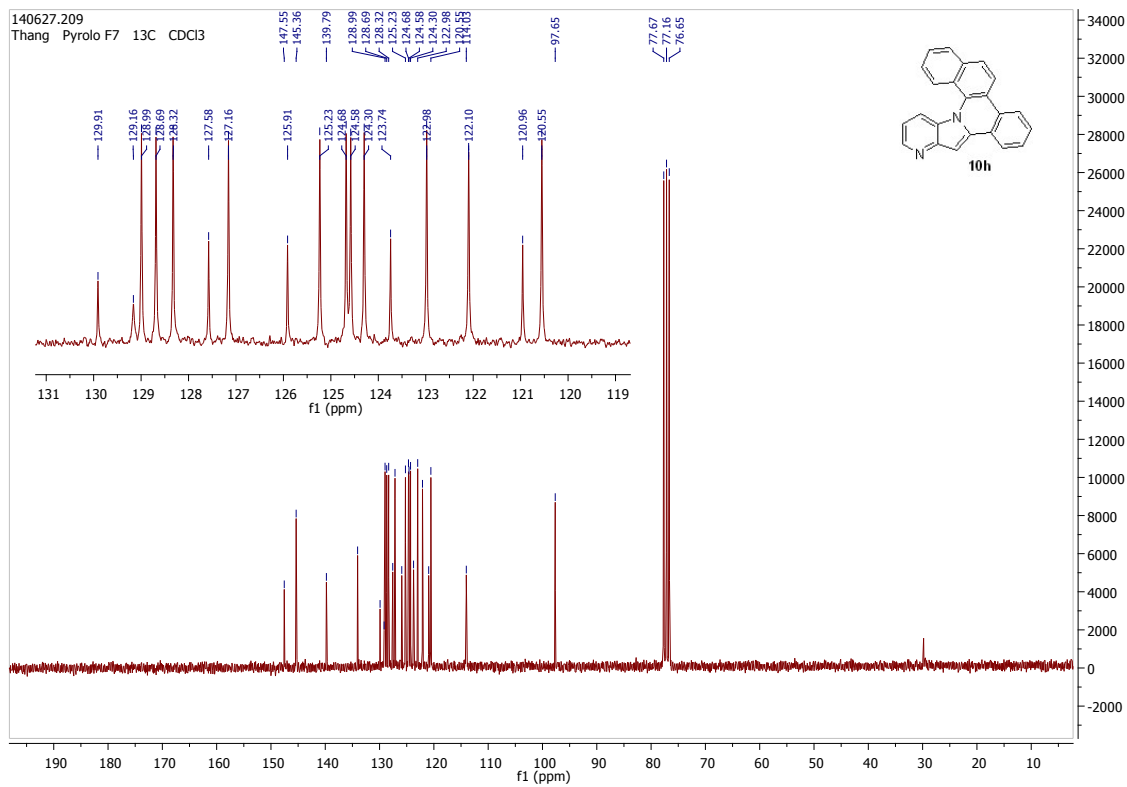
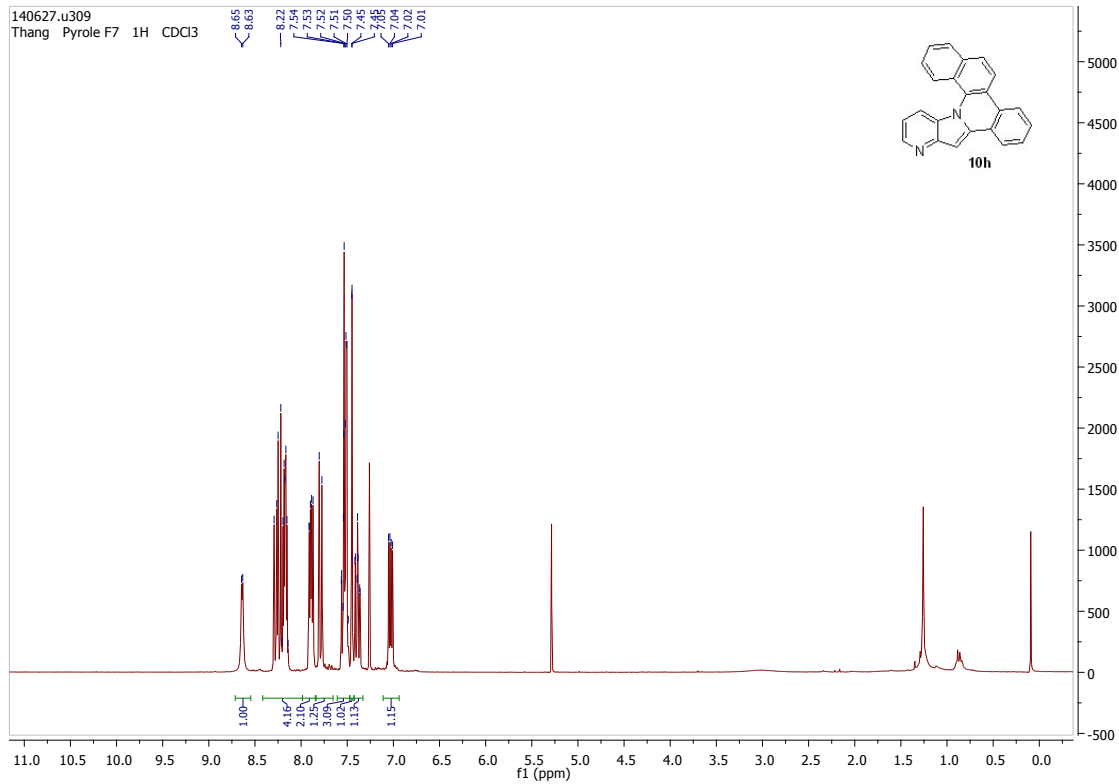


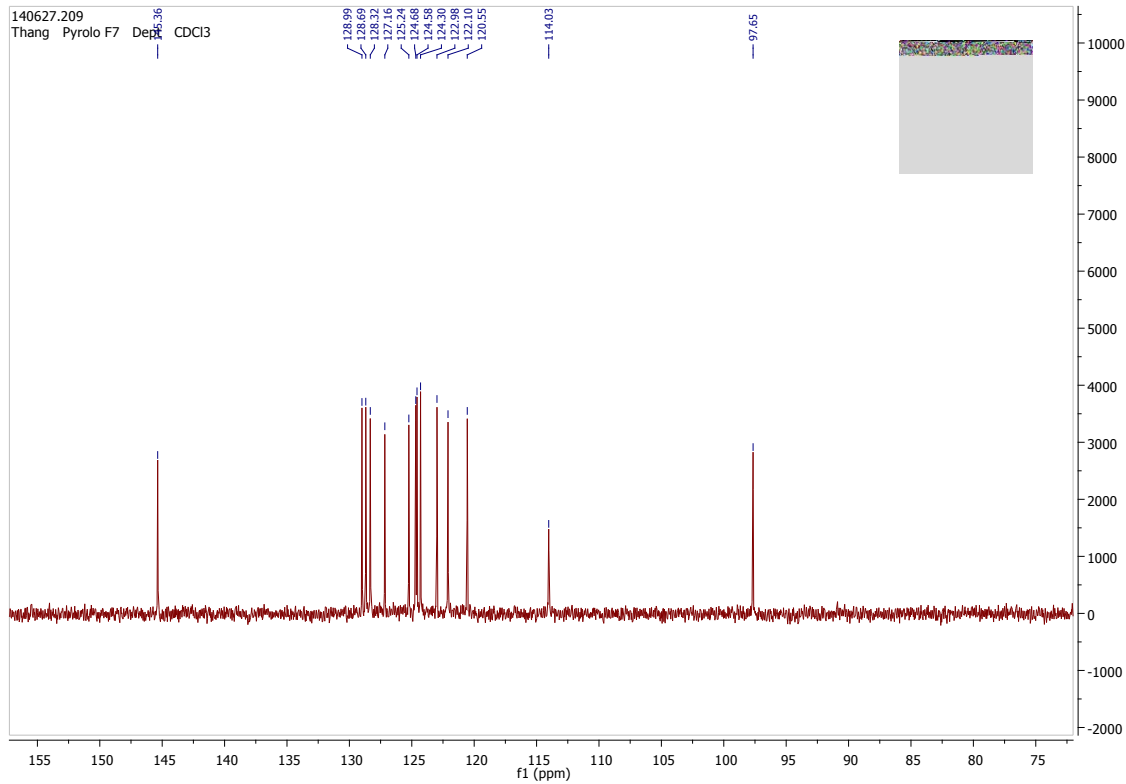
6-(methylthio)pyrido[2',3':4,5]pyrrolo[1,2-f]phenanthridine 10g



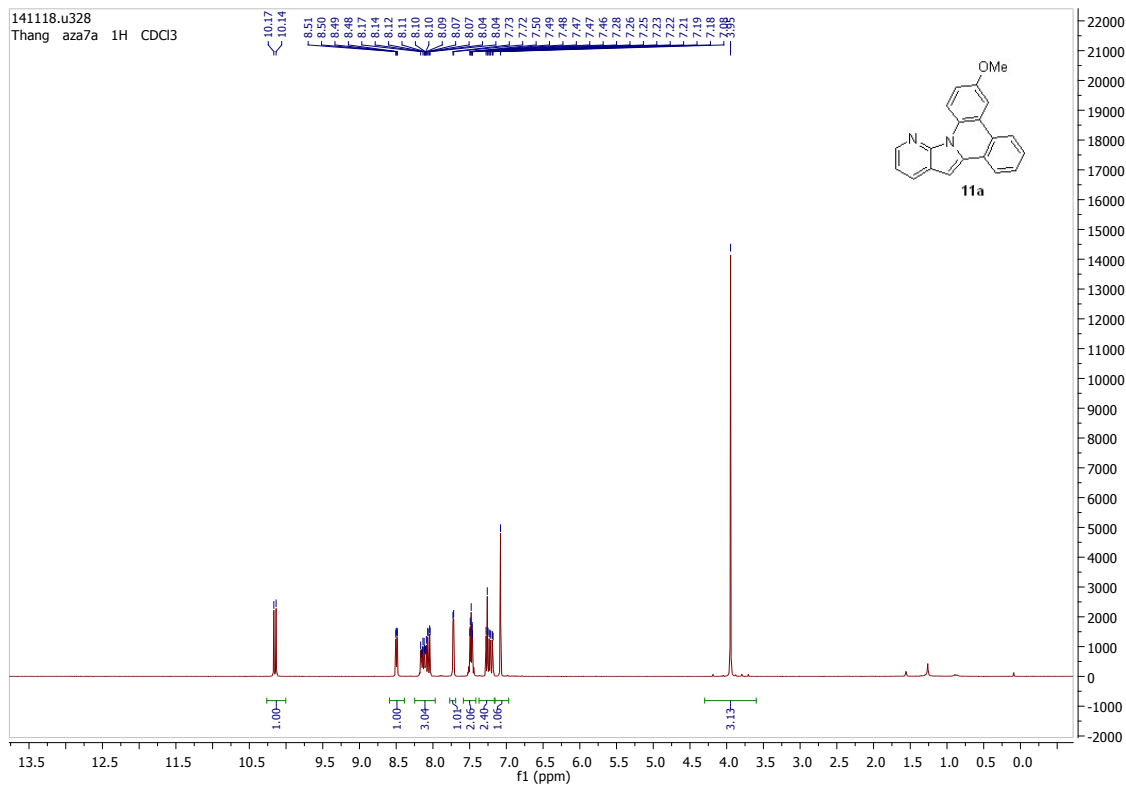


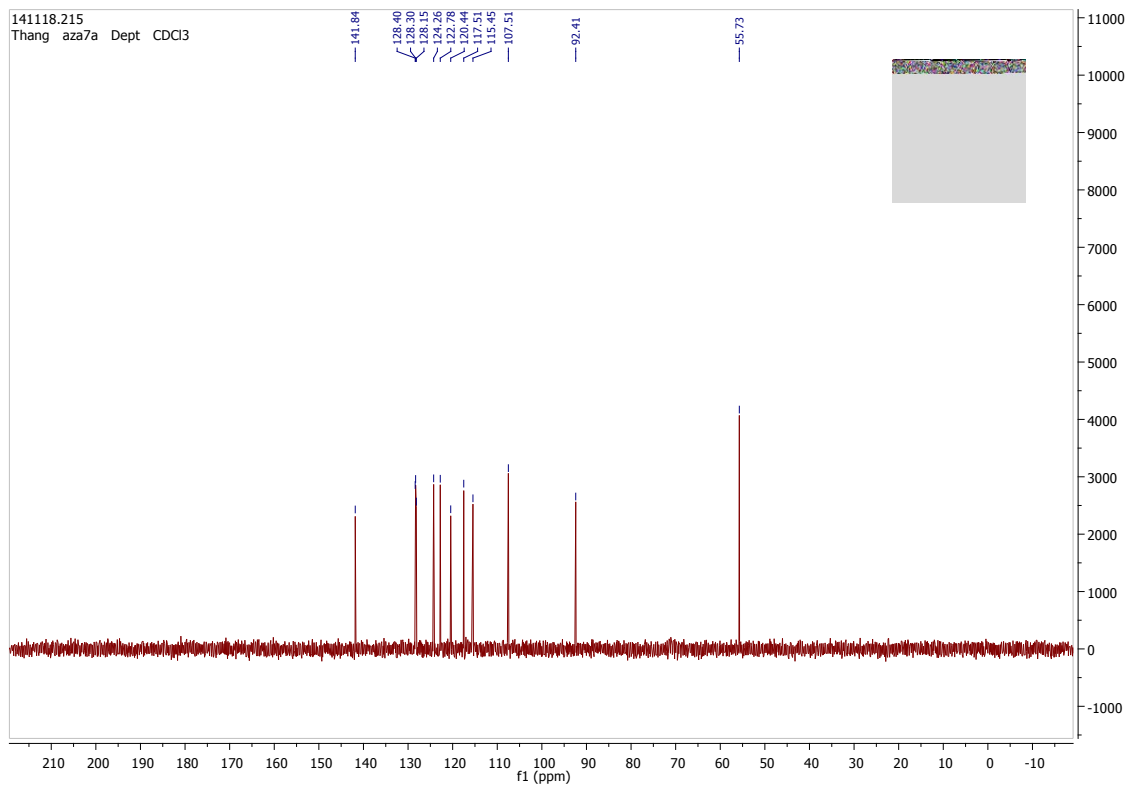
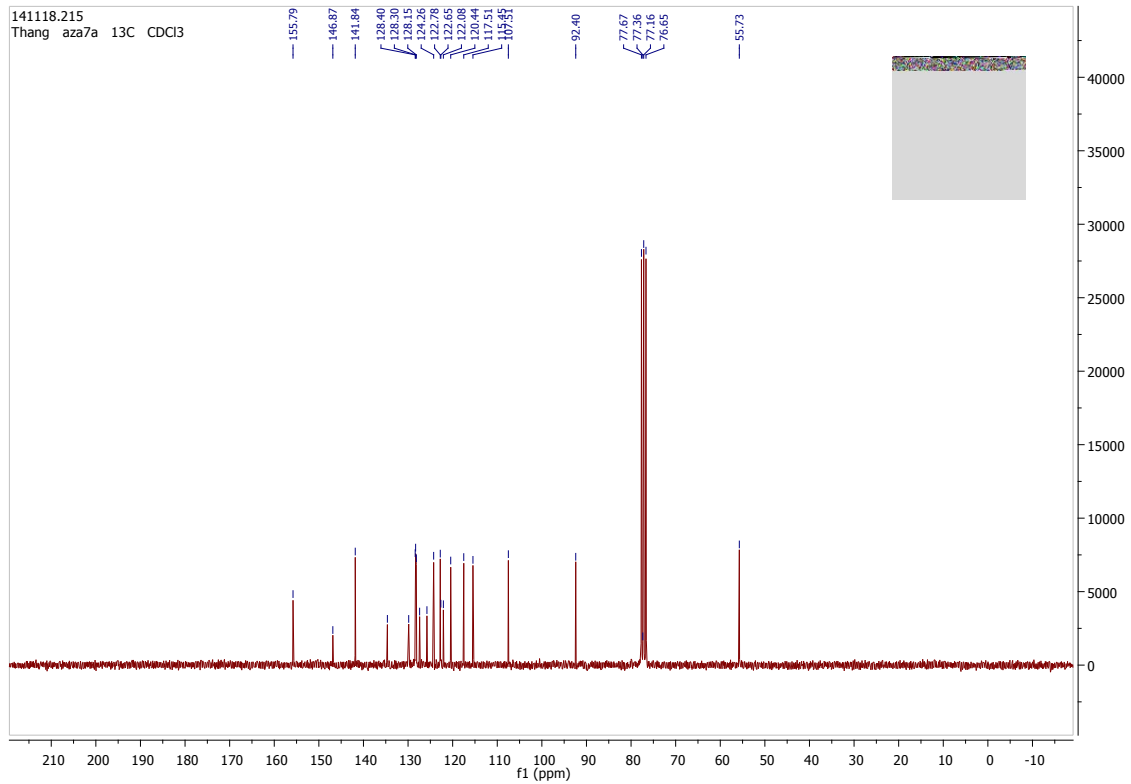
Benzo[*c*]pyrido[2',3':4,5]pyrrolo[1,2-*f*]phenanthridine 10h



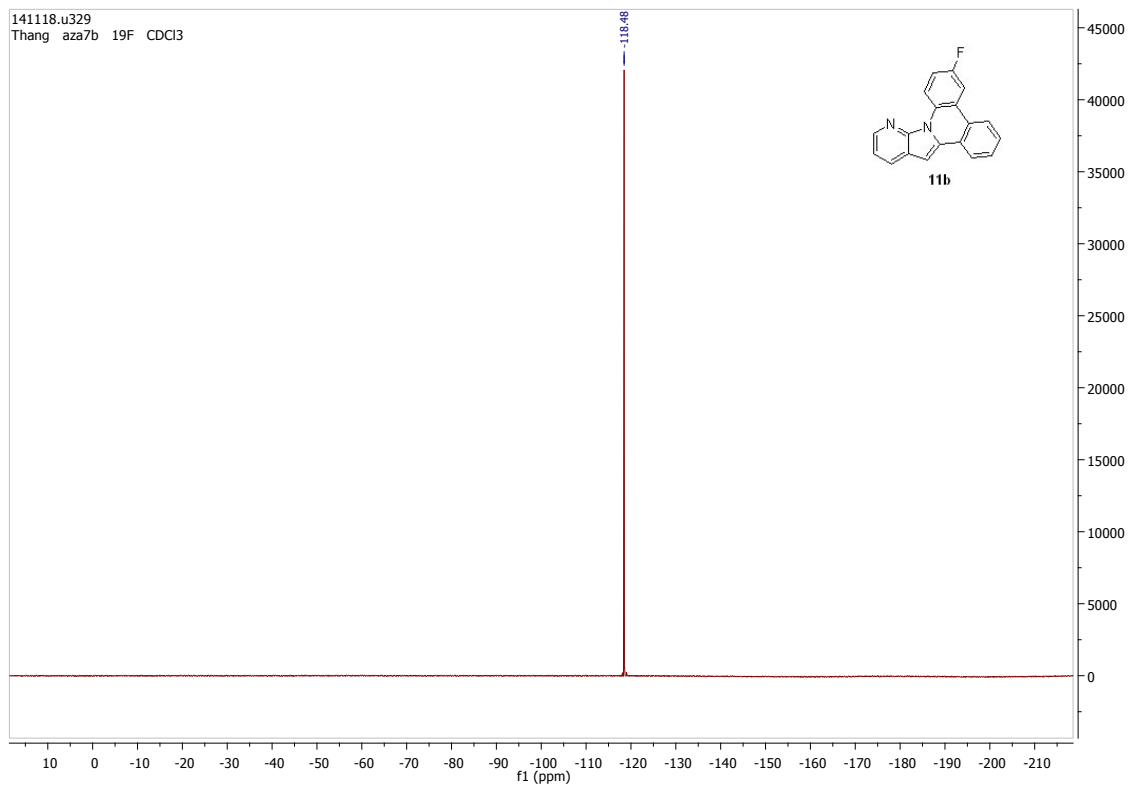
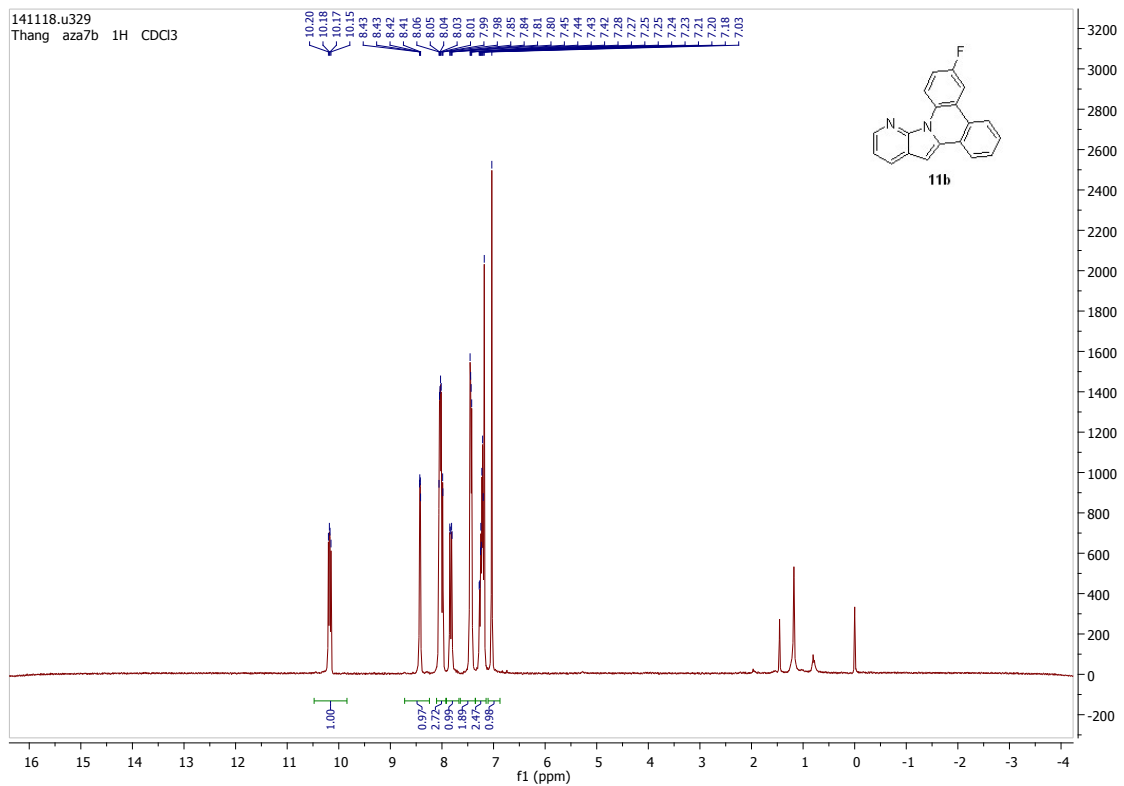


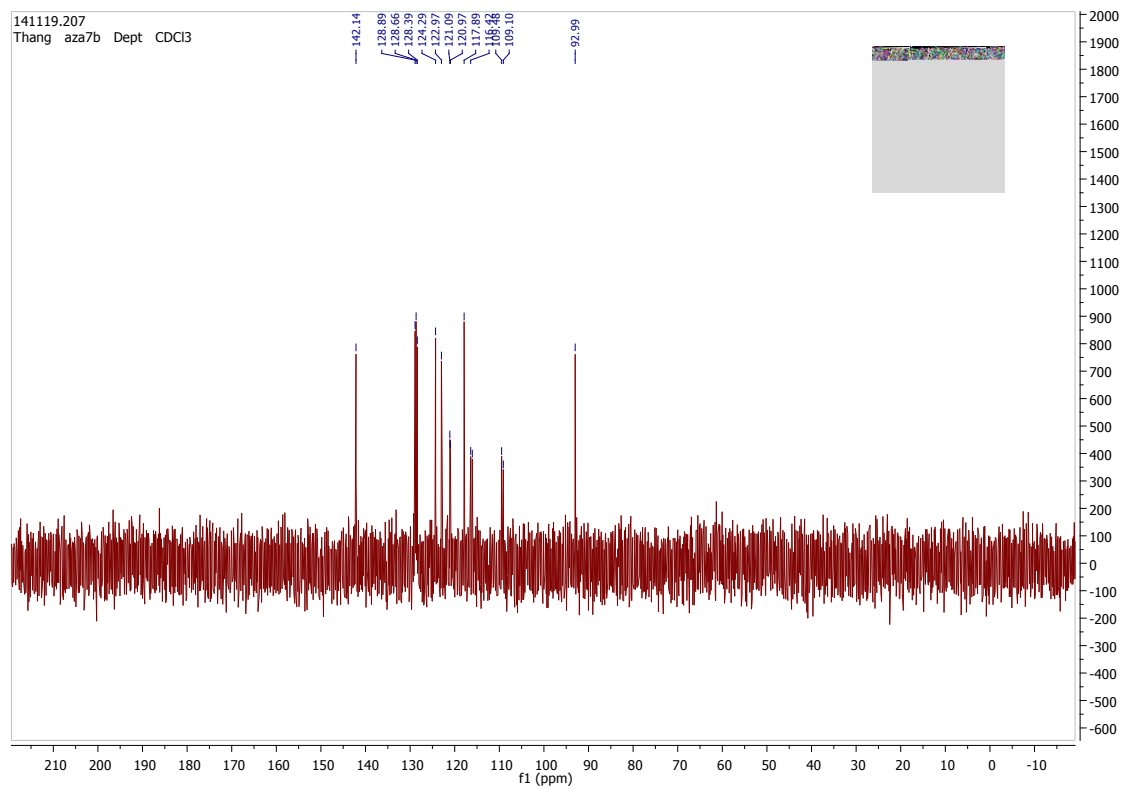
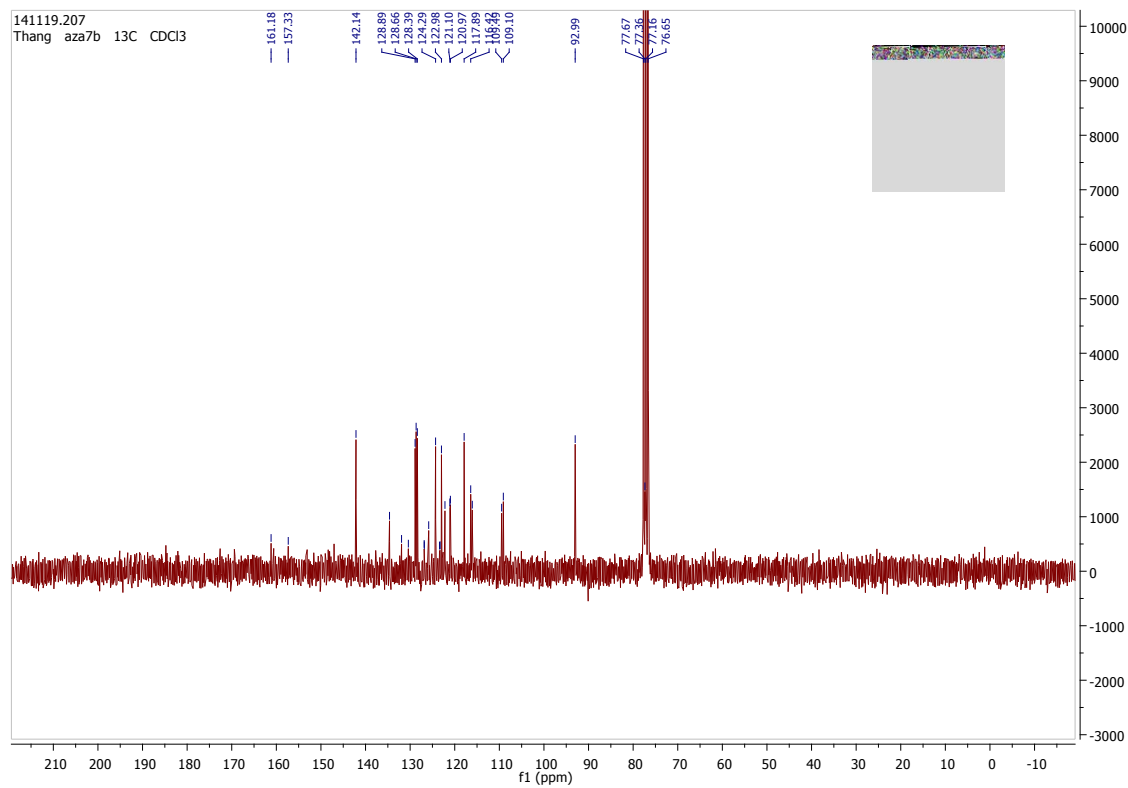
6-methoxypyrido[3',2':4,5]pyrrolo[1,2-f]phenanthridine 11a





6-fluoropyrido[3',2':4,5]pyrrolo[1,2-f]phenanthridine 11b





6-(methylthio)pyrido[3',2':4,5]pyrrolo[1,2-f]phenanthridine 11c

