

Electronic Supplementary Information

LED-Induced Ru-Photoredox Pd-Catalyzed C-H Arylation of (6-Phenylpyridin-2-yl)pyrimidines and Heteroaryl Counterparts

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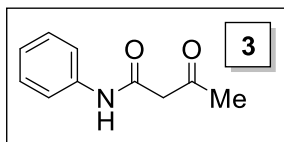
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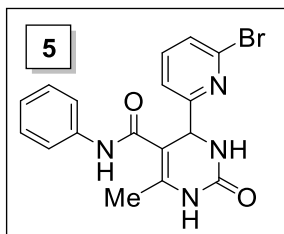
I. Supplementary Synthetic Methods and Characterization Data

• 3-Oxo-*N*-phenylbutanamide (**3**):



Synthesis method: A round-bottom flask was charged with aniline (1.8 mL, 20 mmol, 1 equiv.) and ethyl acetoacetate (3.8 mL, 30 mmol, 1.5 equiv.). A vertical condenser was fitted to the flask and the mixture was heated at 160 °C for 3 h. After cooling down to room temperature, the mixture was dissolved in ethyl acetate and washed with HCl 0.1 M (3 times) and water. The combined organic layer was dried over Na₂SO₄. After filtering out the drying agent, the solution was concentrated under vacuum. The sample was applied to a silica column for flash chromatography. Elution took place with hexane-ethyl acetate step gradient (from 3:1 to 1:1), to afford 1.72 g (9.7 mmol, 49%) of compound **3**, as a white solid. ¹H NMR (CDCl₃): δ_H (ppm) 2.33 (s, 3H), 3.59 (s, 2H), 7.12 (t, 1H, J=7.3 Hz), 7.33 (app. t, 2H, J=7.7 Hz), 7.55 (d, 2H, J=8.1 Hz), 9.11 (bs, 1H). ¹³C NMR (CDCl₃): δ_C (ppm) 31.32, 49.61, 120.14, 124.56, 128.98, 137.45, 163.31, 205.32. FT-IR: wavenumber (cm⁻¹) 1711 (m), 1659 (s), 1597 (s), 1539 (s), 1503 (m), 1445 (s), 1408 (m), 1315 (m), 1163 (s), 1005 (m), 752 (s). MS (ES-API), m/z: calcd for C₁₀H₁₁NO₂: 177.08; found: 178.1 [M+H⁺]. m.p. 82-83 °C.

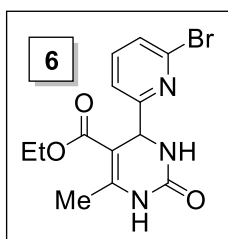
• 4-(6-Bromopyridin-2-yl)-6-methyl-2-oxo-*N*-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxamide (**5**):



Pale yellow solid. Yield: 95%. ¹H NMR (DMSO-d₆): δ_H (ppm) 2.03 (s, 3H), 5.35 (d, 1H, J=3.0 Hz), 7.01 (t, 1H, J=7.4 Hz), 7.26 (app. t, 2H, J=7.9 Hz), 7.31 (d, 1H, J=7.7 Hz), 7.55 (d, 1H, J=7.9 Hz), 7.57 (d, 2H, J=8.4 Hz), 7.70 (dd, 1H, J₁=3.0 Hz, J₂=1.6 Hz), 7.77 (app. t, 1H, J=7.8 Hz), 8.87 (d, 1H, J=1.6 Hz), 9.78 (s, 1H). ¹³C NMR (DMSO-d₆): δ_C (ppm) 17.23, 55.94, 103.91, 119.65, 119.71, 123.09, 126.88, 128.53, 139.26, 140.49, 140.60, 140.83, 152.79, 163.97, 165.02. FT-IR: wavenumber (cm⁻¹) 1697 (m), 1663 (m), 1593 (m), 1555 (m), 1500 (m), 1441 (m), 1327 (m), 1252 (m), 1211 (m), 1011 (m), 748 (s). MS (ES-API), m/z: calcd for C₁₇H₁₅BrN₄O₂: 386.04; found: 387.0 [M+H⁺]. m.p. 233-235 °C.

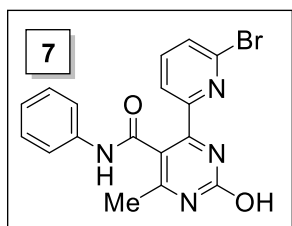
• Ethyl 4-(6-bromopyridin-2-yl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**6**):

White solid. Yield: 68%. ¹H NMR (DMSO-d₆): δ_H (ppm) 1.09 (t, 3H, J=7.1 Hz), 2.23 (s, 3H), 3.99 (q, 2H, J=7.1 Hz), 5.18 (d, 1H, J=3.2 Hz), 7.28 (d, 1H, J=7.4 Hz), 7.52 (d, 1H, J=7.8 Hz), 7.71 (m, 2H, signals overlapping), 9.22 (s, 1H). ¹³C NMR (DMSO-d₆): δ_C (ppm) 14.05, 17.82, 55.28, 59.16, 97.38, 120.25, 126.87, 140.14, 140.92, 149.35, 151.96,



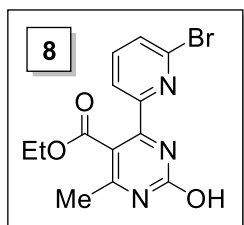
164.03, 165.14. FT-IR: wavenumber (cm^{-1}) 2360 (s), 2341(m), 1702 (w), 1650 (s), 1596 (w), 1577 (w), 1448 (w), 1320 (m), 1277 (s), 945 (m), 936 (m), 919 (m), 813 (w), 766 (m), 704 (s), 695 (s), 670 (w), 638 (s). MS (ES-API), m/z: calcd for $\text{C}_{13}\text{H}_{14}\text{BrN}_3\text{O}_3$: 339.02; found: 340.0 $[\text{M}+\text{H}^+]$. m.p. 157-159 °C.

• **4-(6-Bromopyridin-2-yl)-2-hydroxy-6-methyl-N-phenylpyrimidine-5-carboxamide (7):**



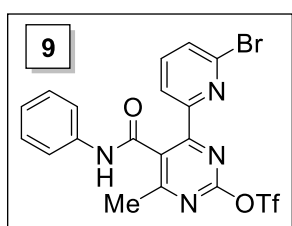
White solid. Yield: 80%. ^1H NMR (DMSO-d_6): δ_{H} (ppm) 2.36 (s, 3H), 7.04 (tt, 1H, $J_1=7.4$ Hz, $J_2=1.0$ Hz), 7.28 (app. t, 2H, $J=7.8$ Hz), 7.54 (dd, 2H, $J_1=8.2$ Hz, $J_2=1.0$ Hz), 7.69 (dd, 1H, $J_1=7.9$ Hz, $J_2=0.7$ Hz), 7.89 (app. t, 1H, $J=7.8$ Hz), 8.07 (d, 1H, $J=7.7$ Hz), 10.17 (bs, 1H). ^{13}C NMR (DMSO-d_6): δ_{C} (ppm) 17.74, 114.34, 119.76, 122.72, 123.36, 128.44, 129.70, 138.97, 139.53, 140.33, 155.22, 156.43, 159.54, 163.70, 165.70. FT-IR: wavenumber (cm^{-1}) 2750 (br), 1649 (s), 1661 (m), 1537 (m), 1456 (m), 1315 (m), 1130 (m), 789 (s), 746 (s), 723 (s). MS (ES-API), m/z: calcd for $\text{C}_{17}\text{H}_{13}\text{BrN}_4\text{O}_2$: 384.02; found: 385.0 $[\text{M}+\text{H}^+]$. m.p. > 250 °C.

• **Ethyl 4-(6-bromopyridin-2-yl)-2-hydroxy-6-methylpyrimidine-5-carboxylate (8):**



Pale yellow solid. Yield: 53%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.22 (t, 3H, $J=7.2$ Hz), 2.60 (s, 3H), 4.37 (q, 2H, $J=7.2$ Hz), 7.59 (d, 1H, $J=7.9$ Hz), 7.71 (app. t, 1H, $J=7.8$ Hz), 8.30 (d, 1H, $J=7.7$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.91, 17.90, 62.00, 112.05, 122.83, 130.32, 139.30, 140.19, 154.27, 158.55, 159.70, 165.85, 168.15. FT-IR: wavenumber (cm^{-1}) 2360 (s), 2343 (m), 1652 (s), 1596 (m), 1577 (w), 1543 (w), 1448 (m), 1321 (m), 1279 (s), 945 (m), 919 (m), 814 (w), 766 (m), 704 (s), 695 (s), 670 (w), 638 (s). MS (ES-API), m/z: calcd for $\text{C}_{13}\text{H}_{12}\text{BrN}_3\text{O}_3$: 337.01; found: 338.1 $[\text{M}+\text{H}^+]$. m.p. 164-166 °C.

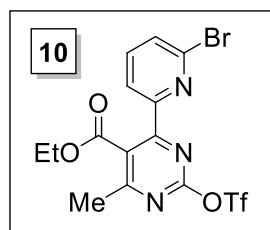
• **4-(6-Bromopyridin-2-yl)-6-methyl-5-(phenylcarbamoyl)pyrimidin-2-yl trifluoromethanesulfonate (9):**



White solid. Yield: 57%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.73 (s, 3H), 7.19 (t, 1H, $J=7.4$ Hz), 7.39 (app. t, 2H, $J=7.7$ Hz), 7.55 (d, 1H, $J=7.9$ Hz), 7.64 (d, 2H, $J=8.0$ Hz), 7.72 (app. t, 1H, 7.8 Hz), 7.77 (bs, 1H), 8.27 (d, 1H, $J=7.7$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.40, 118.50 (CF_3 , q, $J=320.8$ Hz), 120.54, 122.70, 125.11, 128.11, 129.01, 130.88, 137.28, 139.60, 141.11, 152.63, 156.90, 161.05, 163.75, 172.63. FT-IR: wavenumber (cm^{-1}) 1655 (s), 1543 (s), 1408 (s),

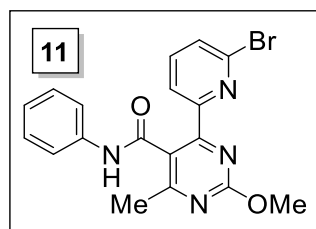
1204 (s), 1144 (s), 1121 (s), 997 (s), 826 (m), 804 (m), 754 (m). MS (ES-API), m/z: calcd for C₁₈H₁₂BrF₃N₄O₄S: 515.97; found: 517.0 [M+H⁺]. m.p. 160-162 °C.

• **Ethyl 4-(6-bromopyridin-2-yl)-6-methyl-2-(((trifluoromethyl)sulfonyl)oxy)pyrimidine-5-carboxylate (10):**



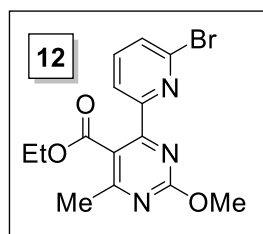
Beige solid. Yield: 54%. ¹H NMR (CDCl₃): δ_H (ppm) 1.38 (t, 3H, J=7.1 Hz), 2.66 (s, 3H), 4.58 (q, 2H, J=7.1 Hz), 7.62 (d, 1H, J=7.9 Hz), 7.76 (app. t, 1H, J=7.8 Hz), 8.35 (d, 1H, J=7.7 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 13.83, 22.19, 62.55, 118.48 (CF₃, q, J=320.9 Hz), 122.40, 125.37, 130.83, 139.70, 140.61, 152.16, 156.87, 161.01, 166.12, 171.67. FT-IR: wavenumber (cm⁻¹) 1736 (s), 1566 (m), 1539 (m), 1422 (s), 1267 (m), 1207 (s), 1124 (s), 1084 (m), 988 (s), 868 (m), 820 (s), 789 (m). MS (ES-API), m/z: calcd for C₁₄H₁₁BrF₃N₃O₅S: 468.96; found: 469.1 [M]. m.p. 89-91 °C.

• **4-(6-Bromopyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (11):**



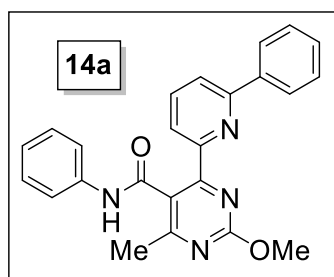
White solid. Yield: 70%. ¹H NMR (CDCl₃): δ_H (ppm) 2.58 (s, 3H), 4.04 (s, 3H), 7.15 (t, 1H, J=7.5 Hz), 7.36 (app. t, 2H, J=7.8 Hz), 7.45 (d, 1H, J=7.9 Hz), 7.61 (app. t, 1H, J=7.8 Hz), 7.66 (d, 2H, J=8.1 Hz), 7.99 (bs, 1H), 8.18 (d, 1H, J=7.7 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 22.32, 55.07, 120.43, 121.98, 123.09, 124.52, 128.84, 129.73, 137.89, 139.09, 140.69, 154.55, 159.67, 164.09, 165.63, 169.75. FT-IR: wavenumber (cm⁻¹) 1657 (s), 1541 (s), 1408 (s), 1202 (s), 1142 (s), 1123 (s), 997 (s), 824 (m), 806 (m), 754 (m). MS (ES-API), m/z: calcd for C₁₈H₁₅BrN₄O₂: 398.04; found: 399.0 [M+H⁺]. m.p. 163-165 °C.

• **Ethyl 4-(6-bromopyridin-2-yl)-2-methoxy-6-methylpyrimidine-5-carboxylate (12):**



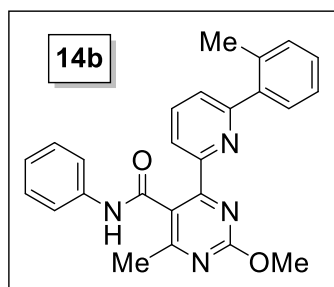
White solid. Yield: 76%. ¹H NMR (CDCl₃): δ_H (ppm) 1.33 (t, 3H, J=7.2 Hz), 2.57 (s, 3H), 4.09 (s, 3H), 4.49 (q, 2H, J=7.2 Hz), 7.55 (dd, 1H, J₁=7.9 Hz, J₂=0.7 Hz), 7.70 (app. t, 1H, J=7.8 Hz), 8.33 (dd, 1H, J₁=7.7 Hz, J₂=0.7 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 14.00, 22.36, 55.11, 61.93, 120.07, 121.80, 129.71, 139.25, 140.39, 154.52, 160.20, 164.33, 168.09, 169.23. FT-IR: wavenumber (cm⁻¹) 2359 (m), 1732 (m), 1650 (m), 1550 (s), 1472 (m), 1448 (m), 1381 (m), 1321 (m), 1276 (s), 1125 (m), 1075 (m), 938 (m), 919 (m), 794 (m), 765 (m), 703 (s), 695 (s), 638 (s). MS (ES-API), m/z: calcd for C₁₄H₁₄BrN₃O₃: 351.02; found: 352.1 [M+H⁺]. m.p. 92-94 °C.

• **2-Methoxy-4-methyl-N-phenyl-6-(6-phenylpyridin-2-yl)pyrimidine-5-carboxamide (14a):**



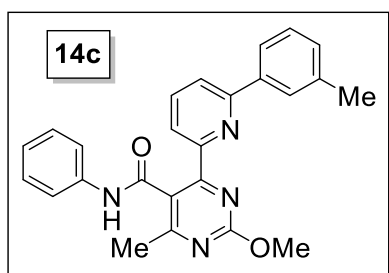
White solid. Yield: 99%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.65 (s, 3H), 4.09 (s, 3H), 7.06-7.12 (m, 3H, 2 signals overlapping), 7.20-7.26 (m, 3H, 2 signals overlapping), 7.51 (d, 2H, $J=8.1$ Hz), 7.76 (d, 1H, $J=7.9$ Hz), 7.82-7.86 (m, 3H, 2 signals overlapping), 7.87 (app. t, 1H, $J=7.8$ Hz), 8.27 (d, 1H, $J=7.7$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.37, 54.95, 119.67, 121.71, 121.87, 122.77, 124.15, 127.23, 128.35, 128.90, 128.98, 137.74, 137.96, 138.46, 153.50, 156.88, 161.37, 164.17, 166.39, 169.73. FT-IR: wavenumber (cm^{-1}) 1643 (m), 1598 (w), 1545 (s), 1470 (m), 1441 (m), 1375 (m), 1317 (s), 1275 (w), 1024 (w), 799 (m), 758 (s), 698 (m). MS (ES-API), m/z : calcd for $\text{C}_{24}\text{H}_{20}\text{N}_4\text{O}_2$: 396.16; found: 397.1 $[\text{M}+\text{H}^+]$. m.p. 191-193 $^{\circ}\text{C}$.

• **2-Methoxy-4-methyl-N-phenyl-6-(6-(*o*-tolyl)pyridin-2-yl)pyrimidine-5-carboxamide (14b):**



White solid. Yield: 96%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.21 (s, 3H), 2.61 (s, 3H), 4.10 (s, 3H), 6.92 (app. t, 1H, $J=7.7$ Hz), 7.01 (t, 1H, $J=7.3$ Hz), 7.07-7.13 (m, 3H, 2 signals overlapping), 7.17 (d, 2H, $J=8.1$ Hz), 7.20-7.26 (m, 2H, 2 signals overlapping), 7.44 (d, 1H, $J=7.9$ Hz), 7.87 (app. t, 1H, $J=7.8$ Hz), 7.93 (bs, 1H), 8.20 (d, 1H, $J=7.7$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 20.14, 22.51, 55.03, 119.79, 121.59, 123.24, 124.06, 125.61, 125.69, 128.35, 128.70, 130.02, 130.45, 135.53, 137.22, 137.77, 139.35, 153.76, 158.92, 161.74, 164.27, 165.92, 169.87. FT-IR: wavenumber (cm^{-1}) 1657 (w), 1557 (s), 1445 (w), 1380 (w), 1323 (m), 750 (m), 746 (w). MS (ES-API), m/z : calcd for $\text{C}_{25}\text{H}_{22}\text{N}_4\text{O}_2$: 410.17; found: 411.1 $[\text{M}+\text{H}^+]$. m.p. 168-170 $^{\circ}\text{C}$.

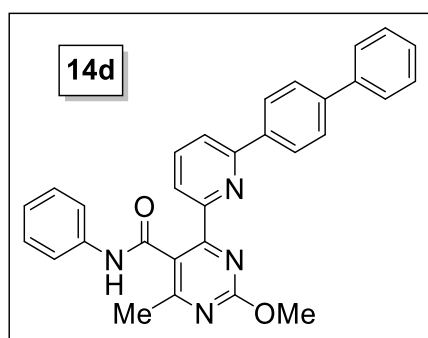
• **2-Methoxy-4-methyl-N-phenyl-6-(6-(*m*-tolyl)pyridin-2-yl)pyrimidine-5-carboxamide (14c):**



White solid. Yield: 98%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.15 (s, 3H), 2.51 (s, 3H), 3.97 (s, 3H), 6.91 (app. t, 1H, $J=7.5$ Hz), 7.02-7.08 (m, 2H, 2 signals overlapping), 7.19 (app. t, 2H, $J=7.6$ Hz), 7.48 (d, 2H, $J=7.9$ Hz), 7.62 (d, 1H, $J=8.1$ Hz), 7.64 (bs, 1H), 7.69 (d, 1H, $J=7.9$ Hz), 7.74 (app. t, 1H, $J=7.8$ Hz), 8.13 (d, 1H, $J=7.7$ Hz), 8.28 (bs, 1H). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 21.14, 22.32, 54.87, 119.86, 121.56, 121.87, 122.86, 124.10, 124.51, 127.74, 128.25, 128.78, 129.76,

137.54, 138.05, 138.07, 138.37, 153.37, 157.03, 161.34, 164.03, 166.38, 169.72. FT-IR: wavenumber (cm⁻¹) 1651 (m), 1597 (m), 1553 (s), 1468 (m), 1441 (m), 1381 (m), 1317 (s), 1254 (m), 1024 (w), 785 (m), 754 (m). MS (ES-API), m/z: calcd for C₂₅H₂₂N₄O₂: 410.17; found: 411.1 [M+H⁺]. m.p. 82-84 °C.

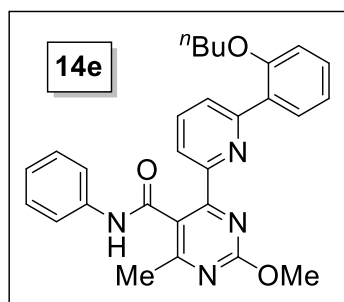
• **4-(6-([1,1'-Biphenyl]-4-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (14d):**



White solid. Yield: 96%. ¹H NMR (CDCl₃): δ_H (ppm) 2.59 (s, 3H), 4.04 (s, 3H), 7.08 (t, 1H, J=7.4 Hz), 7.20-7.26 (m, 4H, 2 signals overlapping), 7.36 (t, 1H, J=7.2 Hz), 7.44 (app. t, 2H, J=7.5 Hz), 7.50 (d, 2H, J=7.8 Hz), 7.55 (d, 2H, J=7.8 Hz), 7.72 (d, 1H, J=7.9 Hz), 7.78 (app. t, 1H, J=7.8 Hz), 7.86 (d, 2H, J=8.1 Hz), 8.09 (bs, 1H), 8.23 (d, 1H, J=7.7 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 22.34, 54.93, 119.82,

121.58, 121.71, 122.69, 124.08, 126.89, 126.91, 127.39, 127.64, 128.73, 128.89, 136.91, 137.64, 138.59, 140.49, 141.44, 153.42, 156.46, 161.18, 164.16, 166.56, 169.69. FT-IR: wavenumber (cm⁻¹) 1651 (m), 1598 (w), 1549 (s), 1472 (m), 1439 (m), 1385 (m), 1317 (s), 1261 (m), 1057 (m), 766 (s). MS (ES-API), m/z: calcd for C₃₀H₂₄N₄O₂: 472.19; found: 473.1 [M+H⁺]. m.p. 234-236 °C.

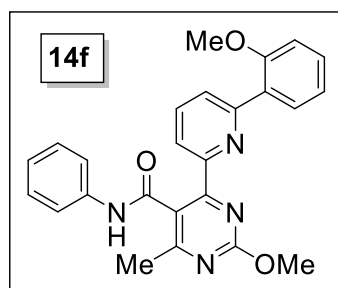
• **4-(6-(2-Butoxyphenyl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (14e):**



White solid. Yield: 98%. ¹H NMR (CDCl₃): δ_H (ppm) 0.90 (t, 3H, J=7.4 Hz), 1.39 (app. sextet, 2H, J=7.5 Hz), 1.68 (app. quint., 2H, J=7.0 Hz), 2.60 (s, 3H), 3.91 (t, 2H, J=6.4 Hz), 4.05 (s, 3H), 6.44 (app. t, 1H, J=7.5 Hz), 6.85 (d, 1H, J=8.2 Hz), 7.05 (t, 1H, J=7.4 Hz), 7.16 (dt, 1H, J₁=7.7 Hz, J₂=1.7 Hz), 7.20 (app. t, 2H, J=7.7 Hz), 7.41 (d, 2H, J=8.0 Hz), 7.67 (dd, 1H, J₁=8.0 Hz, J₂=1.7 Hz), 7.79 (app. t, 1H, J=7.8 Hz),

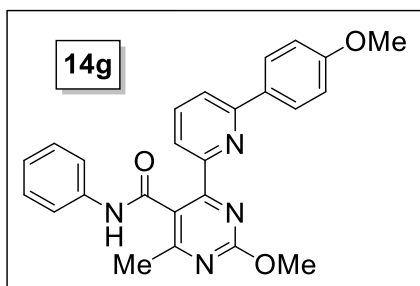
7.98 (dd, 1H, J₁=7.8 Hz, J₂=0.8 Hz), 8.00 (bs, 1H), 8.17 (dd, 1H, J₁=7.8 Hz, J₂=0.8 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 13.76, 19.29, 22.45, 31.27, 54.93, 68.08, 111.91, 119.66, 120.74, 121.33, 122.91, 124.00, 126.86, 127.77, 128.79, 129.91, 132.08, 136.37, 138.35, 153.44, 155.33, 156.34, 161.93, 164.20, 166.31, 169.70. FT-IR: wavenumber (cm⁻¹) 2926 (m), 1651 (m), 1601 (m), 1555 (s), 1466 (m), 1441 (s), 1380 (m), 1319 (s), 1263 (m), 1069 (m), 797 (m), 758 (s). MS (ES-API), m/z: calcd for C₂₈H₂₈N₄O₃: 468.22; found: 469.1 [M+H⁺]. m.p. 118-120 °C.

• **2-Methoxy-4-(6-(2-methoxyphenyl)pyridin-2-yl)-6-methyl-N-phenylpyrimidine-5-carboxamide (14f):**



White solid. Yield: 99%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.57 (s, 3H), 3.75 (s, 3H), 4.03 (s, 3H), 6.46 (app. t, 1H, $J=7.6$ Hz), 6.85 (d, 1H, $J=8.3$ Hz), 7.05 (t, 1H, $J=7.4$ Hz), 7.15-7.21 (m, 3H, 2 signals overlapping), 7.40 (d, 2H, $J=8.0$ Hz), 7.66 (dd, 1H, $J_1=7.6$ Hz, $J_2=1.8$ Hz), 7.76 (app. t, 1H, $J=7.8$ Hz), 7.92 (d, 1H, $J=7.9$ Hz), 8.05 (bs, 1H), 8.17 (d, 1H, $J=7.7$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.39, 54.89, 55.40, 110.89, 119.71, 120.89, 121.33, 122.87, 123.94, 126.75, 127.74, 128.75, 129.88, 132.09, 136.49, 138.36, 153.43, 155.21, 156.76, 161.77, 164.16, 166.33, 169.67. FT-IR: wavenumber (cm^{-1}) 1651 (m), 1597 (m), 1549 (s), 1468 (m), 1466 (m), 1379 (m), 1317 (s), 1260 (s), 1024 (m), 752 (s). MS (ES-API), m/z : calcd for $\text{C}_{25}\text{H}_{22}\text{N}_4\text{O}_3$: 426.17; found: 427.1 [$\text{M}+\text{H}^+$]. m.p. 79-81 $^{\circ}\text{C}$.

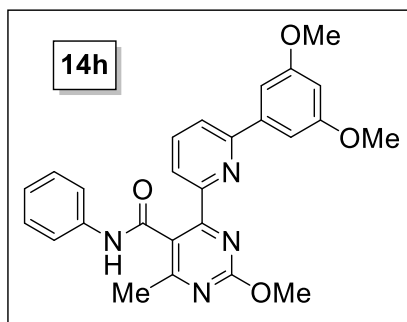
• **2-Methoxy-4-(6-(4-methoxyphenyl)pyridin-2-yl)-6-methyl-N-phenylpyrimidine-5-carboxamide (14g):**



White solid. Yield: 99%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.64 (s, 3H), 3.75 (s, 3H), 4.09 (s, 3H), 6.59 (d, 2H, $J=8.6$ Hz), 7.09 (t, 1H, $J=7.5$ Hz), 7.27 (app. t, 2H, $J=7.8$ Hz), 7.55 (d, 2H, $J=8.1$ Hz), 7.70 (d, 1H, $J=7.9$ Hz), 7.80 (d, 2H, $J=8.6$ Hz), 7.84 (app. t, 1H, $J=7.8$ Hz), 8.06 (bs, 1H), 8.19 (d, 1H, $J=7.7$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.43, 55.05, 55.23, 113.84, 119.79, 121.26, 121.47, 122.96, 124.18, 128.84, 128.93, 129.97, 138.30, 138.47, 153.06, 156.44, 160.75, 161.10, 164.30, 166.31, 169.77. FT-IR: wavenumber (cm^{-1}) 1661 (m), 1599 (m), 1553 (s), 1441 (m), 1379 (m), 1323 (m), 1248 (m), 1179 (m), 1030 (m), 793 (s), 754 (s). MS (ES-API), m/z : calcd for $\text{C}_{25}\text{H}_{22}\text{N}_4\text{O}_3$: 426.17; found: 427.1 [$\text{M}+\text{H}^+$]. m.p. 91-93 $^{\circ}\text{C}$.

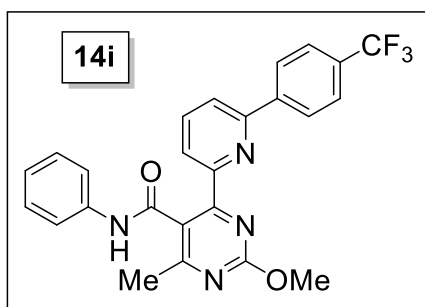
• **4-(6-(3,5-Dimethoxyphenyl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (14h):**

White solid. Yield: 98%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.67 (s, 3H), 3.76 (s, 6H), 4.10 (s, 3H), 6.40 (t, 1H, $J=2.1$ Hz), 7.01 (t, 1H, $J=7.3$ Hz), 7.05 (d, 2H, $J=2.1$ Hz), 7.12 (app. t, 2H, $J=7.6$ Hz), 7.23 (d, 2H, $J=7.9$ Hz), 7.59 (bs, 1H), 7.74 (d, 1H, $J=7.9$ Hz), 7.89 (app. t, 1H, $J=7.8$ Hz), 8.26 (d, 1H, $J=7.7$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.44, 55.06, 55.51, 101.76, 105.49, 121.15, 122.03, 122.25, 122.70, 124.74, 128.59, 137.28, 138.06, 140.07, 153.38, 156.86, 160.89, 161.21, 164.31, 166.48, 170.22. FT-IR: wavenumber (cm^{-1})



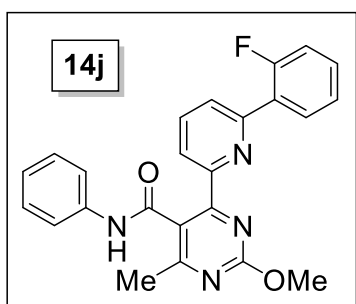
1655 (m), 1595 (m), 1549 (s), 1462 (s), 1379 (m), 1319 (s), 1207 (m), 1155 (s), 1065 (m), 793 (s), 756 (m). MS (ES-API), m/z: calcd for C₂₆H₂₄N₄O₄: 456.18; found: 457.1 [M+H⁺]. m.p. 103-105 °C.

• **2-Methoxy-4-methyl-N-phenyl-6-(6-(4-(trifluoromethyl)phenyl)pyridin-2-yl)pyrimidine-5-carboxamide (14i):**



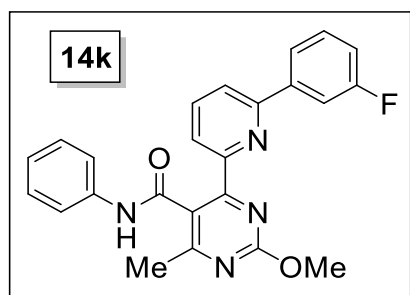
White solid. Yield: 96%. ¹H NMR (CDCl₃): δ_H (ppm) 2.59 (s, 3H), 4.06 (s, 3H), 7.09 (t, 1H, J=7.5 Hz), 7.19 (d, 2H, J=8.2 Hz), 7.23 (app. t, 2H, J=7.7 Hz), 7.45 (d, 2H, J=7.9 Hz), 7.71 (d, 1H, J=7.6 Hz), 7.79-7.89 (m, 2H, 2 signals overlapping), 7.97 (bs, 1H), 8.33 (d, 1H, J=7.8 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 22.28, 55.01, 119.68, 122.22, 122.31, 122.60, 124.46, 125.17 (q, J=3.7 Hz), 127.50, 128.91, 130.57 (q, J=32.4 Hz), 134.09, 137.96, 138.30, 141.25, 153.57, 155.47, 160.71, 164.21, 166.63, 169.75. FT-IR: wavenumber (cm⁻¹) 1553 (s), 1443 (m), 1323 (s), 1255 (m), 1157 (m), 1109 (s), 1074 (m), 1015 (m), 794 (w), 760 (w), 740 (w). MS (ES-API), m/z: calcd for C₂₅H₁₉F₃N₄O₂: 464.15; found: 465.0 [M+H⁺]. m.p. 108-110 °C.

• **4-(6-(2-Fluorophenyl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (14j):**



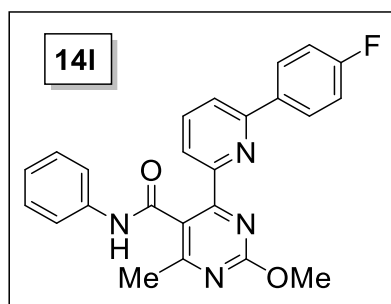
White solid. Yield: 99%. ¹H NMR (CDCl₃): δ_H (ppm) 2.61 (s, 3H), 4.07 (s, 3H), 6.58 (app. t, 1H, J=7.5 Hz), 6.99 (dd, 1H, J₁=11.6 Hz, J₂=8.3 Hz), 7.07 (t, 1H, J=7.4 Hz), 7.16 (m, 1H), 7.22 (app. t, 2H, J=7.6 Hz), 7.46 (d, 2H, J=7.8 Hz), 7.78-7.80 (m, 4H, 4 signals overlapping), 8.28 (dd, 1H, J₁=5.1 Hz, J₂=3.5 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 22.33, 55.00, 115.56 (d, J=22.8 Hz), 119.66, 121.98, 122.77, 124.18, 124.25 (d, J=3.6 Hz), 125.97, 126.10 (d, J=11.3 Hz), 128.88, 130.40 (d, J=8.7 Hz), 131.98 (d, J=2.7 Hz), 137.45, 138.35, 152.73 (d, J=2.7 Hz), 153.58 Hz, 160.33 (d, J=249.3 Hz), 161.24, 164.24, 166.38, 169.72. FT-IR: wavenumber (cm⁻¹) 1643 (m), 1543 (s), 1441 (m), 1317 (m), 1273 (w), 1209 (w), 1167 (w), 758 (s). MS (ES-API), m/z: calcd for C₂₄H₁₉FN₄O₂: 414.15; found: 415.1 [M+H⁺]. m.p. 202-204 °C.

• **4-(6-(3-Fluorophenyl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (14k):**



White solid. Yield: 98%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.49 (s, 3H), 3.96 (s, 3H), 6.85-6.89 (m, 2H, 2 signals overlapping), 7.05 (t, 1H, $J=7.5$ Hz), 7.20 (app. t, 2H, $J=7.8$ Hz), 7.48 (m, 1H), 7.51 (d, 2H, $J=8.1$ Hz), 7.57 (m, 1H), 7.62 (d, 1H, $J=7.9$ Hz), 7.75 (app. t, 1H, $J=7.8$ Hz), 8.17 (d, 1H, $J=7.7$ Hz), 8.35 (bs, 1H). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.27, 54.98, 113.88 (d, $J=22.8$ Hz), 115.82 (d, $J=21.1$ Hz), 119.62, 121.90, 122.17, 122.74, 123.02 (d, $J=2.6$ Hz), 124.23, 128.86, 129.85 (d, $J=8.1$ Hz), 137.89, 138.28, 140.23 (d, $J=7.4$ Hz), 153.52, 155.56 (d, $J=2.5$ Hz), 161.07, 162.94 (d, $J=245.4$ Hz), 164.10, 166.33, 169.74. FT-IR: wavenumber (cm^{-1}) 1651 (m), 1599 (m), 1547 (s), 1468 (m), 1439 (m), 1383 (m), 1317 (s), 1265 (m), 1024 (m), 785 (s), 752 (s). MS (ES-API), m/z : calcd for $\text{C}_{24}\text{H}_{19}\text{FN}_4\text{O}_2$: 414.15; found: 415.1 [$\text{M}+\text{H}^+$]. m.p. 110-112 $^{\circ}\text{C}$.

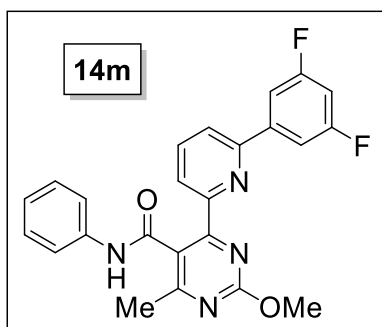
• **4-(6-(4-Fluorophenyl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (14l):**



White solid. Yield: 99%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.58 (s, 3H), 4.04 (s, 3H), 6.67 (app. t, 2H, $J=8.7$ Hz), 7.11 (t, 1H, $J=7.4$ Hz), 7.27 (app. t, 2H, $J=7.6$ Hz), 7.52 (d, 2H, $J=8.0$ Hz), 7.66 (d, 1H, $J=7.9$ Hz), 7.78 (m, 2H), 7.79 (app. t, 1H, $J=7.8$ Hz), 7.99 (bs, 1H), 8.24 (d, 1H, $J=7.7$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.33, 54.97, 115.16 (d, $J=21.7$ Hz), 119.62, 121.51, 121.52, 122.61, 124.31, 128.96, 129.09 (d, $J=8.3$ Hz), 134.13 (d, $J=2.9$ Hz), 137.78, 138.43, 153.39, 155.89, 161.10, 163.42 (d, $J=248.9$ Hz), 164.21, 166.55, 169.72. FT-IR: wavenumber (cm^{-1}) 1645 (m), 1597 (m), 1543 (s), 1510 (m), 1464 (m), 1439 (s), 1379 (m), 1315 (s), 1223 (m), 1167 (m), 795 (s), 760 (s). MS (ES-API), m/z : calcd for $\text{C}_{24}\text{H}_{19}\text{FN}_4\text{O}_2$: 414.15; found: 415.1 [$\text{M}+\text{H}^+$]. m.p. 221-223 $^{\circ}\text{C}$.

• **4-(6-(3,5-Difluorophenyl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (14m):**

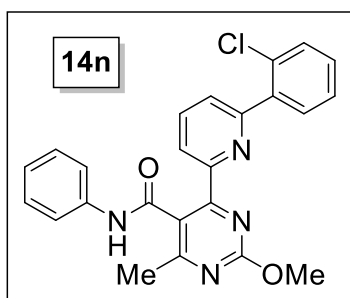
White solid. Yield: 96%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.63 (s, 3H), 4.09 (s, 3H), 6.67 (tt, 1H, $J_1=8.6$ Hz, $J_2=2.2$ Hz), 7.05 (t, 1H, $J=7.5$ Hz), 7.22 (app. t, 2H, $J=7.8$ Hz), 7.40 (d, 2H, $J=7.3$ Hz), 7.47 (d, 2H, $J=8.1$ Hz), 7.66 (bs, 1H), 7.69 (d, 1H, $J=7.9$ Hz), 7.89 (app. t, 1H, $J=7.8$ Hz), 8.35 (d, 1H, $J=7.7$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.36, 55.09, 104.24 (t,



J=25.5 Hz), 110.07 (dd, $J_1=21.1$ Hz, $J_2=6.5$ Hz), 119.52, 121.93, 122.70, 122.78 (t, $J=14.5$ Hz), 124.39, 128.88, 137.92, 138.13, 141.48 (t, $J=9.6$ Hz), 153.73, 154.53, 160.92, 163.05 (dd, $J_1=248.1$ Hz, $J_2=12.9$ Hz), 164.25, 166.31, 169.96. FT-IR: wavenumber (cm^{-1}) 1665 (m), 1598 (m), 1549 (s), 1439 (m), 1380 (m), 1321 (s), 1261 (m), 1121 (m), 988 (m), 795 (m), 756 (s), 698 (m). MS (ES-API), m/z: calcd for $\text{C}_{24}\text{H}_{18}\text{F}_2\text{N}_4\text{O}_2$: 432.14; found:

433.1 $[\text{M}+\text{H}^+]$. m.p. 103-105 °C.

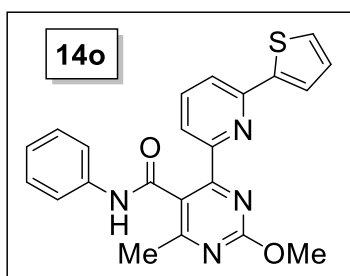
• **4-(6-(2-Chlorophenyl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (14n):**



White solid. Yield: 96%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.61 (s, 3H), 4.09 (s, 3H), 6.77 (app. dt, 1H, $J_1=7.5$ Hz, $J_2=0.9$ Hz), 7.05 (t, 1H, $J=7.4$ Hz), 7.12 (app. dt, 1H, $J_1=7.7$ Hz, $J_2=1.5$ Hz), 7.18 (app. t, 2H, $J=7.7$ Hz), 7.28 (dd, 1H, $J_1=8.1$ Hz, $J_2=0.9$ Hz), 7.35 (d, 2H, $J=8.0$ Hz), 7.40 (dd, 1H, $J_1=7.7$ Hz, $J_2=1.5$ Hz), 7.76 (d, 1H, $J=7.9$ Hz), 7.88 (m, 2H, 2 signals overlapping), 8.28 (d, 1H, $J=7.7$ Hz). ^{13}C NMR

(CDCl_3): δ_{C} (ppm) 22.33, 55.06, 119.63, 122.12, 123.10, 124.06, 126.60, 126.79, 128.79, 129.56, 129.58, 131.50, 132.46, 136.94, 137.63, 138.19, 153.56, 155.65, 161.29, 164.22, 166.22, 169.57. FT-IR: wavenumber (cm^{-1}) 1641 (m), 1597 (m), 1553 (s), 1468 (m), 1443 (m), 1385 (m), 1323 (s), 1271 (m), 1246 (w), 1067 (m), 1040 (m), 880 (m), 799 (m), 750 (s), 692 (s). MS (ES-API), m/z: calcd for $\text{C}_{24}\text{H}_{19}\text{ClN}_4\text{O}_2$: 430.12; found: 431.1 $[\text{M}+\text{H}^+]$. m.p. 176-178 °C.

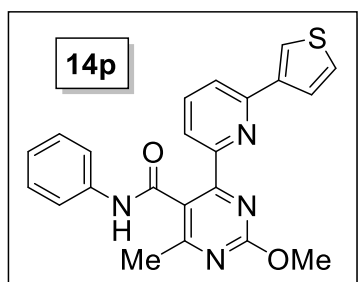
• **2-Methoxy-4-methyl-N-phenyl-6-(6-(thiophen-2-yl)pyridin-2-yl)pyrimidine-5-carboxamide (14o):**



White solid. Yield: 99%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.58 (s, 3H), 4.03 (s, 3H), 6.81 (app. t, 1H, $J=4.3$ Hz), 7.07 (t, 1H, $J=7.4$ Hz), 7.12 (d, 1H, $J=4.9$ Hz), 7.24 (app. t, 2H, $J=7.7$ Hz), 7.48 (d, 1H, $J=3.7$ Hz), 7.57 (m, 3H, 2 signals overlapping), 7.71 (app. t, 1H, $J=7.8$ Hz), 8.06 (d, 1H, $J=7.8$ Hz), 8.10 (bs, 1H). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.43,

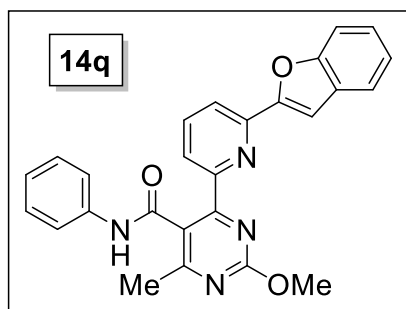
54.95, 119.88, 120.54, 121.43, 122.83, 124.12, 126.10, 127.44, 127.71, 128.74, 137.58, 138.54, 142.96, 152.03, 153.52, 161.17, 164.07, 166.04, 169.81. FT-IR: wavenumber (cm^{-1}) 1661 (m), 1598 (m), 1551 (s), 1468 (m), 1439 (m), 1379 (m), 1317 (s), 1258 (m), 781 (s), 754 (s). MS (ES-API), m/z: calcd for $\text{C}_{22}\text{H}_{18}\text{N}_4\text{O}_2\text{S}$: 402.12; found: 403.1 $[\text{M}+\text{H}^+]$. m.p. 230-232 °C.

• **2-Methoxy-4-methyl-N-phenyl-6-(6-(thiophen-3-yl)pyridin-2-yl)pyrimidine-5-carboxamide (14p):**



White solid. Yield: 99%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.51 (s, 3H), 3.98 (s, 3H), 7.02 (dd, 1H, $J_1=4.9$ Hz, $J_2=3.1$ Hz), 7.08 (t, 1H, $J=7.4$ Hz), 7.23 (app. t, 2H, $J=7.7$ Hz), 7.42 (d, 1H, $J=4.9$ Hz), 7.53 (m, 3H, 2 signals overlapping), 7.69 (dd, 1H, $J_1=7.8$ Hz, $J_2=2.0$ Hz), 7.72 (dd, 1H, $J_1=3.1$ Hz, $J_2=1.3$ Hz), 8.10 (d, 1H, $J=7.8$ Hz), 8.26 (bs, 1H). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.21, 54.87, 119.91, 121.02, 121.49, 122.47, 124.27, 125.07, 125.65, 126.20, 128.81, 137.53, 138.36, 140.70, 152.82, 153.07, 160.89, 163.98, 166.64, 169.69. FT-IR: wavenumber (cm^{-1}) 1651 (m), 1597 (m), 1545 (s), 1466 (m), 1441 (m), 1375 (m), 1323 (s), 1252 (m), 1063 (m), 795 (m), 756 (s), 712 (m). MS (ES-API), m/z : calcd for $\text{C}_{22}\text{H}_{18}\text{N}_4\text{O}_2\text{S}$: 402.12; found: 403.1 [$\text{M}+\text{H}^+$]. m.p. 168-170 $^{\circ}\text{C}$.

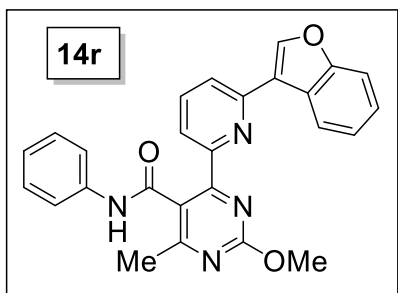
• **4-(6-(Benzofuran-2-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (14q):**



White solid. Yield: 98%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.58 (s, 3H), 4.02 (s, 3H), 6.95 (s, 1H), 7.07-7.17 (m, 3H, 3 signals overlapping), 7.24 (tt, 1H, $J_1=7.5$ Hz, $J_2=1.6$ Hz), 7.29 (app. t, 2H, $J=7.8$ Hz), 7.36 (d, 1H, $J=8.3$ Hz), 7.68 (d, 2H, $J=8.1$ Hz), 7.75 (app. t, 1H, $J=7.8$ Hz), 7.80 (d, 1H, $J=7.9$ Hz), 8.19 (d, 1H, $J=7.7$ Hz), 8.23 (bs, 1H). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.32, 54.98, 106.61, 111.09, 119.82, 120.80, 121.87, 122.00, 122.63, 122.88, 124.40, 125.02, 128.70, 129.07, 137.68, 138.57, 148.63, 153.40, 153.89, 155.03, 160.47, 164.17, 166.58, 169.75. FT-IR: wavenumber (cm^{-1}) 1659 (m), 1601 (m), 1541 (s), 1472 (m), 1439 (m), 1373 (m), 1312 (s), 1258 (s), 1171 (m), 1069 (w), 791 (s), 754 (m), 729 (m). MS (ES-API), m/z : calcd for $\text{C}_{26}\text{H}_{20}\text{N}_4\text{O}_3$: 436.15; found: 437.1 [$\text{M}+\text{H}^+$]. m.p. 196-198 $^{\circ}\text{C}$.

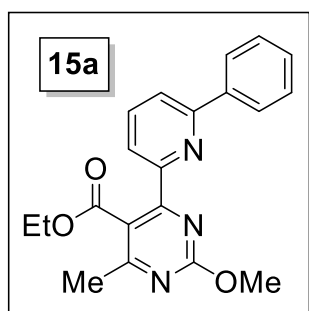
• **4-(6-(Benzofuran-3-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (14r):**

White solid. Yield: 98%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.61 (s, 3H), 4.06 (s, 3H), 7.02 (t, 1H, $J=7.4$ Hz), 7.16 (app. t, 2H, $J=7.7$ Hz), 7.25-7.33 (m, 2H, 2 signals overlapping), 7.39 (d, 2H, $J=8.0$ Hz), 7.47 (dd, 1H, $J_1=7.6$ Hz, $J_2=1.3$ Hz), 7.72 (d, 1H, $J=7.8$ Hz), 7.83-7.87 (m, 2H, 2 signals overlapping), 7.91 (dd, 1H, $J_1=7.4$ Hz, $J_2=1.5$ Hz), 7.99 (s, 1H), 8.19 (d, 1H, $J=7.8$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.27, 54.92, 111.76, 119.74, 120.48, 120.61,



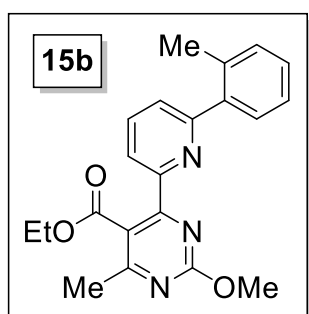
121.18, 122.17, 122.61, 123.11, 124.31, 124.35, 124.86, 128.80, 137.57, 138.04, 146.54, 151.28, 153.54, 155.75, 160.97, 164.07, 166.46, 169.78. FT-IR: wavenumber (cm^{-1}) 1649 (m), 1595 (m), 1545 (s), 1470 (m), 1441 (m), 1373 (m), 1315 (m), 1261 (m), 1103 (m), 795 (m), 745 (s). MS (ES-API), m/z : calcd for $\text{C}_{26}\text{H}_{20}\text{N}_4\text{O}_3$: 436.15; found: 437.1 $[\text{M}+\text{H}^+]$. m.p. 108-110 $^{\circ}\text{C}$.

• **Ethyl 2-methoxy-4-methyl-6-(6-phenylpyridin-2-yl)pyrimidine-5-carboxylate (15a):**



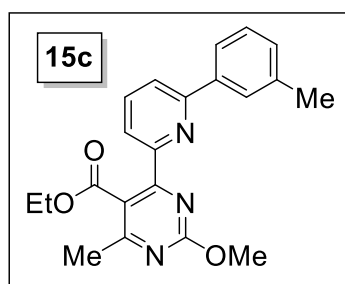
White solid. Yield: 67%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.01 (t, 3H, $J=7.1$ Hz), 2.60 (s, 3H), 4.11 (q, 2H, $J=7.1$ Hz), 4.12 (s, 3H), 7.43 (tt, 1H, $J_1=7.3$ Hz, $J_2=1.5$ Hz), 7.49 (app. t, 2H, $J=7.5$ Hz), 7.84 (dd, 1H, $J_1=7.9$ Hz, $J_2=0.8$ Hz), 7.92 (app. t, 1H, $J=7.8$ Hz), 8.03 (m, 2H), 8.28 (dd, 1H, $J_1=7.7$ Hz, $J_2=0.8$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.73, 22.36, 55.05, 61.41, 119.85, 121.50, 121.69, 127.16, 128.65, 129.32, 137.79, 138.50, 153.64, 156.44, 162.84, 164.34, 168.55, 169.00. FT-IR: wavenumber (cm^{-1}) 1717 (s), 1549 (s), 1470 (m), 1364 (m), 1252 (s), 1200 (m), 1076 (s), 799 (m), 772 (s). MS (ES-API), m/z : calcd for $\text{C}_{20}\text{H}_{19}\text{N}_3\text{O}_3$: 349.14; found: 350.1 $[\text{M}+\text{H}^+]$. m.p. 82-84 $^{\circ}\text{C}$.

• **Ethyl 2-methoxy-4-methyl-6-(6-(*o*-tolyl)pyridin-2-yl)pyrimidine-5-carboxylate (15b):**



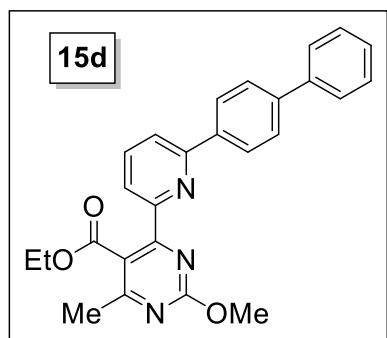
Colorless oil. Yield: 97%. ^1H NMR (CDCl_3): δ_{H} (ppm) 0.93 (t, 3H, $J=7.2$ Hz), 2.32 (s, 3H), 2.52 (s, 3H), 3.82 (q, 2H, $J=7.2$ Hz), 4.10 (s, 3H), 7.22-7.32 (m, 3H, 3 signals overlapping), 7.38 (m, 1H), 7.46 (d, 1H, $J=7.9$ Hz), 7.89 (app. t, 1H, $J=7.9$ Hz), 8.36 (dd, 1H, $J_1=7.9$ Hz, $J_2=0.8$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.53, 20.17, 22.24, 55.00, 61.34, 120.03, 120.86, 125.58, 125.63, 128.44, 129.71, 130.57, 135.97, 137.15, 139.90, 152.73, 158.79, 161.83, 164.34, 168.52, 168.75. FT-IR: wavenumber (cm^{-1}) 1724 (s), 1551 (s), 1470 (s), 1379 (m), 1360 (m), 1265 (s), 1246 (m), 1225 (m), 1167 (m), 1070 (s), 872 (m), 802 (m), 762 (m), 700 (m), 625 (m). MS (ES-API), m/z : calcd for $\text{C}_{21}\text{H}_{21}\text{N}_3\text{O}_3$: 363.16; found: 364.1 $[\text{M}+\text{H}^+]$.

• Ethyl 2-methoxy-4-methyl-6-(6-(*m*-tolyl)pyridin-2-yl)pyrimidine-5-carboxylate (15c):



White solid. Yield: 89%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.01 (t, 3H, $J=7.1$ Hz), 2.46 (s, 3H), 2.60 (s, 3H), 4.11 (s, 3H), 4.12 (q, 2H, $J=7.1$ Hz), 7.25 (d, 1H, $J=7.5$ Hz), 7.37 (app. t, 1H, $J=7.6$ Hz), 7.81 (m, 2H, 2 signals overlapping), 7.87 (s, 1H), 7.89 (app. t, 1H, $J=7.8$ Hz), 8.26 (d, 1H, $J=7.7$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.74, 21.48, 22.33, 55.00, 61.31, 119.81, 121.37, 121.69, 124.22, 127.88, 128.50, 130.03, 137.68, 138.23, 138.41, 153.52, 156.55, 162.84, 164.31, 168.50, 168.95. FT-IR: wavenumber (cm^{-1}) 1721 (s), 1551 (s), 1468 (m), 1377 (m), 1360 (m), 1250 (s), 1072 (s), 787 (s), 746 (m). MS (ES-API), m/z : calcd for $\text{C}_{21}\text{H}_{21}\text{N}_3\text{O}_3$: 363.16; found: 364.1 $[\text{M}+\text{H}^+]$. m.p. 84-86 °C.

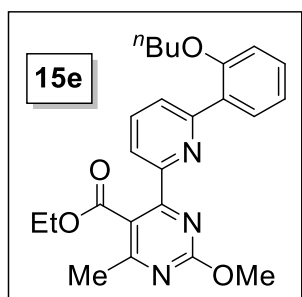
• Ethyl 4-(6-([1,1'-biphenyl]-4-yl)pyridin-2-yl)-2-methoxy-6-methylpyrimidine-5-carboxylate (15d):



White solid. Yield: 98%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.04 (t, 3H, $J=7.2$ Hz), 2.62 (s, 3H), 4.12 (s, 3H), 4.15 (q, 2H, $J=7.2$ Hz), 7.38 (tt, 1H, $J_1=7.4$ Hz, $J_2=1.2$ Hz), 7.48 (app. t, 2H, $J=7.6$ Hz), 7.68 (m, 2H), 7.74 (d, 2H, $J=8.4$ Hz), 7.88 (dd, 1H, $J_1=8.0$ Hz, $J_2=1.0$ Hz), 7.93 (app. t, 1H, $J=7.8$ Hz), 8.12 (d, 2H, $J=8.4$ Hz), 8.29 (dd, 1H, $J_1=7.6$ Hz, $J_2=1.0$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.78, 22.37, 55.03, 61.44, 119.85, 121.51, 121.52, 127.01, 127.30, 127.54, 127.60, 128.84, 137.35, 137.79, 140.37, 141.98, 153.73, 155.98, 162.88, 164.37, 168.56, 169.02. FT-IR: wavenumber (cm^{-1}) 1726 (s), 1553 (s), 1461 (m), 1381 (m), 1358 (m), 1246 (s), 1229 (m), 1184 (m), 1074 (m), 1051 (m), 799 (s), 766 (s), 748 (m). MS (ES-API), m/z : calcd for $\text{C}_{26}\text{H}_{23}\text{N}_3\text{O}_3$: 425.17; found: 426.1 $[\text{M}+\text{H}^+]$. m.p. 142-144 °C.

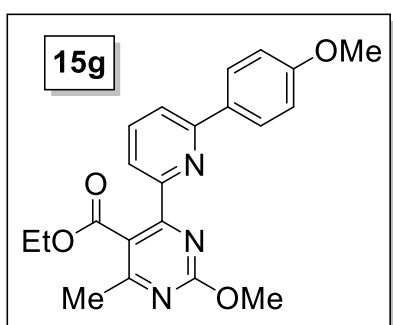
• Ethyl 4-(6-(2-butoxyphenyl)pyridin-2-yl)-2-methoxy-6-methylpyrimidine-5-carboxylate (15e):

Beige solid. Yield: 48%. ^1H NMR (CDCl_3): δ_{H} (ppm) 0.94 (t, 3H, $J=7.4$ Hz), 1.02 (t, 3H, $J=7.1$ Hz), 1.46 (app. sextet, 2H, $J=7.4$ Hz), 1.77 (app. quintet, 2H, $J=7.0$ Hz), 2.57 (s, 3H), 4.03 (t, 2H, $J=6.6$ Hz), 4.05 (q, 2H, $J=7.1$ Hz), 4.12 (s, 3H), 6.98 (d, 1H, $J=8.4$ Hz), 7.09 (dt, 1H, $J_1=7.5$ Hz, $J_2=0.9$ Hz), 7.35 (ddd, 1H, $J_1=8.4$ Hz, $J_2=7.4$ Hz, $J_3=1.7$ Hz), 7.84 (app. t, 1H, $J=7.8$ Hz), 7.88 (dd, 1H, $J_1=7.6$ Hz, $J_2=1.7$ Hz), 8.06 (d, 1H, $J=7.9$ Hz), 8.28 (dd, 1H, $J_1=7.7$ Hz, $J_2=0.7$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.65, 13.77, 19.34, 22.26,



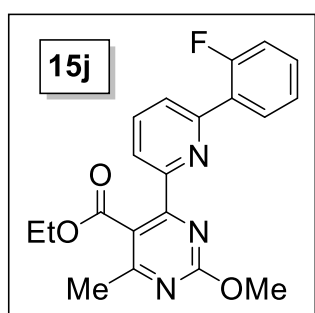
31.27, 55.01, 61.38, 68.11, 112.13, 119.81, 120.64, 120.87, 126.89, 128.12, 130.20, 131.94, 136.33, 152.96, 155.00, 156.64, 162.58, 164.26, 168.56, 168.75. FT-IR: wavenumber (cm^{-1}) 2800 (m), 1721 (s), 1557 (s), 1464 (m), 1358 (m), 1248 (s), 1169 (m), 1072 (m), 1010 (m), 799 (m), 760 (s). MS (ES-API), m/z : calcd for $\text{C}_{24}\text{H}_{27}\text{N}_3\text{O}_4$: 421.20; found: 422.1 $[\text{M}+\text{H}^+]$. m.p. 76-78 °C.

• **Ethyl 2-methoxy-4-(6-(4-methoxyphenyl)pyridin-2-yl)-6-methylpyrimidine-5-carboxylate (15g):**



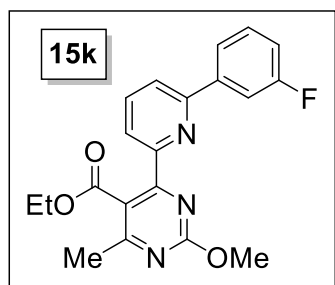
White solid. Yield: 85%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.01 (t, 3H, $J=7.1$ Hz), 2.60 (s, 3H), 3.87 (s, 3H), 4.10 (q, 2H, $J=7.1$ Hz), 4.11 (s, 3H), 7.01 (d, 2H, $J=8.8$ Hz), 7.76 (dd, 1H, $J_1=7.9$ Hz, $J_2=0.7$ Hz), 7.87 (app. t, 1H, $J=7.8$ Hz), 7.99 (d, 2H, $J=8.8$ Hz), 8.20 (dd, 1H, $J_1=7.7$ Hz, $J_2=0.7$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.75, 22.34, 55.02, 55.31, 61.39, 113.98, 119.78, 120.75, 120.84, 128.49, 131.09, 137.66, 153.48, 156.08, 160.67, 163.06, 164.34, 168.61, 168.96. FT-IR: wavenumber (cm^{-1}) 1713 (s), 1547 (s), 1468 (m), 1373 (m), 1244 (s), 1184 (m), 1102 (m), 1063 (m), 1032 (m), 793 (s). MS (ES-API), m/z : calcd for $\text{C}_{21}\text{H}_{21}\text{N}_3\text{O}_4$: 379.15; found: 380.1 $[\text{M}+\text{H}^+]$. m.p. 76-78 °C.

• **Ethyl 4-(6-(2-fluorophenyl)pyridin-2-yl)-2-methoxy-6-methylpyrimidine-5-carboxylate (15j):**



Colorless oil. Yield: 74%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.02 (t, 3H, $J=7.2$ Hz), 2.58 (s, 3H), 4.05 (q, 2H, $J=7.2$ Hz), 4.12 (s, 3H), 7.16 (dd, 1H, $J_1=11.7$ Hz, $J_2=8.2$ Hz, $J_3=1.0$ Hz), 7.30 (dt, 1H, $J_1=7.6$ Hz, $J_2=1.0$ Hz), 7.39 (m, 1H), 7.89-7.95 (m, 2H, 2 signals overlapping), 8.04 (dt, 1H, $J_1=7.9$ Hz, $J_2=1.8$ Hz), 8.33 (dd, 1H, $J_1=6.5$ Hz, $J_2=2.3$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.68, 22.34, 55.05, 61.37, 116.10 (d, $J=22.7$ Hz), 119.79, 121.73, 124.39 (d, $J=3.6$ Hz), 125.98 (d, $J=10.9$ Hz), 126.53 (d, $J=10.9$ Hz), 130.78 (d, $J=8.8$ Hz), 131.69 (d, $J=2.7$ Hz), 137.46, 152.29 (d, $J=2.7$ Hz), 153.61, 160.63 (d, $J=249.9$ Hz), 162.31, 164.36, 168.54, 169.00. FT-IR: wavenumber (cm^{-1}) 1726 (m), 1551 (s), 1462 (s), 1433 (w), 1380 (m), 1360 (m), 1288 (m), 1265 (s), 1246 (m), 1169 (m), 1072 (s), 890 (m), 829 (m), 800 (m), 760 (m), 677 (m). MS (ES-API), m/z : calcd for $\text{C}_{20}\text{H}_{18}\text{FN}_3\text{O}_3$: 367.13; found: 368.1 $[\text{M}+\text{H}^+]$.

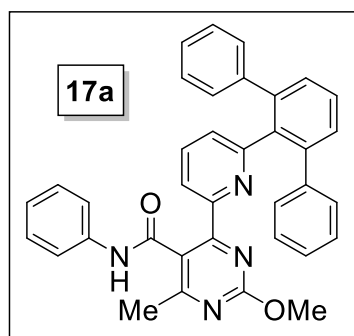
• **Ethyl 4-(6-(3-fluorophenyl)pyridin-2-yl)-2-methoxy-6-methylpyrimidine-5-carboxylate (15k):**



White solid. Yield: 91%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.08 (t, 3H, $J=7.2$ Hz), 2.62 (s, 3H), 4.13 (s, 3H), 4.17 (q, 2H, $J=7.2$ Hz), 7.13 (app. ddt, 1H, $J_1=8.3$ Hz, $J_2=2.5$ Hz, $J_3=0.8$ Hz), 7.46 (app. dt, 1H, $J_1=8.0$ Hz, $J_2=5.9$ Hz), 7.77 (ddd, 1H, $J_1=10.5$ Hz, $J_2=2.5$ Hz, $J_3=1.7$ Hz), 7.80 (ddd, 1H, $J_1=7.9$ Hz, $J_2=1.7$ Hz, $J_3=0.8$ Hz), 7.83 (dd, 1H, $J_1=7.9$ Hz, $J_2=0.8$ Hz), 7.94 (app. t, 1H, $J=7.8$ Hz), 8.31 (dd, 1H, $J=7.7$ Hz, 0.8 Hz).

^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.79, 22.25, 55.18, 61.51, 114.11 (d, $J=23.1$ Hz), 116.22 (d, $J=21.2$ Hz), 119.96, 121.82, 122.16, 122.66 (d, $J=2.9$ Hz), 130.22 (d, $J=8.2$ Hz), 138.03, 140.81 (d, $J=7.7$ Hz), 153.72, 155.11 (d, $J=2.7$ Hz), 162.70, 163.27 (d, $J=245.8$ Hz), 164.17, 168.37, 168.94. FT-IR: wavenumber (cm^{-1}) 1721 (s), 1547 (s), 1470 (m), 1358 (m), 1250 (s), 1190 (m), 1076 (s), 781 (s), 735 (m). MS (ES-API), m/z : calcd for $\text{C}_{20}\text{H}_{18}\text{FN}_3\text{O}_3$: 367.13; found: 368.1 [$\text{M}+\text{H}^+$]. m.p. 106-108 $^{\circ}\text{C}$.

• **4-(6-([1,1':3',1''-Terphenyl]-2'-yl)pyridin-2-yl)-2-methoxy-6-methyl-*N*-phenylpyrimidine-5-carboxamide (17a):**

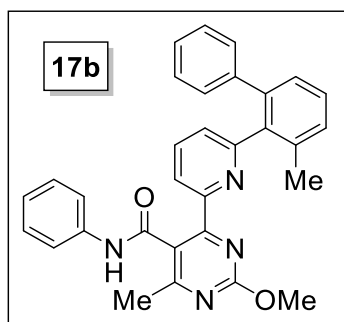


White solid. Yield: 61%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.56 (s, 3H), 4.05 (s, 3H), 6.90 (m, 4H), 6.94 (d, 1H, $J=7.8$ Hz), 7.00 (tt, 1H, $J_1=7.1$ Hz, $J_2=1.3$ Hz), 7.03-7.09 (m, 8H, 3 signals overlapping), 7.10 (app. t, 2H, $J=7.6$ Hz), 7.27 (d, 2H, $J=7.6$ Hz), 7.40 (bs, 1H), 7.43 (t, 1H, $J=7.6$ Hz), 7.46 (app. t, 1H, $J=7.8$ Hz), 7.99 (d, 1H, $J=7.8$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.34, 54.94, 120.48, 120.95, 123.09, 124.22, 126.31, 127.61, 128.21, 128.33, 128.76, 129.25,

129.57, 135.94, 137.29, 137.73, 141.18, 141.69, 152.75, 158.04, 161.30, 164.16, 166.26, 169.03. FT-IR: wavenumber (cm^{-1}) 1645 (m), 1549 (s), 1470 (m), 1439 (m), 1373 (m), 1317 (s), 1271 (w), 1065 (m), 799 (m), 758 (s). MS (ES-API), m/z : calcd for $\text{C}_{36}\text{H}_{28}\text{N}_4\text{O}_2$: 548.22; found: 549.2 [$\text{M}+\text{H}^+$]. m.p. 110-112 $^{\circ}\text{C}$.

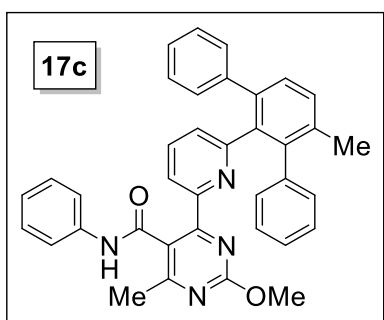
• **2-Methoxy-4-methyl-6-(6-(3-methyl-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-*N*-phenylpyrimidine-5-carboxamide (17b):**

White solid. Yield: 67%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.03 (s, 3H), 2.64 (s, 3H), 4.11 (s, 3H), 6.83 (d, 1H, $J=7.8$ Hz), 6.87 (m, 2H), 6.92 (t, 1H, $J=7.4$ Hz), 7.01 (app. t, 2H, $J=7.7$ Hz), 7.03-7.09 (m, 4H, 3 signals overlapping), 7.09-7.17 (m, 3H, 2 signals overlapping), 7.26 (app. t, 1H, $J=7.6$ Hz), 7.55 (app. t, 1H, $J=7.8$ Hz), 7.68 (bs, 1H), 8.20 (d, 1H, $J=7.8$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 20.45, 22.36, 55.01, 119.73, 121.06, 123.17, 124.00,



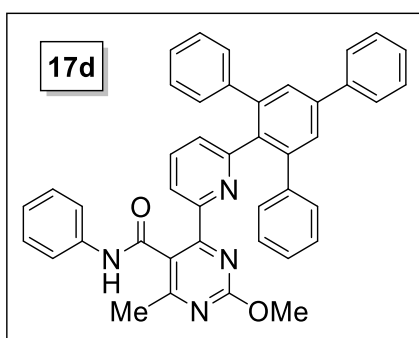
126.21, 127.22, 127.25, 127.58, 128.03, 128.70, 129.27, 129.60, 136.82, 136.85, 136.94, 137.52, 140.99, 141.35, 152.82, 158.69, 161.25, 164.36, 166.35, 169.59. FT-IR: wavenumber (cm^{-1}) 1659 (w), 1599 (w), 1557 (s), 1472 (m), 1445 (m), 1377 (m), 1323 (s), 797 (m), 752 (s), 746 (m). MS (ES-API), m/z : calcd for $\text{C}_{31}\text{H}_{26}\text{N}_4\text{O}_2$: 486.21; found: 487.2 $[\text{M}+\text{H}^+]$. m.p. 99-101 °C.

• **2-Methoxy-4-methyl-6-(6-(4'-methyl-[1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)-N-phenylpyrimidine-5-carboxamide (17c):**



White solid. Yield: 59%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.07 (s, 3H), 2.58 (s, 3H), 4.03 (s, 3H), 6.88 (d, 1H, $J=7.7$ Hz), 6.92 (d, 2H, $J=7.0$ Hz), 6.98-7.06 (m, 7H, 4 signals overlapping), 7.07-7.17 (m, 6H, 4 signals overlapping), 7.21 (d, 1H, $J=7.8$ Hz), 7.33 (d, 1H, $J=7.8$ Hz), 7.37 (app. t, 1H, $J=7.8$ Hz), 7.63 (bs, 1H), 7.87 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 20.72, 22.42, 54.91, 120.35, 120.66, 123.05, 124.17, 126.09, 126.16, 127.45, 127.51, 127.58, 127.89, 128.79, 128.90, 129.49, 130.04, 135.38, 135.55, 137.44, 138.60, 138.92, 139.72, 141.22, 141.30, 152.54, 158.32, 161.27, 164.12, 166.23, 169.26. FT-IR: wavenumber (cm^{-1}) 1649 (m), 1599 (m), 1555 (s), 1470 (m), 1441 (m), 1368 (m), 1315 (s), 1265 (m), 783 (s), 748 (s). MS (ES-API), m/z : calcd for $\text{C}_{37}\text{H}_{30}\text{N}_4\text{O}_2$: 562.24; found: 563.2 $[\text{M}+\text{H}^+]$. m.p. 92-93 °C.

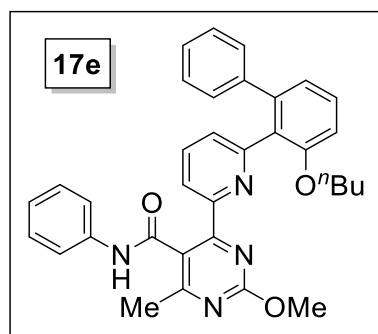
• **2-Methoxy-4-methyl-N-phenyl-6-(6-(5'-phenyl-[1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)pyrimidine-5-carboxamide (17d):**



White solid. Yield: 63%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.56 (s, 3H), 4.06 (s, 3H), 6.87 (t, 1H, $J=7.4$ Hz), 6.98 (dd, 4H, $J_1=7.8$ Hz, $J_2=2.2$ Hz), 6.98-7.02 (m, 3H, signals overlapping), 7.08-7.12 (m, 6H, signals overlapping), 7.17 (d, 2H, $J=7.8$ Hz), 7.37 (bs, 1H), 7.41 (t, 1H, $J=7.6$ Hz), 7.47-7.53 (m, 5H, signals overlapping), 7.67 (d, 2H, $J=7.6$ Hz), 8.03 (dd, 1H, $J_1=7.8$ Hz, $J_2=0.8$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.35, 54.92, 120.42, 120.94, 123.12, 124.22, 126.46, 127.23, 127.64, 127.70, 127.96, 128.22, 128.70, 128.85, 129.61, 135.98, 136.73, 137.26, 140.33, 141.02, 141.16, 142.19, 152.77, 157.93, 161.36, 164.20, 166.35, 168.92. FT-IR: wavenumber (cm^{-1}) 1649 (m), 1599 (m), 1549 (s), 1472 (m), 1441 (m), 1371 (m), 1315 (s), 1263 (m), 1057

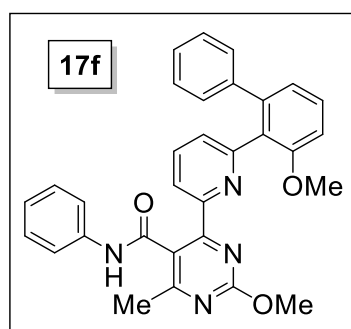
(m), 797 (m), 766 (s). MS (ES-API), m/z: calcd for C₄₂H₃₂N₄O₂: 624.25; found: 625.2 [M+H⁺]. m.p. 148-150 °C.

• **4-(6-(3-Butoxy-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenyl-pyrimidine-5-carboxamide (17e):**



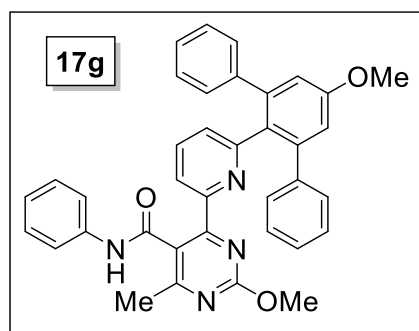
White solid. Yield: 68%. ¹H NMR (CDCl₃): δ_H (ppm) 0.72 (t, 3H, J=7.4 Hz), 1.12 (app. sextet, 2H, J=7.5 Hz), 1.42 (quint., 2H, J=7.0 Hz), 2.61 (s, 3H), 3.63 (t, 2H, J=6.4 Hz), 4.08 (s, 3H), 6.71 (d, 1H, J=8.3 Hz), 6.92 (d, 1H, J=7.7 Hz), 6.93-6.99 (m, 3H, 2 signals overlapping), 7.02-7.08 (m, 6H, 4 signals overlapping), 7.11 (d, 2H, J=8.1 Hz), 7.31 (app. t, 1H, J=8.0 Hz), 7.61 (app. t, 1H, J=7.8 Hz), 8.02 (bs, 1H), 8.07 (d, 1H, J=7.9 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 13.62, 19.00, 22.54, 30.95, 54.95, 68.19, 111.22, 119.89, 121.24, 122.06, 123.34, 123.79, 126.34, 127.50, 127.59, 128.63, 128.87, 129.10, 129.51, 136.29, 137.75, 140.69, 142.51, 153.21, 155.95, 156.77, 161.44, 164.14, 166.13, 169.77. FT-IR: wavenumber (cm⁻¹) 2924 (m), 1651 (m), 1601 (m), 1557 (s), 1467 (m), 1441 (m), 1380 (m), 1319 (s), 1265 (m), 1069 (m), 1026 (m), 797 (m), 758 (s), 748 (m). MS (ES-API), m/z: calcd for C₃₄H₃₂N₄O₃: 544.25; found: 545.1 [M+H⁺]. m.p. 100-102 °C.

• **2-Methoxy-4-(6-(3-methoxy-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-6-methyl-N-phenyl-pyrimidine-5-carboxamide (17f):**



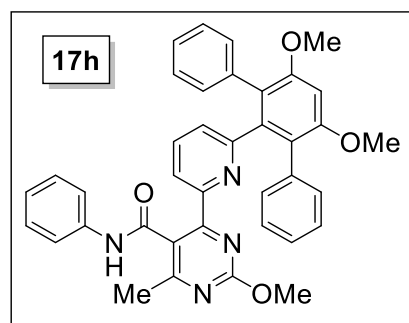
White solid. Yield: 71%. ¹H NMR (CDCl₃): δ_H (ppm) 2.60 (s, 3H), 3.45 (s, 3H), 4.07 (s, 3H), 6.67 (d, 1H, J=8.3 Hz), 6.93 (d, 1H, J=7.7 Hz), 6.94-7.00 (m, 4H, 3 signals overlapping), 7.03-7.11 (m, 5H, 3 signals overlapping), 7.16 (d, 2H, J=8.0 Hz), 7.31 (app. t, 1H, J=8.0 Hz), 7.58 (app. t, 1H, J=7.8 Hz), 7.95 (bs, 1H), 8.12 (d, 1H, J=7.9 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 22.39, 54.91, 55.52, 109.90, 119.87, 121.15, 122.06, 123.30, 123.77, 126.39, 126.85, 127.49, 127.62, 128.66, 129.14, 129.57, 136.56, 137.89, 140.63, 142.51, 153.04, 156.00, 157.14, 161.26, 164.20, 166.26, 169.65. FT-IR: wavenumber (cm⁻¹) 1647 (m), 1597 (m), 1549 (s), 1528 (m), 1470 (m), 1437 (m), 1371 (s), 1317 (s), 1256 (s), 1165 (w), 1070 (w), 1026 (m), 797 (m), 750 (s). MS (ES-API), m/z: calcd for C₃₁H₂₆N₄O₃: 502.20; found: 503.1 [M+H⁺]. m.p. 82-84 °C.

• **2-Methoxy-4-(6-(5'-methoxy-[1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)-6-methyl-N-phenylpyrimidine-5-carboxamide (17g):**



White solid. Yield: 65%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.56 (s, 3H), 3.87 (s, 3H), 4.04 (s, 3H), 6.78 (s, 2H), 6.91 (m, 5H, 2 signals overlapping), 7.01 (t, 1H, $J=7.3$ Hz), 7.05-7.09 (m, 6H, 2 signals overlapping), 7.11 (app. t, 2H, $J=7.7$ Hz), 7.16 (d, 2H, $J=8.1$ Hz), 7.40 (bs, 1H), 7.43 (app. t, 1H, $J=7.8$ Hz), 7.96 (d, 1H, $J=7.8$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.34, 54.93, 55.34, 114.65, 120.45, 120.68, 123.13, 124.08, 126.44, 127.63, 128.45, 128.68, 129.45, 130.80, 135.84, 137.41, 141.20, 143.06, 152.67, 157.96, 158.96, 161.47, 164.15, 166.33, 168.95. FT-IR: wavenumber (cm^{-1}) 1659 (m), 1599 (m), 1553 (s), 1514 (m), 1441 (m), 1323 (s), 1248 (s), 1179 (m), 1032 (m), 793 (s), 754 (s). MS (ES-API), m/z : calcd for $\text{C}_{37}\text{H}_{30}\text{N}_4\text{O}_3$: 578.23; found: 579.2 $[\text{M}+\text{H}^+]$. m.p. 94-96 $^{\circ}\text{C}$.

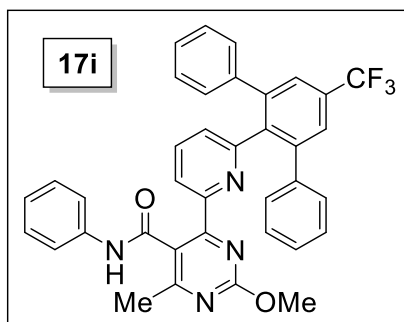
• **4-(6-(4',6'-Dimethoxy-[1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (17h):**



White solid. Yield: 55%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.59 (s, 3H), 3.77 (s, 6H), 4.04 (s, 3H), 6.61 (s, 1H), 6.81 (d, 1H, $J=7.7$ Hz), 6.90 (d, 4H, $J=6.5$ Hz), 6.97 (t, 2H, $J=7.2$ Hz), 7.00-7.06 (m, 5H, 2 signals overlapping), 7.15 (app. t, 2H, $J=7.7$ Hz), 7.28 (d, 2H, $J=8.1$ Hz), 7.32 (app. t, 1H, $J=7.8$ Hz), 7.57 (bs, 1H), 7.85 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.40, 54.96, 56.00, 96.08, 120.47, 120.49, 123.06, 124.01, 125.99, 127.18, 127.82, 128.71, 131.04, 131.10, 135.45, 136.40, 137.71, 141.56, 152.26, 156.74, 157.64, 161.27, 164.10, 166.37, 169.08. FT-IR: wavenumber (cm^{-1}) 1655 (m), 1595 (m), 1549 (s), 1462 (s), 1459 (m), 1375 (m), 1319 (s), 1260 (m), 1200 (m), 1155 (s), 1069 (m), 793 (s), 756 (s). MS (ES-API), m/z : calcd for $\text{C}_{38}\text{H}_{32}\text{N}_4\text{O}_4$: 608.24; found: 609.2 $[\text{M}+\text{H}^+]$. m.p. 107-109 $^{\circ}\text{C}$.

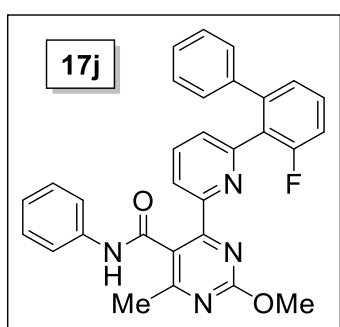
• **2-Methoxy-4-methyl-N-phenyl-6-(6-(5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)pyrimidine-5-carboxamide (17i):**

Beige solid. Yield: 51%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.54 (s, 3H), 4.04 (s, 3H), 6.89-6.95 (m, 5H, 2 signals overlapping), 7.01 (t, 1H, $J=7.5$ Hz), 7.08 (app. t, 2H, $J=7.7$ Hz), 7.09-7.13 (m, 6H, 2 signals overlapping), 7.17 (d, 2H, $J=7.9$ Hz), 7.24 (bs, 1H), 7.47 (s, 2H), 7.49 (app. t, 1H, $J=7.8$ Hz), 8.08 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.22,



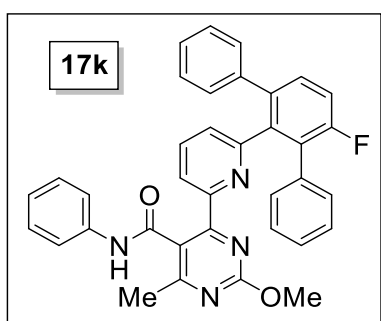
54.96, 119.76, 121.27, 122.85, 123.09, 124.42, 125.02, 125.79, 126.99, 127.85, 128.72, 129.46, 130.42, 136.23, 137.33, 139.80, 140.97, 142.45, 152.78, 156.95, 161.07, 164.25, 166.24, 168.84. FT-IR: wavenumber (cm^{-1}) 1553 (s), 1443 (m), 1323 (s), 1256 (m), 1157 (m), 1109 (s), 1074 (m), 1015 (m), 760 (m). MS (ES-API), m/z : calcd for $\text{C}_{37}\text{H}_{27}\text{F}_3\text{N}_4\text{O}_2$: 616.21; found: 617.1 $[\text{M}+\text{H}^+]$. m.p. 96-98 °C.

• **4-(6-(3-Fluoro-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (17j):**



White solid. Yield: 61%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.62 (s, 3H), 4.10 (s, 3H), 6.75 (app. t, 1H, $J=8.9$ Hz), 6.91 (d, 1H, $J=7.7$ Hz), 6.94-6.98 (m, 3H, 2 signals overlapping), 7.06 (m, 3H, 2 signals overlapping), 7.12 (m, 3H, 2 signals overlapping), 7.24 (m, 1H), 7.28 (d, 2H, $J=8.1$ Hz), 7.59 (app. t, 1H, $J=7.8$ Hz), 7.72 (bs, 1H), 8.20 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.29, 54.96, 114.32 (d, $J=22.0$ Hz), 119.37, 121.53, 123.37, 123.72, 125.21 (d, $J=2.9$ Hz), 126.90, 127.05, 127.17, 127.27, 127.88, 128.63, 129.48 (d, $J=9.2$ Hz), 129.60, 136.75, 138.01, 139.47 (d, $J=2.6$ Hz), 142.94 (d, $J=2.2$ Hz), 153.34 (d, $J=25.3$ Hz), 160.10 (d, $J=248.0$ Hz), 161.13, 164.26, 166.33, 169.42. FT-IR: wavenumber (cm^{-1}) 1641 (m), 1609 (w), 1543 (s), 1474 (m), 1317 (s), 1277 (m), 1209 (w), 1171 (w), 1067 (w), 799 (m), 758 (s). MS (ES-API), m/z : calcd for $\text{C}_{30}\text{H}_{23}\text{FN}_4\text{O}_2$: 490.18; found: 491.1 $[\text{M}+\text{H}^+]$. m.p. 104-106 °C.

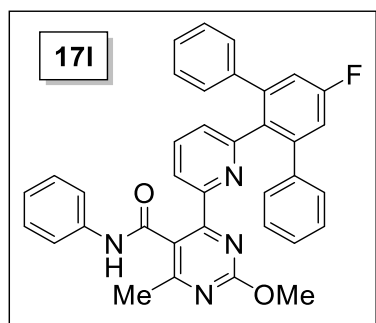
• **4-(6-(4'-Fluoro-[1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (17k):**



White solid. Yield: 60%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.57 (s, 3H), 4.04 (s, 3H), 6.89 (m, 3H, 2 signals overlapping), 6.93 (d, 2H, $J=6.4$ Hz), 7.03 (t, 1H, $J=7.4$ Hz), 7.06-7.10 (m, 6H, 4 signals overlapping), 7.14 (app. t, 2H, $J=7.7$ Hz), 7.16 (app. t, 1H, $J=8.9$ Hz), 7.19-7.23 (m, 3H, 2 signals overlapping), 7.36 (bs, 1H), 7.44 (app. t, 1H, $J=7.8$ Hz), 7.98 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.32, 54.97, 115.57 (d, $J=22.6$ Hz), 120.08, 121.09, 123.05, 124.33, 126.43, 127.01, 127.28, 127.55, 127.70, 127.92, 128.81, 128.98 (d, $J=7.4$ Hz), 129.54, 130.41, 130.49, 133.76, 136.05, 137.41, 137.58 (d, $J=3.6$ Hz), 140.34, 152.61, 156.84, 158.92 (d, $J=246.1$ Hz), 161.14, 164.18, 166.20,

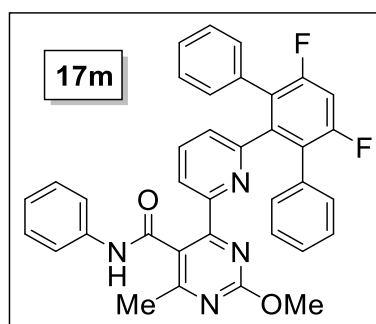
168.97. FT-IR: wavenumber (cm^{-1}) 1651 (m), 1597 (m), 1549 (s), 1470 (m), 1441 (m), 1379 (m), 1317 (s), 1267 (m), 1194 (w), 1070 (m), 785 (s), 758 (s). MS (ES-API), m/z : calcd for $\text{C}_{36}\text{H}_{27}\text{FN}_4\text{O}_2$: 566.21; found: 567.1 $[\text{M}+\text{H}^+]$. m.p. 114-116 $^\circ\text{C}$.

• **4-(6-(5'-Fluoro-[1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (17l):**



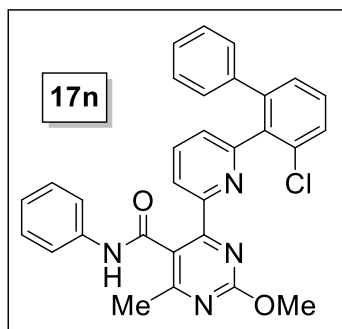
Beige solid. Yield: 52%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.56 (s, 3H), 4.05 (s, 3H), 6.86-6.92 (m, 5H, 2 signals overlapping), 6.94 (d, 2H, $J=9.3$ Hz), 7.05-7.11 (m, 8H, 4 signals overlapping), 7.14 (app. t, 2H, $J=7.7$ Hz), 7.18 (d, 2H, $J=8.1$ Hz), 7.46 (app. t, 1H, $J=7.8$ Hz), 8.02 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.28, 54.95, 115.75 (d, $J=21.3$ Hz), 120.08, 120.94, 123.08, 124.27, 126.80, 127.74, 128.28, 128.74, 129.37, 134.00, 136.05, 137.37, 140.14, 143.79 (d, $J=8.2$ Hz), 152.69, 157.33, 161.26, 161.92 (d, $J=247.8$ Hz), 164.20, 166.29, 168.85. FT-IR: wavenumber (cm^{-1}) 1643 (m), 1597 (m), 1541 (s), 1508 (m), 1470 (m), 1439 (m), 1379 (m), 1317 (s), 1223 (m), 1167 (m), 1065 (m), 795 (s), 760 (s). MS (ES-API), m/z : calcd for $\text{C}_{36}\text{H}_{27}\text{FN}_4\text{O}_2$: 566.21; found: 567.2 $[\text{M}+\text{H}^+]$. m.p. 115-117 $^\circ\text{C}$.

• **4-(6-(4',6'-Difluoro-[1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (17m):**



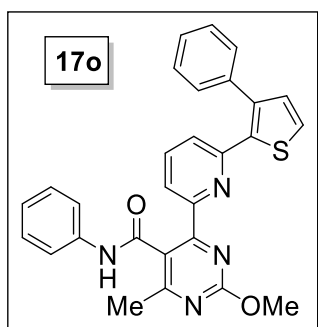
White solid. Yield: 53%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.58 (s, 3H), 4.04 (s, 3H), 6.84 (d, 1H, $J=7.7$ Hz), 6.91-6.95 (m, 5H, 2 signals overlapping), 7.03-7.15 (m, 7H, 3 signals overlapping), 7.20 (app. t, 2H, $J=7.7$ Hz), 7.31 (d, 2H, $J=8.1$ Hz), 7.33 (bs, 1H), 7.42 (app. t, 1H, $J=7.8$ Hz), 7.98 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.34, 55.01, 104.01 (d, $J=27.1$ Hz), 119.70, 121.22, 123.05, 124.46, 127.16, 127.44, 127.60, 127.66, 128.89, 130.56, 133.05, 136.08, 137.61, 142.17, 152.58, 155.74, 158.69 (dd, $J_1=248.7$ Hz, $J_2=12.9$ Hz), 161.05, 164.25, 166.23, 168.96. FT-IR: wavenumber (cm^{-1}) 1665 (m), 1597 (m), 1547 (s), 1470 (m), 1439 (m), 1379 (m), 1321 (m), 1260 (m), 1119 (m), 988 (m), 793 (m), 756 (s), 698 (m). MS (ES-API), m/z : calcd for $\text{C}_{36}\text{H}_{26}\text{F}_2\text{N}_4\text{O}_2$: 584.20; found: 585.2 $[\text{M}+\text{H}^+]$. m.p. 116-118 $^\circ\text{C}$.

• **4-(6-(3-Chloro-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (17n):**



Beige solid. Yield: 71%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.62 (s, 3H), 4.10 (s, 3H), 6.88 (d, 1H, $J=7.7$ Hz), 6.93 (t, 1H, $J=7.4$ Hz), 6.99 (m, 2H), 7.04 (app. t, 2H, $J=7.7$ Hz), 7.08 (app. dt, 1H, $J_1=7.6$ Hz, $J_2=1.5$ Hz), 7.10-7.12 (m, 3H, 2 signals overlapping), 7.16 (dd, 1H, $J_1=7.8$ Hz, $J_2=1.5$ Hz), 7.19 (t, 1H, $J=7.7$ Hz), 7.27 (d, 2H, $J=8.0$ Hz), 7.60 (app. t, 1H, $J=7.8$ Hz), 7.68 (bs, 1H), 8.25 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.27, 55.01, 119.33, 121.51, 123.43, 123.66, 126.79, 126.87, 127.82, 128.08, 128.32, 128.61, 129.10, 129.57, 133.50, 137.13, 137.50, 137.92, 143.03, 152.77, 156.18, 160.86, 164.34, 166.44, 169.42. FT-IR: wavenumber (cm^{-1}) 1641 (m), 1596 (m), 1549 (s), 1468 (m), 1443 (m), 1383 (m), 1323 (s), 1271 (m), 1072 (m), 1040 (m), 880 (m), 799 (m), 750 (s), 692 (m). MS (ES-API), m/z : calcd for $\text{C}_{30}\text{H}_{23}\text{ClN}_4\text{O}_2$: 506.15; found: 507.2 [$\text{M}+\text{H}^+$]. m.p. 112-114 $^{\circ}\text{C}$.

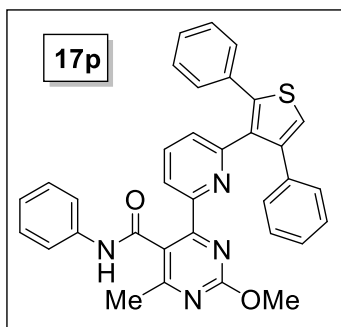
• **2-Methoxy-4-methyl-N-phenyl-6-(6-(3-phenylthiophen-2-yl)pyridin-2-yl)pyrimidine-5-carboxamide (17o):**



Beige solid. Yield: 71%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.62 (s, 3H), 4.05 (s, 3H), 6.96 (d, 1H, $J=5.1$ Hz), 6.98 (d, 1H, $J=7.9$ Hz), 7.02 (t, 1H, $J=7.4$ Hz), 7.12-7.22 (m, 5H, 3 signals overlapping), 7.27-7.31 (m, 3H, 2 signals overlapping), 7.45-7.53 (m, 3H, 2 signals overlapping), 7.97 (d, 1H, $J=7.7$ Hz), 8.14 (bs, 1H). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.56, 55.02, 119.86, 121.60, 123.13, 123.64, 124.14, 127.06, 127.43, 128.60, 128.69, 128.99, 130.51, 136.62, 136.91, 137.95, 138.36, 140.21, 152.35, 153.94, 161.69, 164.09, 165.62, 169.97. FT-IR: wavenumber (cm^{-1}) 1661 (m), 1597 (m), 1551 (s), 1472 (m), 1441 (m), 1377 (m), 1317 (s), 1258 (m), 1057 (m), 781 (s), 754 (s), 706 (m). MS (ES-API), m/z : calcd for $\text{C}_{28}\text{H}_{22}\text{N}_4\text{O}_2\text{S}$: 478.15; found: 479.1 [$\text{M}+\text{H}^+$]. m.p. 131-133 $^{\circ}\text{C}$.

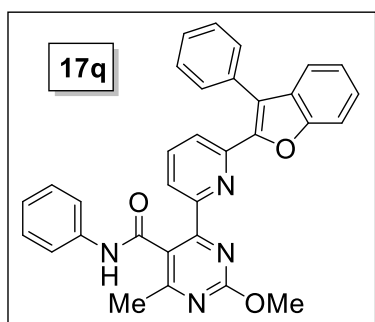
• **4-(6-(2,4-Diphenylthiophen-3-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (17p):**

Beige solid. Yield: 70%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.54 (s, 3H), 4.05 (s, 3H), 6.89 (m, 2H), 7.01 (m, 2H), 7.03 (tt, 1H, $J_1=6.8$ Hz, $J_2=2.0$ Hz), 7.06 (dd, 1H, $J_1=7.8$ Hz, $J_2=0.9$ Hz), 7.08-7.20 (m, 11H, 7 signals overlapping), 7.50 (bs, 1H), 7.64 (app. t, 1H, $J=7.8$ Hz), 8.13 (dd, 1H, $J_1=7.8$ Hz, $J_2=0.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.34, 54.97, 120.35, 121.70, 121.93, 123.32, 124.24, 126.70, 127.38, 127.39, 127.90, 128.23, 128.64, 128.69,



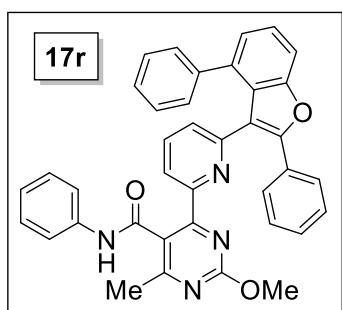
129.09, 133.84, 136.15, 136.33, 137.01, 137.40, 142.80, 143.51, 153.76, 154.81, 161.40, 164.19, 166.14, 169.18. FT-IR: wavenumber (cm^{-1}) 1651 (s), 1599 (m), 1545 (s), 1468 (s), 1439 (s), 1373 (m), 1321 (s), 1285 (m), 1063 (m), 795 (m), 756 (s). MS (ES-API), m/z : calcd for $\text{C}_{34}\text{H}_{26}\text{N}_4\text{O}_2\text{S}$: 554.18; found: 555.1 $[\text{M}+\text{H}^+]$. m.p. 122-124 °C.

• **2-Methoxy-4-methyl-N-phenyl-6-(6-(3-phenylbenzofuran-2-yl)pyridin-2-yl)pyrimidine-5-carboxamide (17q):**



White solid. Yield: 53%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.68 (s, 3H), 4.12 (s, 3H), 6.94 (t, 1H, $J=7.4$ Hz), 7.05 (app. t, 2H, $J=7.8$ Hz), 7.15 (d, 1H, $J=8.1$ Hz), 7.24 (t, 1H, $J=7.4$ Hz), 7.31 (app. t, 1H, $J=8.0$ Hz), 7.34 (m, 2H), 7.39-7.43 (m, 4H, 3 signals overlapping), 7.44-7.46 (m, 3H, 2 signals overlapping), 7.70 (app. t, 1H, $J=7.8$ Hz), 8.03 (d, 1H, $J=7.8$ Hz), 8.21 (bs, 1H). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.62, 55.21, 111.85, 119.16, 119.85, 120.11, 120.35, 120.55, 122.98, 123.25, 123.71, 124.10, 124.37, 126.02, 128.14, 128.74, 128.80, 129.03, 129.25, 129.67, 131.81, 137.88, 138.01, 148.17, 154.42, 164.15, 165.43, 169.92. FT-IR: wavenumber (cm^{-1}) 1657 (m), 1649 (m), 1599 (m), 1547 (s), 1491 (w), 1470 (m), 1441 (m), 1375 (m), 1319 (s), 1260 (m), 1236 (m), 1171 (m), 1088 (s), 880 (s), 795 (m), 750 (m), 729 (m). MS (ES-API), m/z : calcd for $\text{C}_{32}\text{H}_{24}\text{N}_4\text{O}_3$: 512.18; found: 513.2 $[\text{M}+\text{H}^+]$. m.p. 111-113 °C.

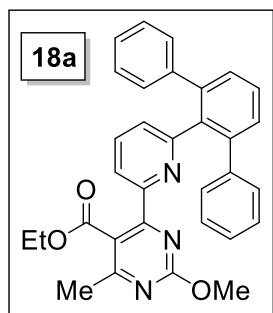
• **4-(6-(2,4-Diphenylbenzofuran-3-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (17r):**



White solid. Yield: 71%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.58 (s, 3H), 4.13 (s, 3H), 6.78-6.94 (m, 9H, signals overlapping), 6.98 (d, 2H, $J=7.6$ Hz), 7.09 (dd, 1H, $J_1=7.4$ Hz, $J_2=0.8$ Hz), 7.20 (m, 3H, signals overlapping), 7.28 (dd, 2H, $J_1=7.3$ Hz, $J_2=1.8$ Hz), 7.34 (t, 1H, $J=7.8$ Hz), 7.40 (t, 1H, $J=7.8$ Hz), 7.48 (bs, 1H), 7.50 (d, 1H, $J=8.2$ Hz), 8.04 (dd, 1H, $J_1=7.9$ Hz, $J_2=0.8$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 22.32, 55.01, 110.04, 117.06, 119.16, 121.59, 123.61, 123.81, 124.18, 124.39, 126.25, 126.72, 127.02, 127.04, 127.12, 128.20, 128.24, 128.38, 128.66, 130.01, 136.23, 136.61, 137.37, 139.11, 152.08, 152.13, 153.71, 153.93, 161.38, 164.17, 166.22, 169.02. FT-IR: wavenumber (cm^{-1}) 1651 (m), 1599 (m), 1537 (s), 1470 (m), 1441 (m), 1375 (m), 1315 (s), 1261 (m), 1225 (m), 1103 (m), 1069 (m), 795 (m),

743 (s). MS (ES-API), m/z: calcd for C₃₈H₂₈N₄O₃: 588.22; found: 589.2 [M+H⁺]. m.p. 109-111 °C.

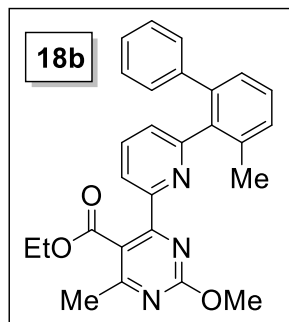
• **Ethyl 4-(6-([1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)-2-methoxy-6-methyl-pyrimidine-5-carboxylate (18a):**



White solid. Yield: 58%. ¹H NMR (CDCl₃): δ_H (ppm) 1.07 (t, 3H, J=7.2 Hz), 2.49 (s, 3H), 3.87 (q, 2H, J=7.2 Hz), 4.07 (s, 3H), 6.87 (dd, 1H, J₁=7.7 Hz, J₂=0.9 Hz), 7.08 (tt, 2H, J₁=7.1 Hz, J₂=2.0 Hz), 7.12 (app. t, 4H, J=7.3 Hz), 7.16 (m, 4H), 7.42 (app. t, 1H, J=7.8 Hz), 7.44 (d, 2H, J=7.7 Hz), 7.54 (t, 1H, J=7.7 Hz), 8.10 (dd, 1H, J₁=7.9 Hz, J₂=0.9 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 13.76, 22.11, 54.91, 61.12, 120.23, 120.29, 126.43, 127.46, 127.53, 128.15, 129.06, 129.81, 136.14, 138.14, 140.89, 141.86, 151.21,

157.89, 160.94, 164.17, 168.11, 168.60. FT-IR: wavenumber (cm⁻¹) 1721 (s), 1547 (s), 1470 (m), 1375 (m), 1252 (s), 1198 (m), 1169 (m), 1078 (s), 772 (s). MS (ES-API), m/z: calcd for C₃₂H₂₇N₃O₃: 501.21; found: 502.2 [M+H⁺]. m.p. 82-84 °C.

• **Ethyl 2-methoxy-4-methyl-6-(6-(3-methyl-[1,1'-biphenyl]-2-yl)pyridin-2-yl)pyrimidine-5-carboxylate (18b):**

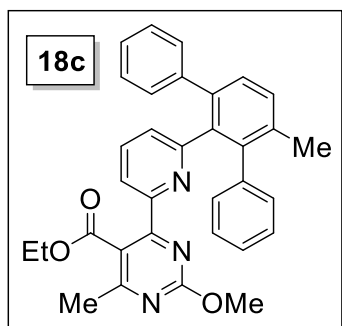


White solid. Yield: 56%. ¹H NMR (CDCl₃): δ_H (ppm) 1.04 (t, 3H, J=7.2 Hz), 2.15 (s, 3H), 2.52 (s, 3H), 3.83 (bd, 2H), 4.12 (s, 3H), 6.84 (dd, 1H, J₁=7.7 Hz, J₂=1.0 Hz), 7.06 (m, 2H), 7.10-7.16 (m, 3H, signals overlapping), 7.28 (d, 1H, J=7.8 Hz), 7.31 (d, 1H, J=7.4 Hz), 7.38 (app. t, 1H, J=7.6 Hz), 7.56 (app. t, 1H, J=7.8 Hz), 8.31 (dd, 1H, J₁=7.9 Hz, J₂=1.0 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 13.63, 20.39, 22.08, 54.97, 61.37, 120.25, 120.34, 126.39, 126.94, 127.35, 127.76, 128.17, 129.15, 129.70,

136.93, 137.26, 138.78, 141.03, 141.16, 151.72, 158.30, 160.84, 164.39, 168.33, 169.05. FT-IR: wavenumber (cm⁻¹) 1724 (s), 1551 (s), 1470 (s), 1379 (m), 1360 (m), 1265 (s), 1246 (m), 1225 (m), 1167 (m), 1094 (m), 1070 (s), 874 (m), 802 (m), 764 (m), 700 (m), 627 (m). MS (ES-API), m/z: calcd for C₂₇H₂₅N₃O₃: 439.19; found: 440.1 [M+H⁺]. m.p. 76-78 °C.

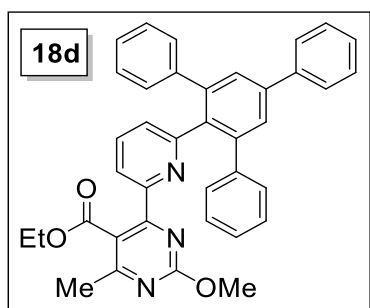
• **Ethyl 2-methoxy-4-methyl-6-(6-(4'-methyl-[1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)pyrimidine-5-carboxylate (18c):**

White solid. Yield: 61%. ¹H NMR (CDCl₃): δ_H (ppm) 1.11 (t, 3H, J=7.1 Hz), 2.17 (s, 3H), 2.50 (s, 3H), 3.88 (q, 2H, J=7.1 Hz), 4.05 (s, 3H), 6.78 (dd, 1H, J₁=7.8 Hz, J₂=0.8 Hz), 6.95 (t, 1H, J=6.7 Hz), 7.01 (t, 2H, J=7.1 Hz), 7.08 (d, 2H, J=7.5 Hz), 7.11 (t, 2H, J=7.0 Hz), 7.16



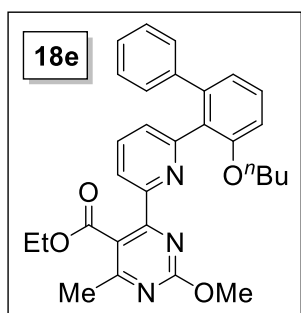
(d, 2H, $J=7.5$ Hz), 7.21 (t, 1H, $J=6.5$ Hz), 7.33 (t, 1H, $J=7.9$ Hz), 7.36 (d, 1H, $J=8.0$ Hz), 7.41 (d, 1H, $J=8.0$ Hz), 8.00 (dd, 1H, $J_1=8.0$ Hz, $J_2=0.8$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.76, 20.76, 22.12, 54.87, 61.13, 119.87, 120.17, 126.17, 126.26, 127.05, 127.15, 127.53, 127.57, 128.64, 129.22, 129.69, 129.80, 130.84, 138.68, 138.83, 139.47, 140.93, 141.64, 150.88, 158.15, 161.00, 164.18, 168.05, 168.74. FT-IR: wavenumber (cm^{-1}) 1721 (s), 1549 (s), 1468 (m), 1379 (m), 1360 (m), 1250 (s), 1192 (m), 1074 (s), 787 (s). MS (ES-API), m/z : calcd for $\text{C}_{33}\text{H}_{29}\text{N}_3\text{O}_3$: 515.22; found: 516.2 $[\text{M}+\text{H}^+]$. m.p. 84-86 °C.

• **Ethyl 2-methoxy-4-methyl-6-(6-(5'-phenyl-[1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)pyrimidine-5-carboxylate (18d):**



White solid. Yield: 63%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.08 (t, 3H, $J=7.2$ Hz), 2.49 (s, 3H), 3.92 (q, 2H, $J=7.2$ Hz), 4.07 (s, 3H), 6.91 (dd, 1H, $J_1=7.7$ Hz, $J_2=0.9$ Hz), 7.11 (tt, 2H, $J_1=7.0$ Hz, $J_2=2.0$ Hz), 7.15 (app. t, 4H, $J=7.2$ Hz), 7.22 (m, 4H), 7.40 (tt, 1H, $J_1=7.4$ Hz, $J_2=1.5$ Hz), 7.44 (app. t, 1H, $J=7.8$ Hz), 7.49 (app. t, 2H, $J=7.7$ Hz), 7.70 (s, 2H), 7.73 (m, 2H), 8.12 (dd, 1H, $J_1=7.9$ Hz, $J_2=0.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.77, 22.12, 54.93, 61.21, 120.26, 120.37, 126.58, 127.18, 127.54, 127.62, 127.63, 127.72, 128.92, 129.83, 136.20, 137.18, 140.34, 140.87, 140.89, 142.45, 151.36, 157.75, 161.01, 164.17, 168.12, 168.62. FT-IR: wavenumber (cm^{-1}) 1724 (s), 1549 (s), 1474 (m), 1362 (m), 1358 (m), 1248 (s), 1175 (m), 1076 (m), 1053 (m), 824 (m), 799 (s), 764 (s). MS (ES-API), m/z : calcd for $\text{C}_{38}\text{H}_{31}\text{N}_3\text{O}_3$: 577.24; found: 578.2 $[\text{M}+\text{H}^+]$. m.p. 142-144 °C.

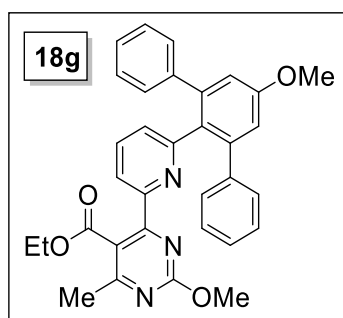
• **Ethyl 4-(6-(3-butoxy-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-2-methoxy-6-methylpyrimidine-5-carboxylate (18e):**



White wax. Yield: 58%. ^1H NMR (CDCl_3): δ_{H} (ppm) 0.73 (t, 3H, $J=7.5$ Hz), 1.01 (t, 3H, $J=7.1$ Hz), 1.17 (app. sextet, 2H, $J=7.5$ Hz), 1.52 (app. quintet, 2H, $J=7.0$ Hz), 2.50 (s, 3H), 3.83 (q, 2H, $J=7.1$ Hz), 3.94 (t, 2H, $J=6.5$ Hz), 4.10 (s, 3H), 6.98 (d, 1H, $J=8.1$ Hz), 7.02 (d, 1H, $J=7.7$ Hz), 7.05 (d, 1H, $J=7.7$ Hz), 7.09 (m, 1H), 7.10-7.14 (m, 4H, signals overlapping), 7.41 (app. t, 1H, $J=7.9$ Hz), 7.60 (app. t, 1H, $J=7.8$ Hz), 8.24 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.59, 13.60, 18.94, 22.12, 31.01, 54.89, 61.09, 68.54, 111.09, 120.24, 120.30, 122.07, 126.43, 127.25, 127.59, 129.09, 129.32, 129.66, 136.29, 140.52, 142.56, 151.79, 155.90, 157.09, 161.47,

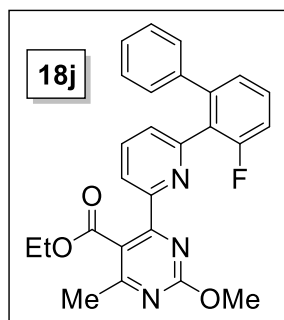
164.27, 168.14, 168.55. FT-IR: wavenumber (cm^{-1}) 2800 (m), 1721 (s), 1553 (s), 1462 (m), 1360 (m), 1269 (s), 1225 (s), 1179 (m), 1072 (m), 1007 (m), 799 (m), 762 (s). MS (ES-API), m/z : calcd for $\text{C}_{30}\text{H}_{31}\text{N}_3\text{O}_4$: 497.23; found: 498.2 $[\text{M}+\text{H}^+]$.

• **Ethyl 2-methoxy-4-(6-(5'-methoxy-[1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)-6-methylpyrimidine-5-carboxylate (18g):**



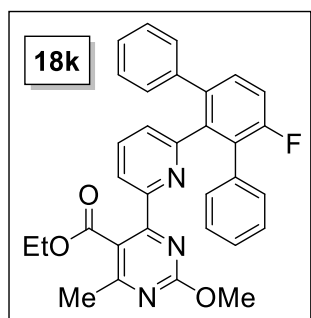
White solid. Yield: 56%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.12 (t, 3H, $J=7.2$ Hz), 2.49 (s, 3H), 3.92 (s, 3H), 3.94 (q, 2H, $J=7.2$ Hz), 4.06 (s, 3H), 6.83 (dd, 1H, $J_1=7.7$ Hz, $J_2=1.0$ Hz), 6.99 (s, 2H), 7.08 (tt, 2H, $J_1=7.0$ Hz, $J_2=2.0$ Hz), 7.12 (app. t, 4H, $J=7.3$ Hz), 7.17 (m, 4H), 7.39 (app. t, 1H, $J=7.8$ Hz), 8.07 (dd, 1H, $J_1=7.9$ Hz, $J_2=1.0$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.81, 22.14, 54.90, 55.50, 61.17, 114.42, 120.12, 120.18, 126.55, 127.54, 127.93, 129.70, 131.25, 136.04, 140.91, 143.31, 151.23, 157.83, 158.81, 161.01, 164.19, 168.11, 168.63. FT-IR: wavenumber (cm^{-1}) 1711 (s), 1553 (s), 1470 (m), 1373 (m), 1292 (m), 1244 (s), 1182 (m), 1076 (m), 1030 (m), 793 (s). MS (ES-API), m/z : calcd for $\text{C}_{33}\text{H}_{29}\text{N}_3\text{O}_4$: 531.22; found: 532.2 $[\text{M}+\text{H}^+]$. m.p. 76-78 $^{\circ}\text{C}$.

• **Ethyl 4-(6-(3-fluoro-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-2-methoxy-6-methylpyrimidine-5-carboxylate (18j):**



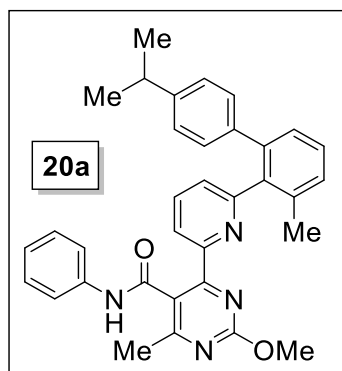
White solid. Yield: 53%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.12 (t, 3H, $J=7.2$ Hz), 2.53 (s, 3H), 3.97 (q, 2H, $J=7.2$ Hz), 4.10 (s, 3H), 6.96 (dd, 1H, $J_1=7.7$ Hz, $J_2=1.0$ Hz), 7.09 (m, 2H), 7.15-7.17 (m, 3H, signals overlapping), 7.19 (app. dt, 1H, $J_1=8.6$ Hz, $J_2=1.0$ Hz), 7.26 (dd, 1H, $J_1=7.6$ Hz, $J_2=1.0$ Hz), 7.46 (dt, 1H, $J_1=8.1$ Hz, $J_2=5.6$ Hz), 7.61 (app. t, 1H, $J=7.8$ Hz), 8.28 (dd, 1H, $J_1=7.9$ Hz, $J_2=1.0$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.63, 22.21, 55.00, 61.28, 114.39 (d, $J=22.9$ Hz), 120.24, 121.22, 125.56 (d, $J=2.8$ Hz), 127.06, 127.31, 127.44, 127.96, 129.63, 129.73 (d, $J=8.7$ Hz), 136.81, 139.35 (d, $J=2.8$ Hz), 143.45 (d, $J=2.8$ Hz), 152.60, 153.17, 160.28 (d, $J=249.1$ Hz), 161.32, 164.34, 168.53, 168.58. FT-IR: wavenumber (cm^{-1}) 1726 (m), 1612 (w), 1551 (s), 1462 (s), 1433 (w), 1379 (m), 1360 (m), 1288 (m), 1265 (s), 1246 (m), 1198 (w), 1169 (m), 1072 (s), 889 (m), 829 (m), 800 (m), 760 (m), 677 (m). MS (ES-API), m/z : calcd for $\text{C}_{26}\text{H}_{22}\text{FN}_3\text{O}_3$: 443.16; found: 444.1 $[\text{M}+\text{H}^+]$. m.p. 78-80 $^{\circ}\text{C}$.

• **Ethyl 4-(6-(4'-fluoro-[1,1':3',1''-terphenyl]-2'-yl)pyridin-2-yl)-2-methoxy-6-methylpyrimidine-5-carboxylate (18k):**



White solid. Yield: 55%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.15 (t, 3H, $J=6.6$ Hz), 2.51 (s, 3H), 3.95 (q, 2H, $J=6.6$ Hz), 4.06 (s, 3H), 6.82 (dd, 1H, $J_1=7.0$ Hz, $J_2=0.8$ Hz), 7.06-7.22 (m, 10H, signals overlapping), 7.31 (t, 1H, $J=8.5$ Hz), 7.42 (m, 2H, signals overlapping), 8.08 (dd, 1H, $J_1=7.6$ Hz, $J_2=0.8$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 13.78, 22.16, 54.90, 61.14, 115.37 (d, $J=23.0$ Hz), 120.17, 120.47, 126.57, 127.06, 127.08, 127.46, 127.66, 129.41 (d, $J=16.5$ Hz), 129.78, 130.36 (d, $J=7.8$ Hz), 130.61, 133.47, 136.21, 137.70 (d, $J=3.4$ Hz), 140.04, 140.60 (d, $J=2.5$ Hz), 151.31, 156.61 (d, $J=2.5$ Hz), 158.92 (d, $J=246.9$ Hz), 160.78, 164.22, 168.19, 168.65. FT-IR: wavenumber (cm^{-1}) 1721 (s), 1547 (s), 1472 (m), 1377 (m), 1252 (s), 1190 (m), 1070 (s), 995 (m), 783 (s), 735 (m). MS (ES-API), m/z : calcd for $\text{C}_{32}\text{H}_{26}\text{FN}_3\text{O}_3$: 519.20; found: 520.1 [$\text{M}+\text{H}^+$]. m.p. 106-108 °C.

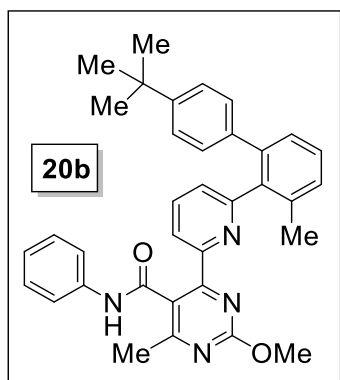
• **4-(6-(4'-isopropyl-3-methyl-[1,1'-biphenyl]-2'-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (20a):**



Beige solid. Yield: 76%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.13 (d, 6H, $J=6.8$ Hz), 2.03 (s, 3H), 2.64 (s, 3H), 2.75 (hept, 1H, $J=6.8$ Hz), 4.11 (s, 3H), 6.80 (d, 2H, $J=8.2$ Hz), 6.83 (dd, 1H, $J_1=7.7$ Hz, $J_2=0.8$ Hz), 6.88-6.94 (m, 3H, 2 signals overlapping), 6.98-7.04 (m, 3H, 2 signals overlapping), 7.11-7.15 (m, 3H, 2 signals overlapping), 7.24 (t, 1H, $J=7.7$ Hz), 7.54 (t, 1H, $J=7.8$ Hz), 7.72 (bs, 1H), 8.20 (dd, 1H, $J_1=7.9$ Hz, $J_2=0.8$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 20.43, 22.37, 23.87, 33.54, 55.01, 119.81, 121.02, 123.21, 123.99, 125.65, 127.22, 127.29, 127.94, 128.70, 129.05, 129.50, 136.65, 136.87, 137.50, 138.64, 138.74, 141.00, 146.77, 152.86, 158.91, 161.38, 164.35, 166.38, 169.58. FT-IR: wavenumber (cm^{-1}) 1685 (m), 1654 (m), 1599 (m), 1555 (s), 1471 (s), 1441 (m), 1379 (s), 1316 (s), 1263 (m), 1070 (m), 840 (w), 799 (m), 751 (s). MS (ES-API), m/z : calcd for $\text{C}_{34}\text{H}_{32}\text{N}_4\text{O}_2$: 528.25; found: 529.2 [$\text{M}+\text{H}^+$]. m.p. 99-101 °C.

• **4-(6-(4'-(tert-butyl)-3-methyl-[1,1'-biphenyl]-2'-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (20b):**

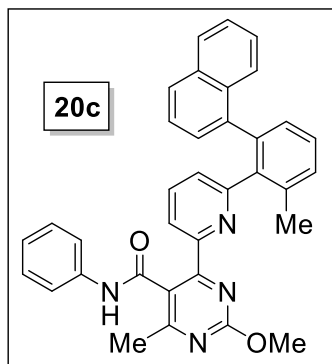
Beige solid. Yield: 79%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.20 (s, 9H), 2.03 (s, 3H), 2.61 (s, 3H), 4.06 (s, 3H), 6.79-6.87 (m, 3H, 2 signals overlapping), 6.91 (t, 1H, $J=7.5$ Hz), 6.97-7.03 (m, 3H, 2 signals overlapping), 7.07 (d, 2H, $J=8.3$ Hz), 7.10-7.18 (m, 3H, 2 signals



overlapping), 7.24 (app. t, 1H, $J=7.6$ Hz), 7.53 (app. t, 1H, $J=7.8$ Hz), 7.87 (bs, 1H), 8.21 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 20.44, 22.32, 31.23, 34.27, 54.94, 119.75, 120.93, 123.14, 123.95, 124.50, 127.25, 127.28, 127.92, 128.65, 129.01, 129.21, 136.61, 136.85, 137.56, 138.34, 138.60, 140.86, 149.02, 152.70, 158.89, 161.26, 164.24, 166.37, 169.49. FT-IR: wavenumber (cm^{-1}) 1669 (m), 1600 (m), 1559 (s), 1500 (m), 1470 (m), 1441 (m), 1381 (s), 1316 (s), 1263 (m), 1070 (w), 839 (w), 799 (m),

757 (s). MS (ES-API), m/z : calcd for $\text{C}_{35}\text{H}_{34}\text{N}_4\text{O}_2$: 542.27; found: 543.1 $[\text{M}+\text{H}^+]$. m.p. 109-111 $^{\circ}\text{C}$.

• **2-Methoxy-4-methyl-6-(6-(2-methyl-6-(naphthalen-1-yl)phenyl)pyridin-2-yl)-*N*-phenylpyrimidine-5-carboxamide (20c):**

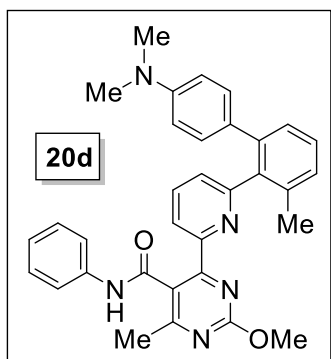


Colorless wax. Yield: 47%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.14 (s, 3H), 2.60 (s, 3H), 4.01 (s, 3H), 6.51-6.91 (bs, 2H, 2 signals overlapping), 6.98 (app. t, 1H, $J=6.8$ Hz), 7.05-7.15 (m, 4H, signals overlapping), 7.18-7.26 (m, 3H, signals overlapping), 7.27-7.43 (m, 4H, signals overlapping), 7.57 (d, 1H, $J=8.0$ Hz), 7.72 (bs, 2H, 2 signals overlapping), 7.92 (bs, 1H), 8.01 (bs, 1H). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 20.59, 22.35, 54.91, 119.82, 121.03, 123.01, 124.10, 124.85, 125.35, 125.65, 126.21, 126.94, 127.57, 127.99, 128.23,

128.41, 128.76, 128.82, 129.57, 132.35, 133.18, 136.53, 137.19, 137.71, 138.62, 139.17, 139.58, 152.55, 158.16, 160.84, 164.16, 166.09, 169.63. FT-IR: wavenumber (cm^{-1}) 1656 (m), 1599 (m), 1553 (s), 1499 (w), 1470 (m), 1443 (m), 1381 (m), 1317 (s), 1265 (m), 1163 (w), 1084 (s), 1047 (s), 995 (w), 880 (m), 799 (m), 779 (m), 754 (m), 691 (m). MS (ES-API), m/z : calcd for $\text{C}_{35}\text{H}_{28}\text{N}_4\text{O}_2$: 536.22; found: 537.2 $[\text{M}+\text{H}^+]$. m.p. 108-110 $^{\circ}\text{C}$.

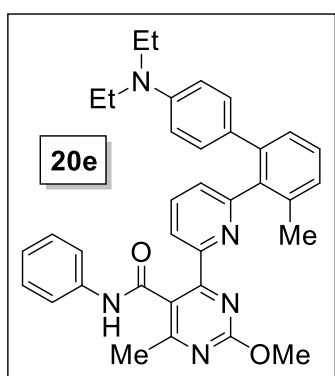
• **4-(6-(4'-(Dimethylamino)-3-methyl-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-2-methoxy-6-methyl-*N*-phenylpyrimidine-5-carboxamide (20d):**

Yellow solid. Yield: 89%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.01 (s, 3H), 2.64 (s, 3H), 2.83 (s, 6H), 4.11 (s, 3H), 6.43 (d, 2H, $J=8.5$ Hz), 6.76 (d, 2H, $J=8.5$ Hz), 6.87 (d, 1H, $J=7.7$ Hz), 6.91 (t, 1H, $J=7.3$ Hz), 6.96-7.02 (m, 3H, 2 signals overlapping), 7.09-7.15 (m, 3H, 2 signals overlapping), 7.22 (t, 1H, $J=7.6$ Hz), 7.57 (t, 1H, $J=7.8$ Hz), 7.77 (bs, 1H), 8.19 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 20.46, 22.36, 40.43, 54.99, 111.80, 119.84, 120.90, 123.23, 123.99, 127.25, 127.30, 127.94, 128.45, 128.66, 129.48, 130.36, 136.76, 136.79, 137.47, 138.49, 141.01, 148.86, 152.88, 159.35, 161.51, 164.35,



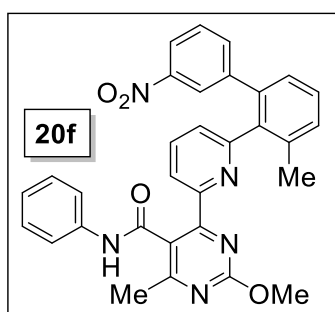
166.44, 169.53. FT-IR: wavenumber (cm^{-1}) 1683 (m), 1654 (m), 1599 (m), 1557 (s), 1471 (m), 1444 (m), 1379 (s), 1316 (m), 1263 (m), 1070 (w), 799 (w), 754 (s). MS (ES-API), m/z : calcd for $\text{C}_{33}\text{H}_{31}\text{N}_5\text{O}_2$: 529.25; found: 530.1 $[\text{M}+\text{H}^+]$. m.p. 124-126 °C.

• **4-(6-(4'-(Diethylamino)-3-methyl-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-2-methoxy-6-methyl-*N*-phenylpyrimidine-5-carboxamide (20e):**



Dark yellow solid. Yield: 84%. ^1H NMR (CDCl_3): δ_{H} (ppm) 1.06 (t, 6H, $J=7.1$ Hz), 2.00 (s, 3H), 2.64 (s, 3H), 3.23 (q, 4H, $J=7.1$ Hz), 4.11 (s, 3H), 6.37 (d, 2H, $J=8.6$ Hz), 6.73 (d, 2H, $J=8.6$ Hz), 6.89 (d, 1H, $J=7.7$ Hz), 6.92 (t, 1H, $J=7.4$ Hz), 6.94 (d, 1H, $J=7.4$ Hz), 7.00 (app. t, 2H, $J=7.8$ Hz), 7.11-7.15 (m, 3H, 2 signals overlapping), 7.21 (app. t, 1H, $J=7.5$ Hz), 7.59 (app. t, 1H, $J=7.8$ Hz), 7.77 (bs, 1H), 8.20 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 12.53, 20.50, 22.38, 44.12, 54.96, 111.04, 119.89, 120.86, 123.20, 124.01, 127.24, 127.36, 127.93, 128.25, 128.28, 128.65, 130.57, 136.74, 136.80, 137.44, 138.37, 141.09, 146.17, 152.85, 159.44, 161.53, 164.33, 166.47, 169.52. FT-IR: wavenumber (cm^{-1}) 1683 (m), 1653 (m), 1599 (m), 1559 (s), 1544 (m), 1498 (w), 1472 (m), 1380 (s), 1317 (s), 1261 (m), 1070 (w), 799 (w), 756 (s). MS (ES-API), m/z : calcd for $\text{C}_{35}\text{H}_{35}\text{N}_5\text{O}_2$: 557.28; found: 558.2 $[\text{M}+\text{H}^+]$. m.p. 129-131 °C.

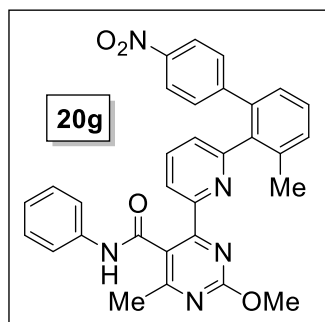
• **2-Methoxy-4-methyl-6-(6-(3-methyl-3'-nitro-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-*N*-phenylpyrimidine-5-carboxamide (20f):**



Beige solid. Yield: 59%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.13 (s, 3H), 2.63 (s, 3H), 4.11 (s, 3H), 6.81 (d, 1H, $J=7.7$ Hz), 6.84 (t, 1H, $J=7.0$ Hz), 6.92 (app. t, 2H, $J=7.4$ Hz), 7.04 (d, 1H, $J=7.5$ Hz), 7.11 (d, 2H, $J=7.8$ Hz), 7.24 (app. t, 1H, $J=7.8$ Hz), 7.25 (d, 1H, $J=7.5$ Hz), 7.32 (d, 1H, $J=7.7$ Hz), 7.34 (app. t, 1H, $J=7.5$ Hz), 7.57 (app. t, 1H, $J=7.8$ Hz), 7.58 (bs, 1H), 7.71 (bs, 1H), 7.87 (d, 1H, $J=7.9$ Hz), 8.31 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 20.36, 22.23, 55.00, 119.58, 121.12, 121.14, 122.80, 123.83, 124.74, 126.83, 126.86, 128.29, 128.56, 128.69, 130.19, 135.39, 137.17, 137.41, 137.60, 138.30, 138.85, 142.91, 147.09, 152.83, 157.97, 160.50, 164.36, 166.41, 169.66. FT-IR: wavenumber (cm^{-1}) 1685 (m), 1656 (m),

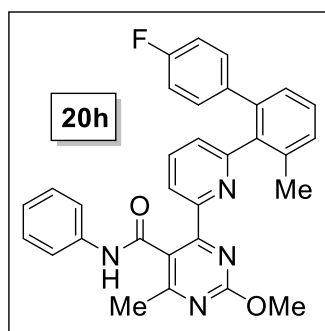
1599 (m), 1558 (s), 1529 (s), 1470 (m), 1441 (m), 1376 (m), 1351 (s), 1316 (m), 1247 (m), 1070 (m), 799 (m), 756 (s). MS (ES-API), m/z: calcd for C₃₁H₂₅N₅O₄: 531.19; found: 532.1 [M+H⁺]. m.p. 155-157 °C.

• **2-Methoxy-4-methyl-6-(6-(3-methyl-4'-nitro-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-N-phenylpyrimidine-5-carboxamide (20g):**



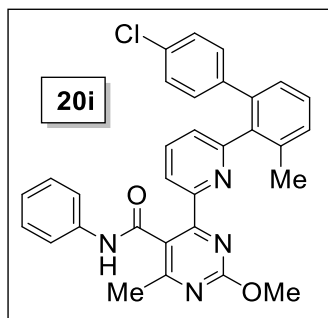
Pale yellow solid. Yield: 58%. ¹H NMR (CDCl₃): δ_H (ppm) 2.02 (s, 3H), 2.62 (s, 3H), 4.09 (s, 3H), 6.83 (dd, 1H, J₁=7.7 Hz, J₂=0.8 Hz), 6.91 (t, 1H, J=7.2 Hz), 7.00 (app. t, 2H, J=8.0 Hz), 7.04 (d, 2H, J=9.0 Hz), 7.08 (d, 1H, J=7.5 Hz), 7.13 (m, 3H, 2 signals overlapping), 7.30 (app. t, 1H, J=7.7 Hz), 7.59 (app. t, 1H, J=7.8 Hz), 7.67 (bs, 1H), 7.90 (d, 2H, J=8.8 Hz), 8.25 (dd, 1H, J₁=7.9 Hz, J₂=0.8 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 20.30, 22.26, 55.02, 119.44, 121.36, 122.84, 123.07, 123.98, 126.84, 126.87, 128.25, 128.74, 130.40, 130.42, 137.16, 137.33, 137.59, 138.59, 138.76, 146.28, 148.29, 153.11, 157.93, 160.99, 164.38, 166.34, 169.44. FT-IR: wavenumber (cm⁻¹) 1686 (m), 1656 (m), 1599 (m), 1560 (s), 1528 (s), 1468 (m), 1441 (m), 1378 (m), 1351 (s), 1316 (m), 1247 (w), 1070 (m), 799 (m), 757 (s), 738 (m). MS (ES-API), m/z: calcd for C₃₁H₂₅N₅O₄: 531.19; found: 532.1 [M+H⁺]. m.p. 139-141 °C.

• **4-(6-(4'-Fluoro-3-methyl-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (20h):**



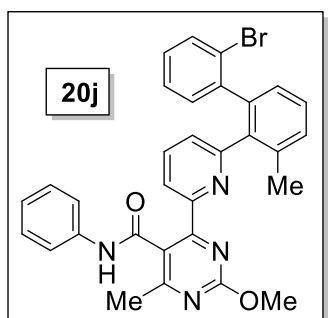
Beige solid. Yield: 70%. ¹H NMR (CDCl₃): δ_H (ppm) 2.01 (s, 3H), 2.61 (s, 3H), 4.08 (s, 3H), 6.73 (app. t, 2H, J=8.7 Hz), 6.83 (m, 3H, 2 signals overlapping), 6.92 (t, 1H, J=7.3 Hz), 7.01 (app. t, 2H, J=7.7 Hz), 7.05 (d, J=7.7 Hz), 7.07 (d, J=7.5 Hz), 7.13 (d, 2H, J=8.1 Hz), 7.25 (app. t, 1H, J=7.6 Hz), 7.57 (app. t, 1H, J=7.8 Hz), 7.76 (bs, 1H), 8.22 (dd, 1H, J₁=7.9 Hz, J₂=0.8 Hz). ¹³C NMR (CDCl₃): δ_C (ppm) 20.39, 22.29, 54.97, 114.45 (d, J=21.1 Hz), 119.59, 121.00, 123.09, 123.94, 127.05, 127.16, 127.99, 128.69, 129.32, 131.12 (d, J=8.2 Hz), 136.83, 136.94, 137.31 (d, J=3.6 Hz), 137.58, 138.68, 139.92, 152.88 (d, J=3.9 Hz), 158.62, 161.16, 161.47 (d, J=245.4 Hz), 164.30, 166.31, 169.47. FT-IR: wavenumber (cm⁻¹) 1663 (m), 1655 (m), 1600 (m), 1558 (s), 1508 (m), 1500 (m), 1471 (m), 1442 (m), 1380 (s), 1316 (s), 1222 (m), 1158 (m), 1068 (m), 840 (m), 798 (m), 756 (s). MS (ES-API), m/z: calcd for C₃₁H₂₅FN₄O₂: 504.20; found: 505.1 [M+H⁺]. m.p. 108-110 °C.

• **4-(6-(4'-Chloro-3-methyl-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (20i):**



Beige solid. Yield: 66%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.01 (s, 3H), 2.62 (s, 3H), 4.10 (s, 3H), 6.79 (d, 2H, $J=8.3$ Hz), 6.83 (d, 1H, $J=7.7$ Hz), 6.92 (t, 1H, $J=7.5$ Hz), 7.00 (app. t, 2H, $J=7.6$ Hz), 7.01 (d, 2H, $J=8.3$ Hz), 7.06 (d, 1H, $J=7.6$ Hz), 7.07 (d, 1H, $J=7.6$ Hz), 7.12 (d, 2H, $J=7.7$ Hz), 7.26 (t, 1H, $J=7.6$ Hz), 7.59 (t, 1H, $J=7.8$ Hz), 7.68 (bs, 1H), 8.23 (d, 1H, $J=7.9$ Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 20.40, 22.33, 55.00, 119.58, 121.14, 123.12, 123.98, 127.04, 127.08, 127.77, 128.07, 128.72, 129.52, 130.87, 132.37, 136.97, 137.05, 137.54, 138.59, 139.72, 139.81, 152.97, 158.49, 161.22, 164.38, 166.33, 169.51. FT-IR: wavenumber (cm^{-1}) 1685 (m), 1655 (m), 1600 (m), 1558 (s), 1543 (m), 1472 (m), 1458 (m), 1376 (s), 1318 (s), 1263 (w), 1091 (w), 1071 (w), 834 (w), 799 (m), 756 (s). MS (ES-API), m/z : calcd for $\text{C}_{31}\text{H}_{25}\text{ClN}_4\text{O}_2$: 520.17; found: 521.1 [$\text{M}+\text{H}^+$]. m.p. 112-114 $^{\circ}\text{C}$.

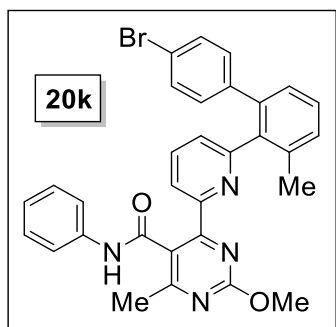
• **4-(6-(2'-Bromo-3-methyl-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (20j):**



Beige solid. Yield: 54%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.04 (s, 3H), 2.62 (s, 3H), 4.06 (s, 3H), 6.50 (bs, 1H), 6.87 (bs, 1H), 6.90 (app. t, 1H, $J=7.2$ Hz), 6.96 (t, 1H, $J=7.3$ Hz), 7.03-7.07 (m, 4H, 3 signals overlapping), 7.11 (d, 1H, $J=7.9$ Hz), 7.14 (d, 2H, $J=7.9$ Hz), 7.28 (app. t, 1H, $J=7.7$ Hz), 7.43 (bs, 1H), 7.55 (app. t, 1H, $J=7.8$ Hz), 7.76 (bs, 1H), 8.12 (bs, 1H). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 20.36, 22.37, 54.97, 119.68, 121.17, 123.10, 123.50, 124.03, 126.22, 126.51, 127.40, 127.58, 128.18, 128.80, 129.82, 131.95, 132.28, 136.72, 136.78, 137.62, 138.74, 140.00, 141.73, 152.82, 158.01, 161.19, 164.25, 166.21, 169.63. FT-IR: wavenumber (cm^{-1}) 1684 (m), 1654 (m), 1663 (m), 1655 (m), 1599 (m), 1560 (s), 1555 (s), 1498 (m), 1470 (m), 1442 (m), 1380 (s), 1316 (s), 1262 (m), 1070 (m), 1011 (m), 824 (m), 797 (m), 787 (w), 754 (s). MS (ES-API), m/z : calcd for $\text{C}_{31}\text{H}_{25}\text{BrN}_4\text{O}_2$: 531.19; found: 532.1 [$\text{M}+\text{H}^+$]. m.p. 139-141 $^{\circ}\text{C}$.

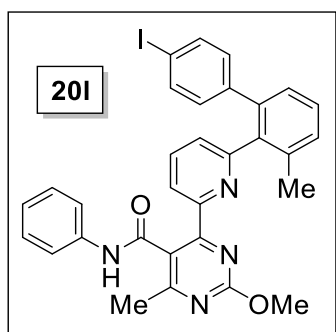
• **4-(6-(4'-Bromo-3-methyl-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (20k):**

Beige solid. Yield: 62%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.01 (s, 3H), 2.61 (s, 3H), 4.08 (s, 3H), 6.74 (d, 2H, $J=8.2$ Hz), 6.83 (d, 1H, $J=7.7$ Hz), 6.91 (t, 1H, $J=7.3$ Hz), 6.99 (app. t, 2H, $J=7.5$ Hz), 7.06 (m, 2H, 2 signals overlapping), 7.12 (d, 2H, $J=7.7$ Hz), 7.17 (d, 2H, $J=8.2$



Hz), 7.25 (app. t, 1H, J=7.7 Hz), 7.59 (app. t, 1H, J=7.8 Hz), 7.72 (bs, 1H), 8.23 (d, 1H, J=7.9 Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 20.37, 22.29, 54.99, 119.55, 120.59, 121.11, 123.08, 123.94, 127.00, 127.04, 128.07, 128.70, 129.54, 130.71, 131.22, 136.98, 137.08, 137.56, 138.52, 139.68, 140.28, 152.91, 158.45, 161.13, 164.33, 166.30, 169.49. FT-IR: wavenumber (cm^{-1}) 1685 (m), 1655 (m), 1599 (m), 1555 (s), 1498 (m), 1470 (m), 1442 (m), 1380 (s), 1316 (s), 1261 (m), 1070 (m), 1011 (m), 824 (m), 797 (m), 754 (s). MS (ES-API), m/z: calcd for $\text{C}_{31}\text{H}_{25}\text{BrN}_4\text{O}_2$: 564.12; found: 565.0 $[\text{M}+\text{H}^+]$. m.p. 115-117 °C.

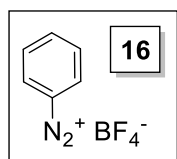
• **4-(6-(4'-Iodo-3-methyl-[1,1'-biphenyl]-2-yl)pyridin-2-yl)-2-methoxy-6-methyl-N-phenylpyrimidine-5-carboxamide (20l):**



Beige solid. Yield: 60%. ^1H NMR (CDCl_3): δ_{H} (ppm) 2.01 (s, 3H), 2.63 (s, 3H), 4.11 (s, 3H), 6.61 (d, 2H, J=8.3 Hz), 6.84 (d, 1H, J=8.3 Hz), 6.91 (t, 1H, J=7.3 Hz), 7.00 (app. t, 2H, J=7.6 Hz), 7.05 (d, 1H, J=7.7 Hz), 7.07 (d, 1H, J=7.5 Hz), 7.11 (d, 2H, J=7.9 Hz), 7.25 (app. t, 1H, J=7.6 Hz), 7.37 (d, 2H, J=8.3 Hz), 7.60 (app. t, 1H, J=7.8 Hz), 7.64 (bs, 1H), 8.23 (d, 1H, J=7.9 Hz). ^{13}C NMR (CDCl_3): δ_{C} (ppm) 20.39, 22.32, 55.02, 92.25, 119.56, 121.17, 123.10, 123.98, 126.99, 127.03, 128.10, 128.71, 129.55, 131.49, 136.69, 137.03, 137.09, 137.51, 138.47, 139.74, 140.88, 152.95, 158.43, 161.21, 164.37, 166.32, 169.50. FT-IR: wavenumber (cm^{-1}) 1663 (m), 1657 (m), 1599 (m), 1555 (s), 1498 (m), 1469 (m), 1442 (m), 1379 (s), 1317 (s), 1261 (m), 1070 (m), 1011 (m), 824 (m), 797 (m), 755 (s). MS (ES-API), m/z: calcd for $\text{C}_{31}\text{H}_{25}\text{IN}_4\text{O}_2$: 612.10; found: 613.1 $[\text{M}+\text{H}^+]$. m.p. 116-118 °C.

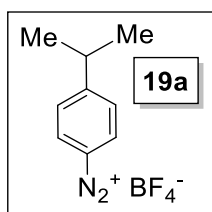
◆ **General method for synthesis of diazonium tetrafluoroborate salts:** In a round-bottom flask open to air, an aniline (0.1 mol, 1 equiv.) was dissolved in a mixture of water (40 mL) and 50% wt. aqueous HBF_4 solution (25.4 mL of solution, 17.56 g HBF_4 , 0.2 mol, 2 equiv.). In case the aniline was not fully soluble, drops of MeOH were added until the solution became transparent. The resulting solution was cooled at 0 °C, followed by dropwise addition of a solution of NaNO_2 (7.59 g, 0.11 mol, 1.1 equiv.) in 15 mL of water, while the temperature was maintained at 0-5 °C. Stirring continued at the same temperature for 2 more hours. The crude solid precipitate was collected by filtration and washed with a small amount of cold water. It was then dissolved in acetone and precipitated again by addition of diethyl ether. The solid was collected by filtration and dried under house vacuum. It was stored in small portions in a fridge until use.

• **Benzenediazonium tetrafluoroborate (16):**



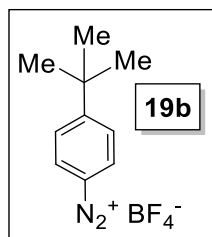
Grey solid. Yield: 85%. ^1H NMR (DMSO- d_6): δ_{H} (ppm) 7.98 (app. t, 2H, $J=8.0$ Hz), 8.26 (tt, 1H, $J_1=7.7$ Hz, $J_2=1.1$ Hz), 8.66 (d, 2H, $J_1=8.3$ Hz, $J_2=1.1$ Hz). ^{13}C NMR (DMSO- d_6): δ_{C} (ppm) 131.26, 132.69, 140.86, 157.30. FT-IR: wavenumber (cm^{-1}) 2295 (m), 1570 (m), 1462 (m), 1312 (m), 1026 (s), 756 (m), 665 (m), 515 (m). MS (ES-API), m/z : calcd for $\text{C}_6\text{H}_5\text{N}_2^+$: 105.04; found: 105.1 [M].

• **4-Isopropylbenzenediazonium tetrafluoroborate (19a):**



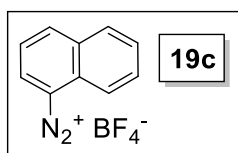
White solid. Yield: 71%. ^1H NMR (DMSO- d_6): δ_{H} (ppm) 1.25 (d, 6H, $J=6.9$ Hz), 3.16 (hept., 1H, $J=6.9$ Hz), 7.89 (d, 2H, $J=8.8$ Hz), 8.58 (d, 2H, $J=8.8$ Hz). ^{13}C NMR (DMSO- d_6): δ_{C} (ppm) 22.82, 34.48, 112.31, 129.45, 133.06, 163.49. FT-IR: wavenumber (cm^{-1}) 2270 (m), 1580 (m), 1462 (w), 1288 (w), 1037 (s), 843 (m), 542 (m). MS (ES-API), m/z : calcd for $\text{C}_9\text{H}_{11}\text{N}_2^+$: 147.09; found: 147.0 [M].

• **4-(*Tert*-butyl)benzenediazonium tetrafluoroborate (19b):**



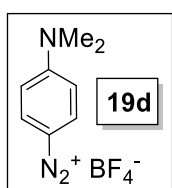
White solid. Yield: 63%. ^1H NMR (DMSO- d_6): δ_{H} (ppm) 1.34 (s, 9H), 8.03 (d, 2H, $J=9.1$ Hz), 8.59 (d, 2H, $J=9.1$ Hz). ^{13}C NMR (DMSO- d_6): δ_{C} (ppm) 30.20, 36.51, 112.32, 128.56, 132.85, 165.55. FT-IR: wavenumber (cm^{-1}) 2270 (m), 1580 (m), 1038 (s), 843 (m), 542 (m). MS (ES-API), m/z : calcd for $\text{C}_{10}\text{H}_{13}\text{N}_2^+$: 161.11; found: 161.1 [M].

• **Naphthalene-1-diazonium tetrafluoroborate (19c):**



Brown solid. Yield: 86%. ^1H NMR (DMSO- d_6): δ_{H} (ppm) 7.98 (m, 1H), 8.06 (m, 1H), 8.12 (m, 1H), 8.43 (dd, 1H, $J_1=8.0$ Hz, $J_2=3.7$ Hz), 8.51 (dd, 1H, $J_1=8.0$ Hz, $J_2=3.7$ Hz), 8.94 (dd, 1H, $J_1=8.0$ Hz, $J_2=3.7$ Hz), 9.20 (dd, 1H, $J_1=8.0$ Hz, $J_2=3.7$ Hz). ^{13}C NMR (DMSO- d_6): δ_{C} (ppm) 111.10, 122.46, 126.42, 127.14, 129.93, 130.34, 132.24, 132.60, 137.21, 142.66. FT-IR: wavenumber (cm^{-1}) 2264 (m), 1369 (m), 1198 (m), 1033 (s), 808 (m), 768 (m). MS (ES-API), m/z : calcd for $\text{C}_{10}\text{H}_7\text{N}_2^+$: 155.06; found: 155.0 [M].

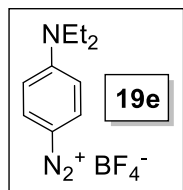
• **4-(Dimethylamino)benzenediazonium tetrafluoroborate (19d):**



Yellow solid. Yield: 91%. ^1H NMR (DMSO- d_6): δ_{H} (ppm) 3.26 (s, 6H), 7.06 (d, 2H, $J=9.7$ Hz), 8.22 (d, 2H, $J=9.7$ Hz). ^{13}C NMR (DMSO- d_6): δ_{C} (ppm) 40.52, 88.98, 113.90, 134.03, 156.17. FT-IR: wavenumber (cm^{-1}) 2156

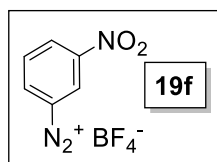
(s), 1582 (s), 1389 (m), 1113 (m), 1029 (s), 932 (m), 826 (m). MS (ES-API), m/z: calcd for $C_8H_{10}N_3^+$: 148.09; found: 148.0 [M].

• **4-(Diethylamino)benzenediazonium tetrafluoroborate (19e):**



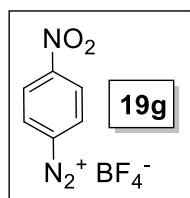
Yellow solid. Yield: 89%. 1H NMR (DMSO- d_6): δ_H (ppm) 1.17 (t, 6H, $J=7.1$ Hz), 3.62 (q, 4H, $J=7.1$ Hz), 7.09 (d, 2H, $J=9.7$ Hz), 8.21 (d, 2H, $J=9.7$ Hz). ^{13}C NMR (DMSO- d_6): δ_C (ppm) 12.16, 45.37, 88.63, 113.84, 134.40, 154.60. FT-IR: wavenumber (cm^{-1}) 2154 (s), 1580 (s), 1389 (m), 1113 (m), 1028 (s), 932 (m), 824 (m), 781 (w). MS (ES-API), m/z: calcd for $C_{10}H_{14}N_3^+$: 176.12; found: 176.1 [M].

• **3-Nitrobenzenediazonium tetrafluoroborate (19f):**



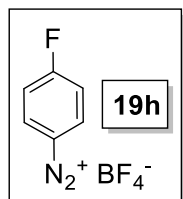
Yellow solid. Yield: 81%. 1H NMR (DMSO- d_6): δ_H (ppm) 8.24 (app. t, 1H, $J=8.4$ Hz), 8.99 (dd, 1H, $J_1=8.5$ Hz, $J_2=2.3$ Hz), 9.02 (dd, 1H, $J_1=8.3$ Hz, $J_2=1.7$ Hz), 9.61 (app. t, 1H, $J=2.0$ Hz). ^{13}C NMR (DMSO- d_6): δ_C (ppm) 118.25, 128.17, 132.76, 135.02, 137.89, 147.65. FT-IR: wavenumber (cm^{-1}) 2305 (w), 1605 (m), 1539 (m), 1352 (m), 1072 (m), 1034 (s), 999 (m), 905 (m), 818 (m), 775 (m), 733 (m). MS (ES-API), m/z: calcd for $C_6H_4N_3O_2^+$: 150.03; found: 150 [M].

• **4-Nitrobenzenediazonium tetrafluoroborate (19g):**



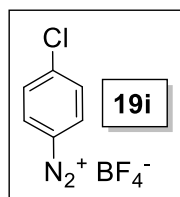
Yellow solid. Yield: 78%. 1H NMR (DMSO- d_6): δ_H (ppm) 8.72 (d, 2H, $J=9.4$ Hz), 8.93 (d, 2H, $J=9.4$ Hz). ^{13}C NMR (DMSO- d_6): δ_C (ppm) 121.90, 126.03, 134.51, 153.22. FT-IR: wavenumber (cm^{-1}) 2305 (w), 1605 (m), 1539 (m), 1352 (m), 1033 (s), 999 (m), 905 (m), 818 (m), 775 (m), 733 (m), 646 (m). MS (ES-API), m/z: calcd for $C_6H_4N_3O_2^+$: 150.03; found: 150.0 [M].

• **4-Fluorobenzenediazonium tetrafluoroborate (19h):**



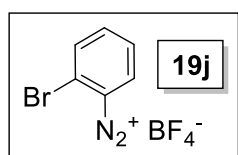
White solid. Yield: 88%. 1H NMR (DMSO- d_6): δ_H (ppm) 7.89 (dd, 2H, $J_1=9.2$ Hz, $J_2=8.4$ Hz), 8.80 (dd, 2H, $J_1=9.2$ Hz, $J_2=4.5$ Hz). ^{13}C NMR (DMSO- d_6): δ_C (ppm) 111.87 (d, $J=2.6$ Hz), 119.40 (d, $J=25.7$ Hz), 136.99 (d, $J=12.6$ Hz), 168.39 (d, $J=267.0$ Hz). FT-IR: wavenumber (cm^{-1}) 2293 (m), 1578 (m), 1483 (m), 1250 (m), 1013 (s), 851 (m), 832 (m), 696 (m). MS (ES-API), m/z: calcd for $C_6H_4FN_2^+$: 123.04; found: 123.1 [M].

• **4-Chlorobenzenediazonium tetrafluoroborate (19i):**



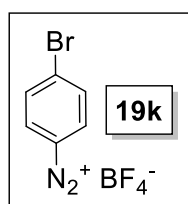
White solid. Yield: 92%. ^1H NMR (DMSO- d_6): δ_{H} (ppm) 8.11 (d, 2H, $J=9.1$ Hz), 8.69 (d, 2H, $J=9.1$ Hz). ^{13}C NMR (DMSO- d_6): δ_{C} (ppm) 114.78, 131.61, 134.41, 146.50. FT-IR: wavenumber (cm^{-1}) 2290 (m), 1562 (m), 1412 (w), 1312 (w), 1078 (m), 1026 (s), 835 (s), 775 (m). MS (ES-API), m/z : calcd for $\text{C}_6\text{H}_4\text{ClN}_2^+$: 139.01; found: 139.0 [M].

• **2-Bromobenzenediazonium tetrafluoroborate (19j):**



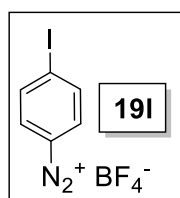
White solid. Yield: 88%. ^1H NMR (DMSO- d_6): δ_{H} (ppm) 7.99 (app. dt, 1H, $J_1=7.9$ Hz, $J_2=0.7$ Hz), 8.17 (app. dt, 1H, $J_1=7.9$ Hz, $J_2=1.5$ Hz), 8.31 (d, 1H, $J_1=8.3$ Hz), 8.84 (dd, 1H, $J_1=8.3$ Hz, $J_2=1.5$ Hz). ^{13}C NMR (DMSO- d_6): δ_{C} (ppm) 118.72, 124.43, 130.41, 135.06, 135.29, 141.86. FT-IR: wavenumber (cm^{-1}) 2361 (s), 2340 (s), 1562 (m), 1468 (m), 1302 (m), 1269 (m), 1051 (s), 1031 (s), 772 (s), 664 (w). MS (ES-API), m/z : calcd for $\text{C}_6\text{H}_4\text{BrN}_2^+$: 182.96; found: 182.9 [M].

• **4-Bromobenzenediazonium tetrafluoroborate (19k):**



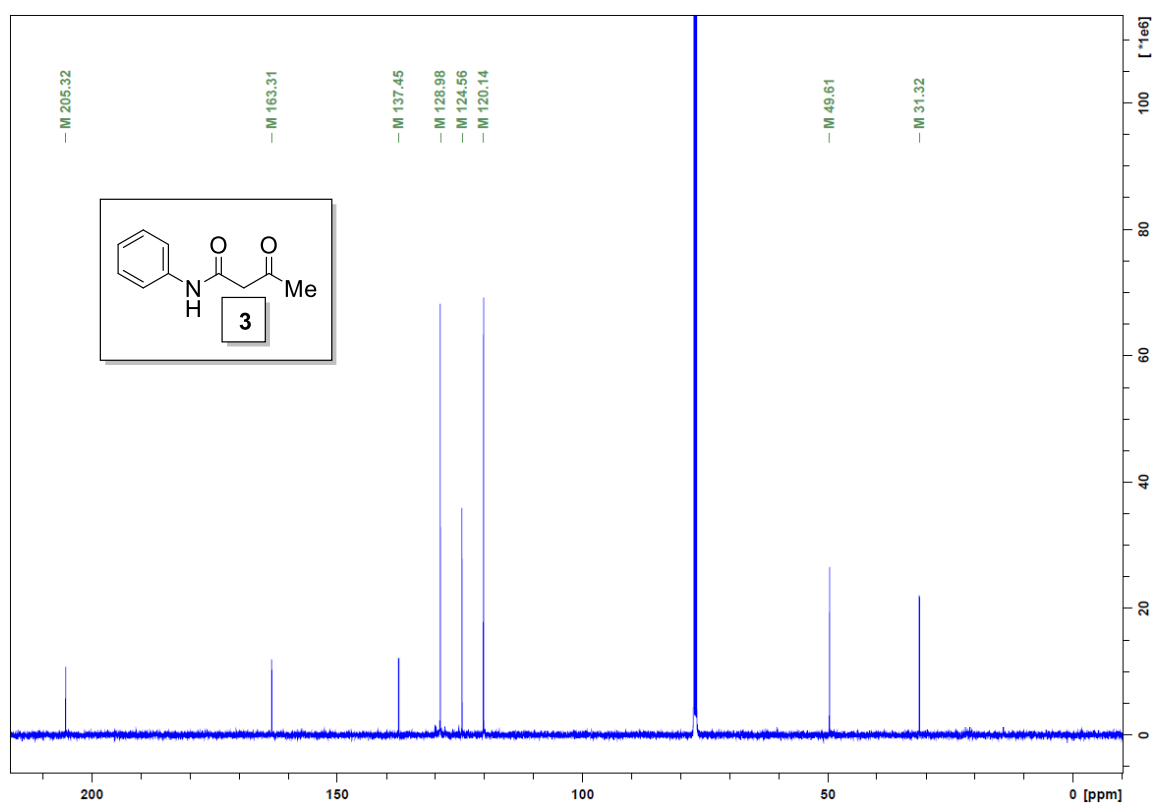
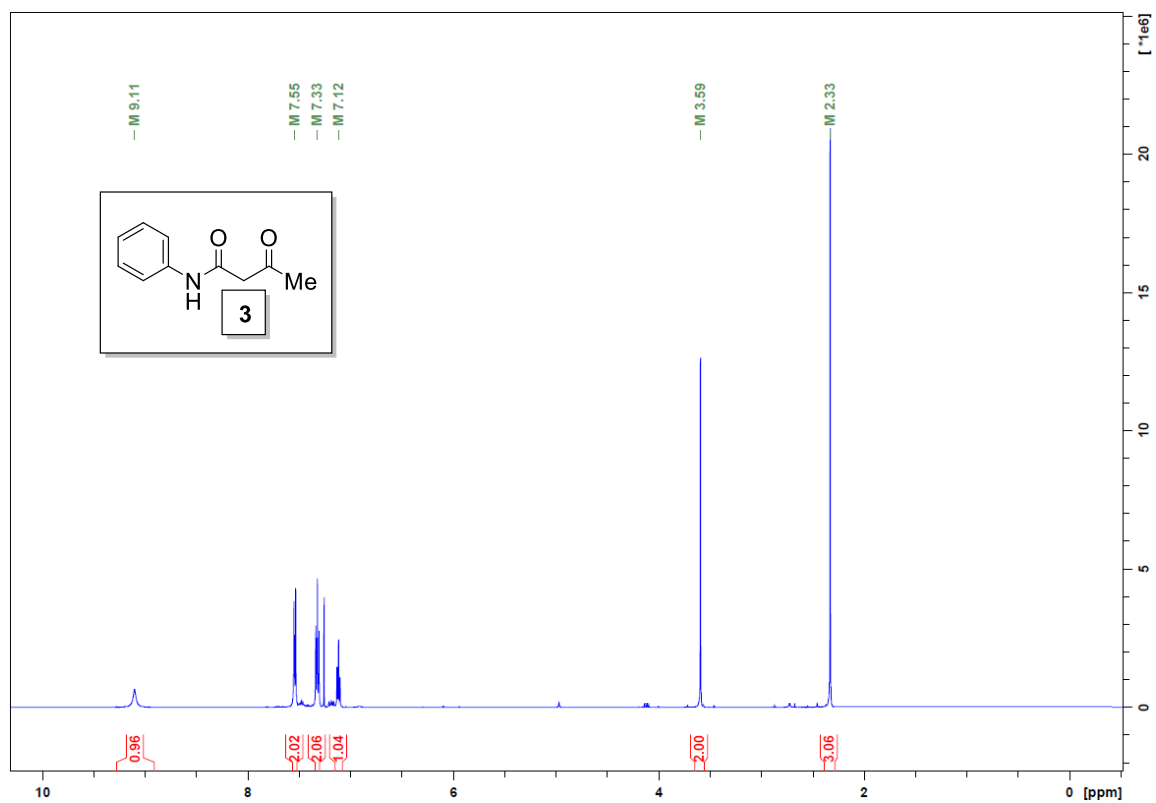
White solid. Yield: 90%. ^1H NMR (DMSO- d_6): δ_{H} (ppm) 8.26 (d, 2H, $J=8.9$ Hz), 8.57 (d, 2H, $J=8.9$ Hz). ^{13}C NMR (DMSO- d_6): δ_{C} (ppm) 115.15, 133.97, 134.53, 136.54. FT-IR: wavenumber (cm^{-1}) 2290 (m), 1562 (m), 1468 (m), 1302 (m), 1269 (m), 1051 (s), 1031 (s), 772 (s), 656 (m), 525 (m). MS (ES-API), m/z : calcd for $\text{C}_6\text{H}_4\text{BrN}_2^+$: 182.96; found: 182.9 [M].

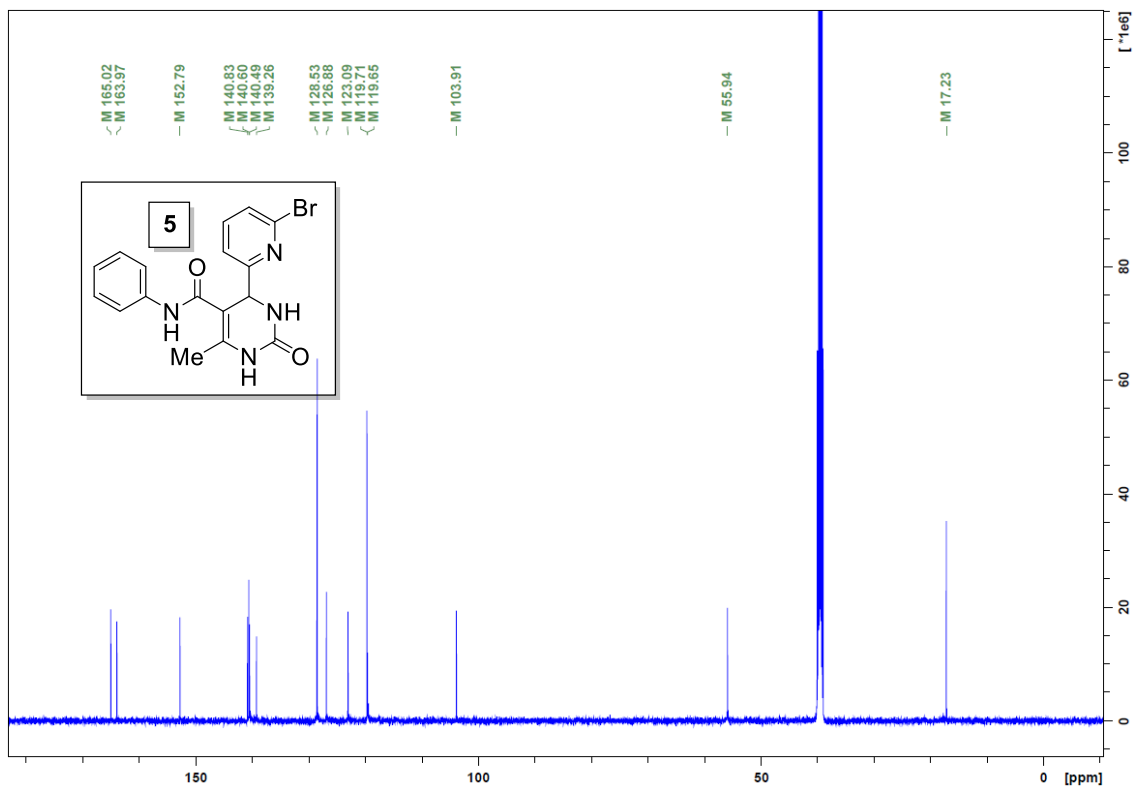
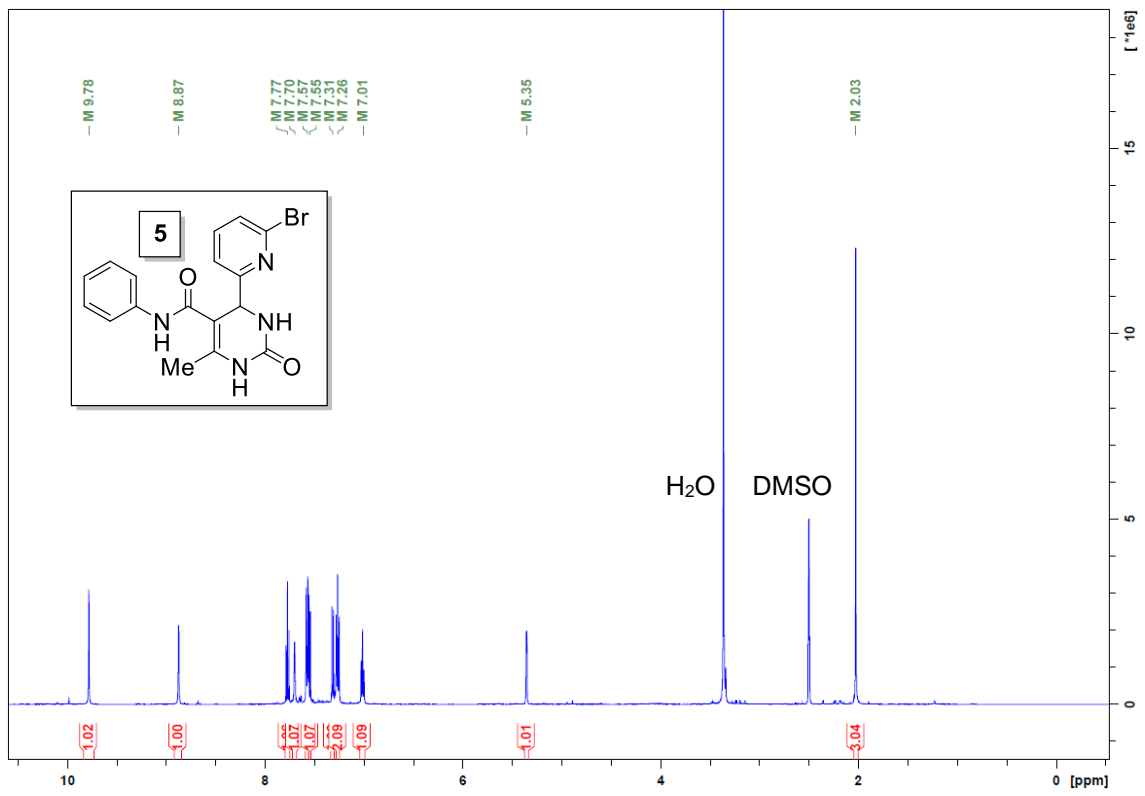
• **4-Iodobenzenediazonium tetrafluoroborate (19l):**

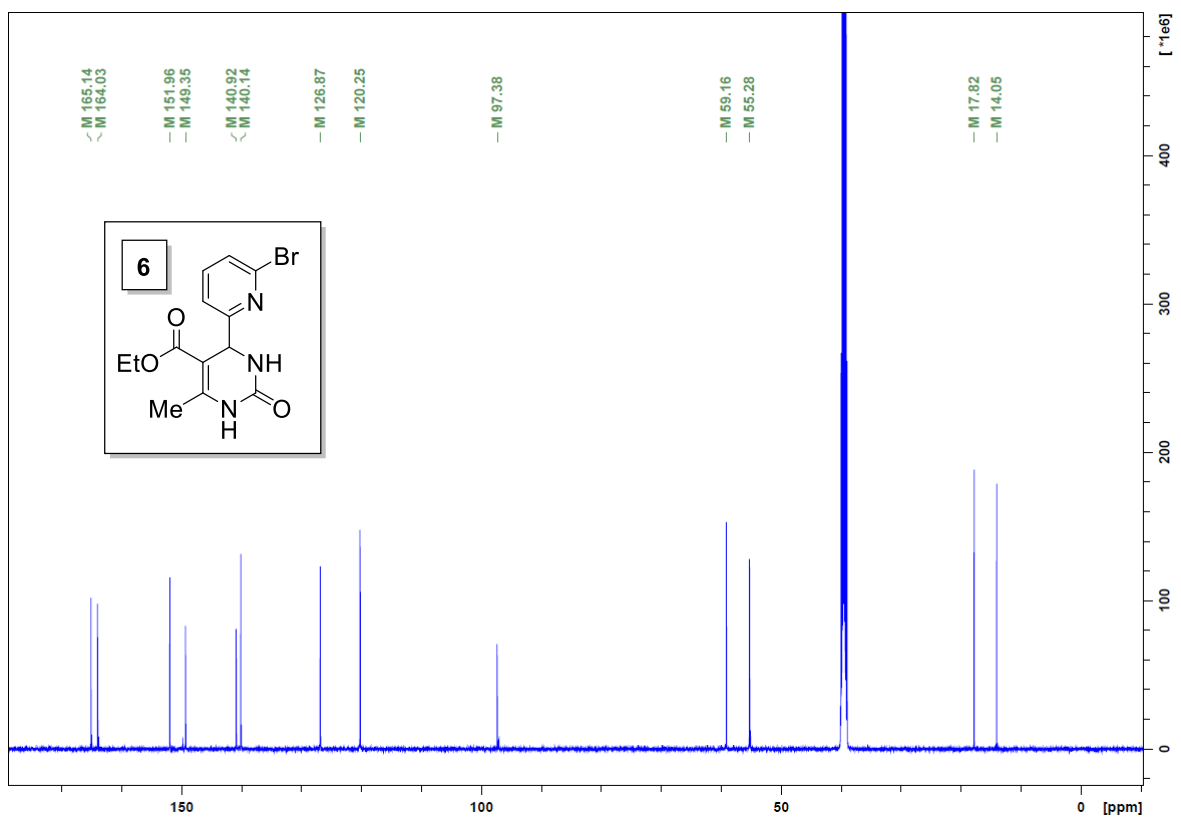
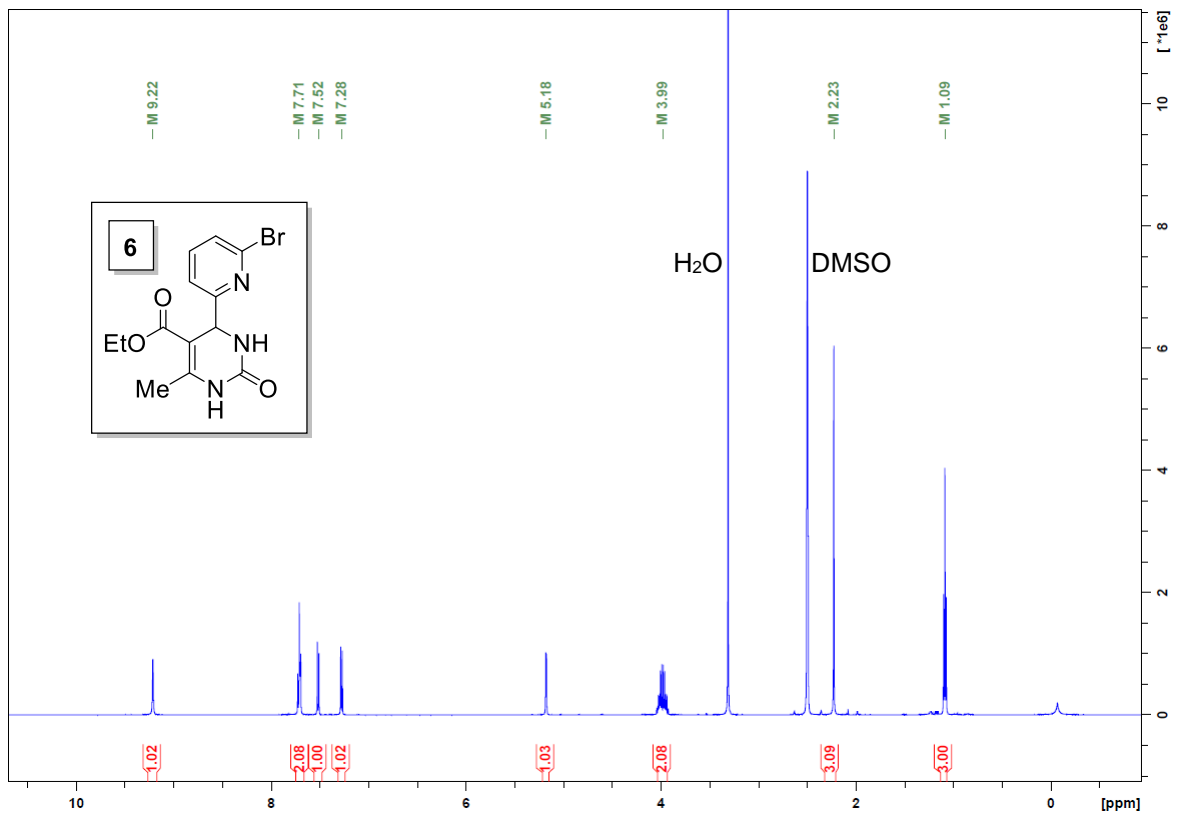


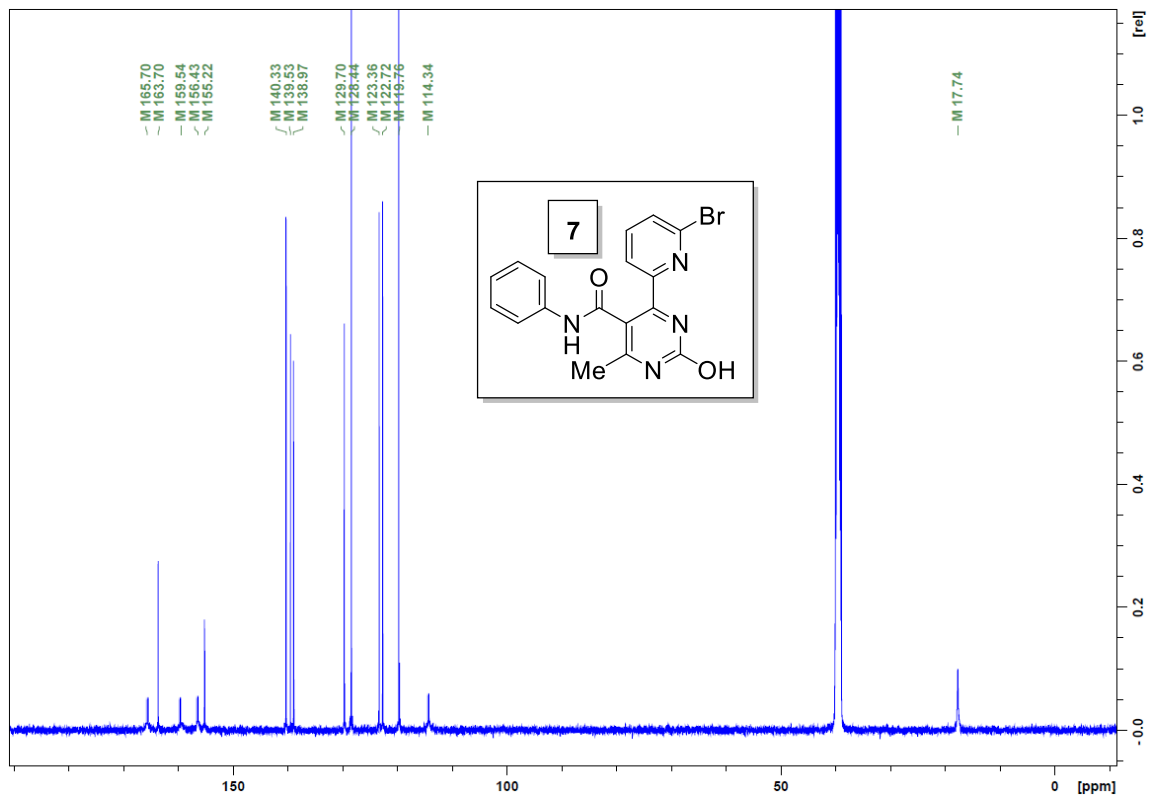
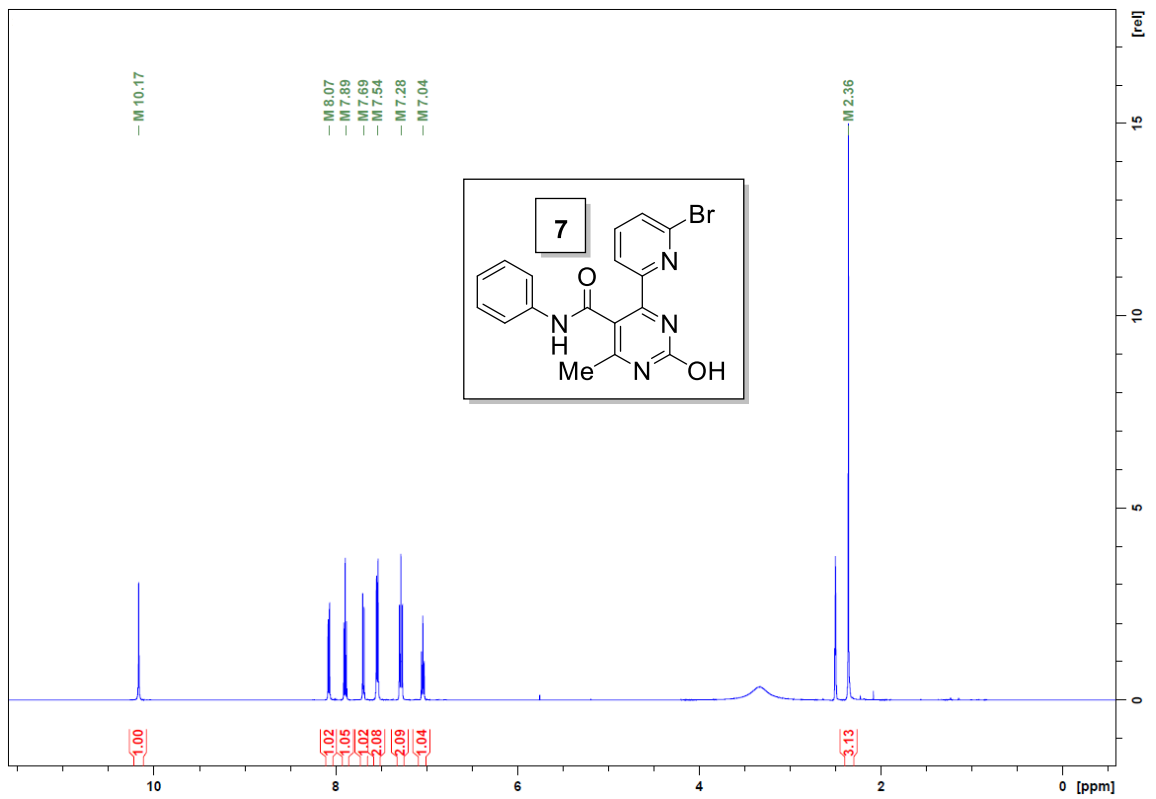
White solid. Yield: 72%. ^1H NMR (DMSO- d_6): δ_{H} (ppm) 8.34 (d, 2H, $J=8.9$ Hz), 8.43 (d, 2H, $J=8.9$ Hz). ^{13}C NMR (DMSO- d_6): δ_{C} (ppm) 113.69, 115.19, 132.89, 140.26. FT-IR: wavenumber (cm^{-1}) 2284 (m), 1547 (m), 1462 (m), 1406 (m), 1288 (m), 1031 (s), 1004 (m), 826 (s), 758 (m). MS (ES-API), m/z : calcd for $\text{C}_6\text{H}_4\text{IN}_2^+$: 230.94; found: 230.9 [M].

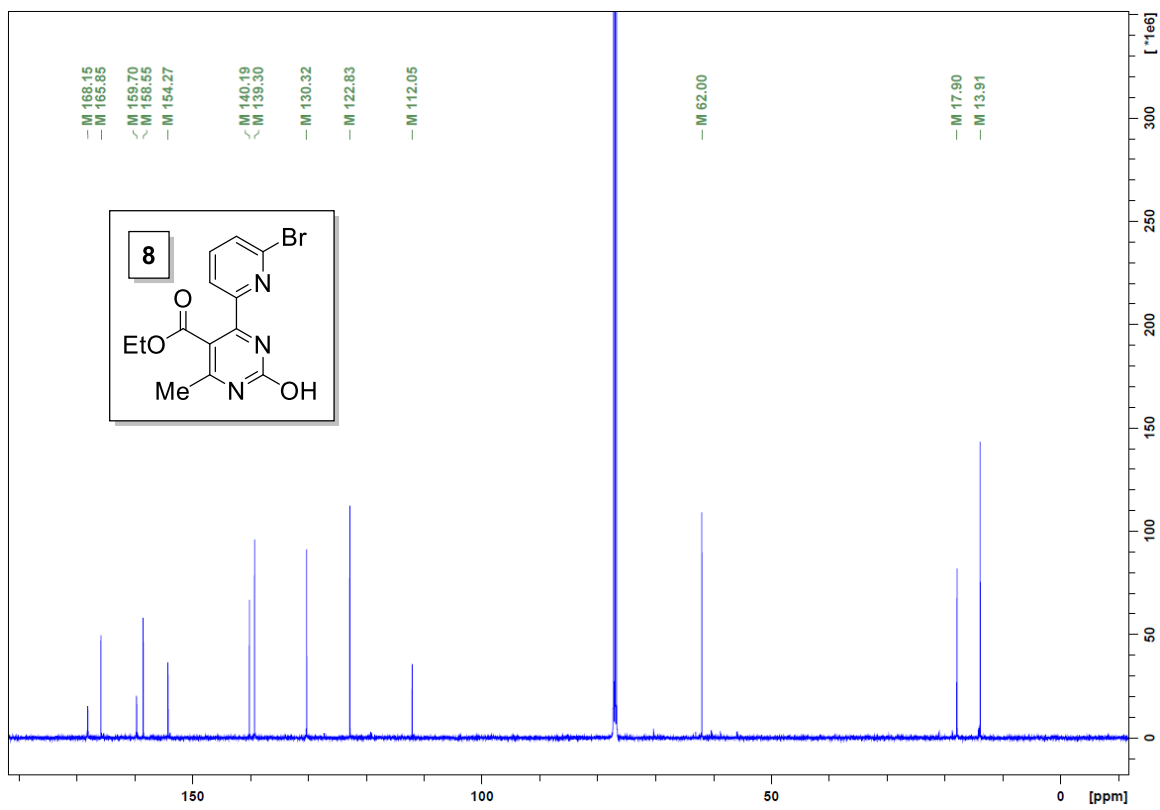
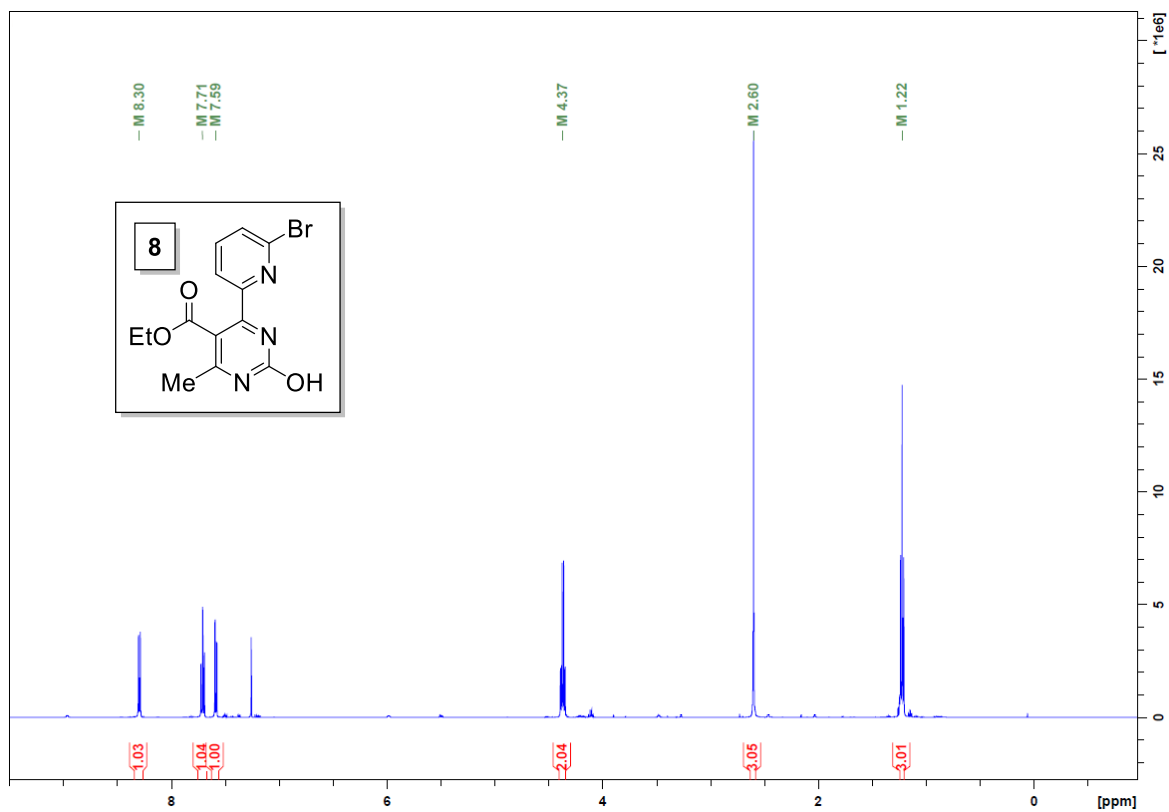
II. ¹H and ¹³C NMR Spectra of Synthesized Compounds

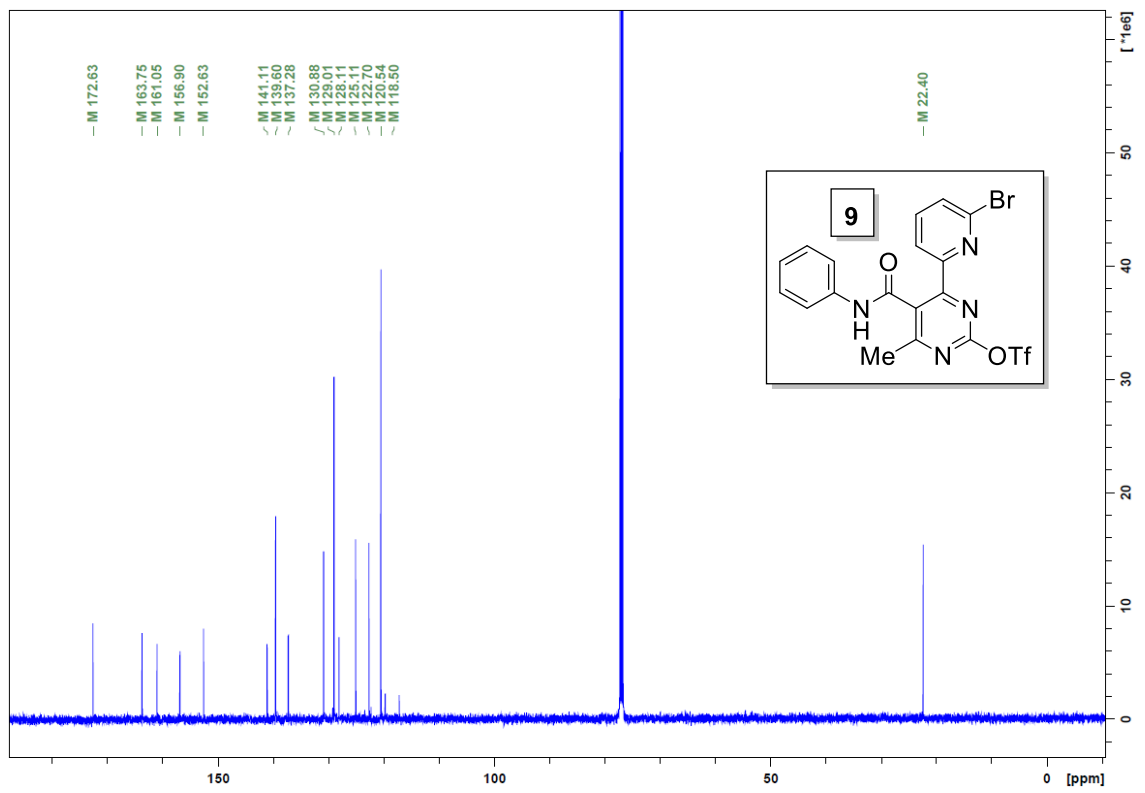
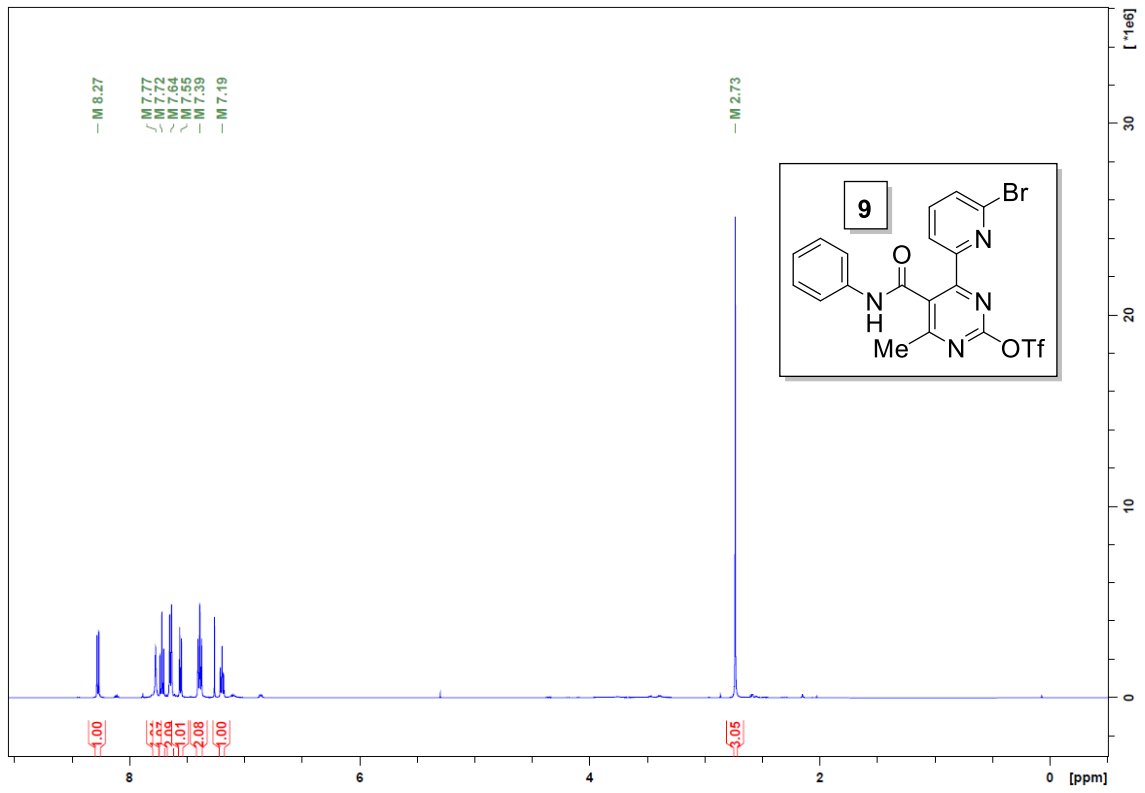


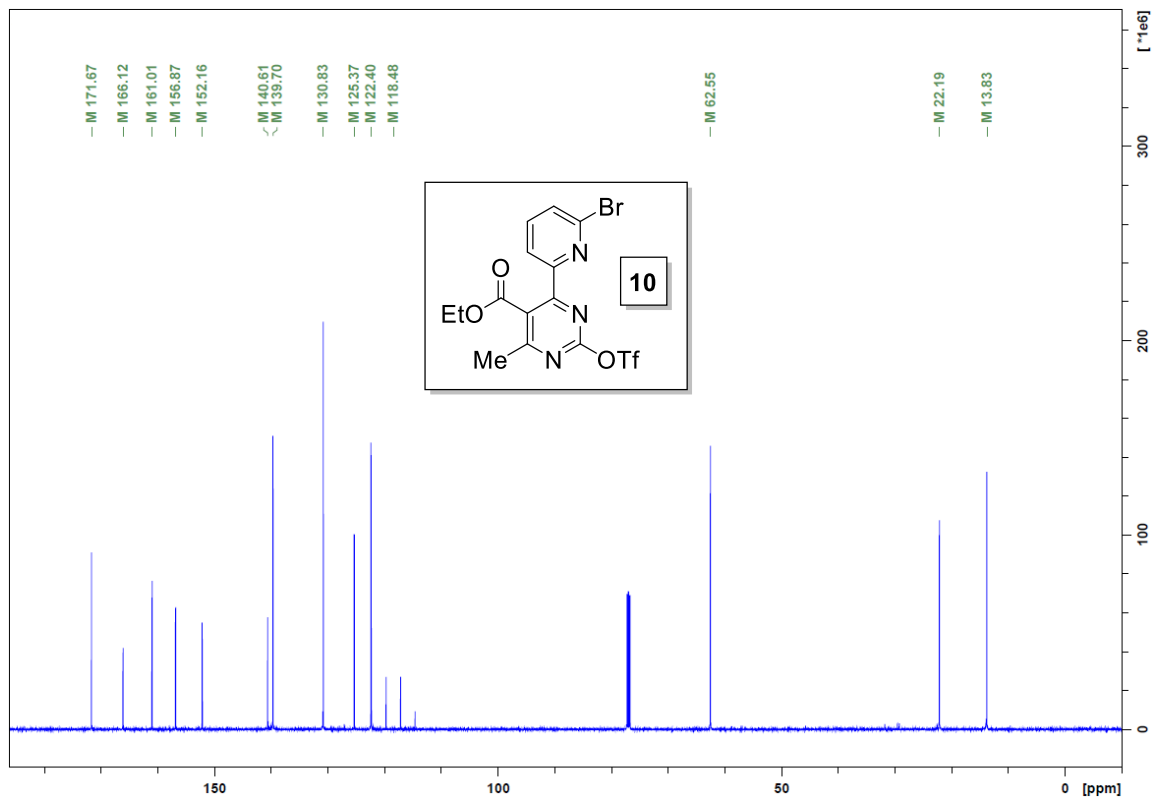
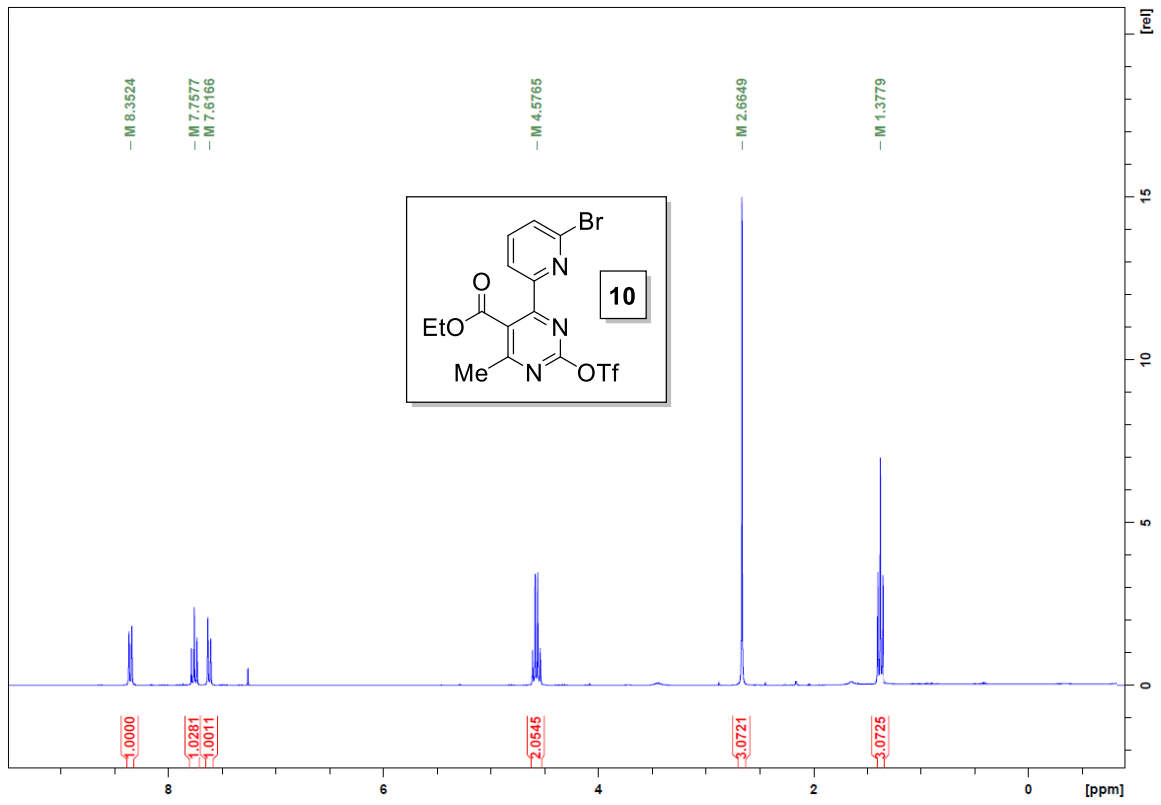


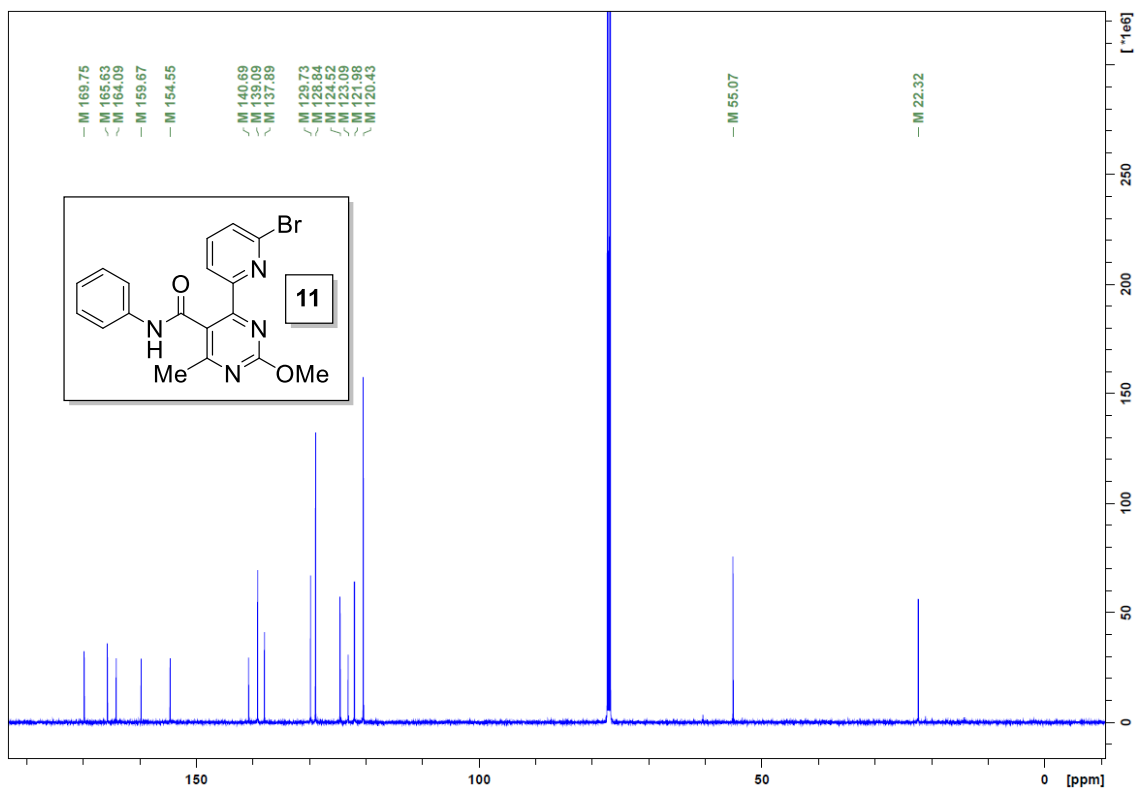
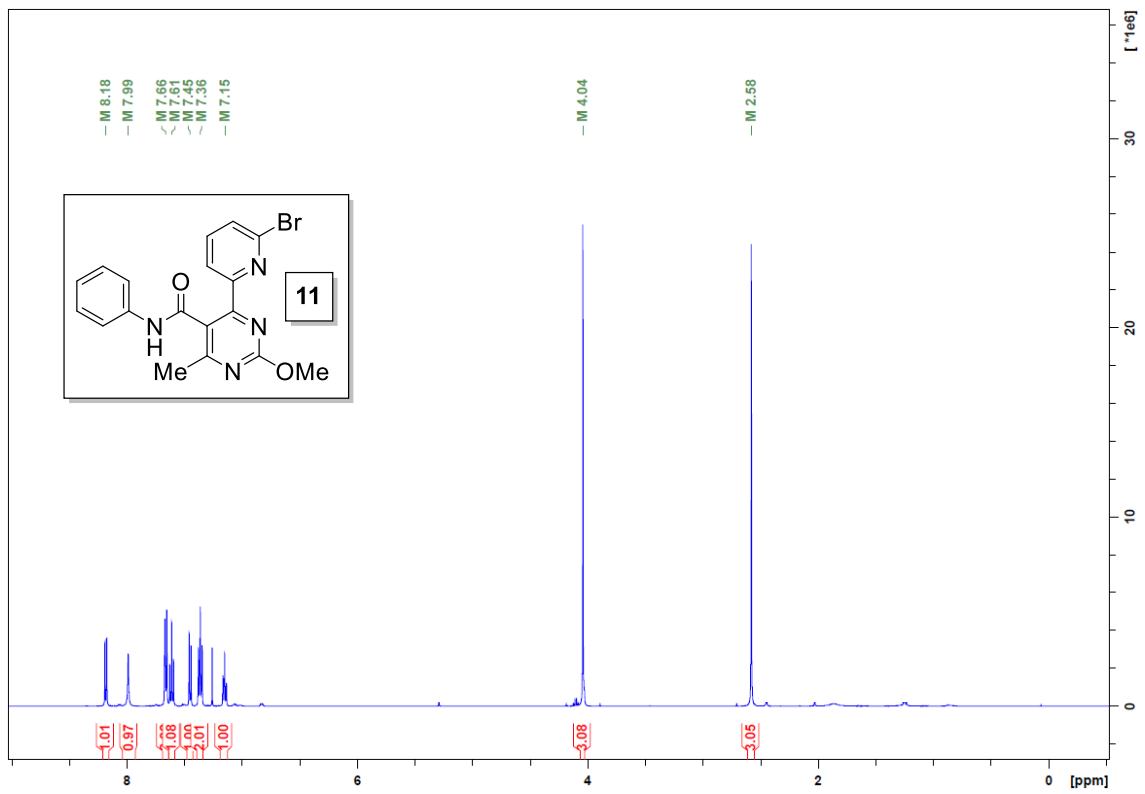


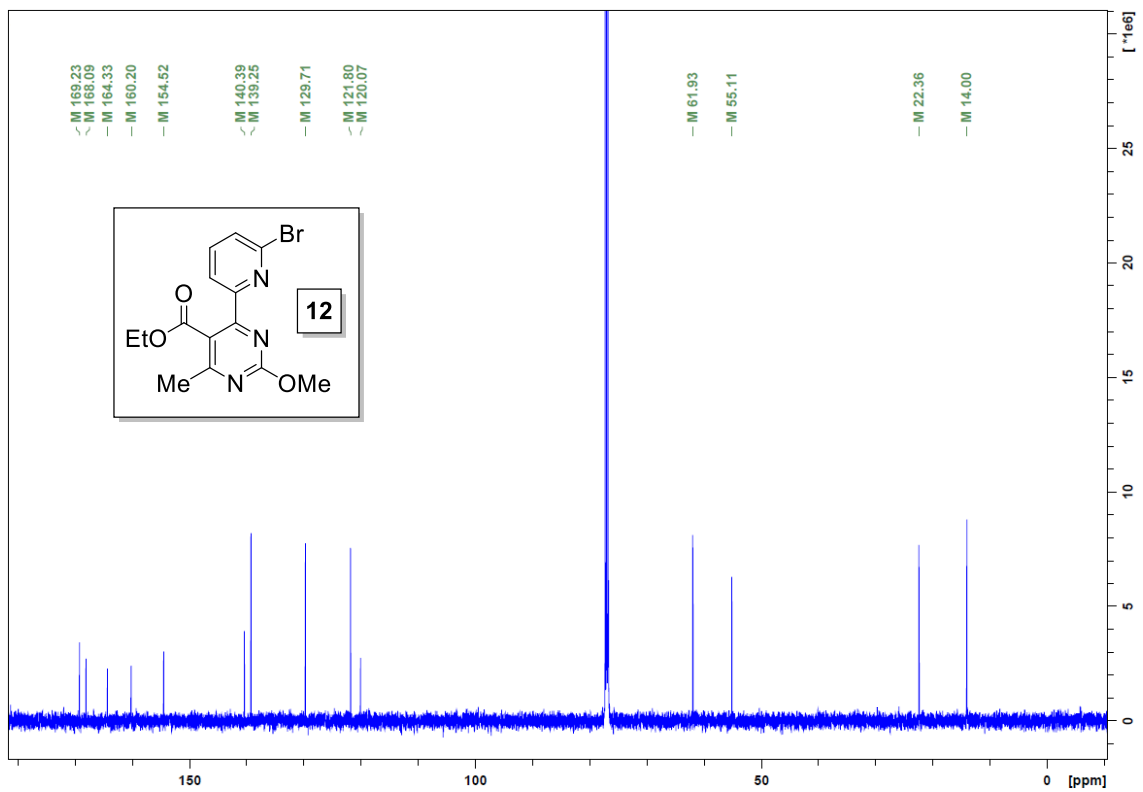
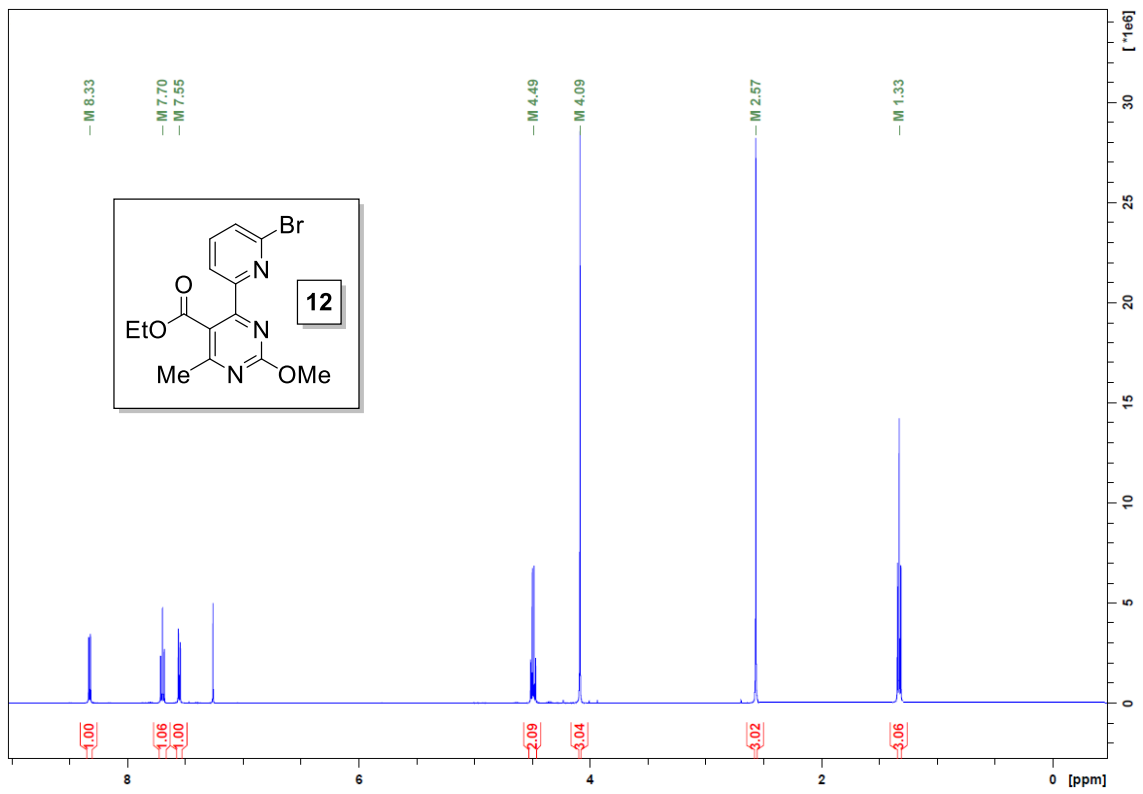


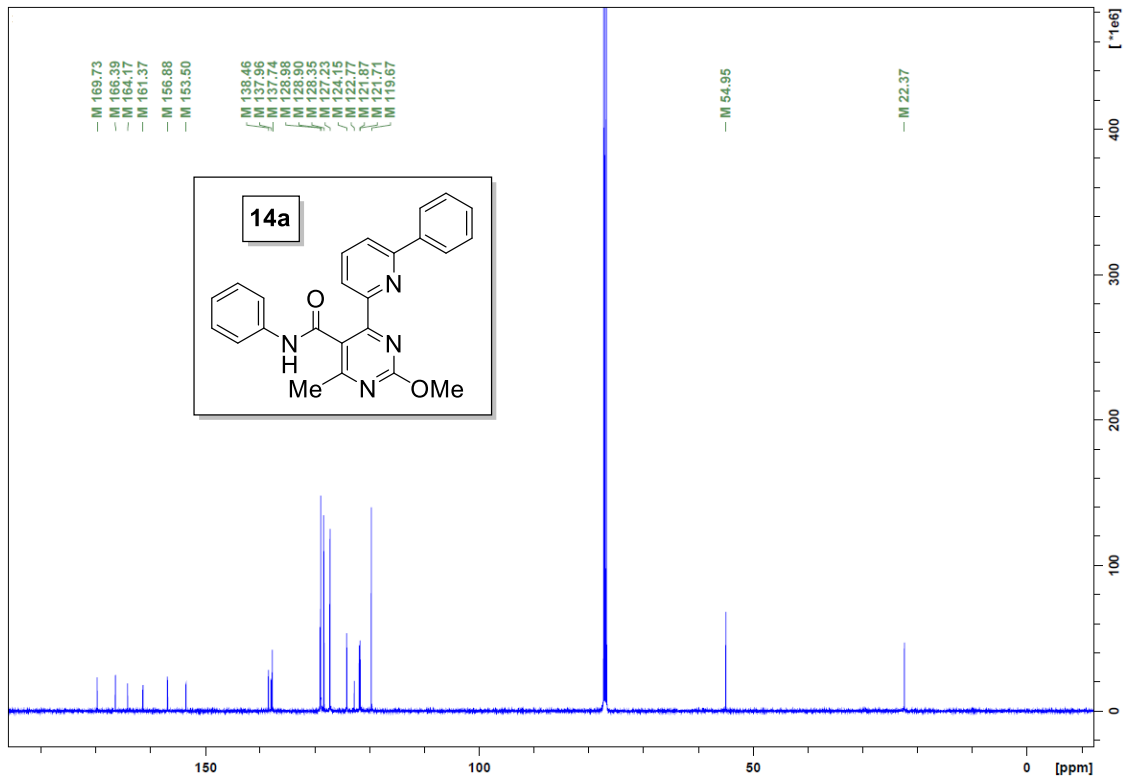
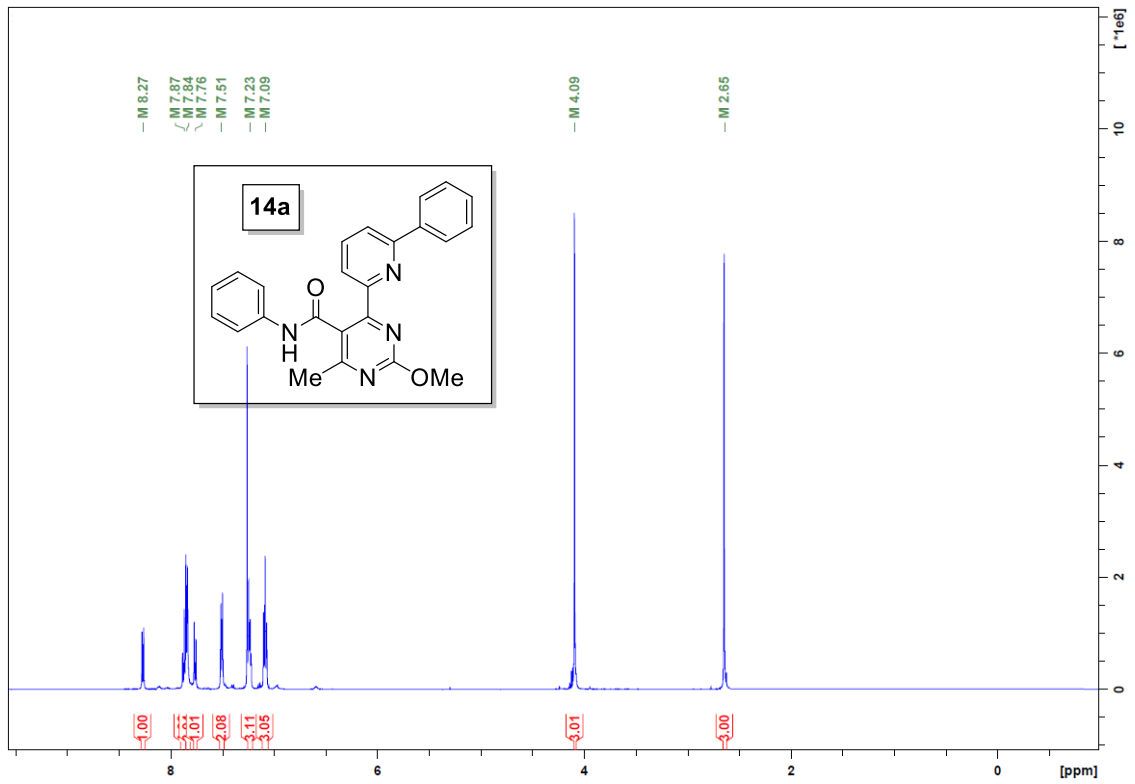


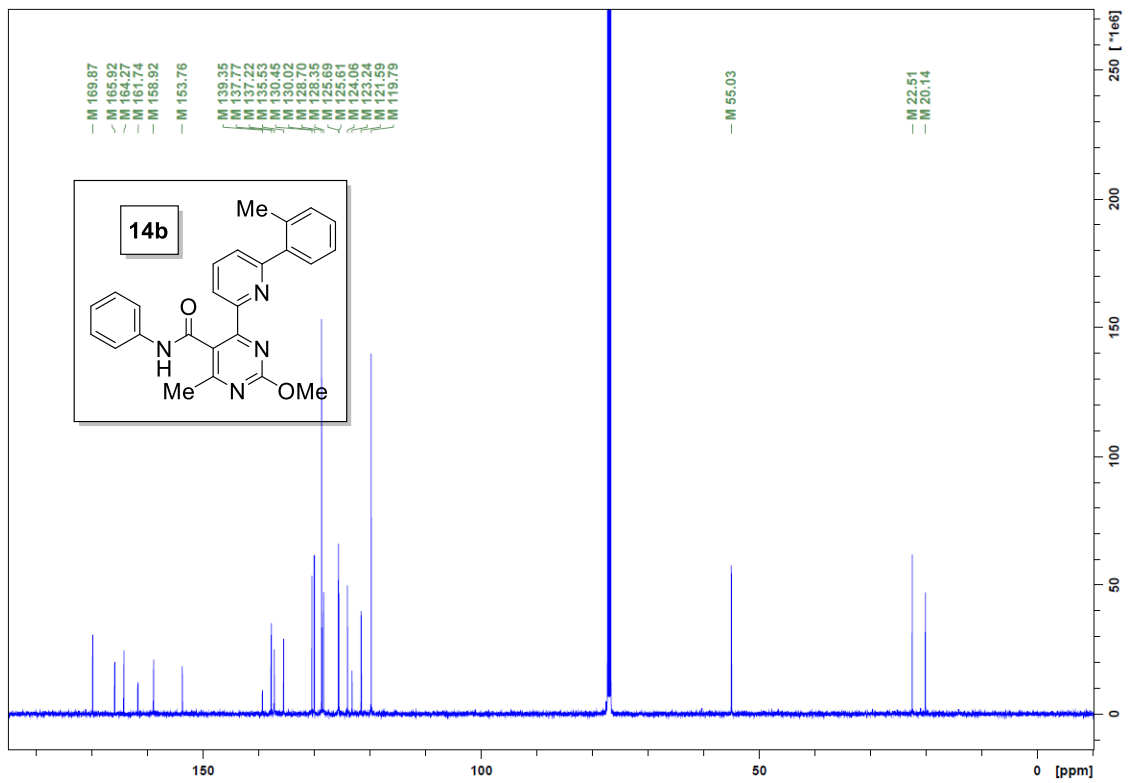
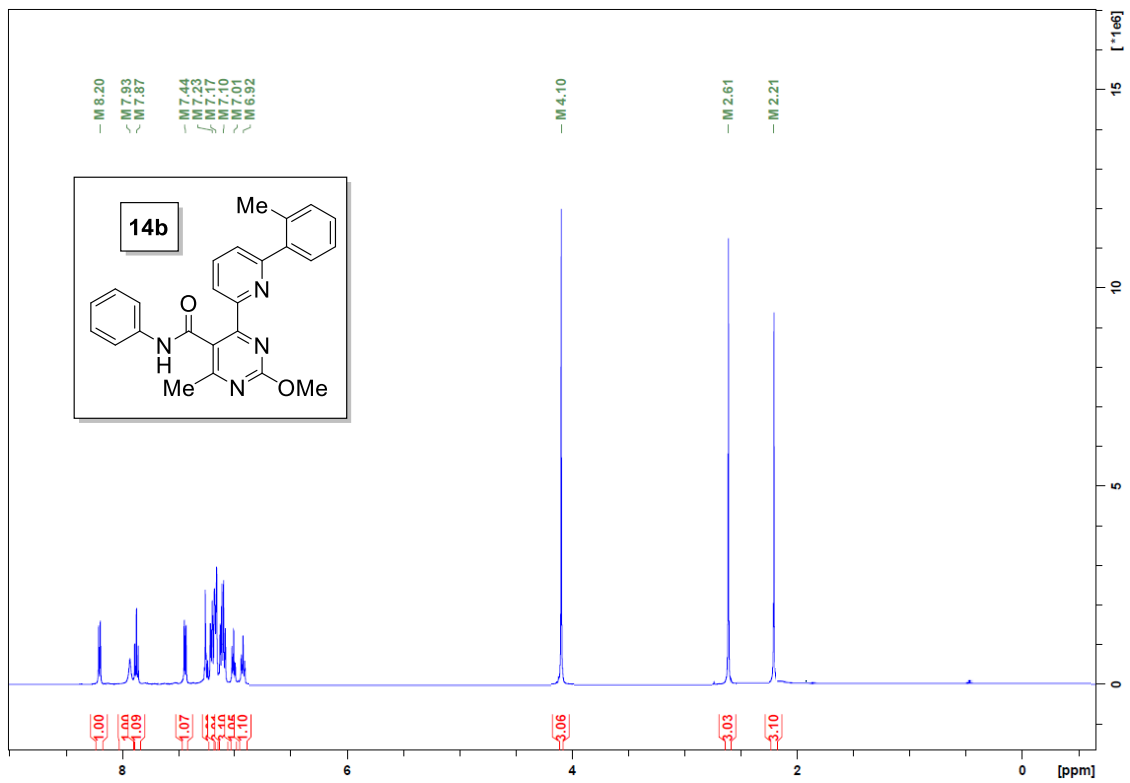


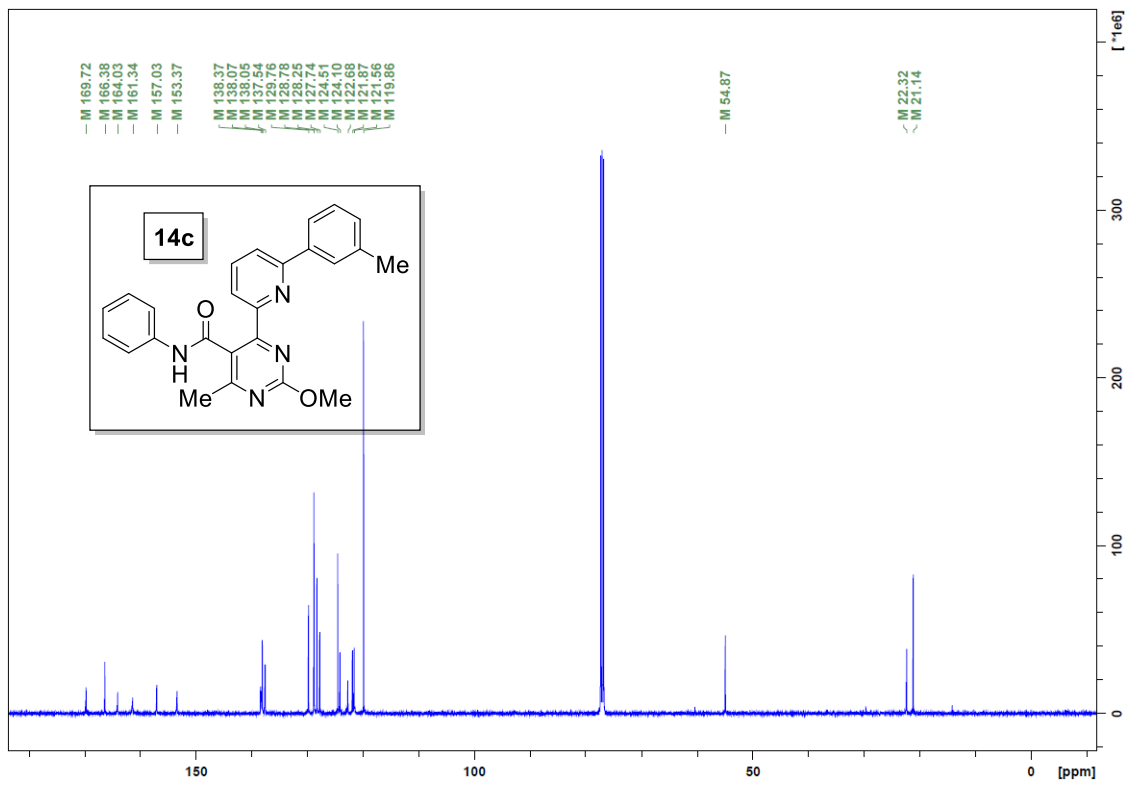
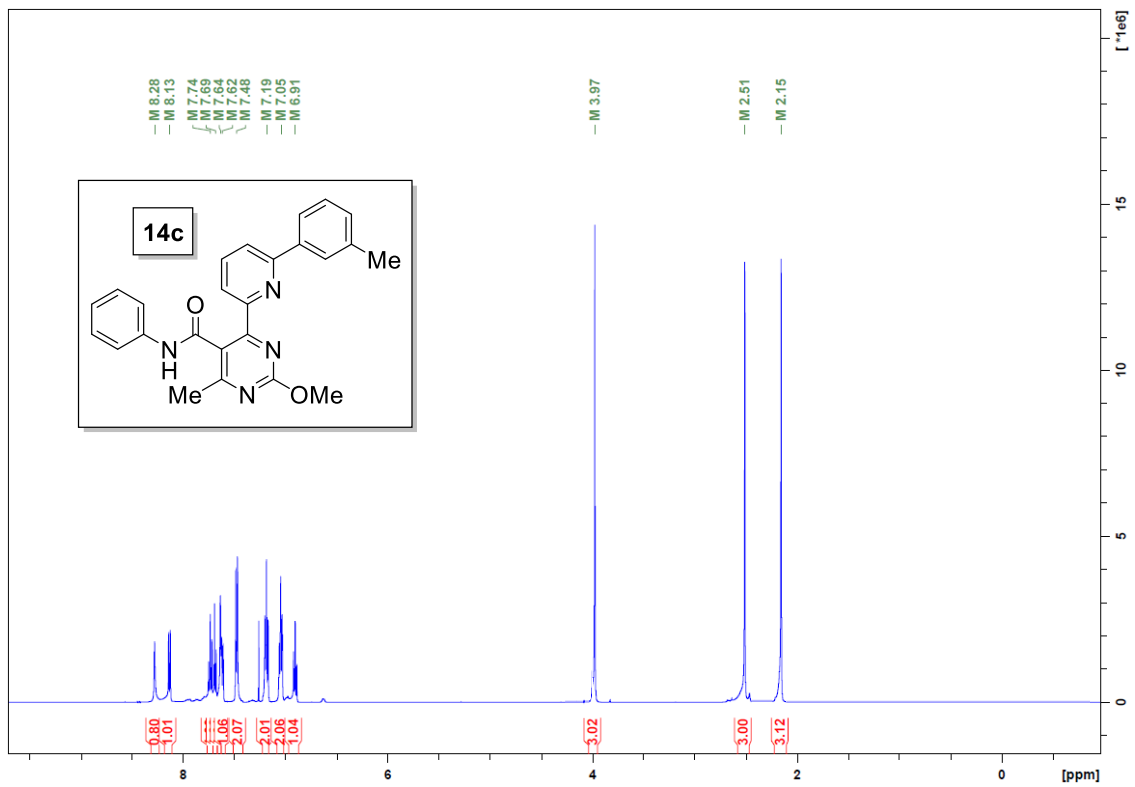


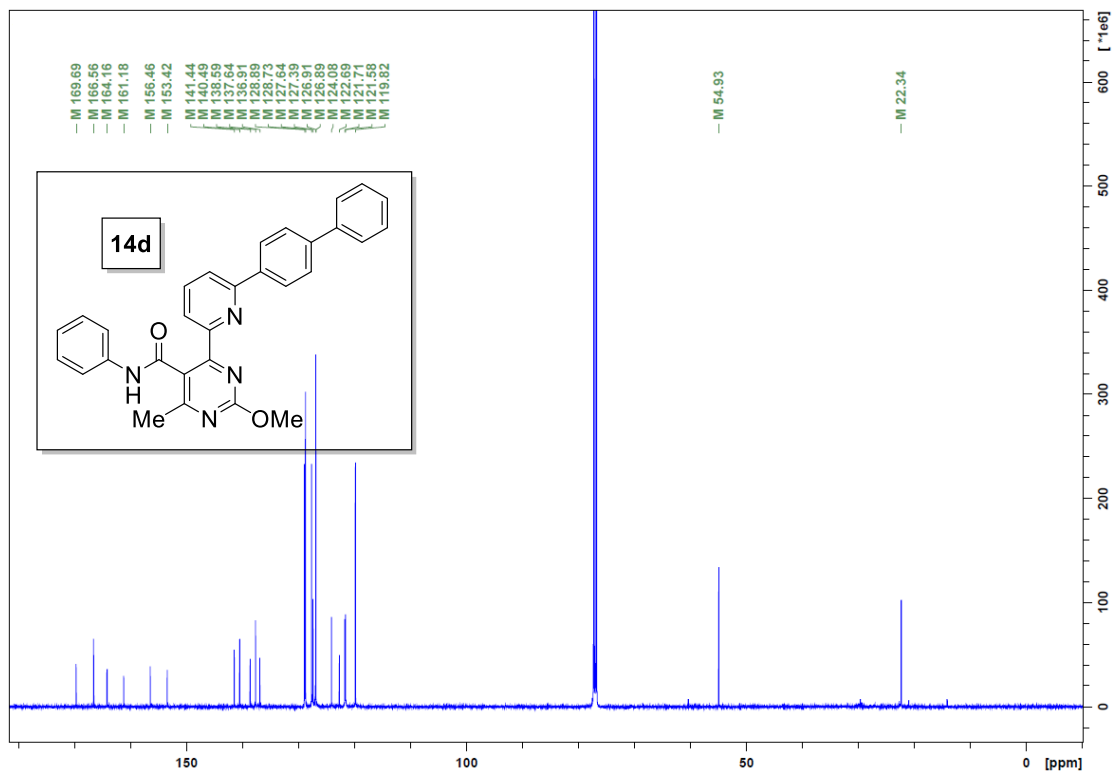
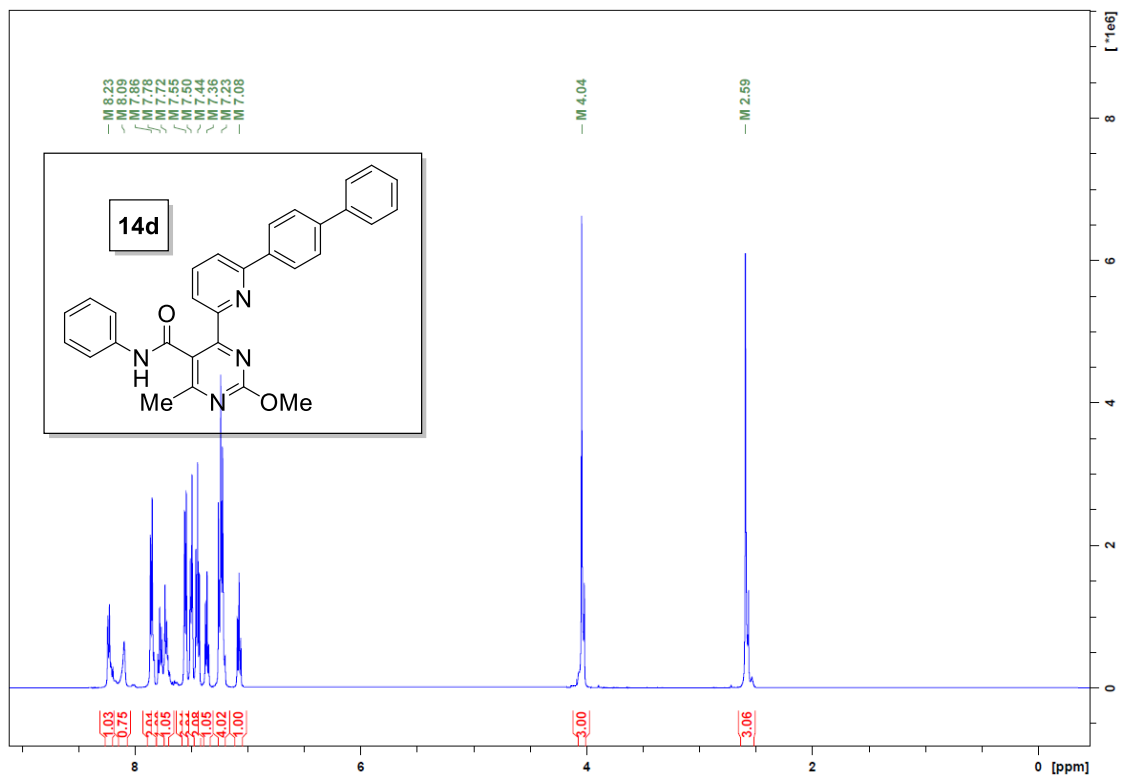


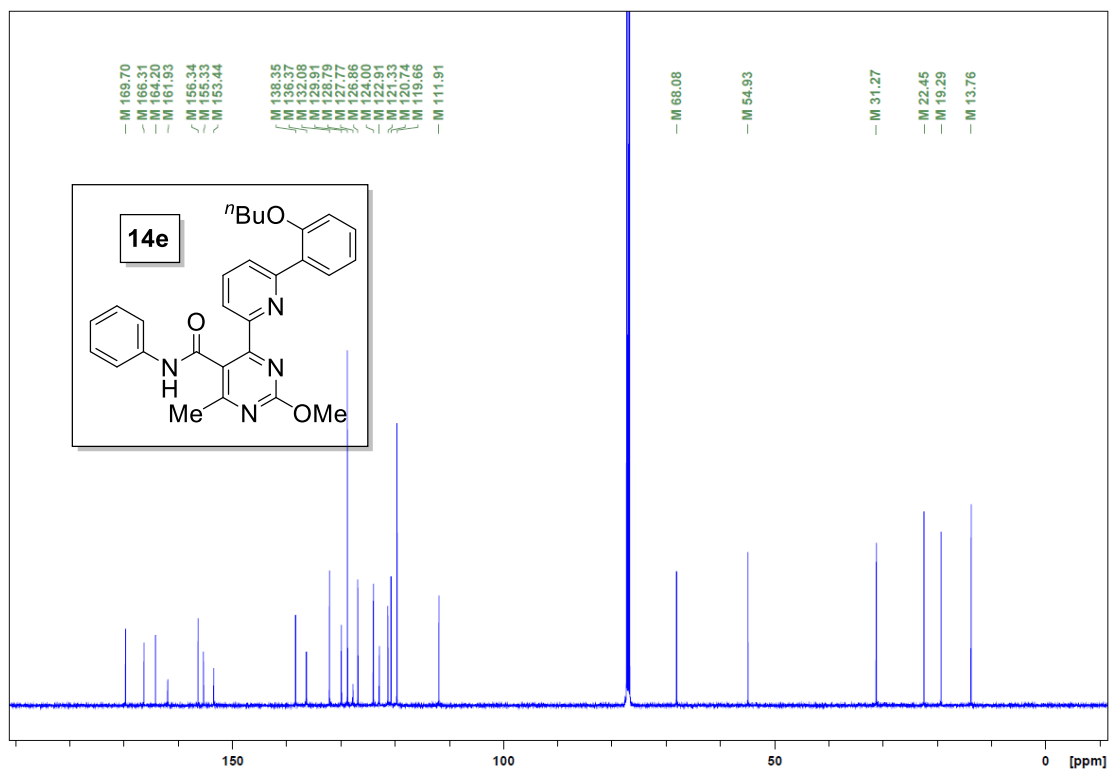
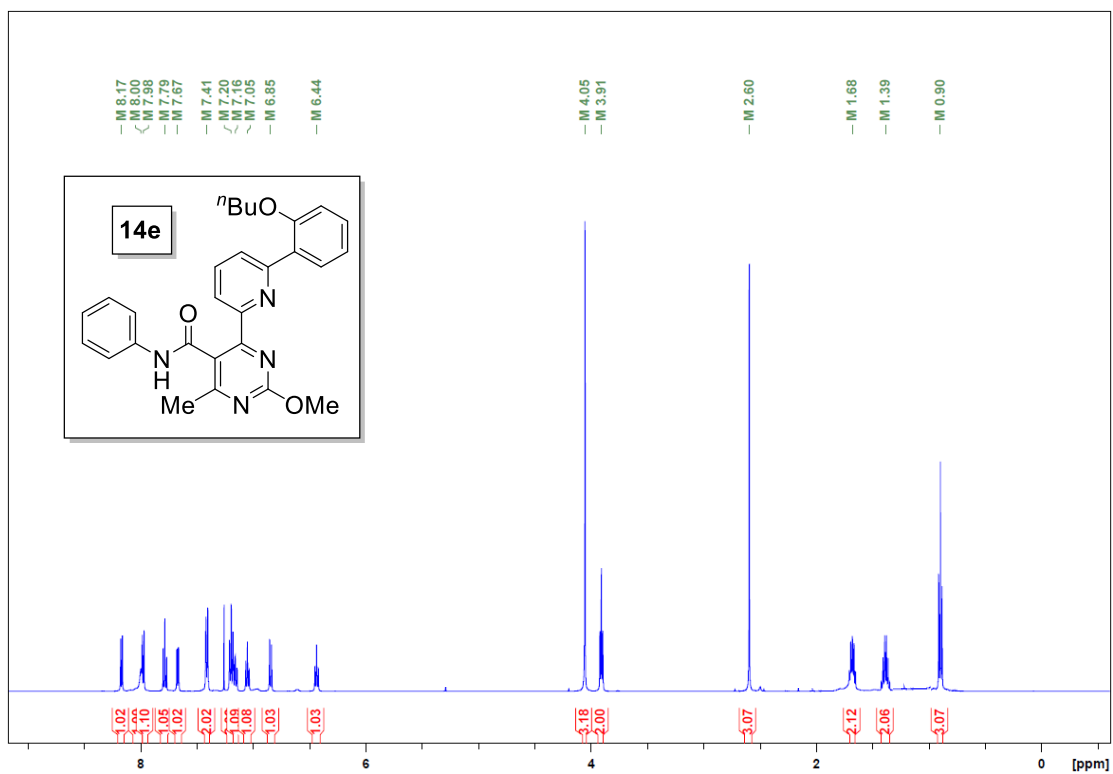


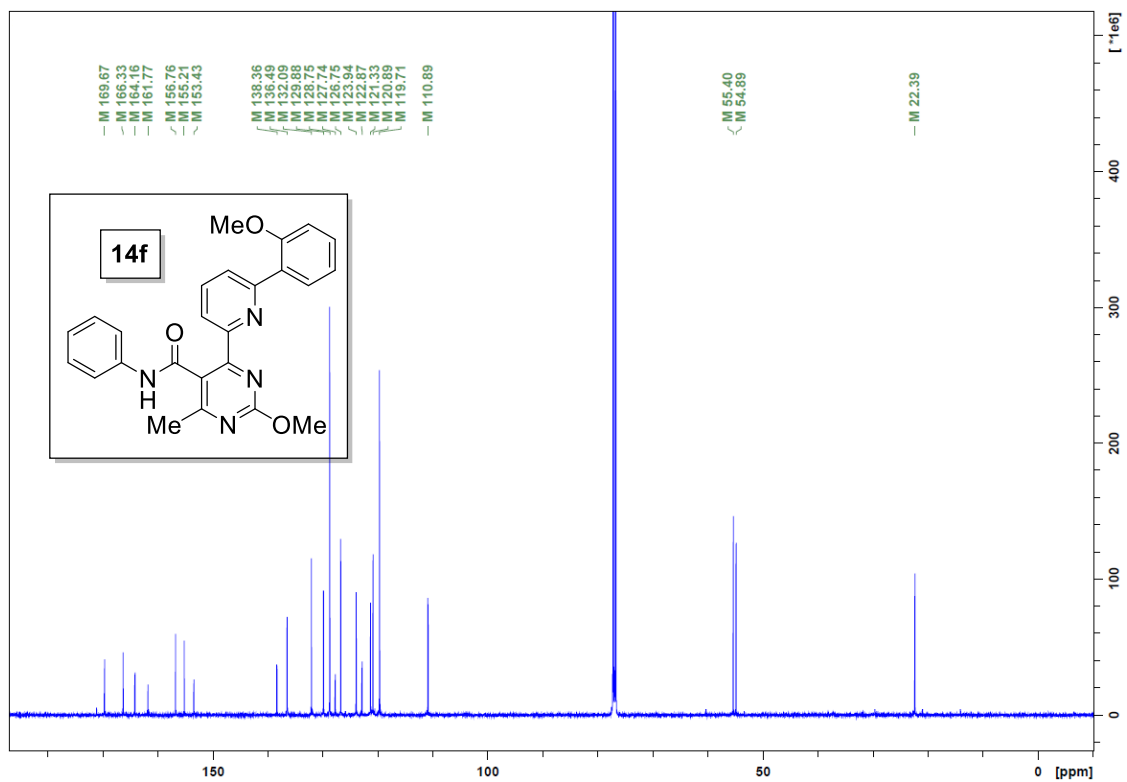
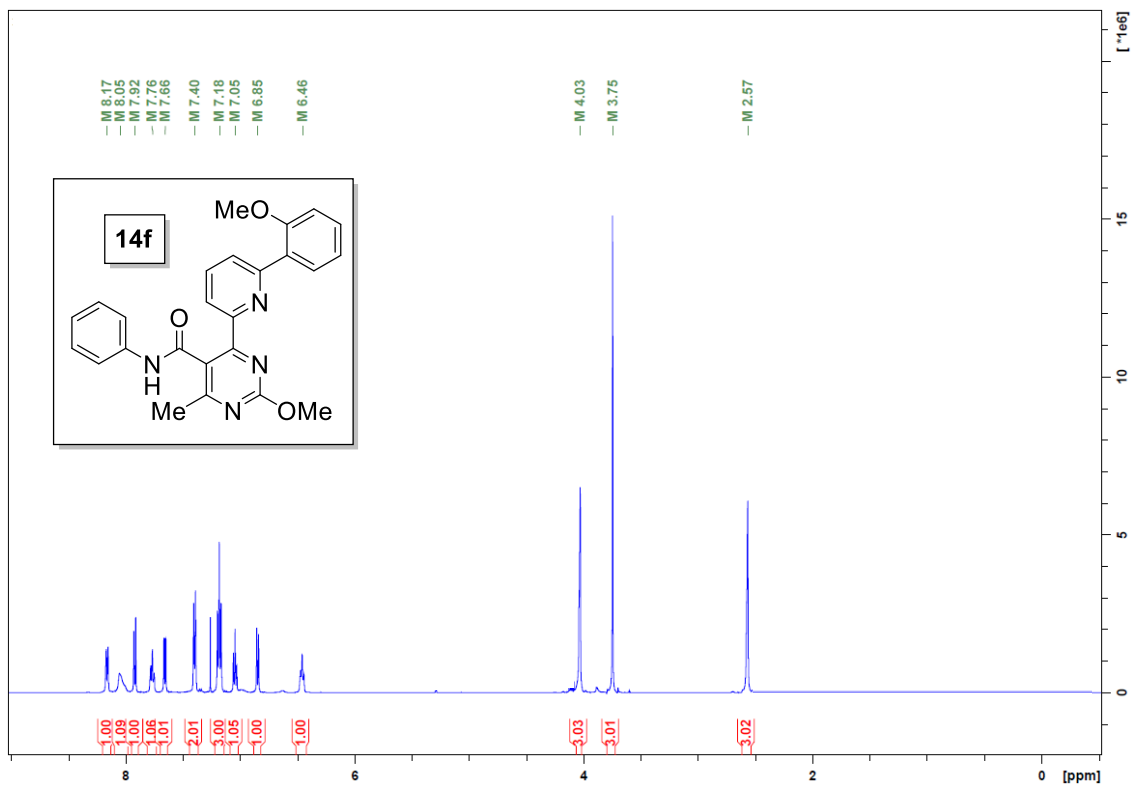


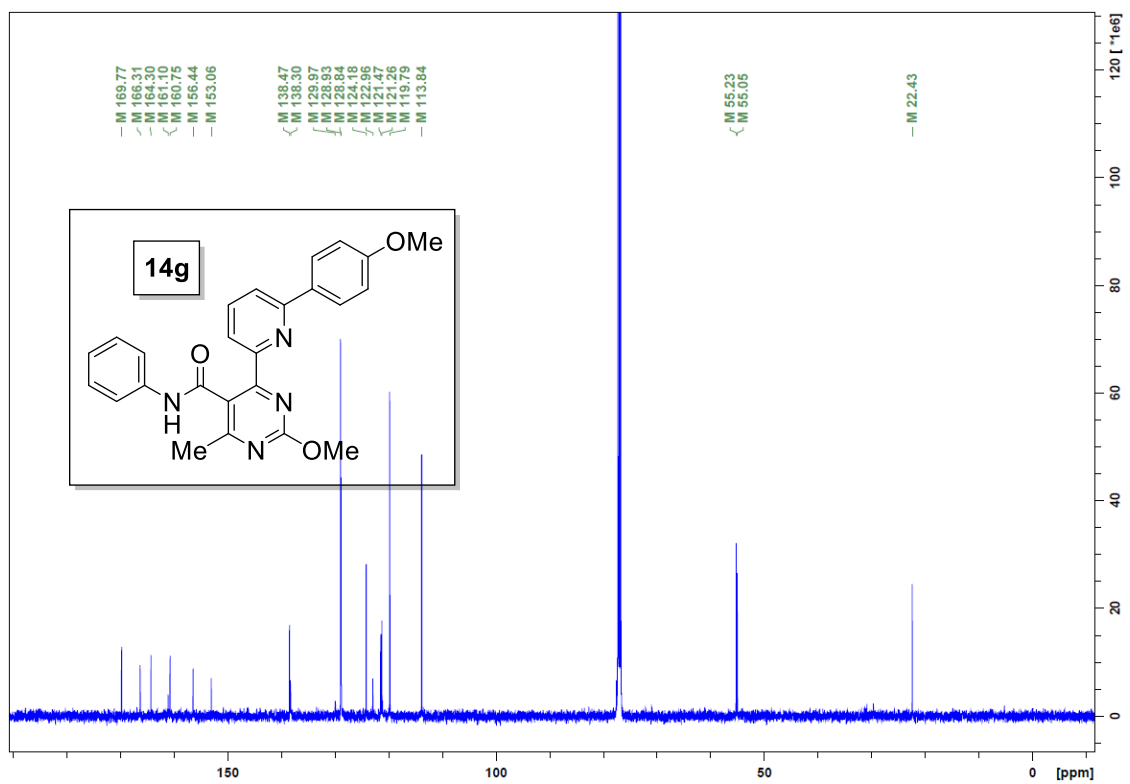
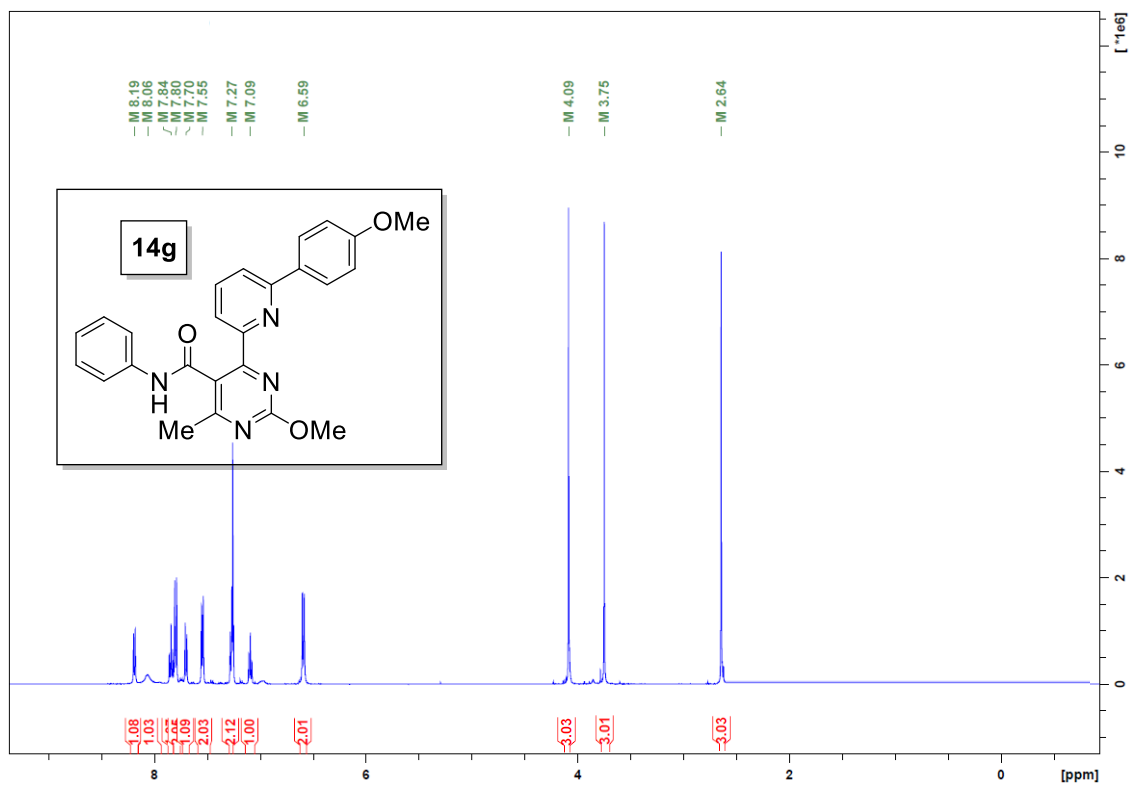


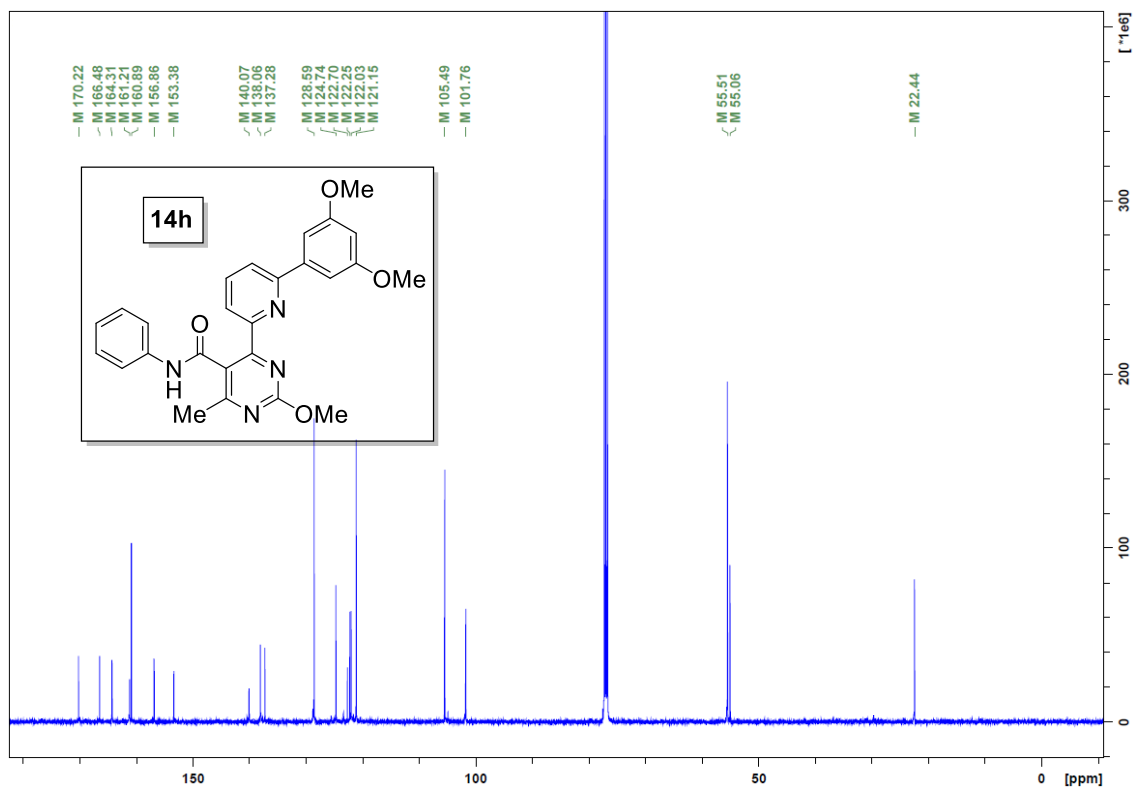
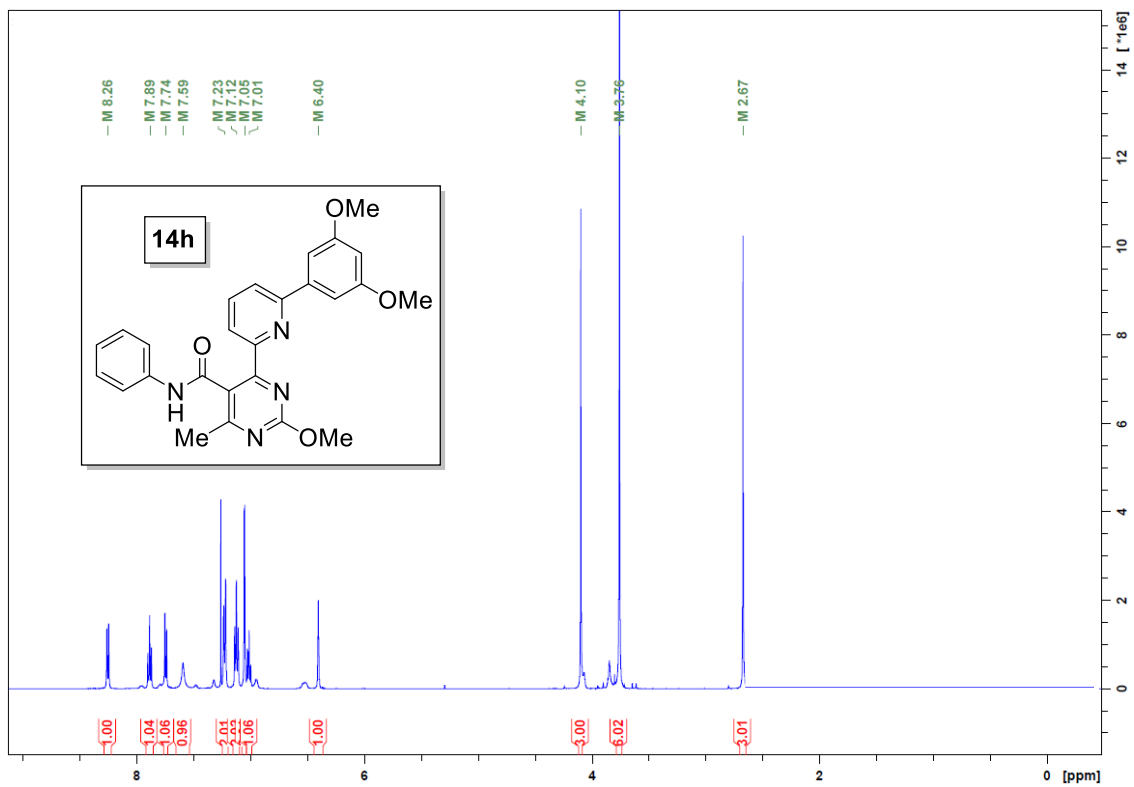


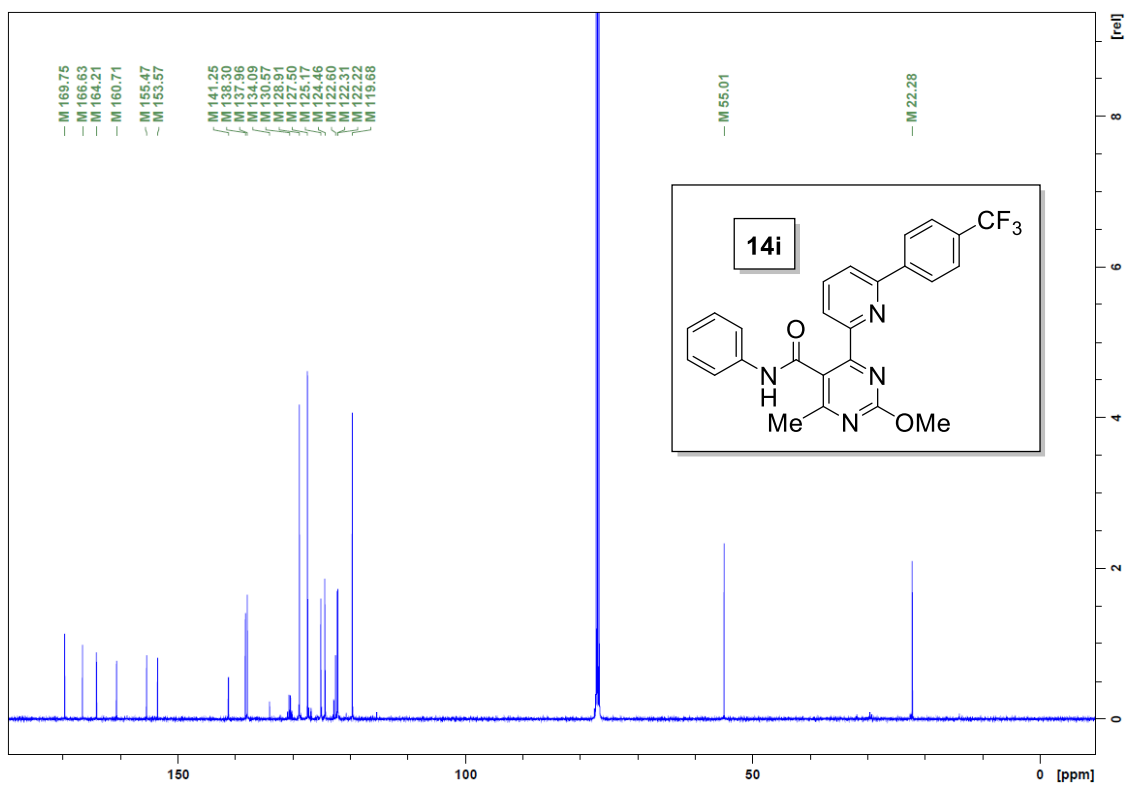
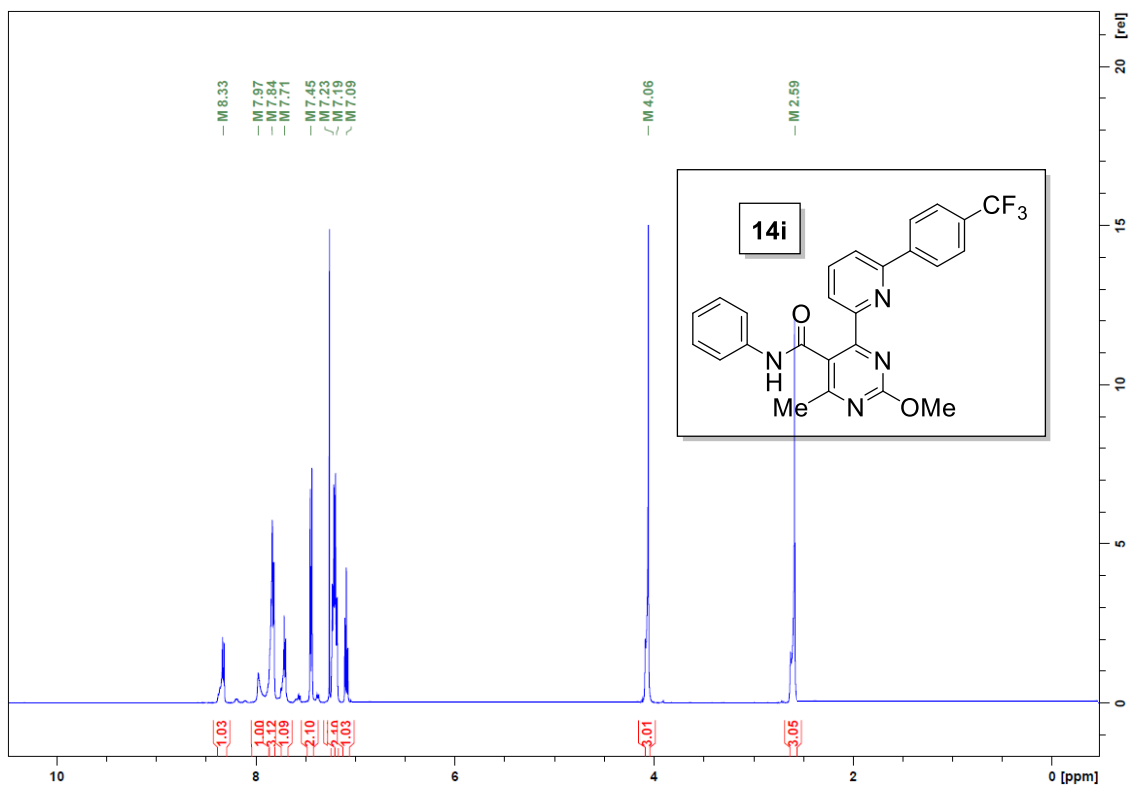


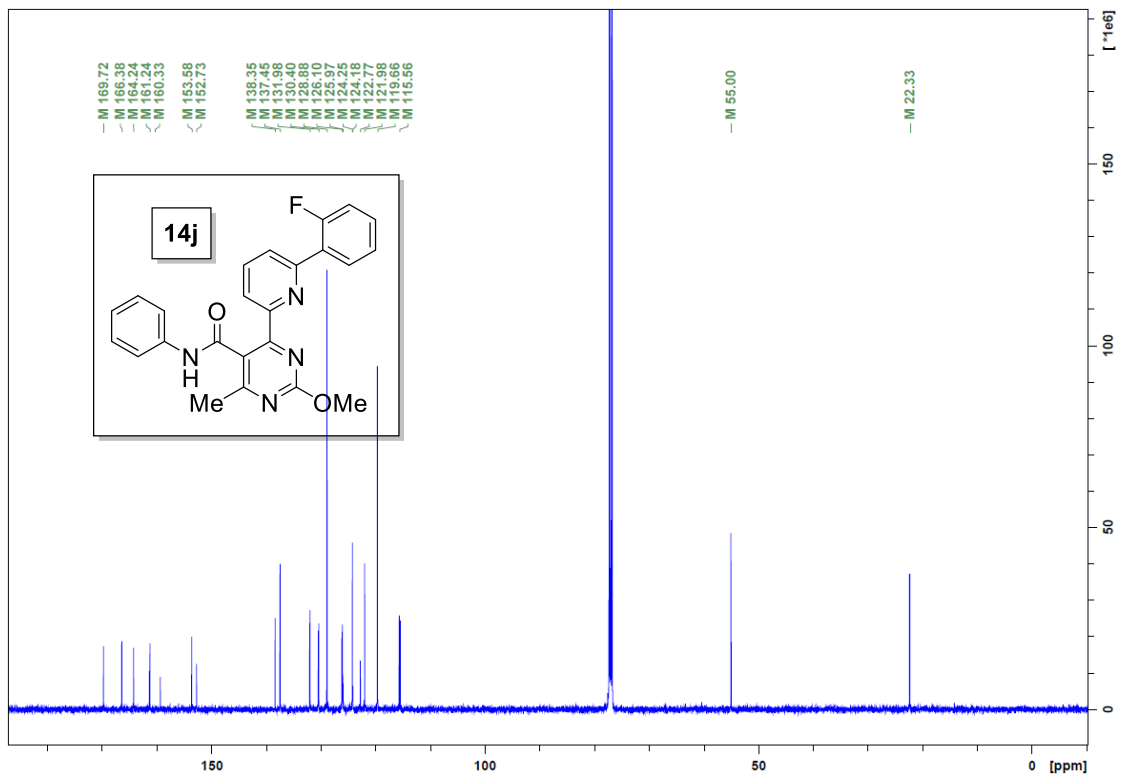
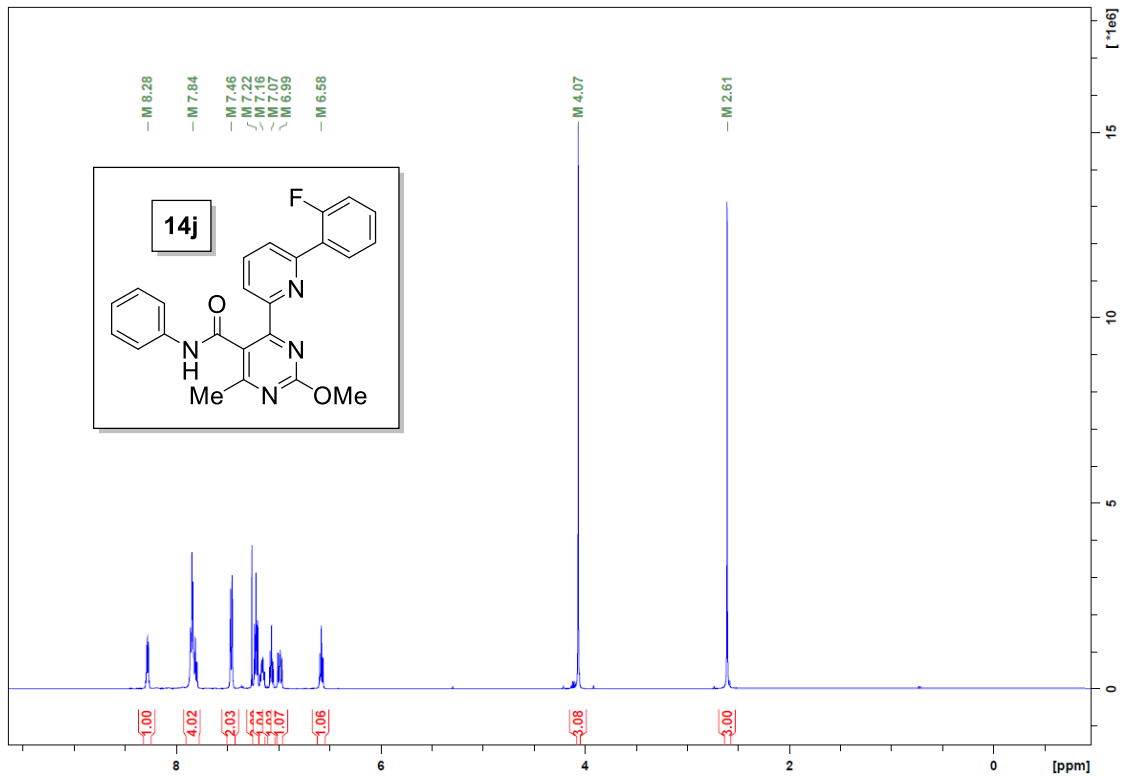


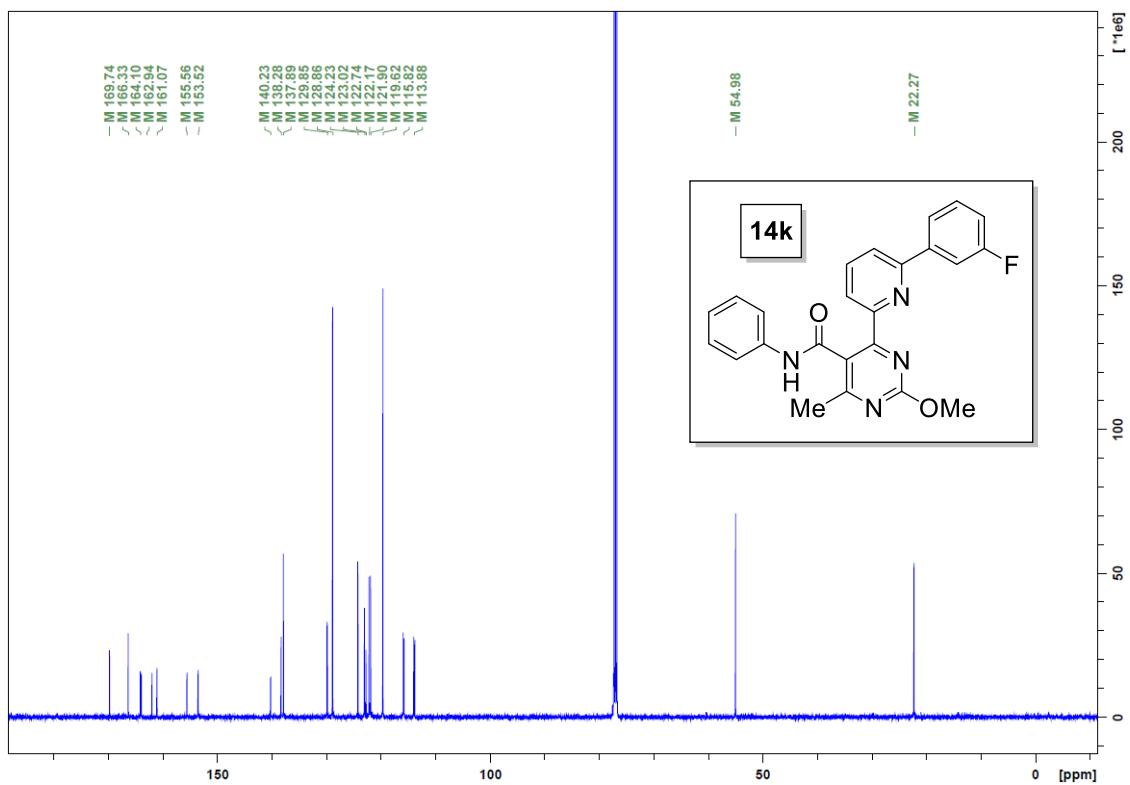
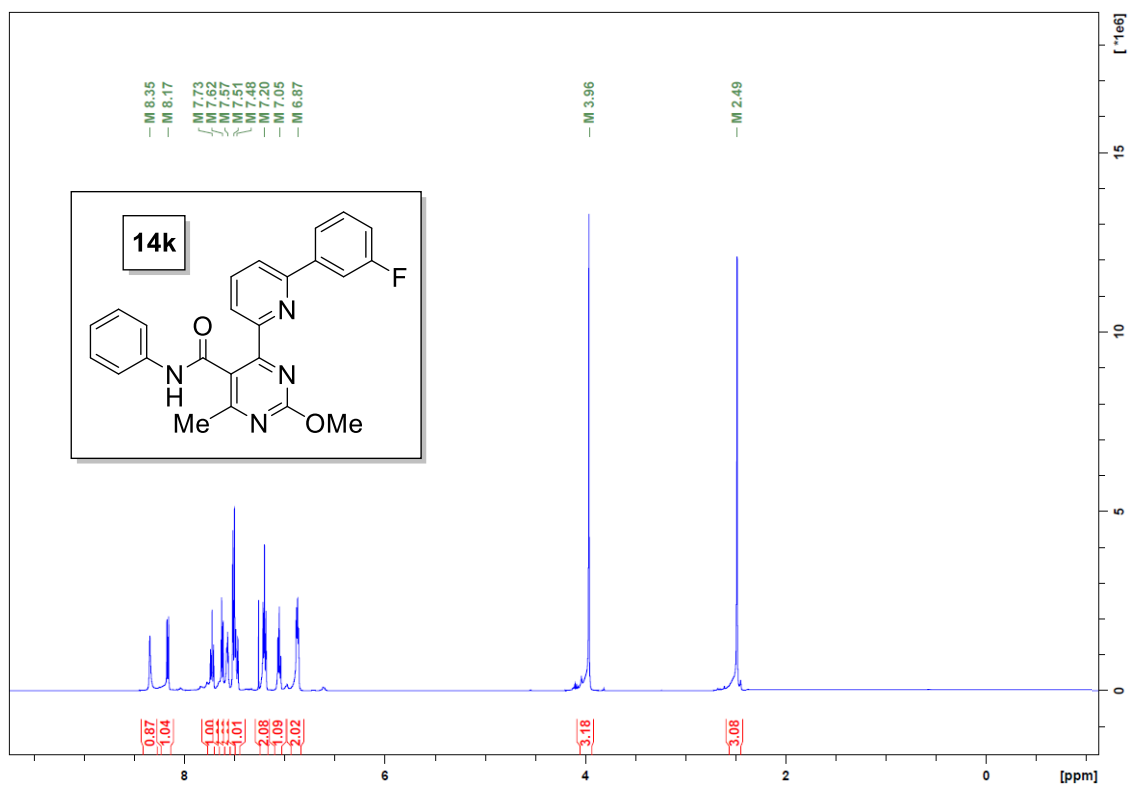


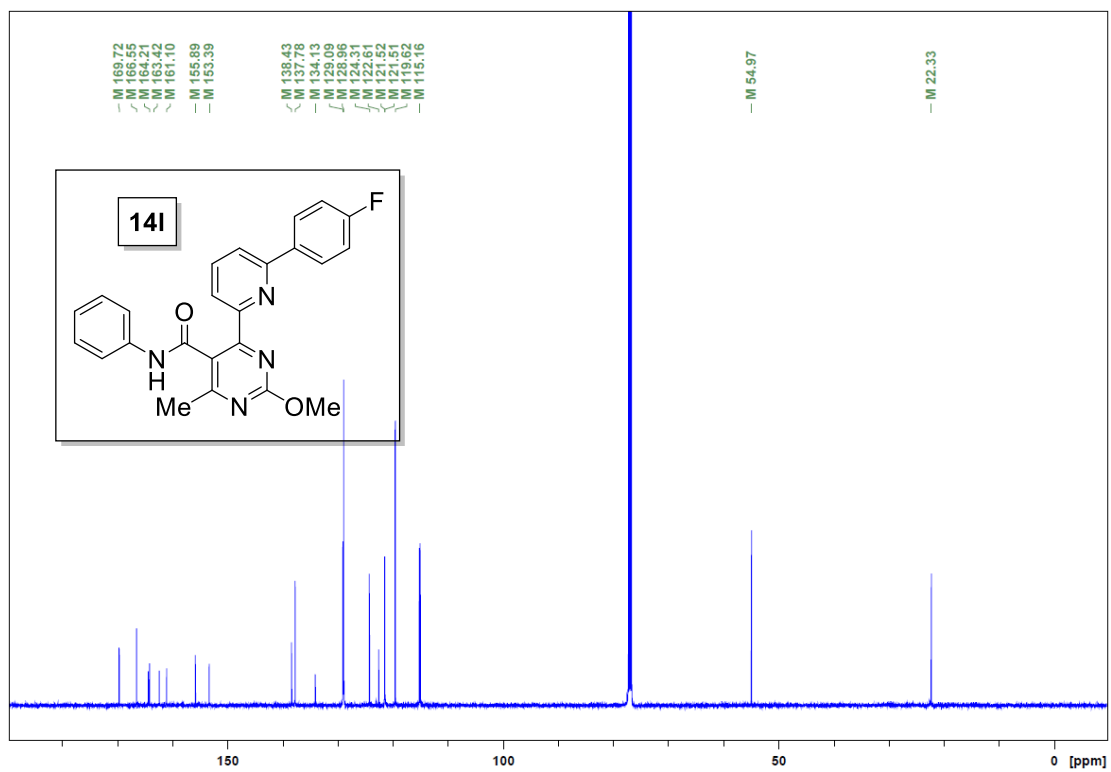
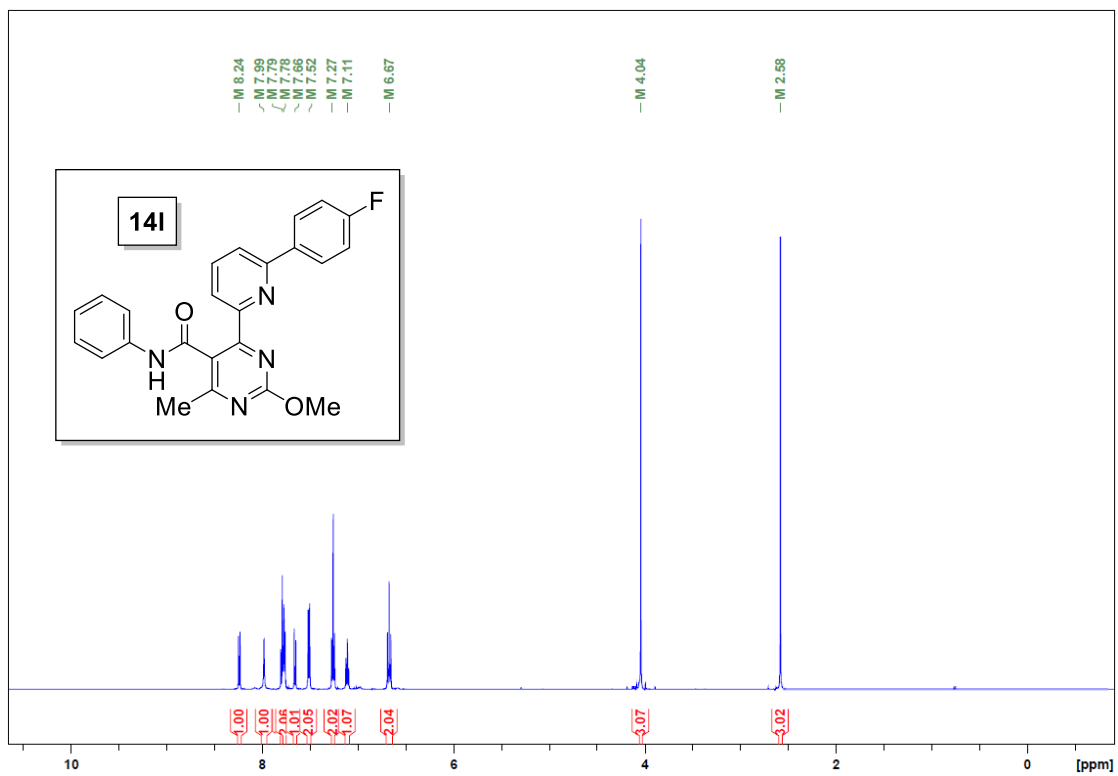


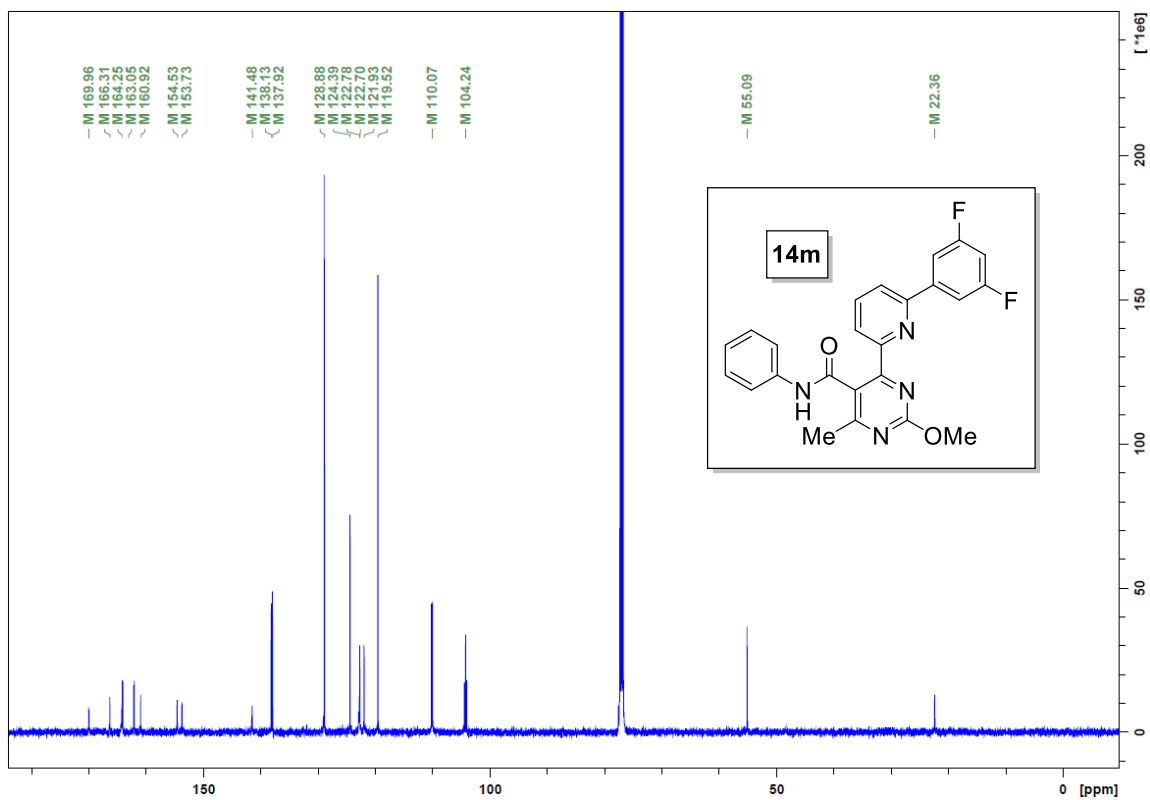
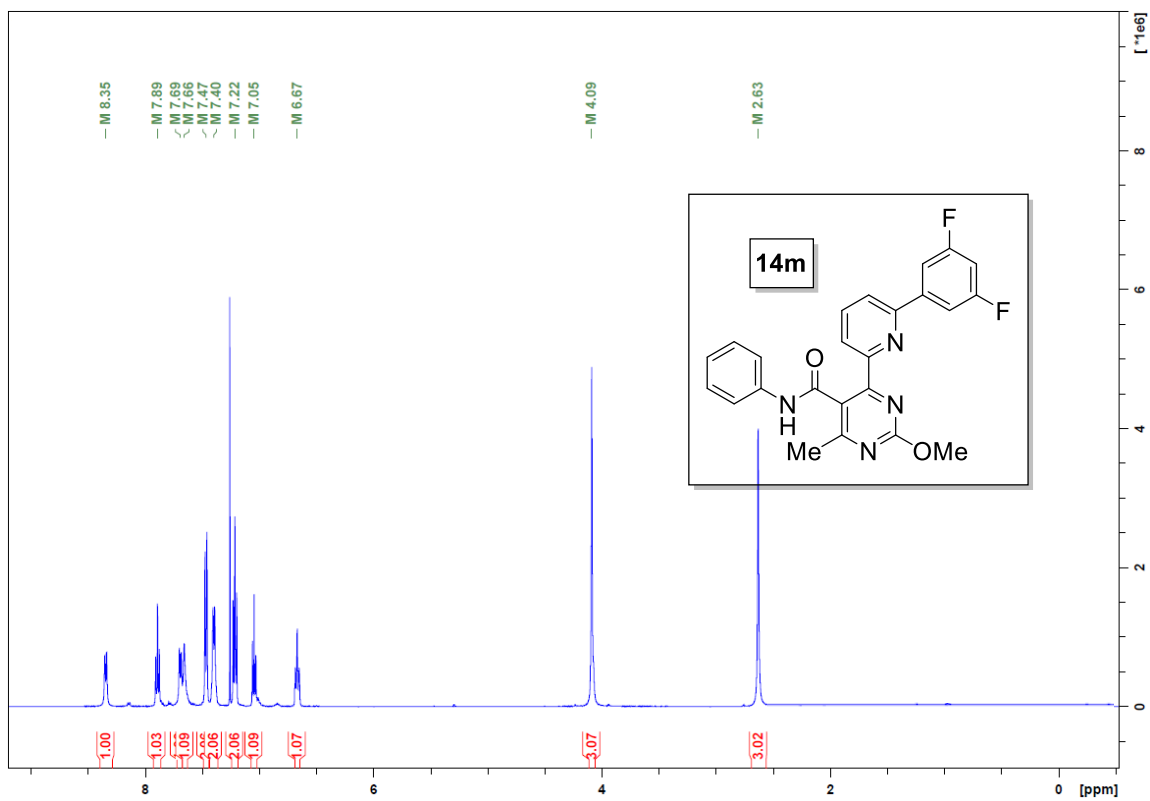


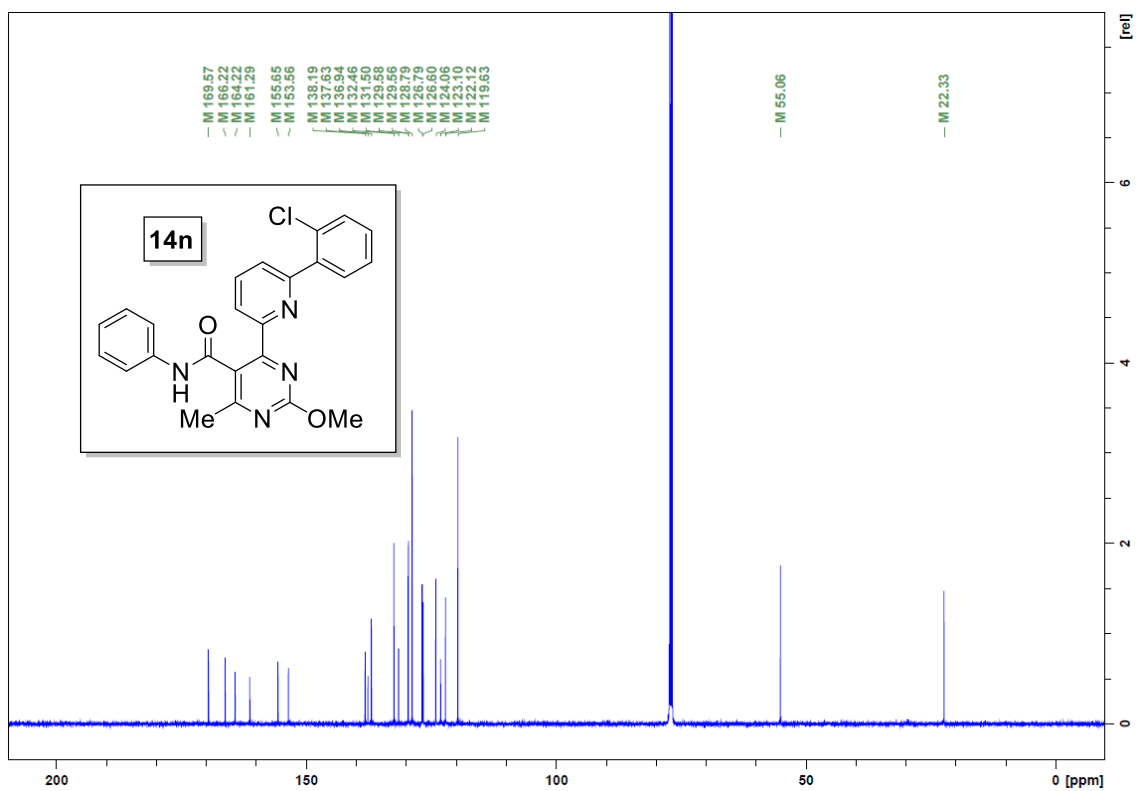
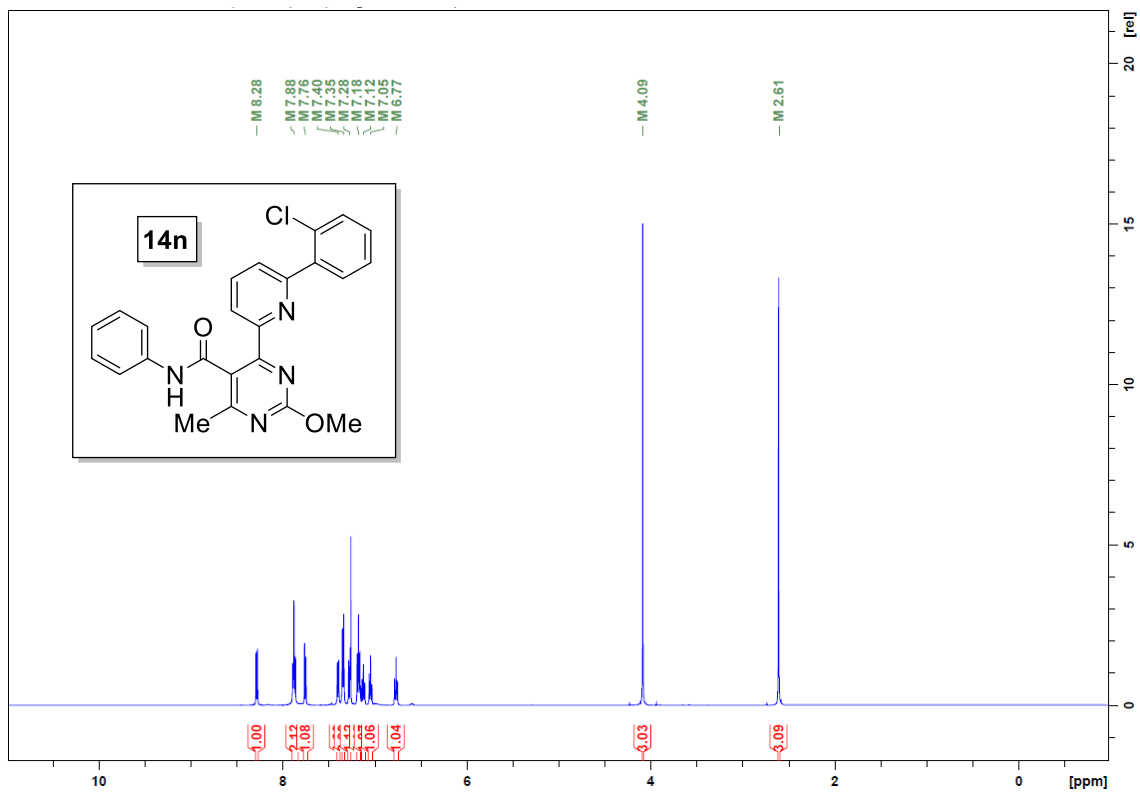


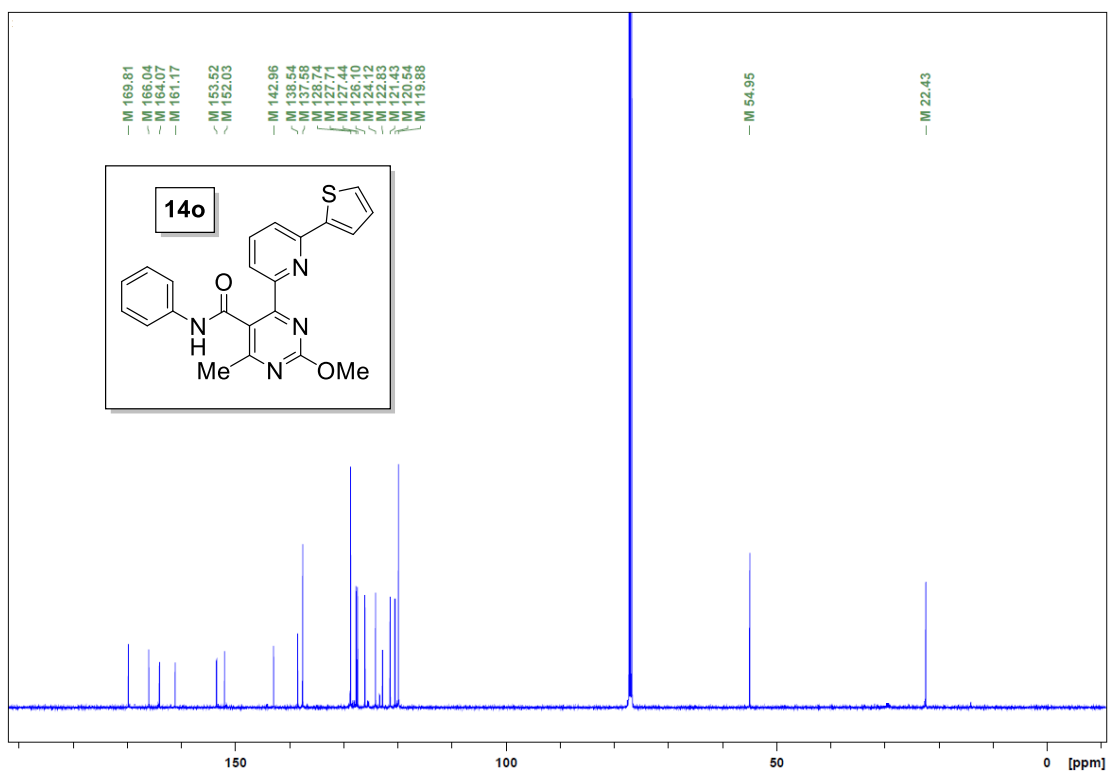
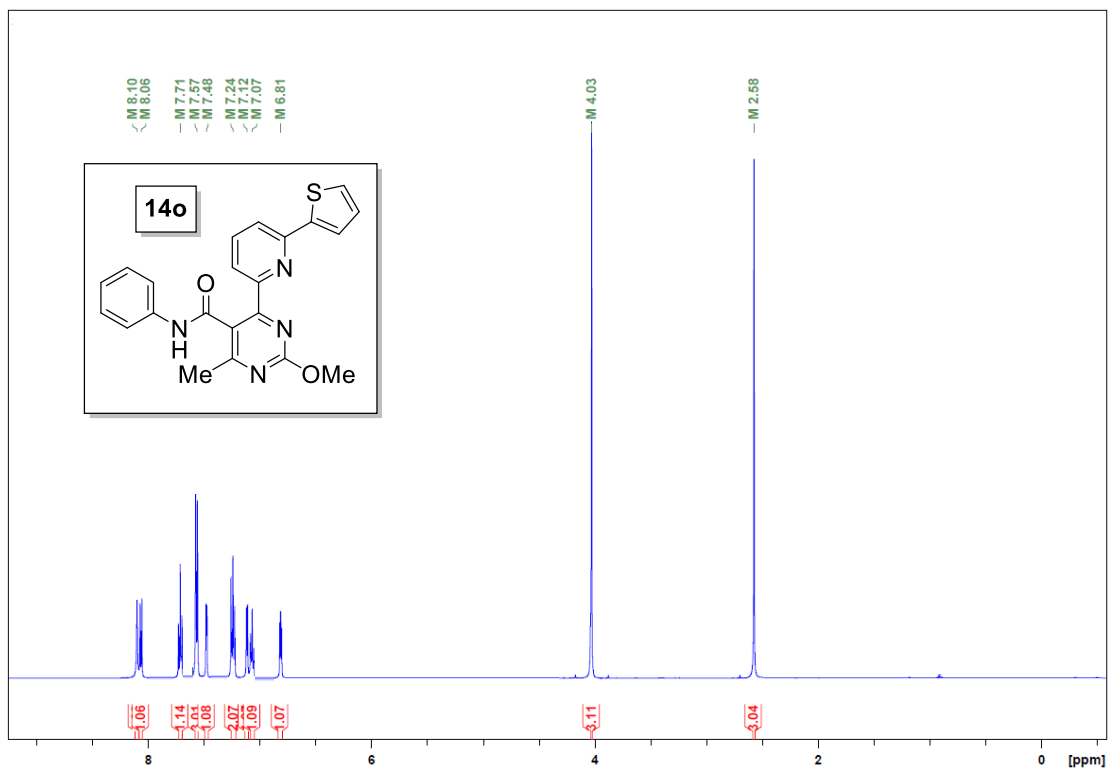


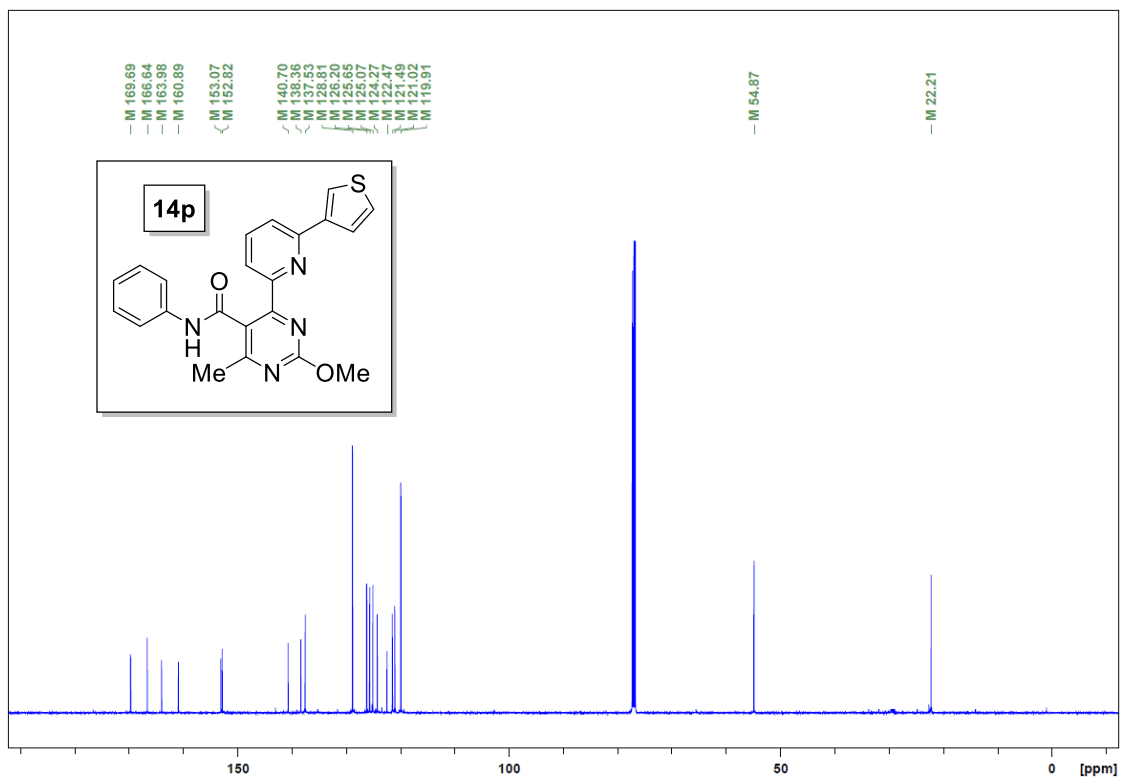
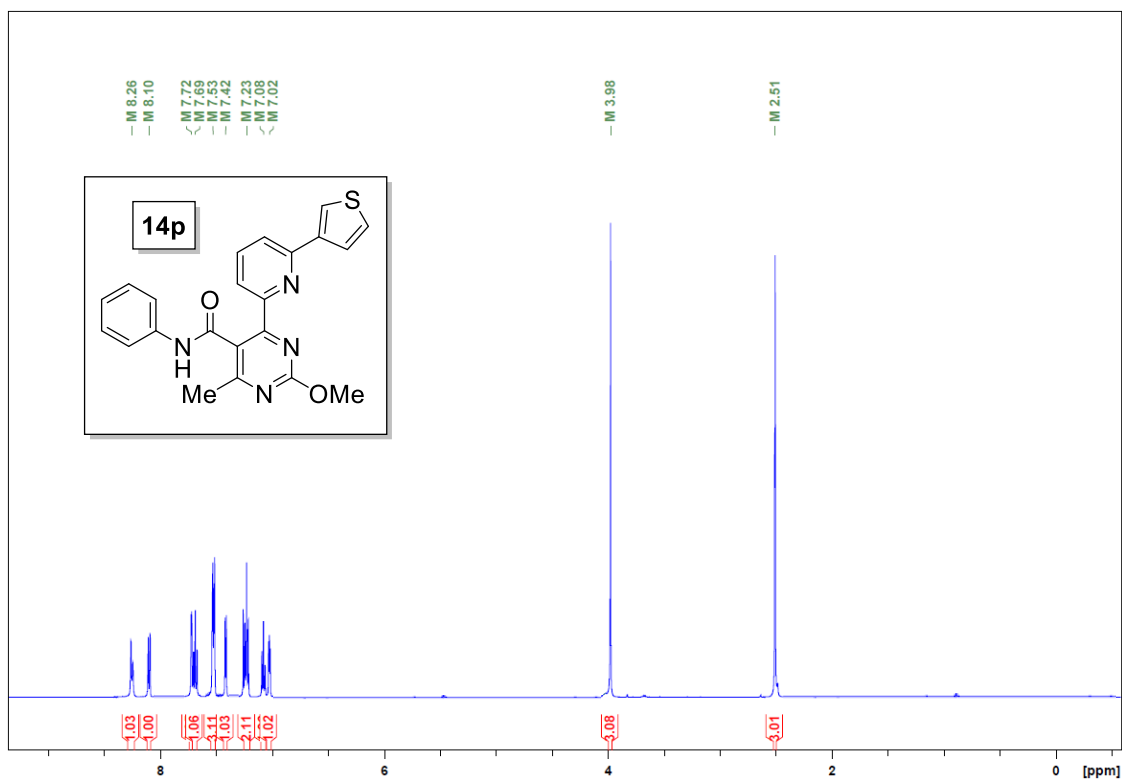


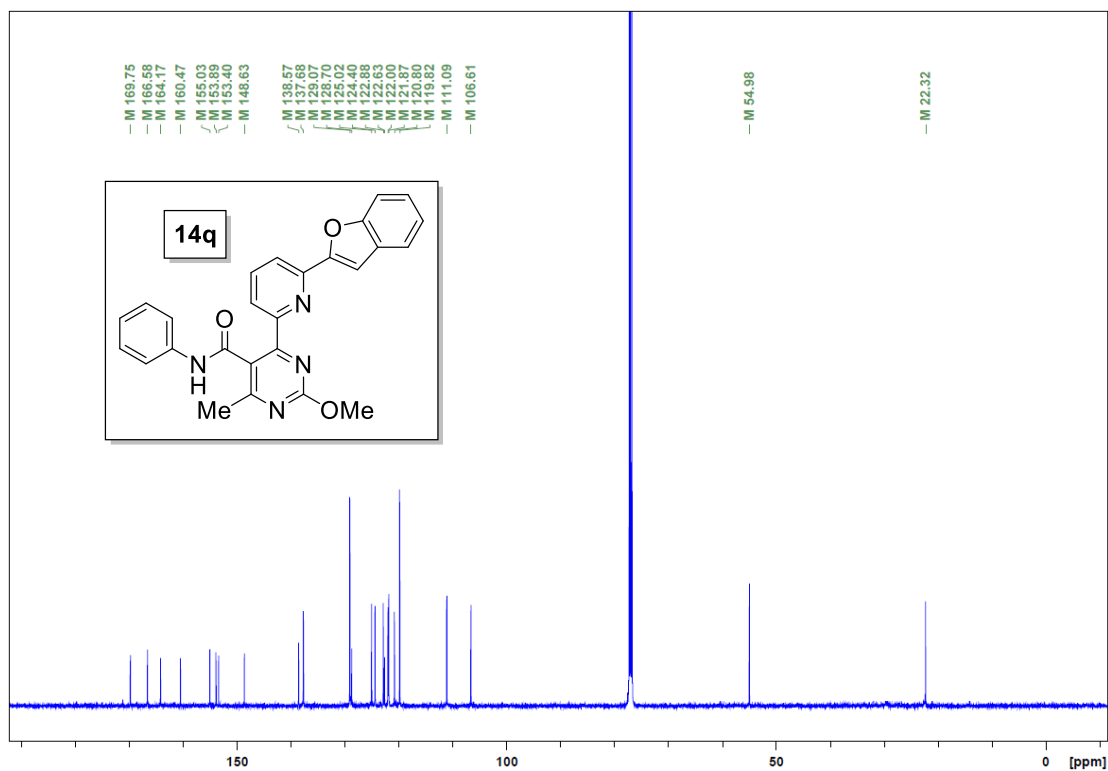
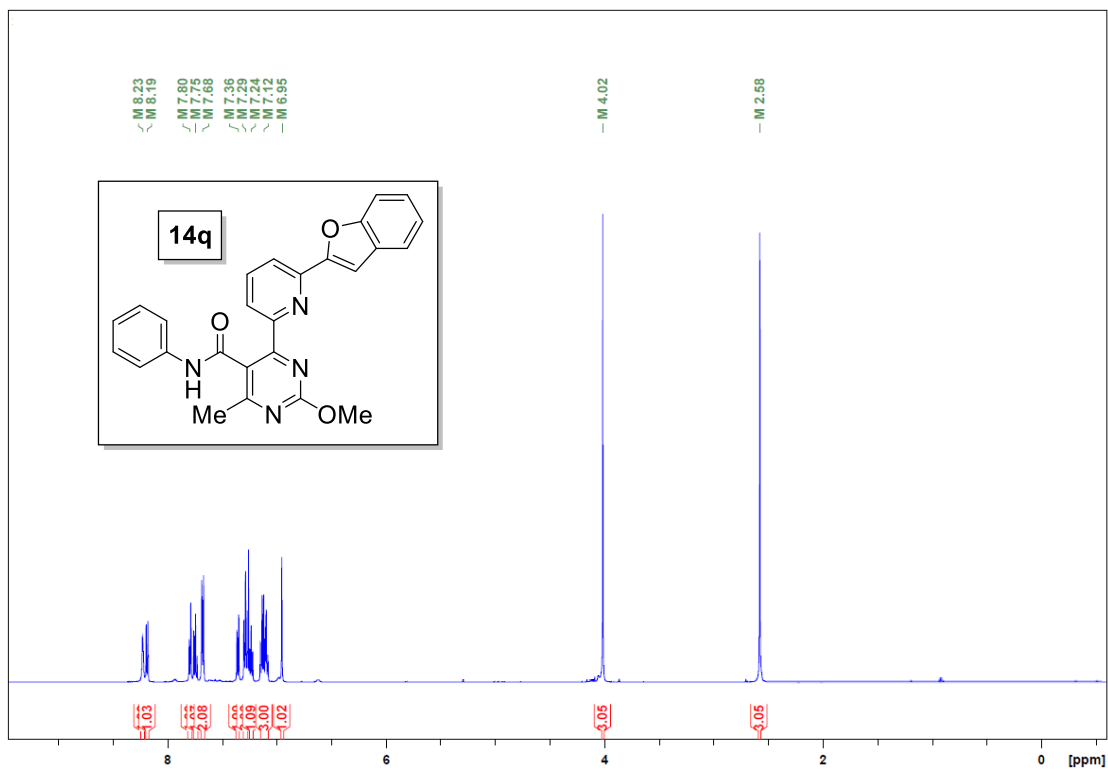


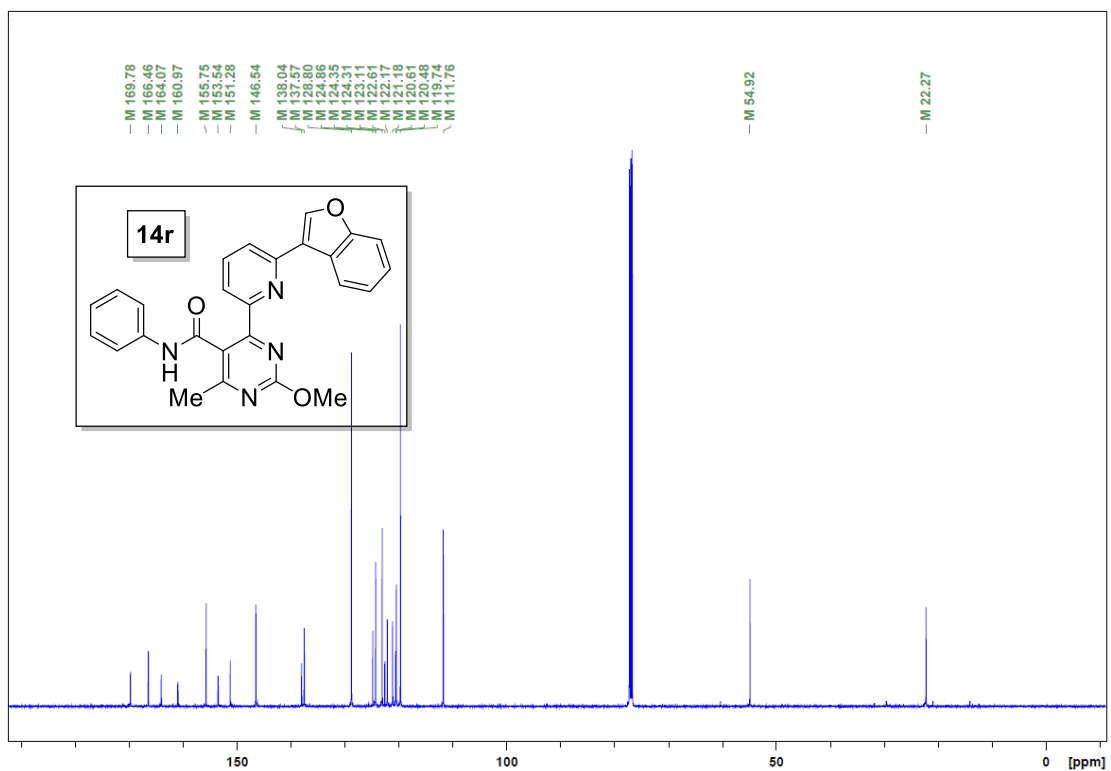
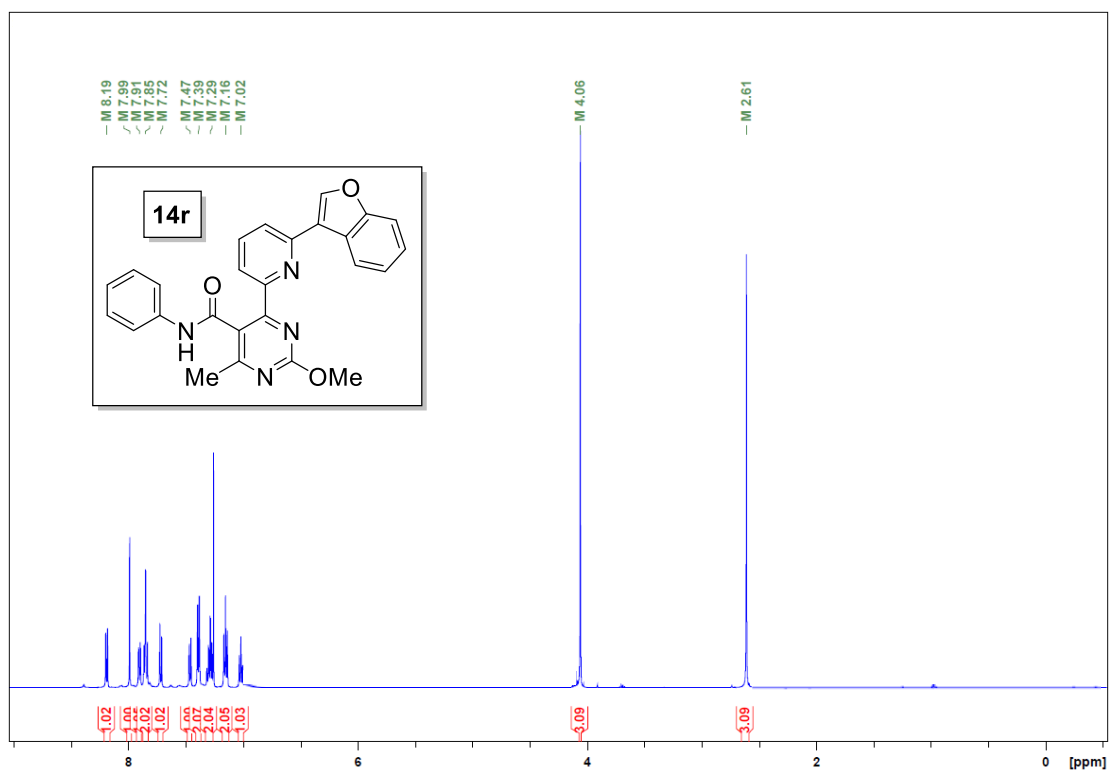


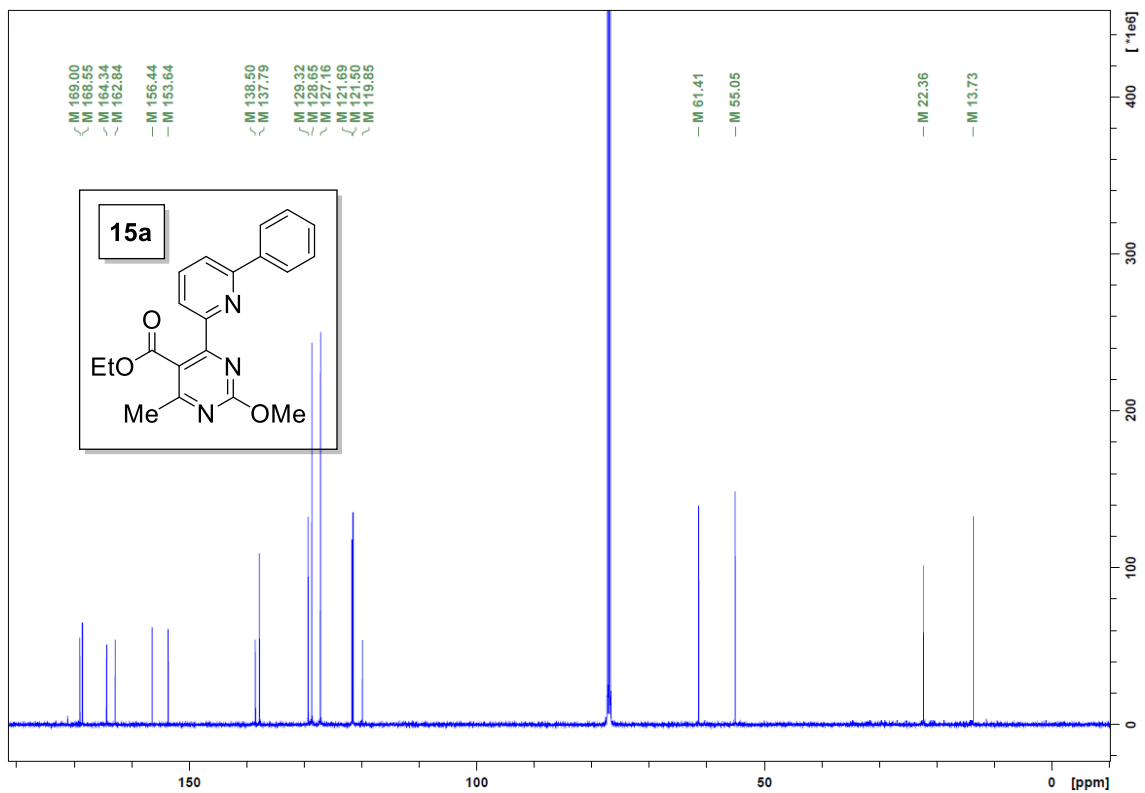
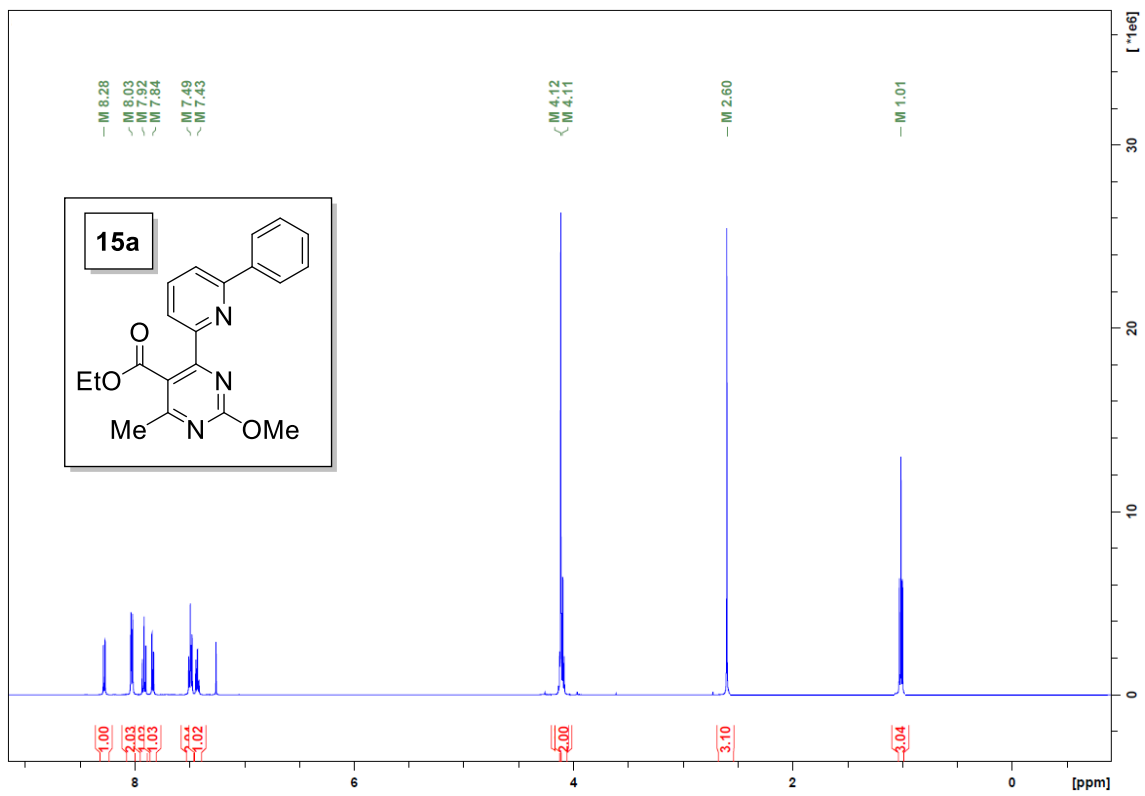


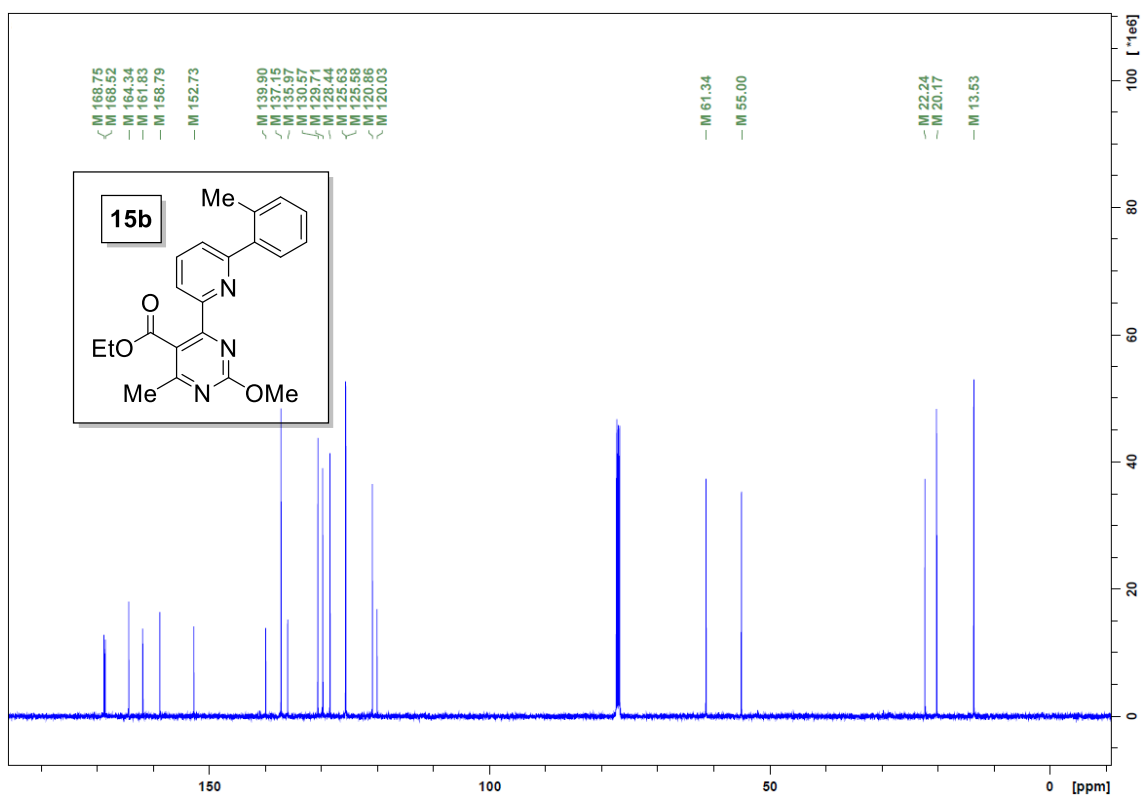
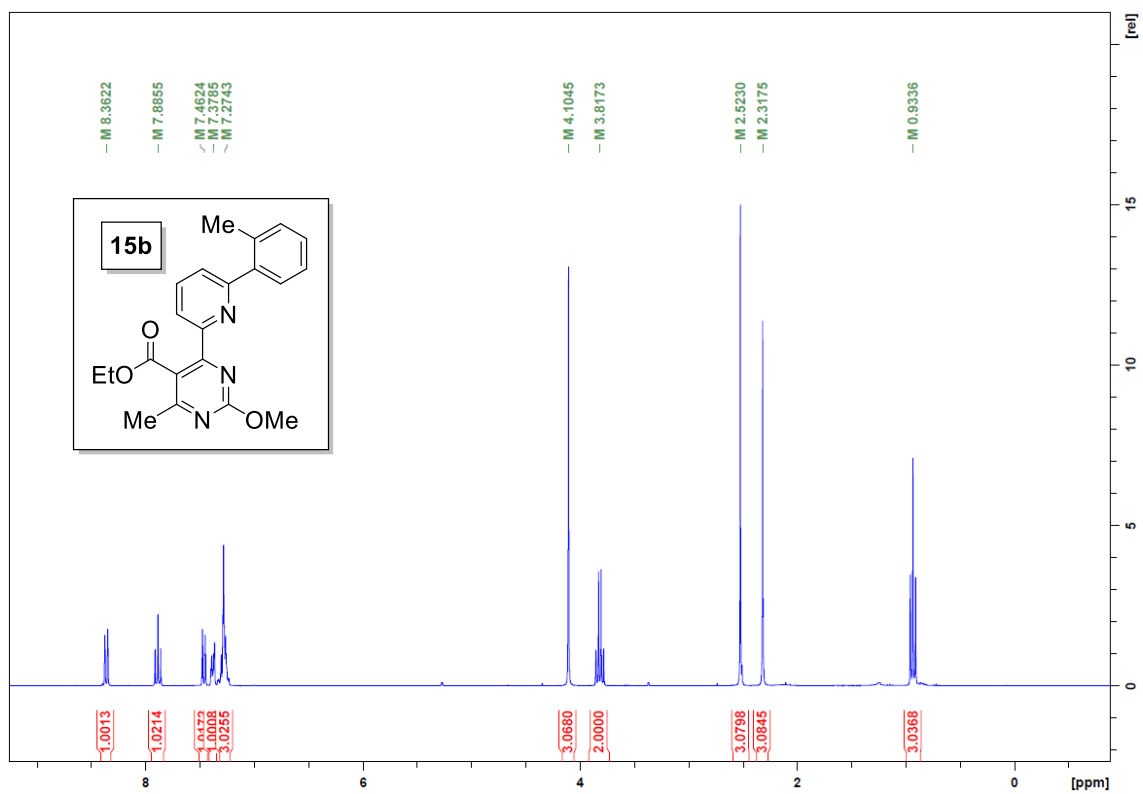


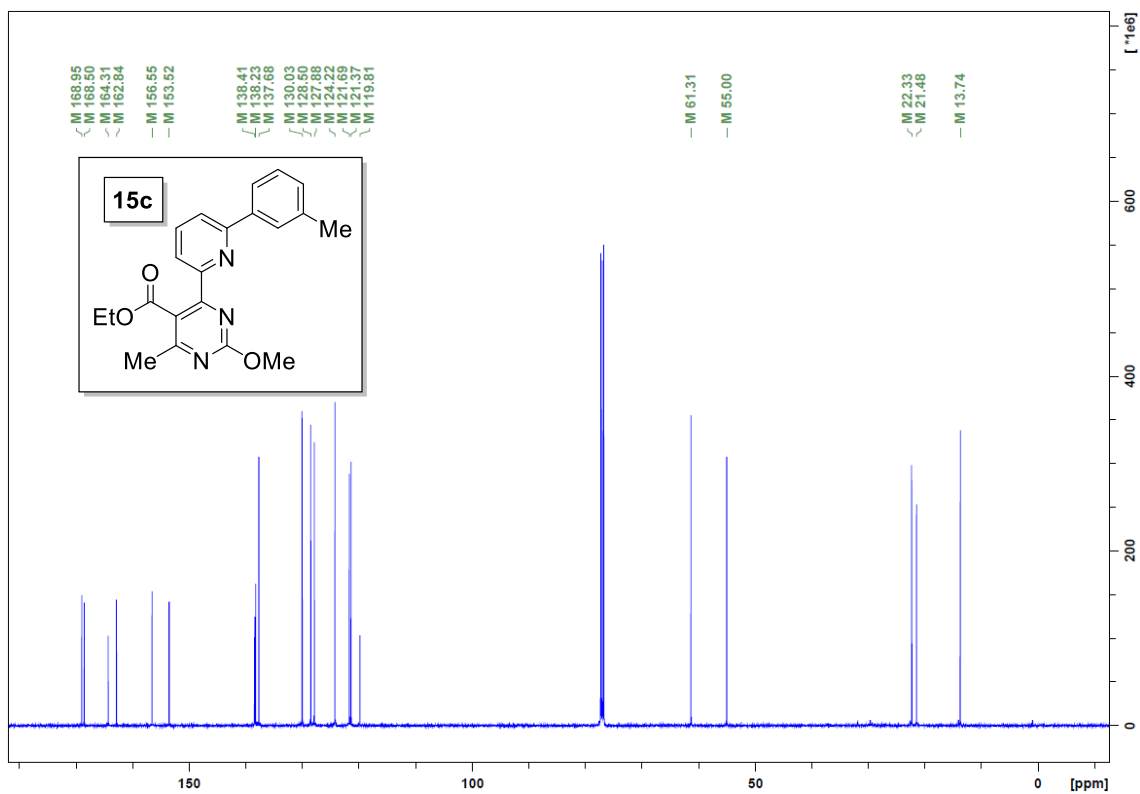
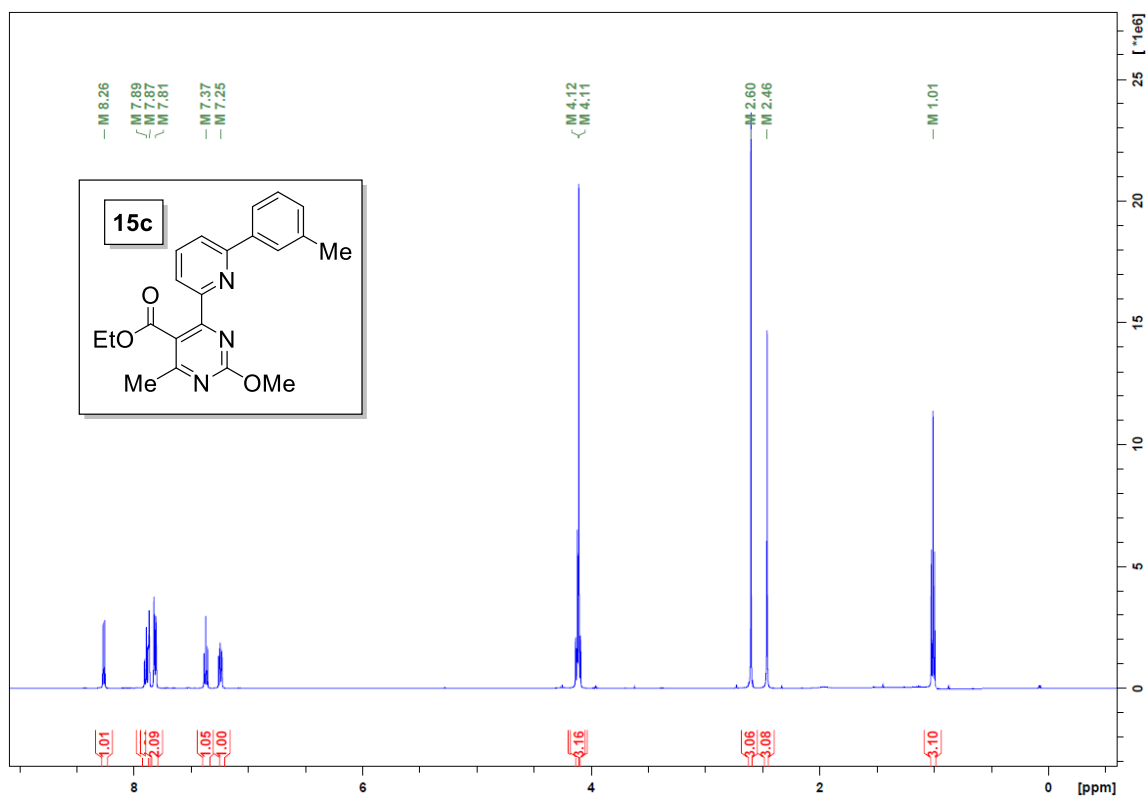


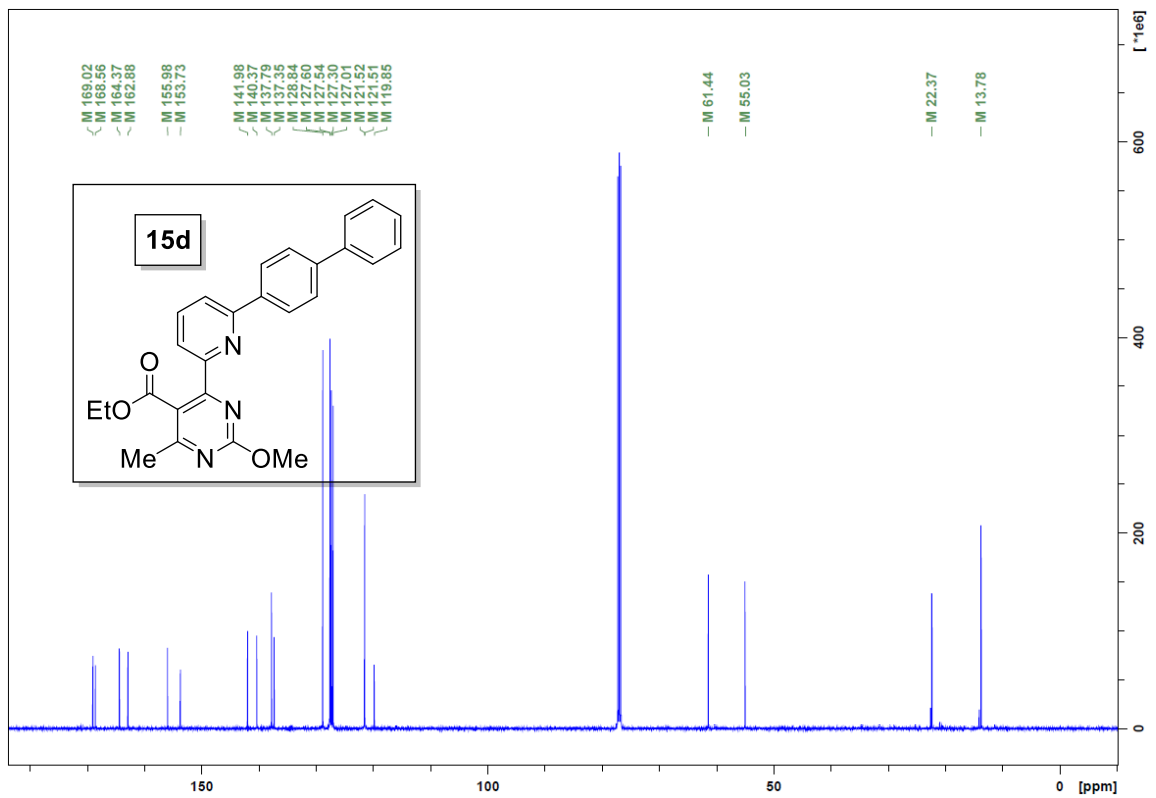
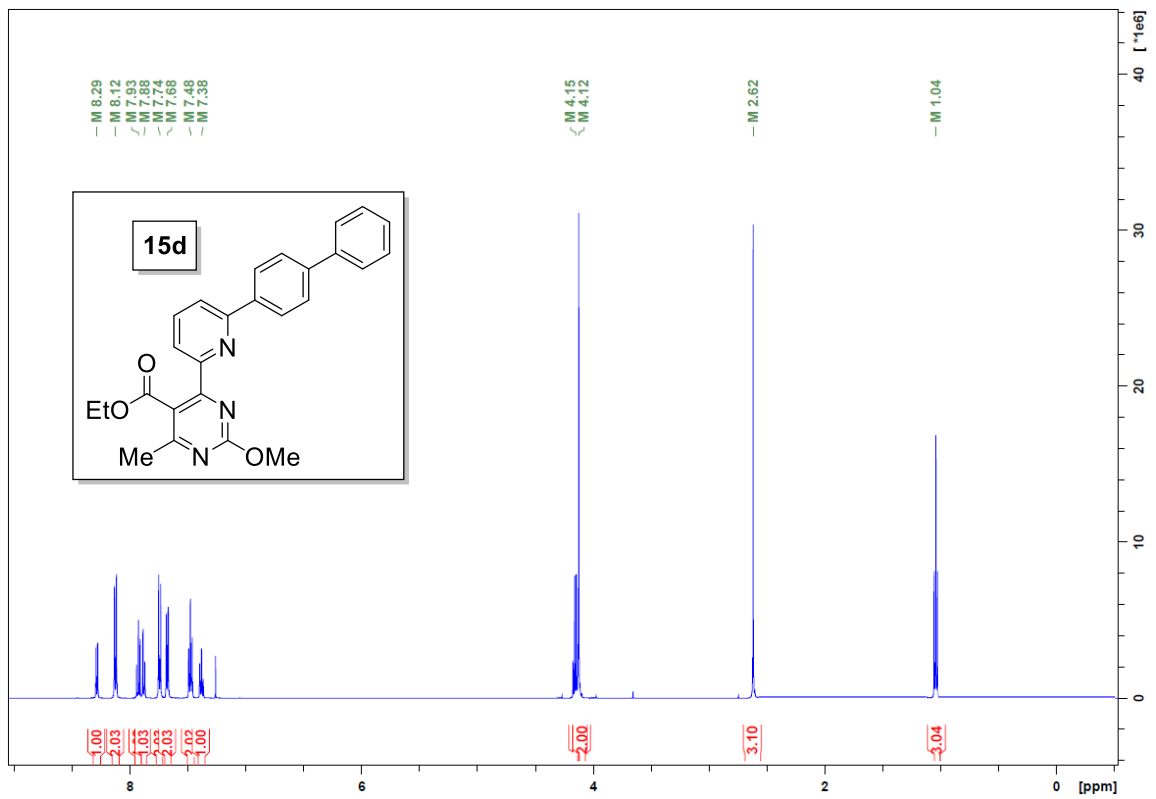


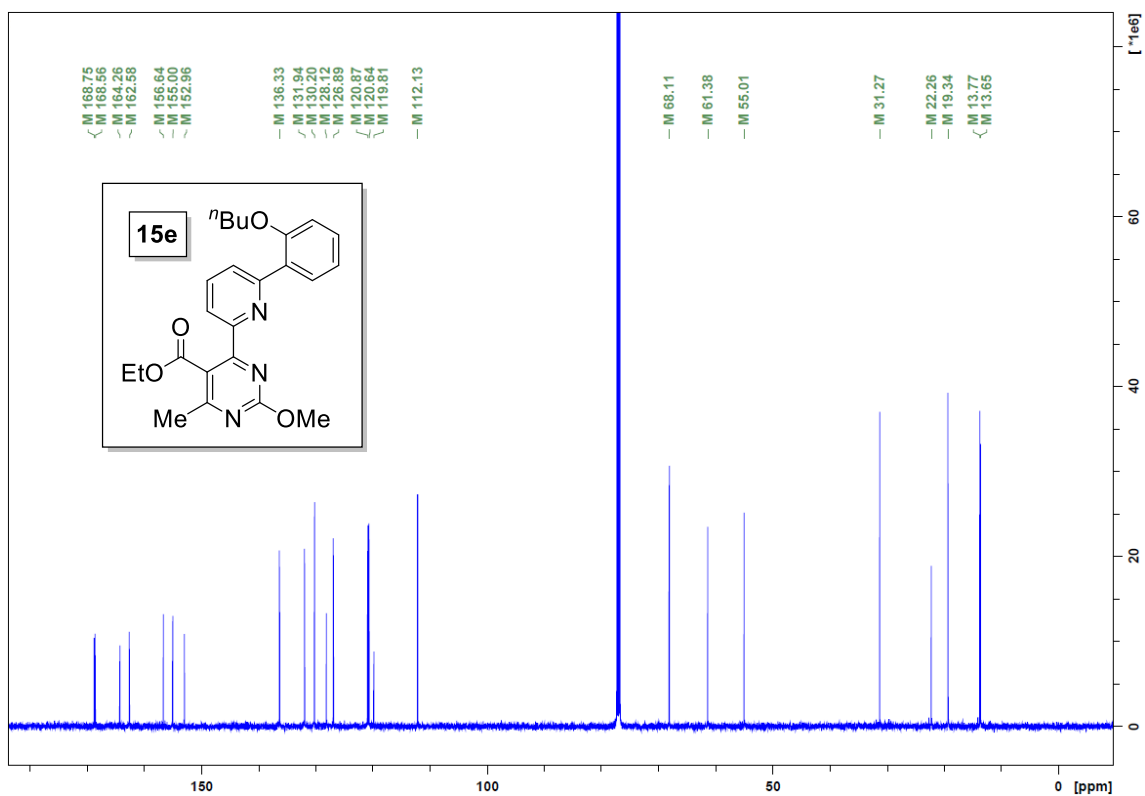
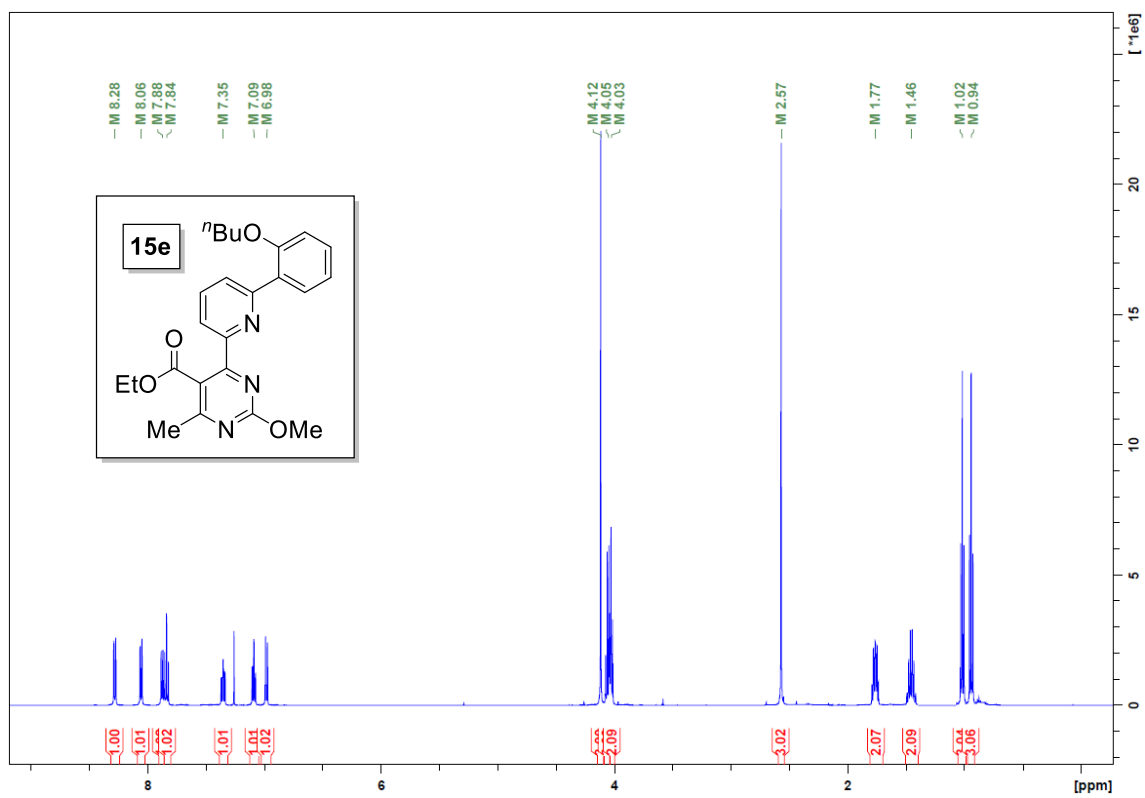


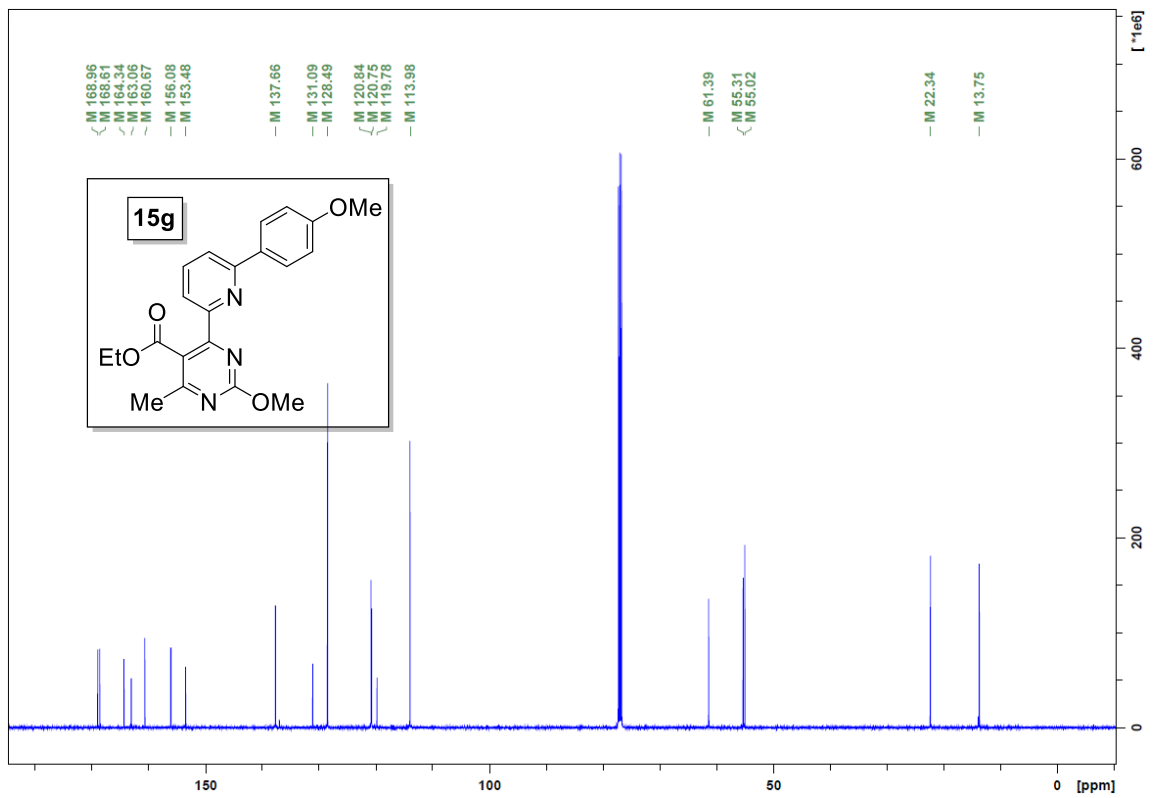
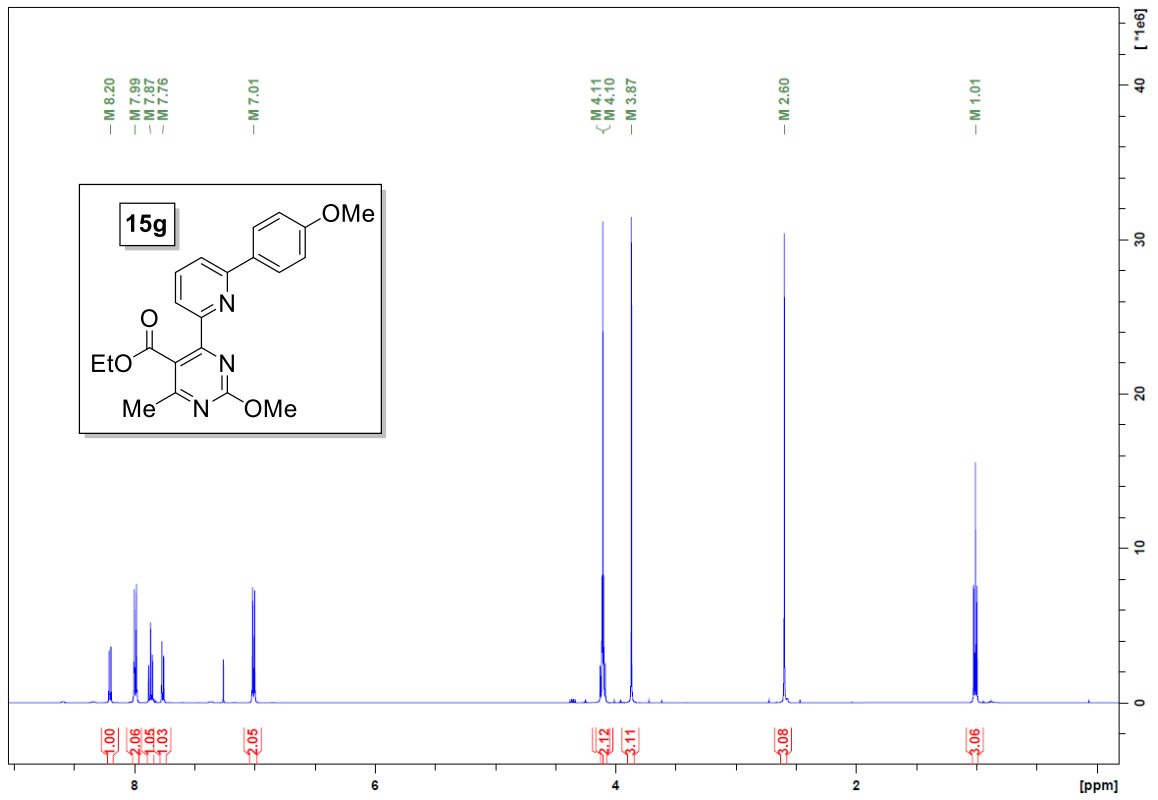


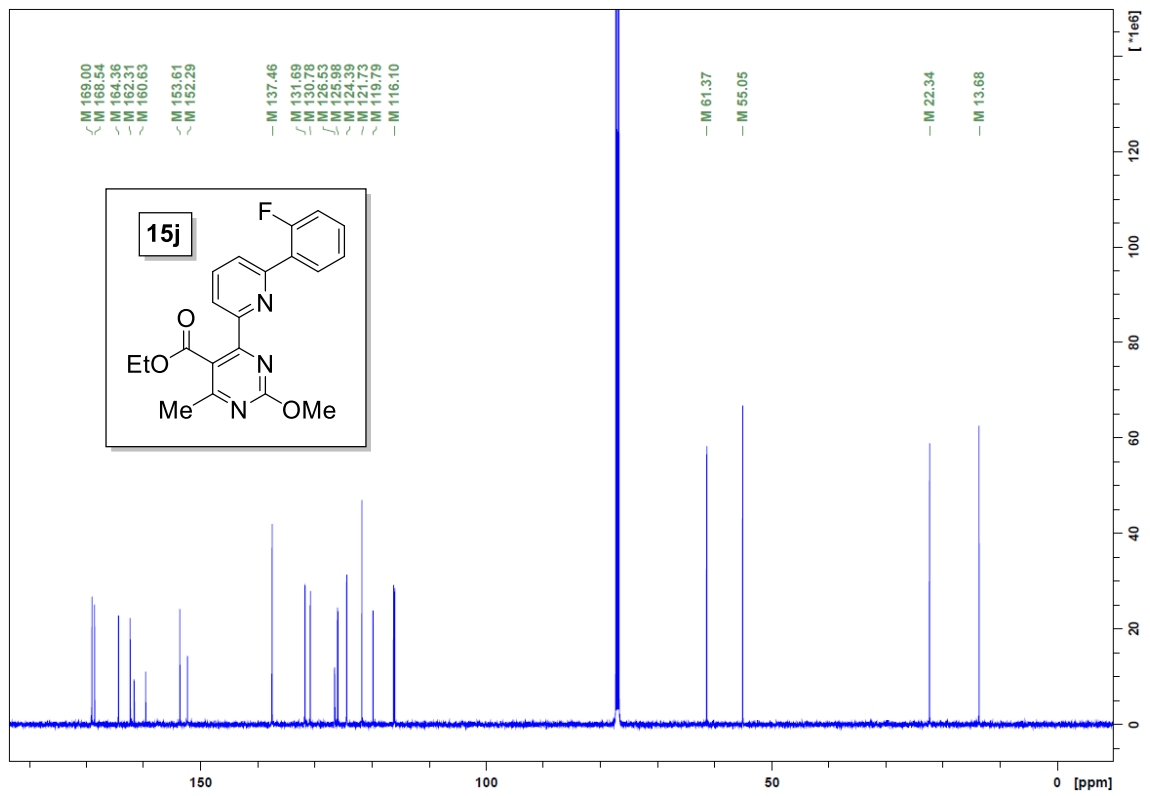
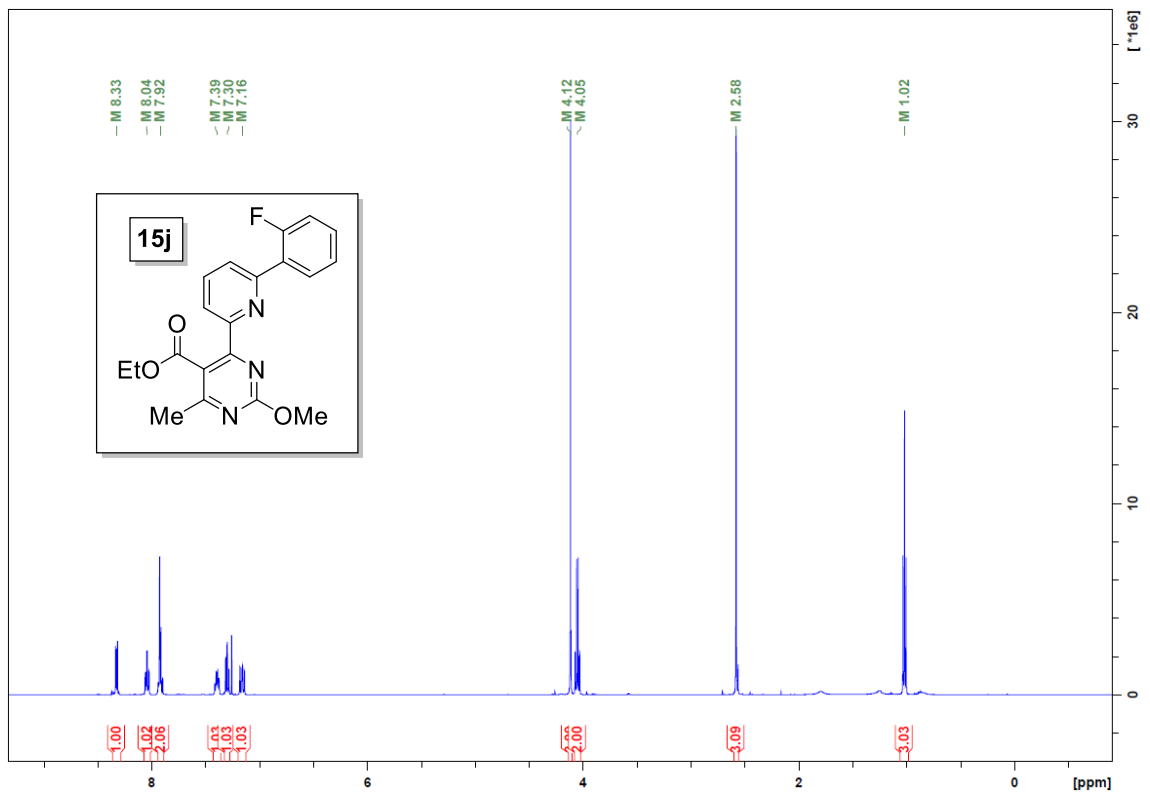


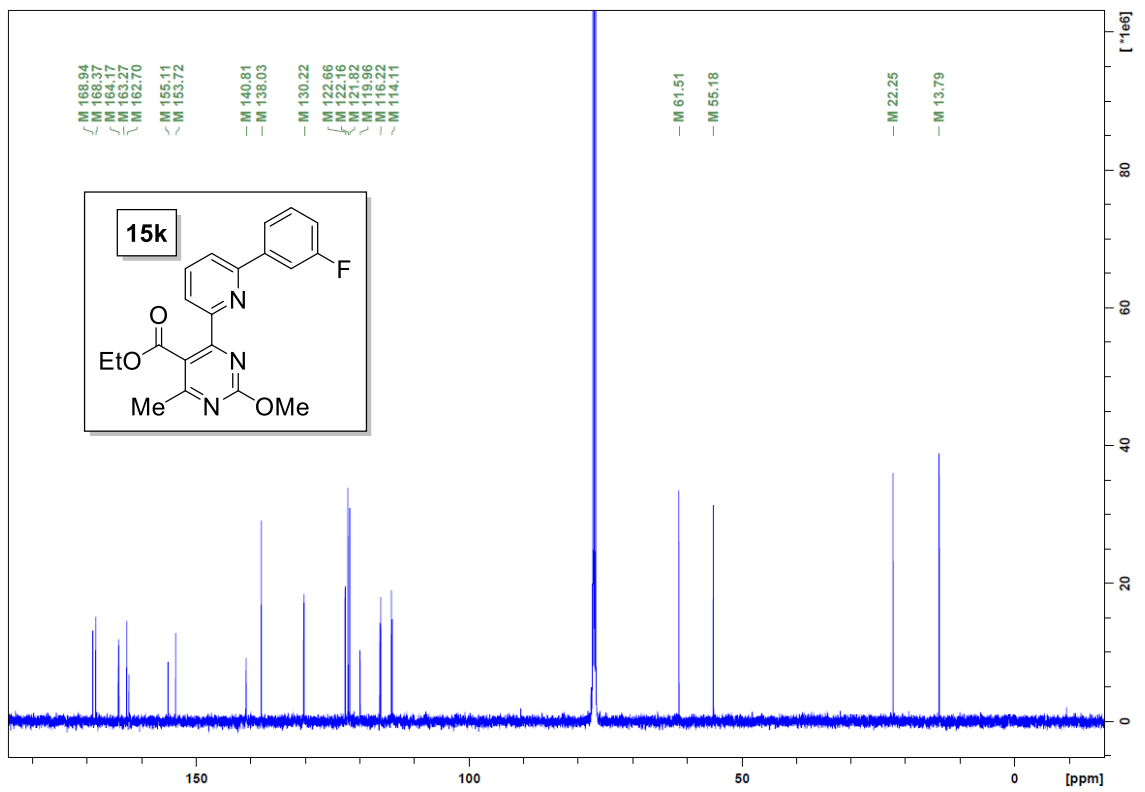
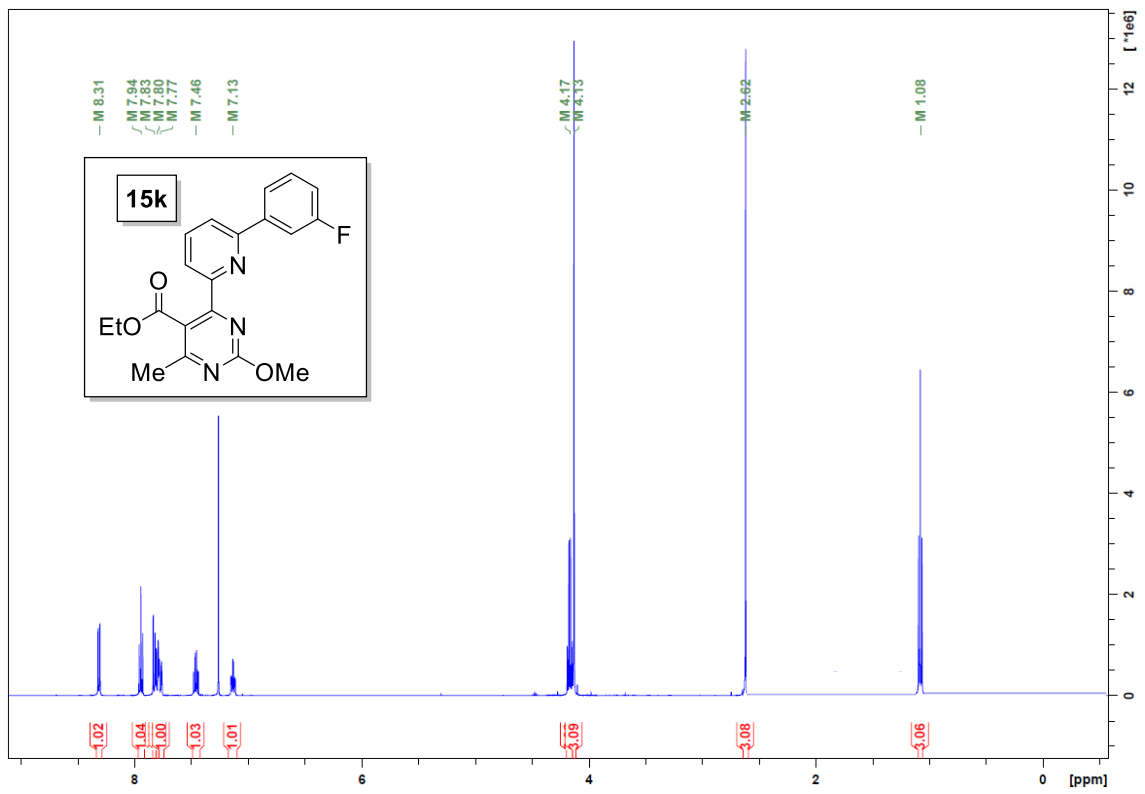


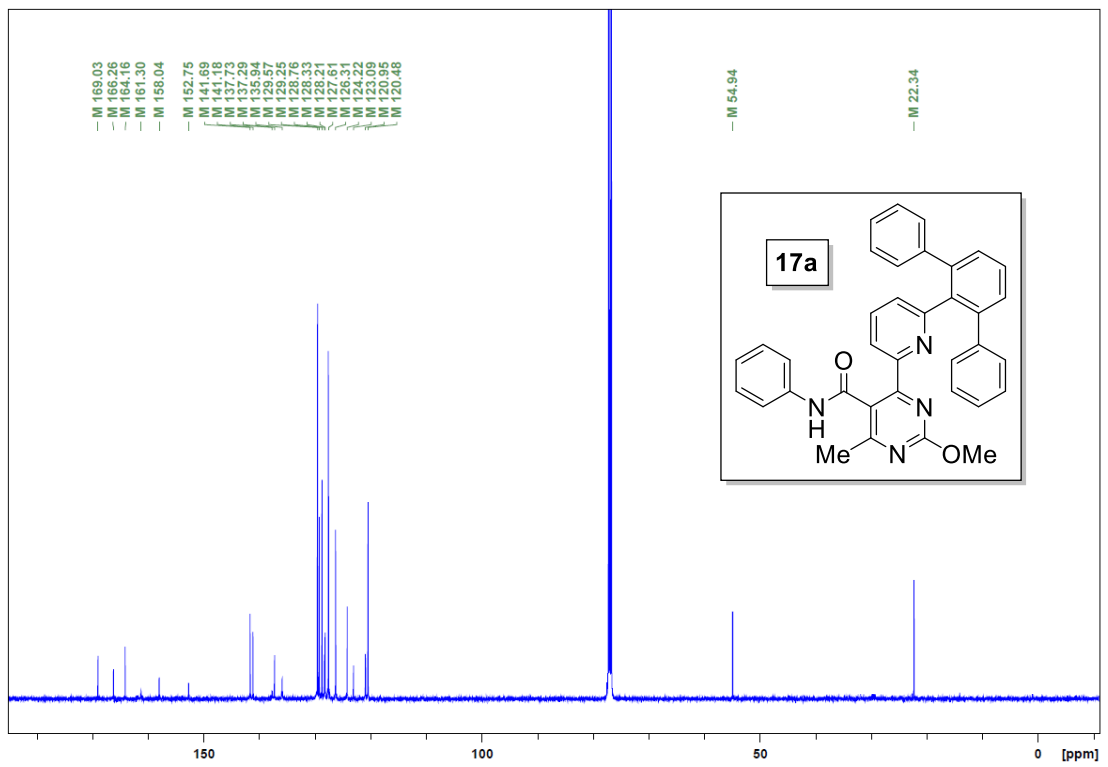
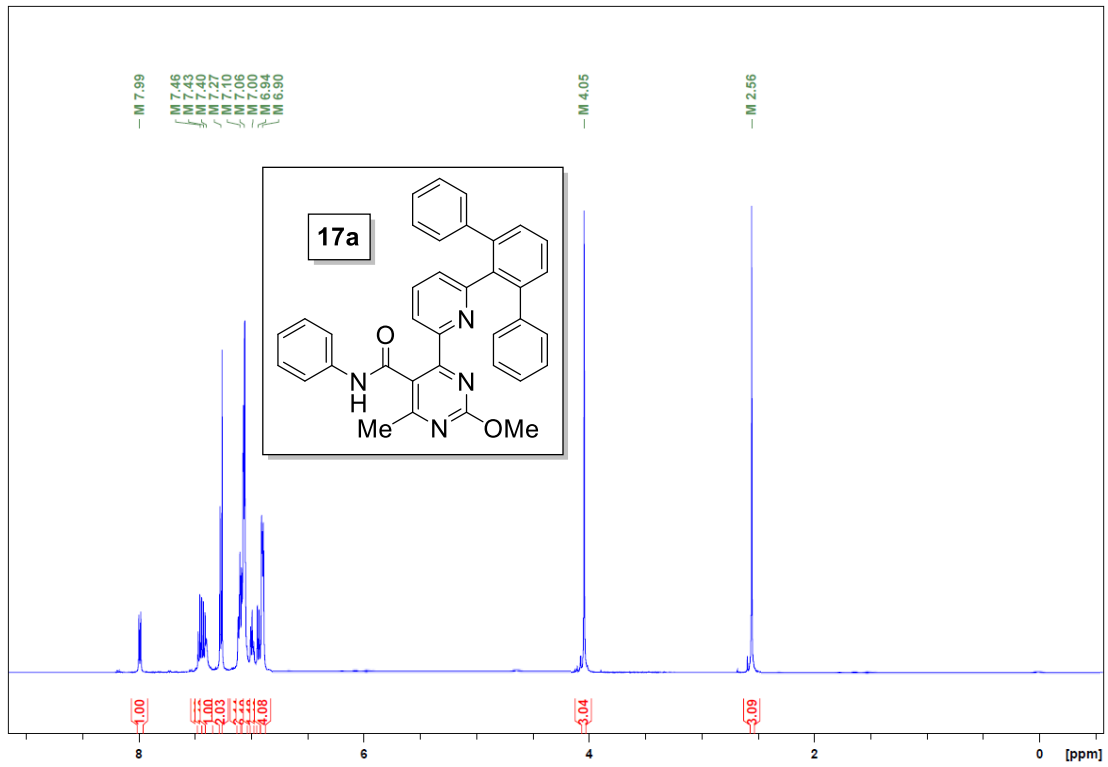


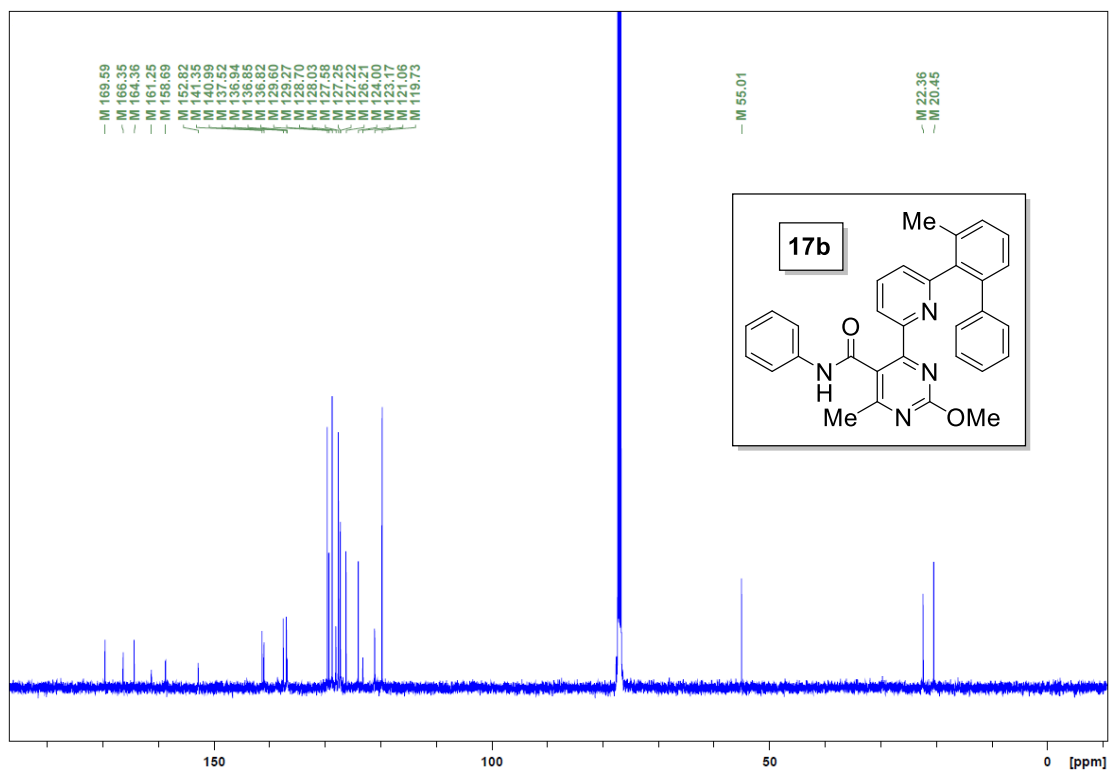
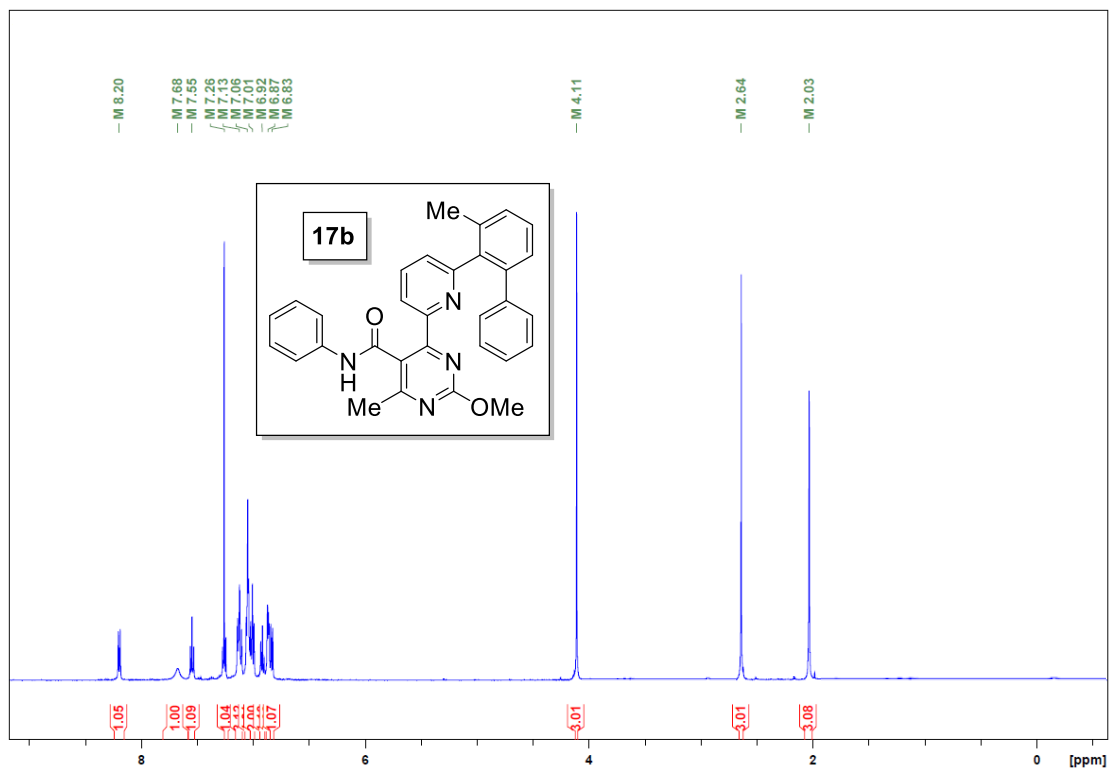


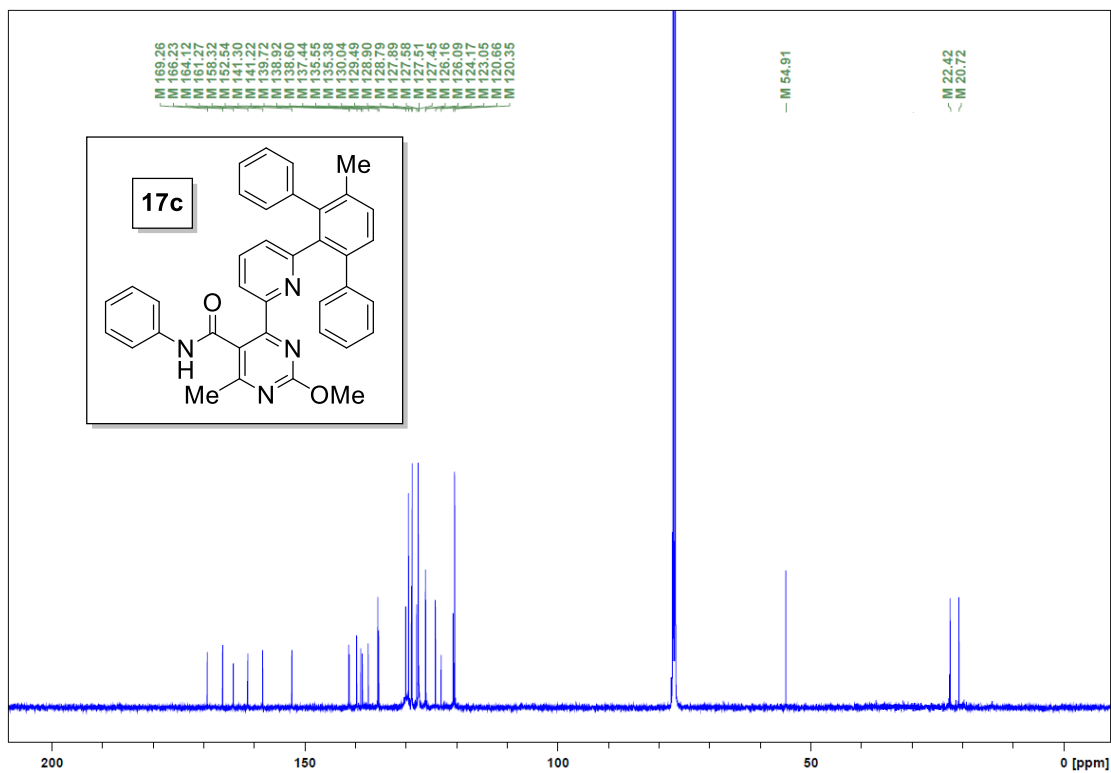
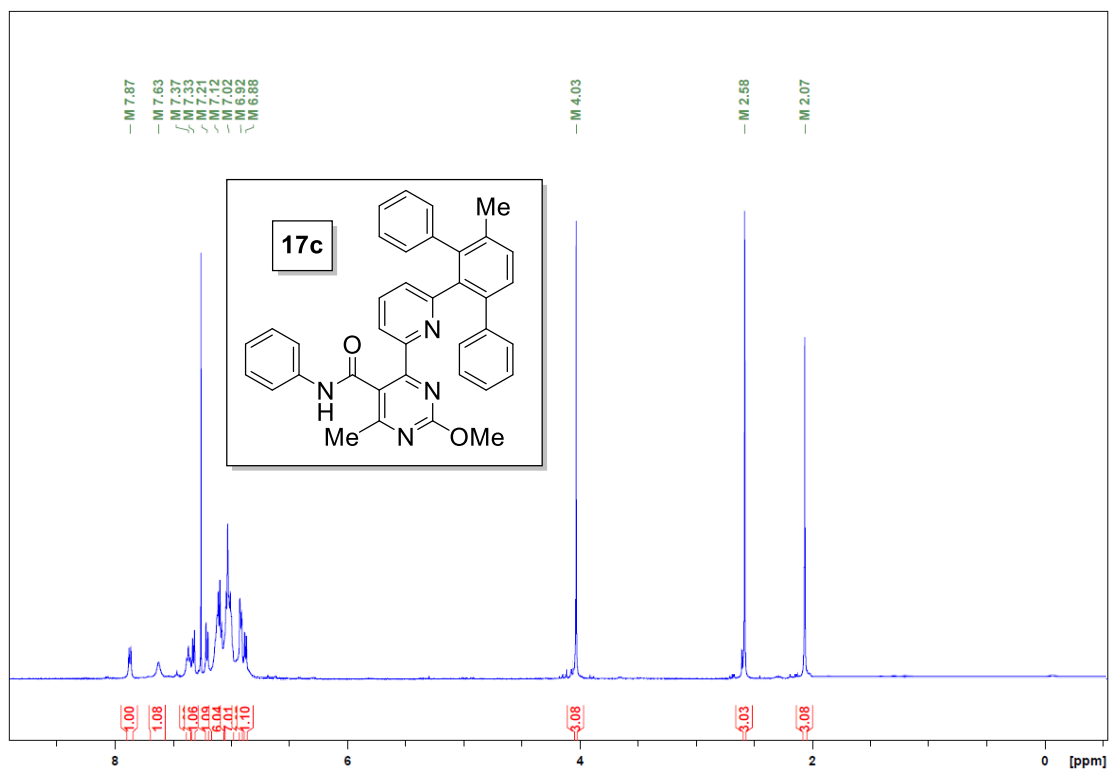


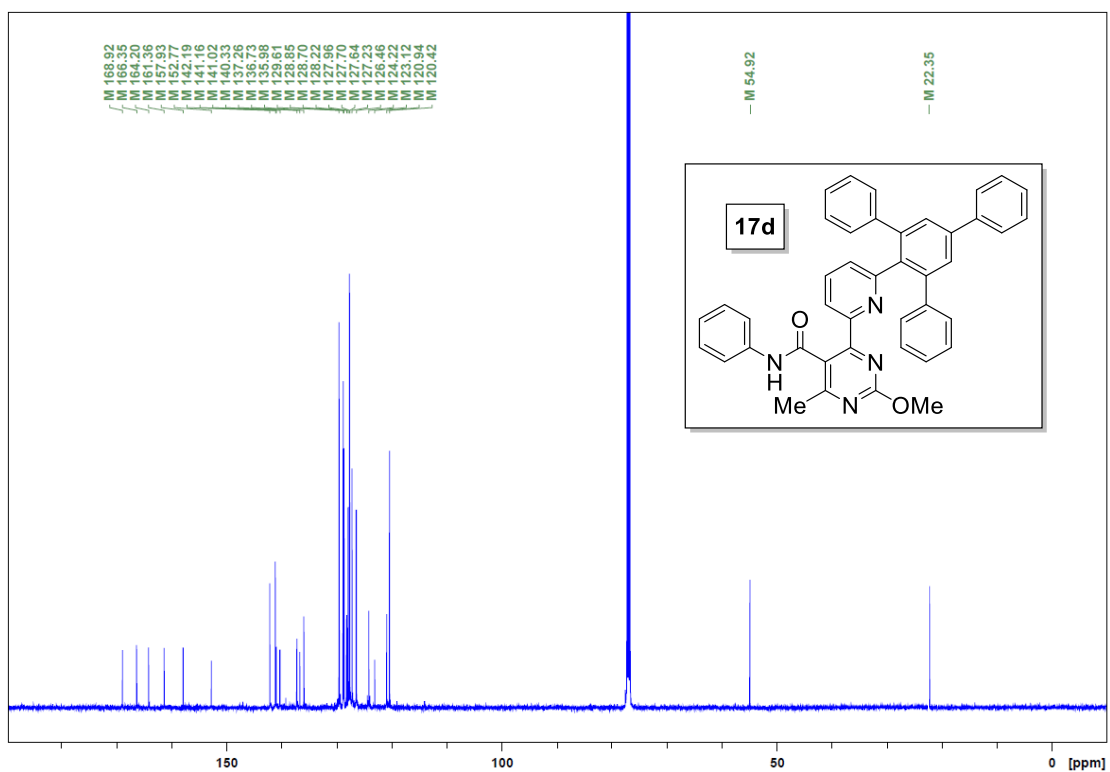
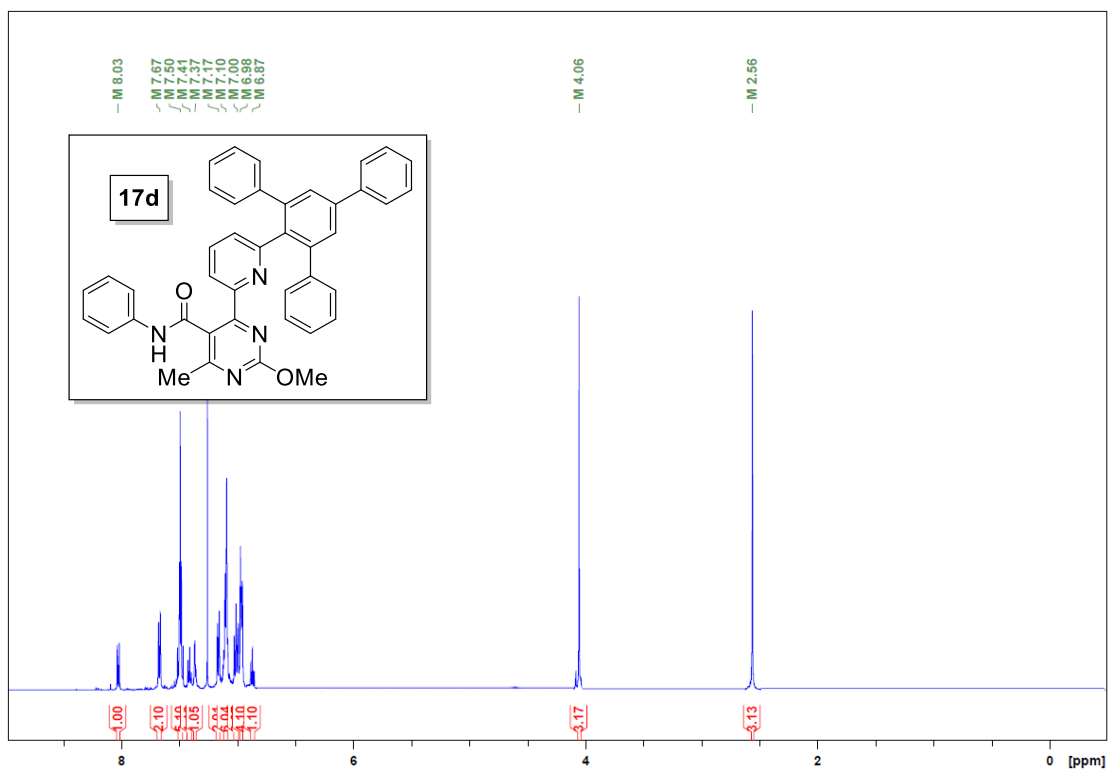


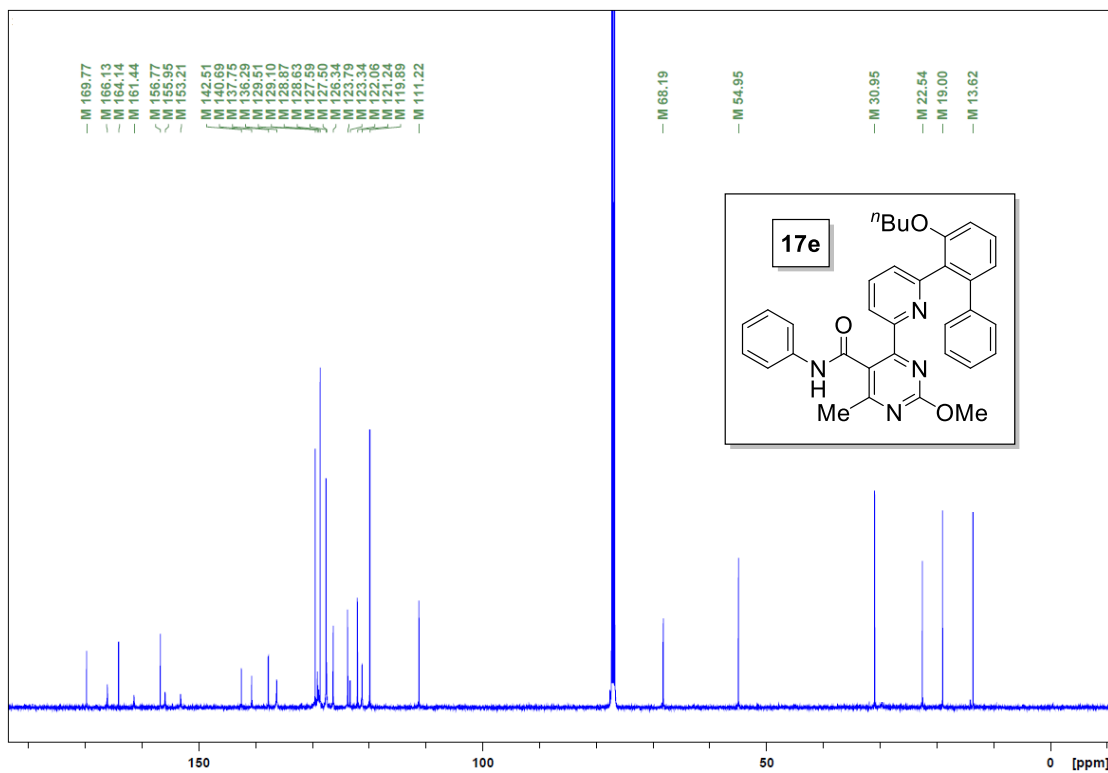
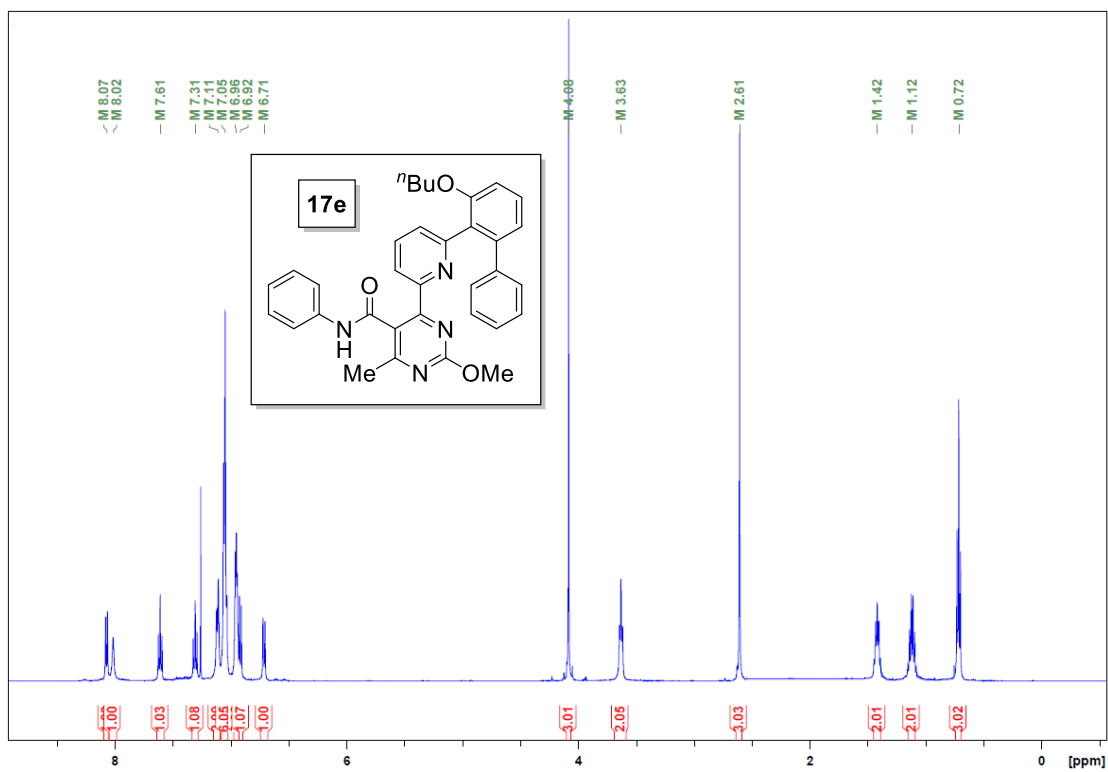


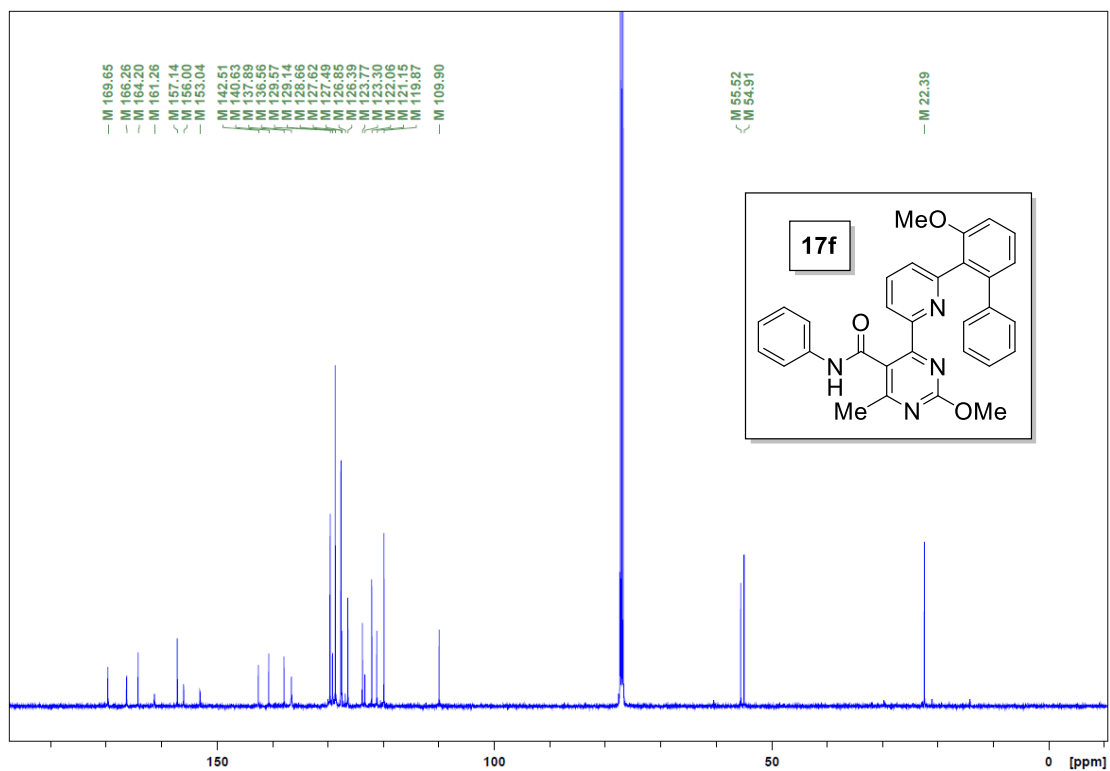
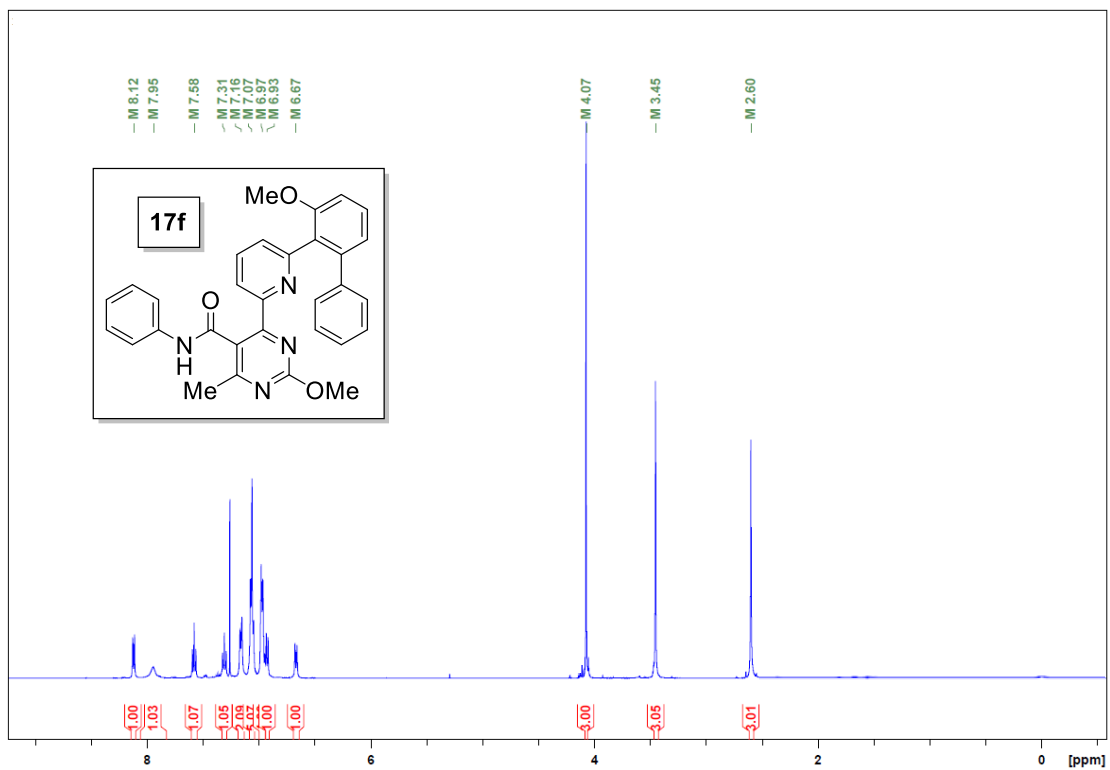


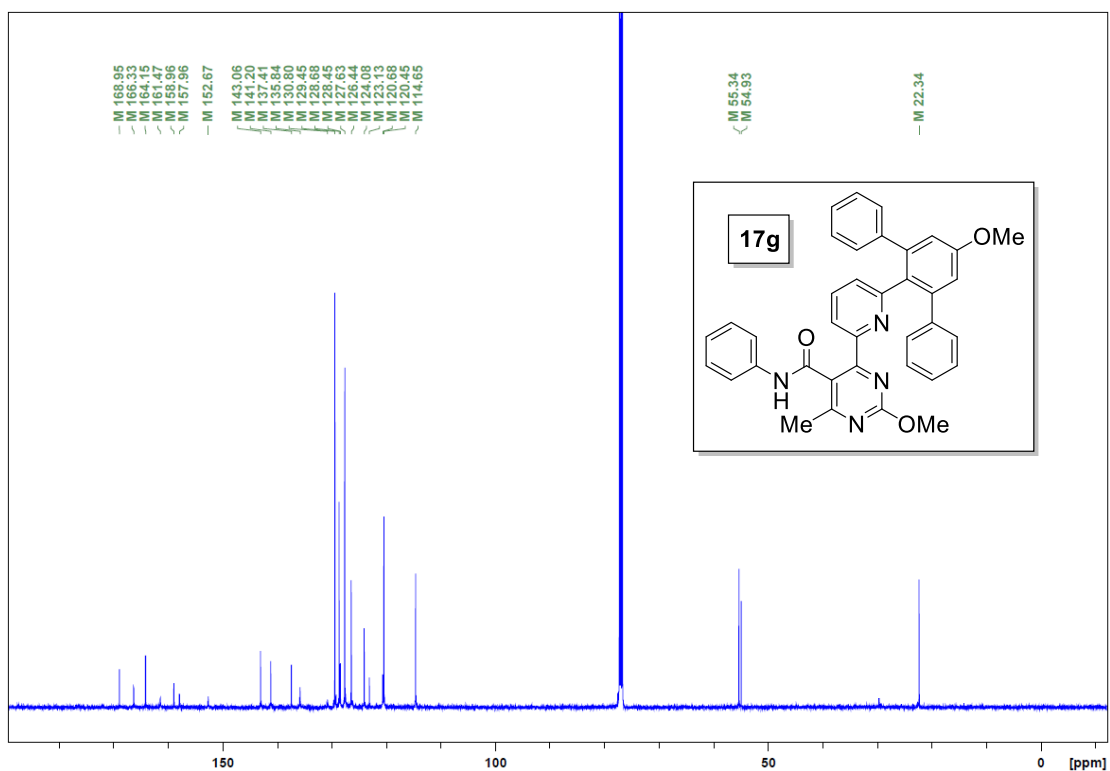
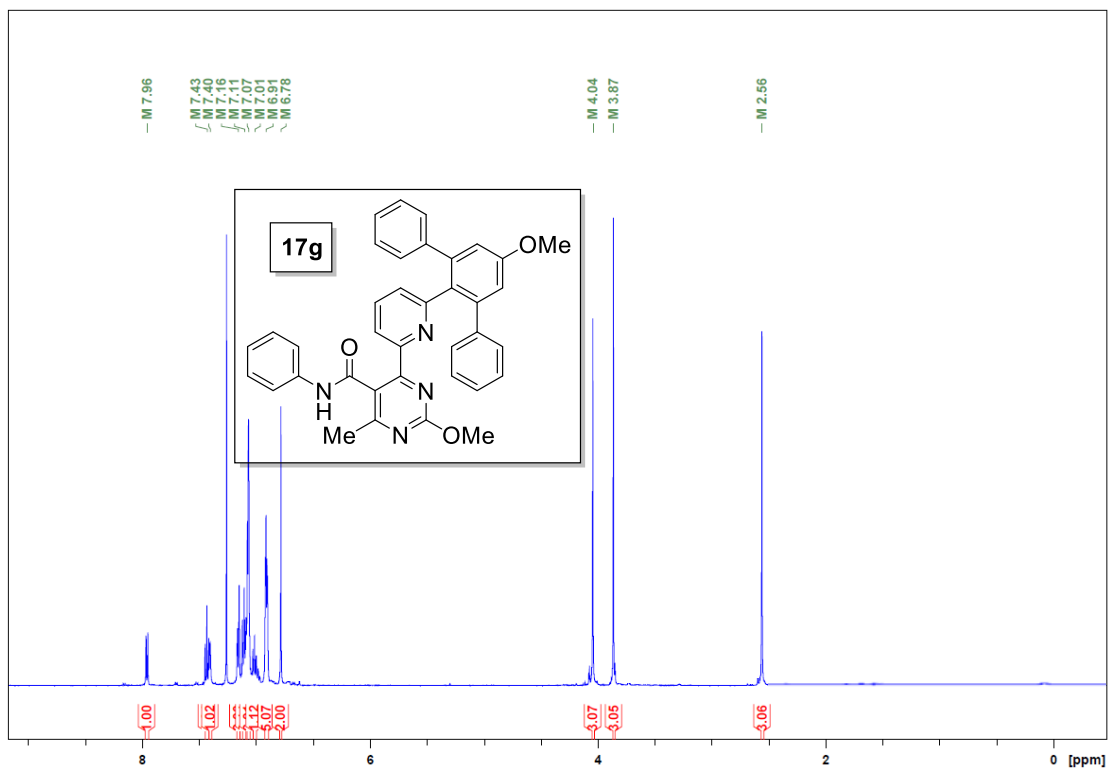


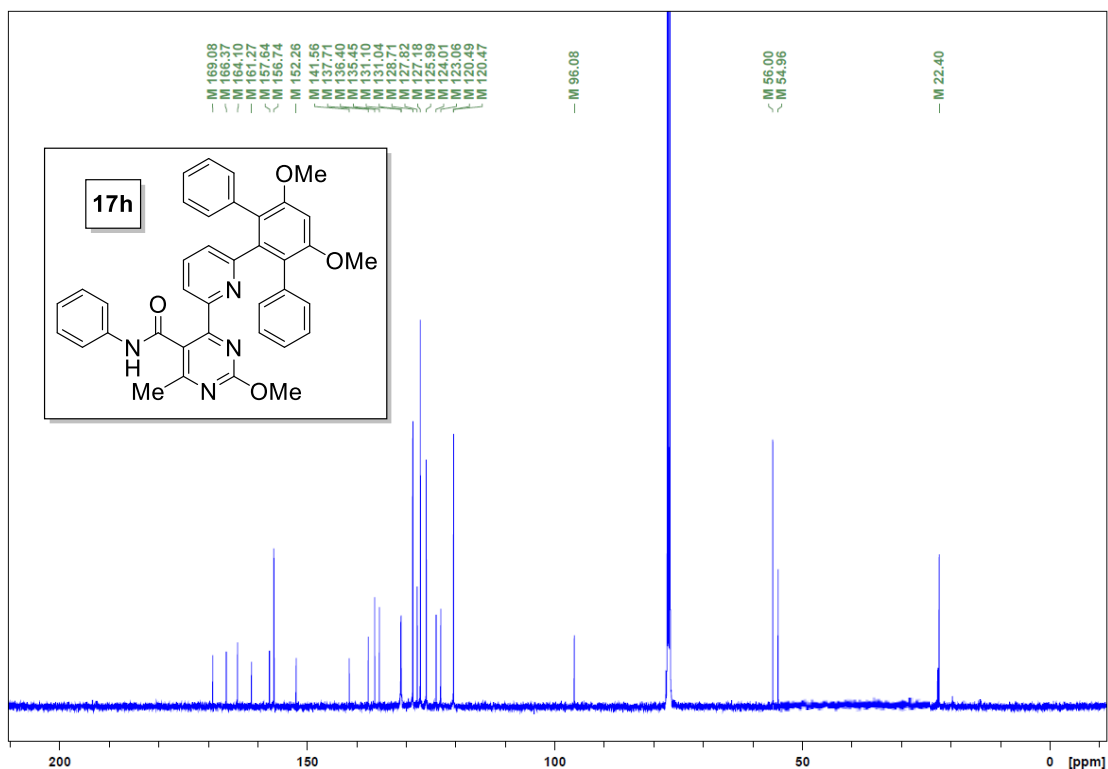
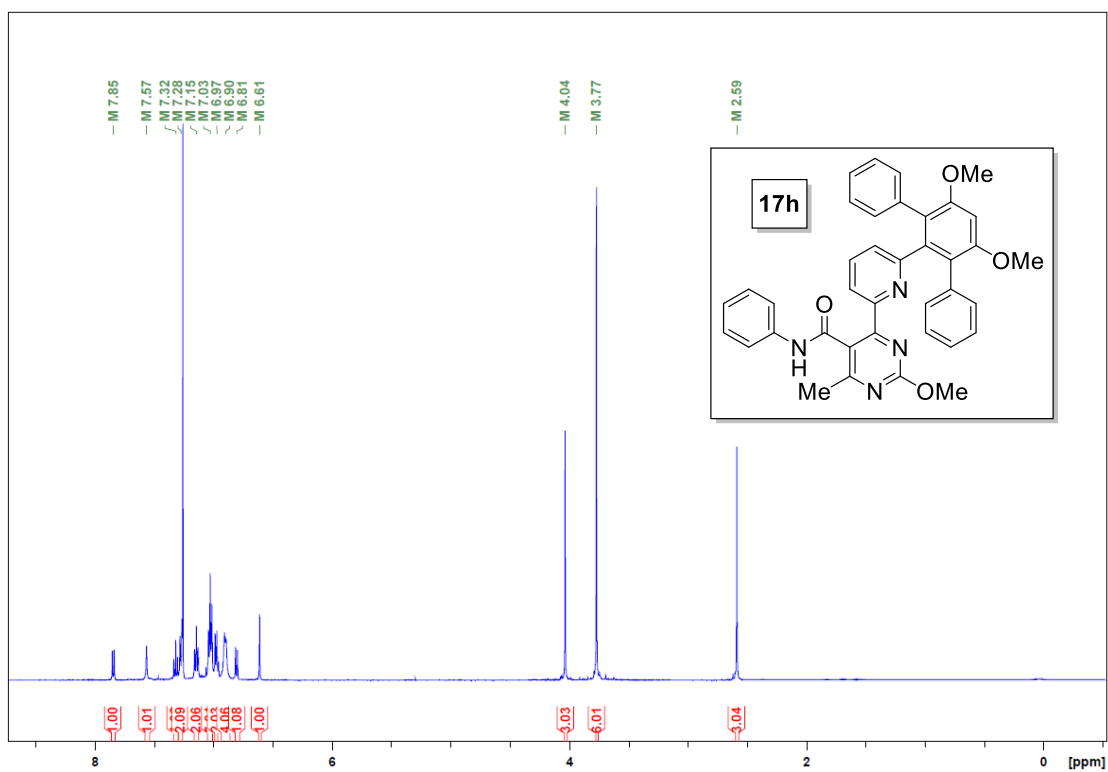


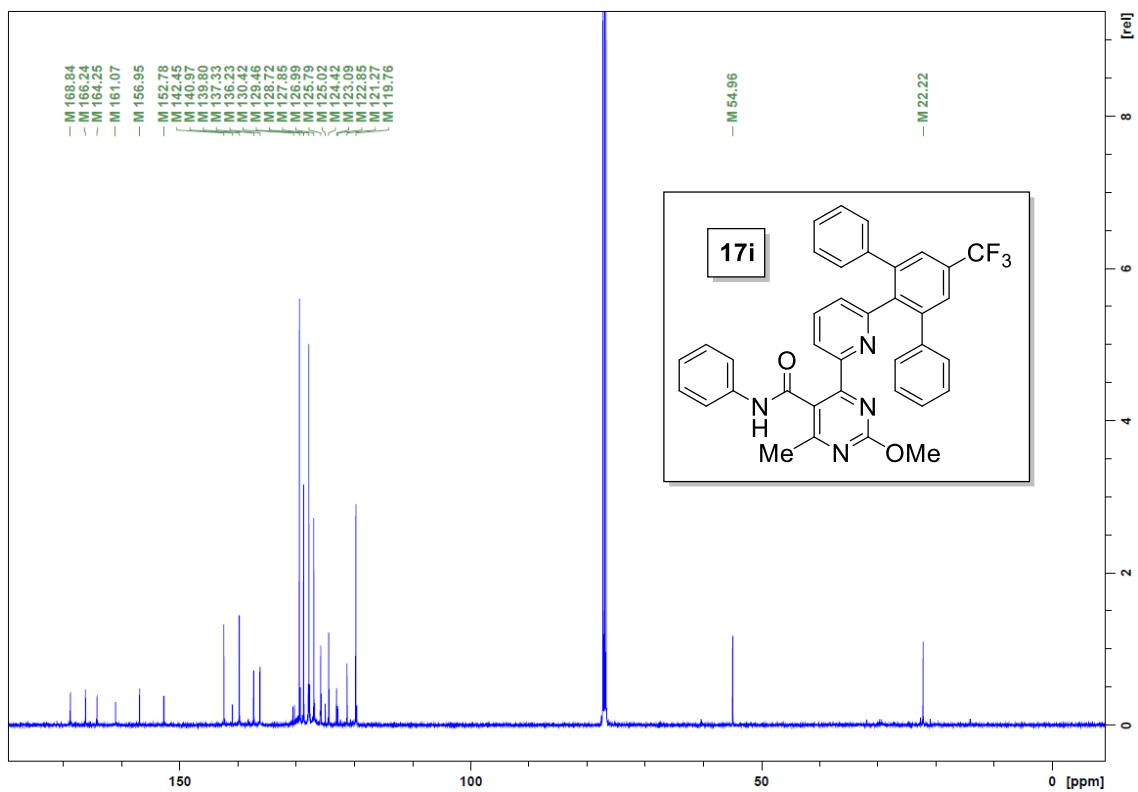
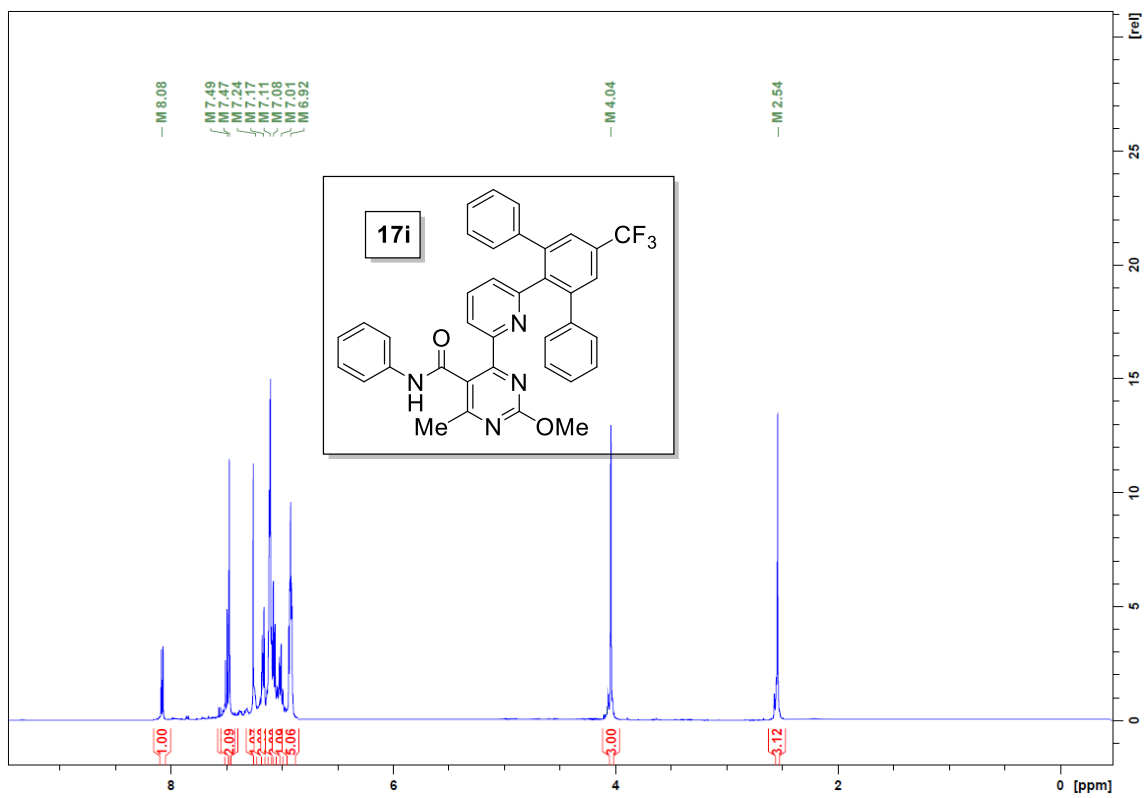


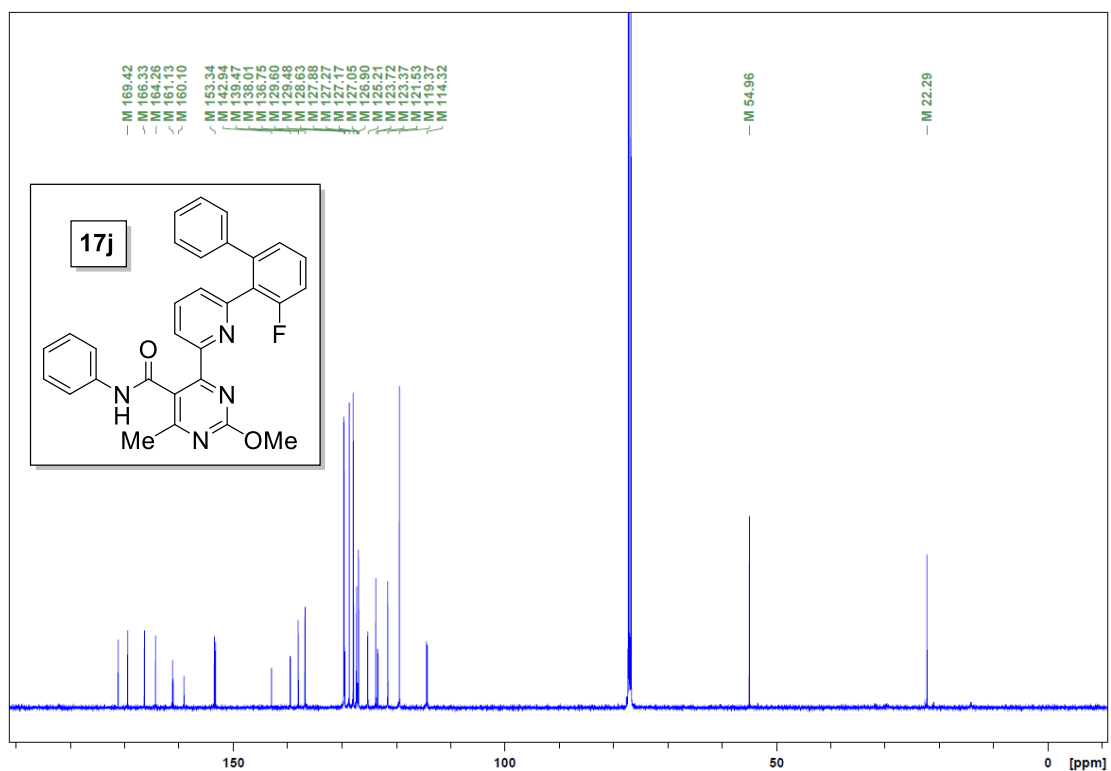
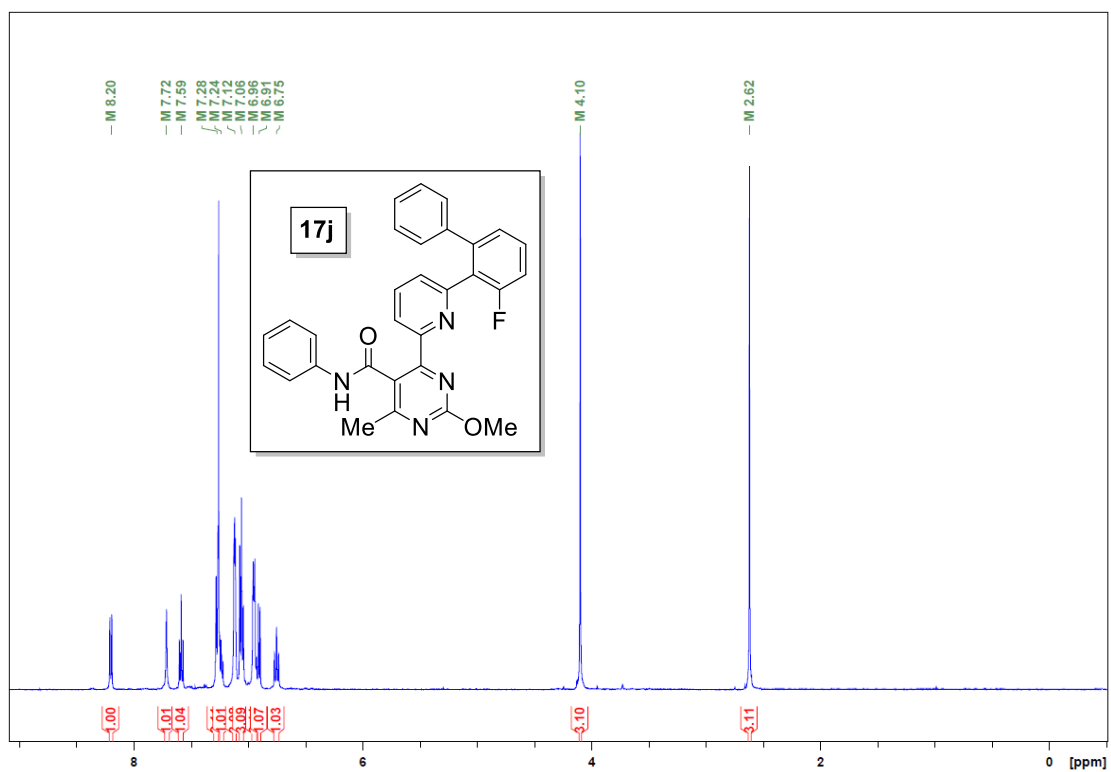


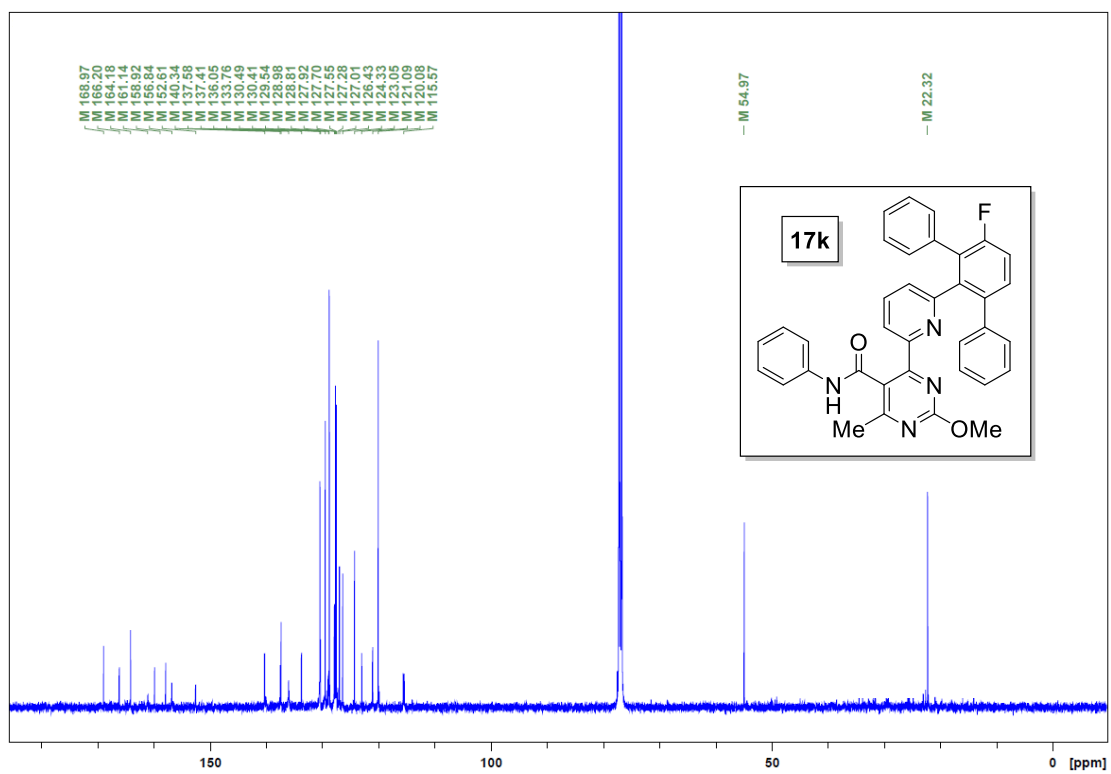
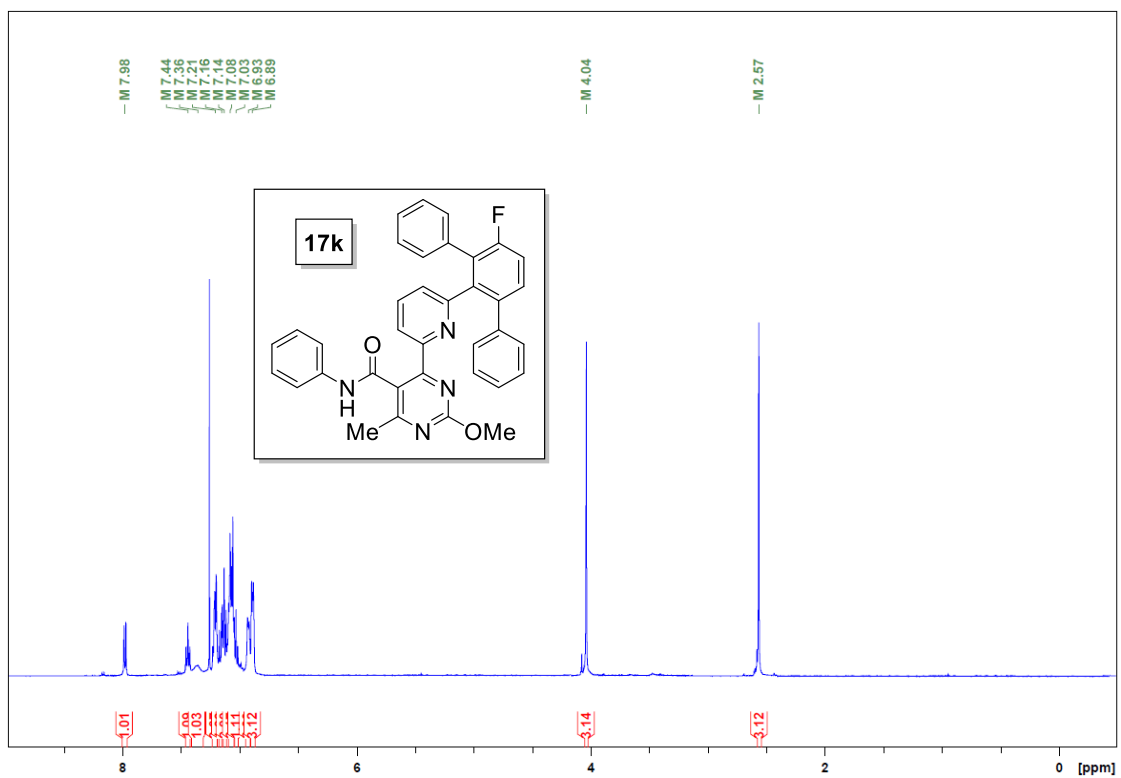


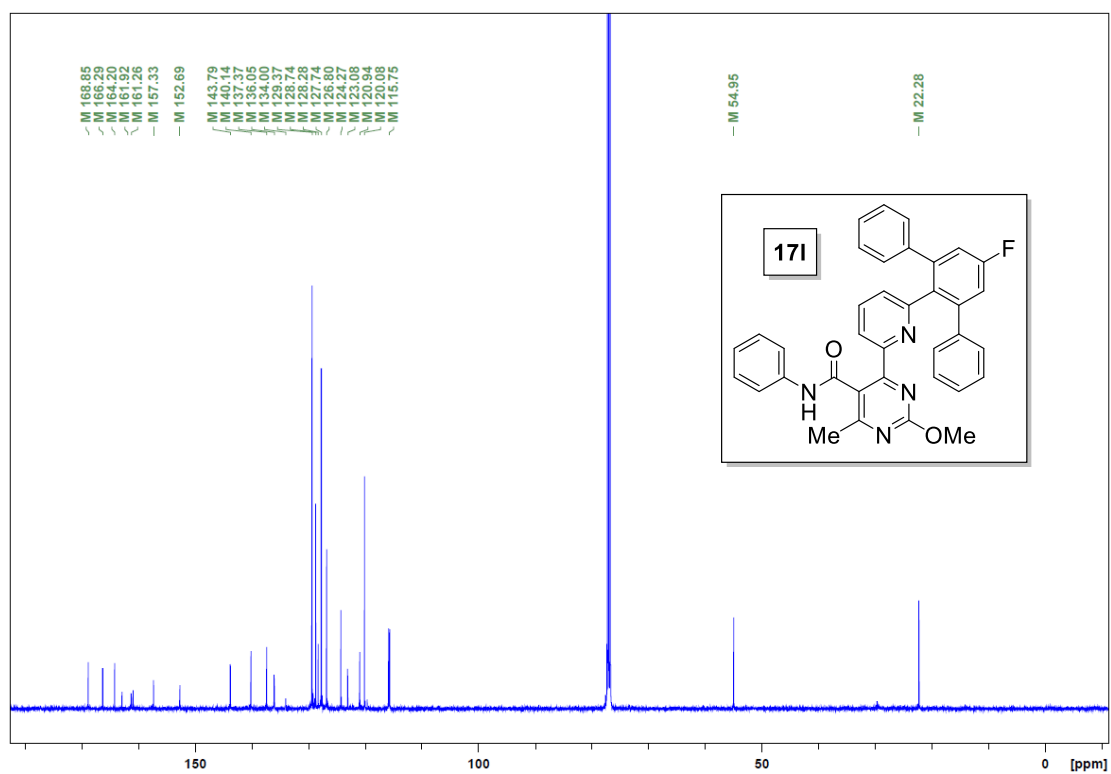
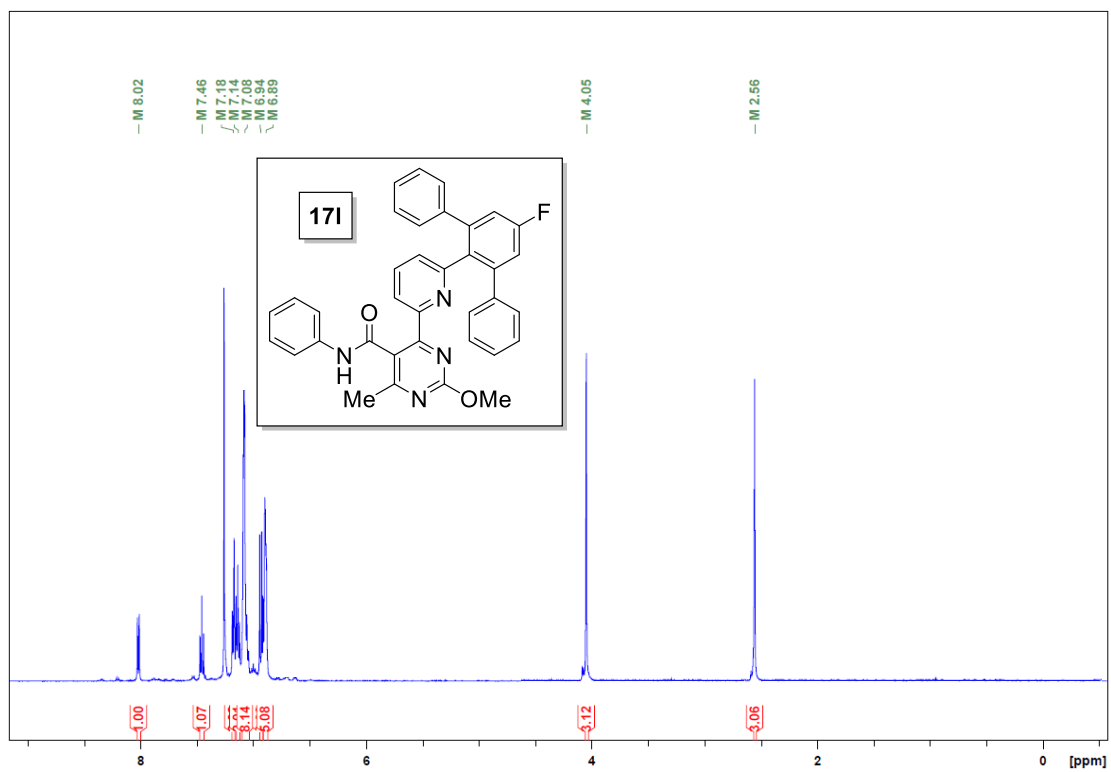


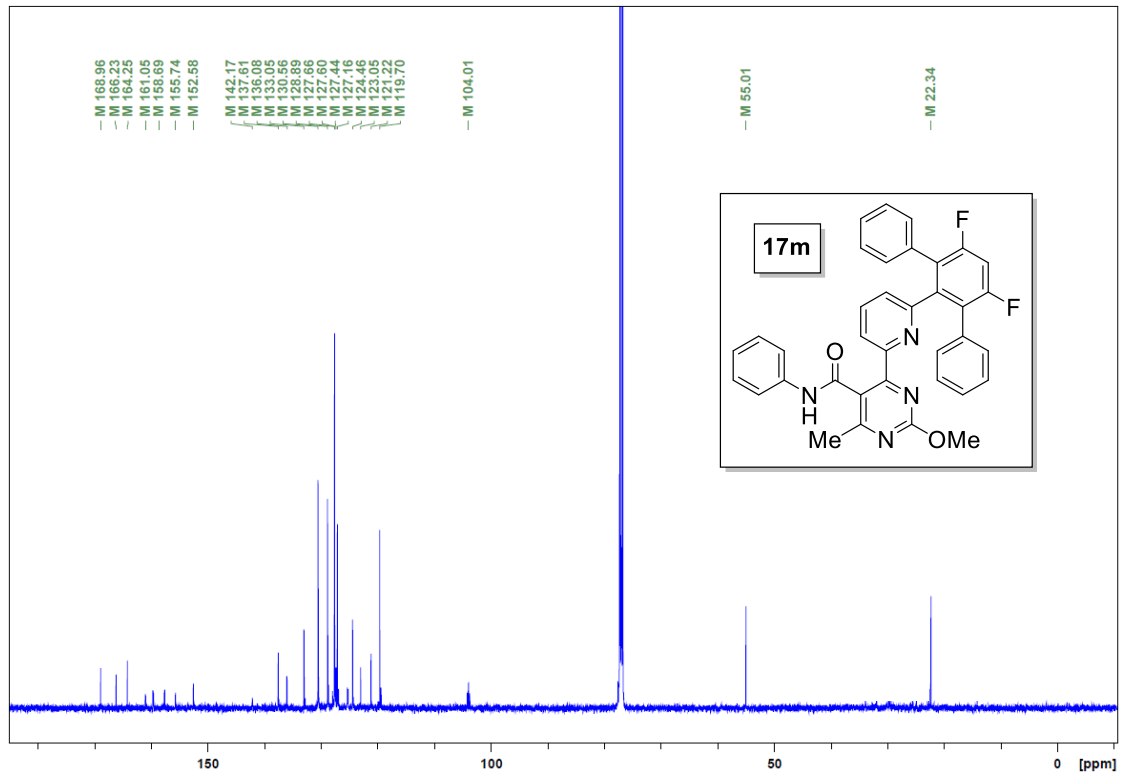
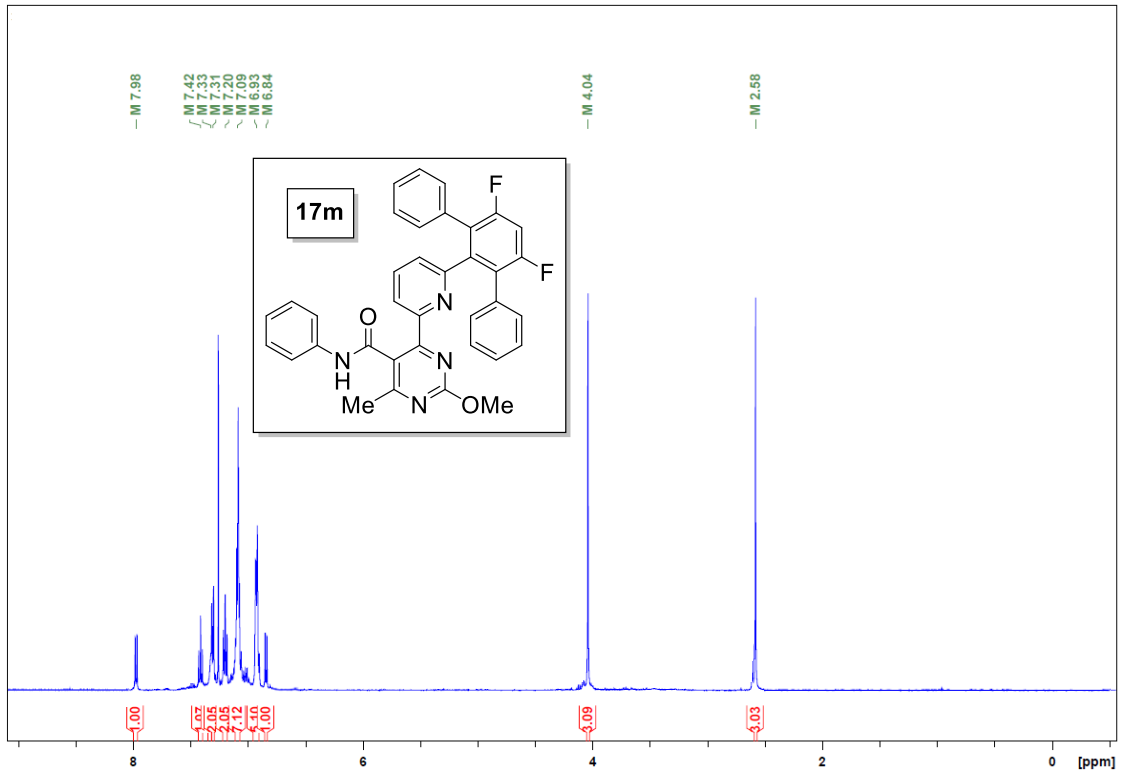


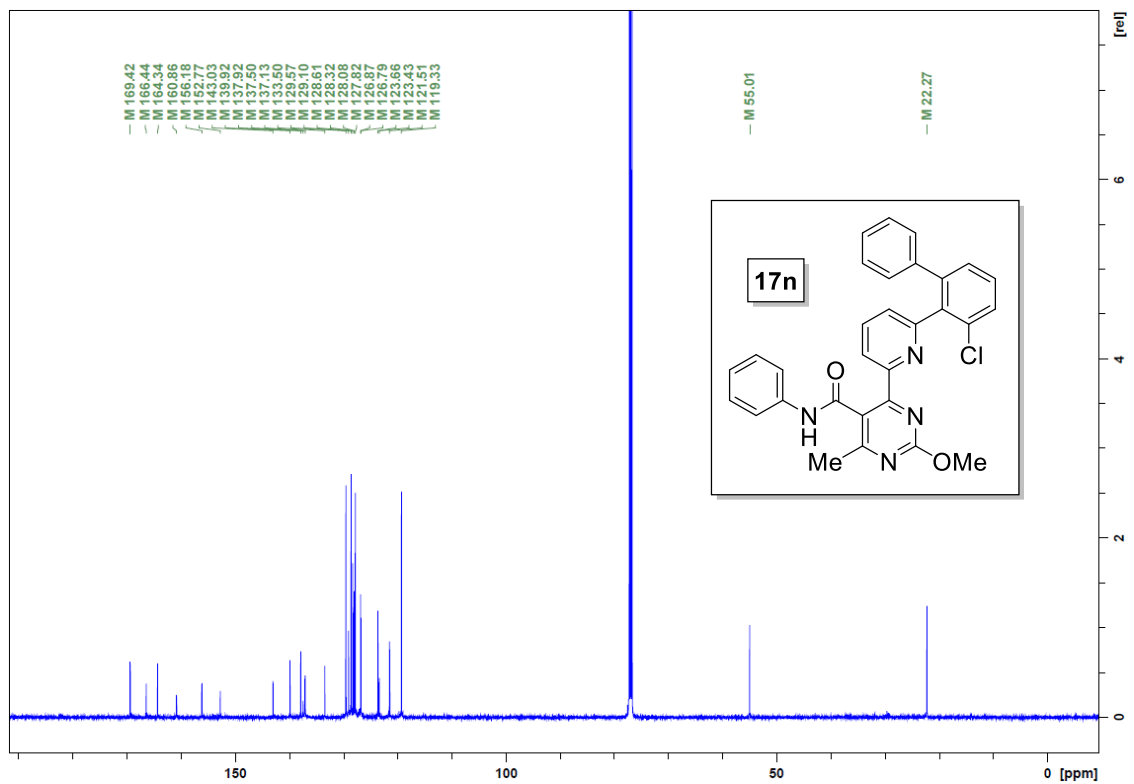
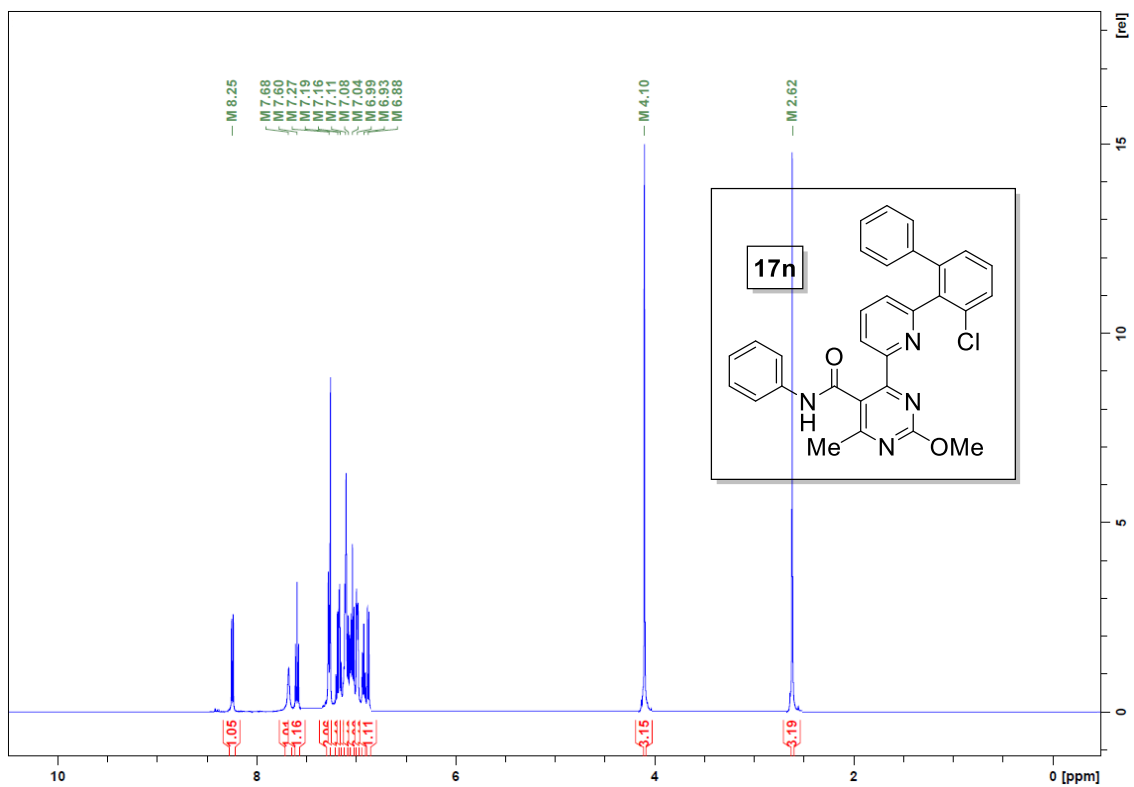


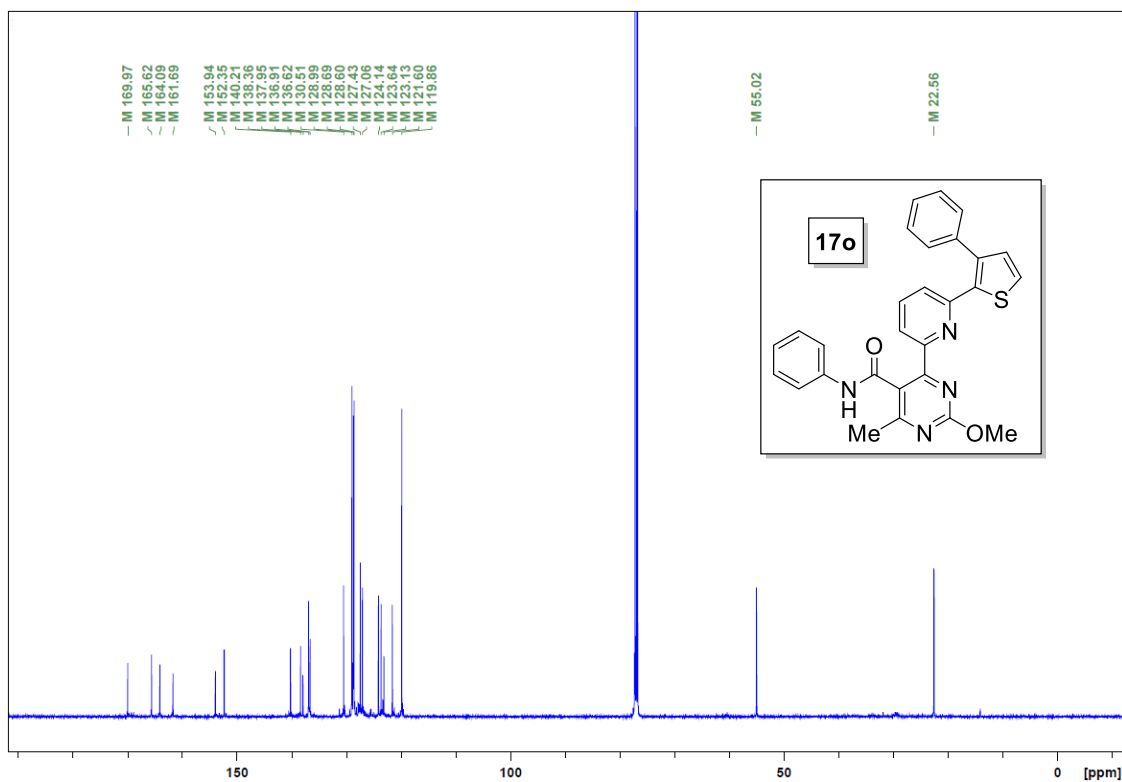
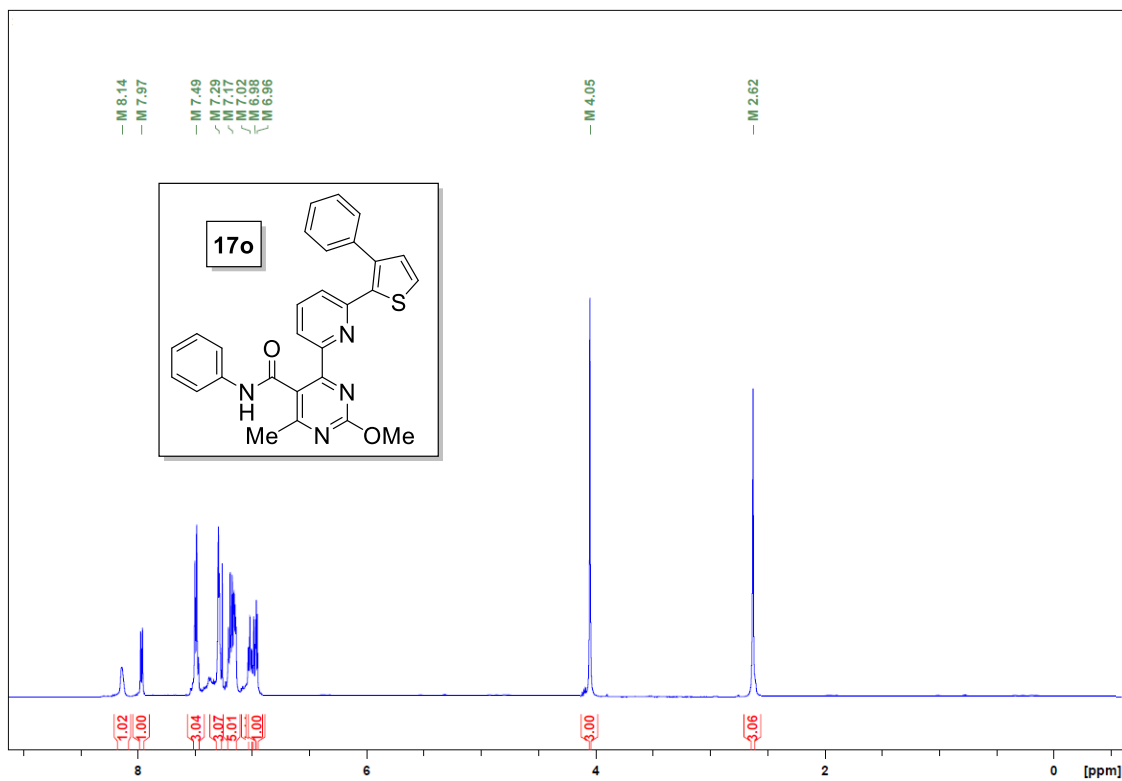


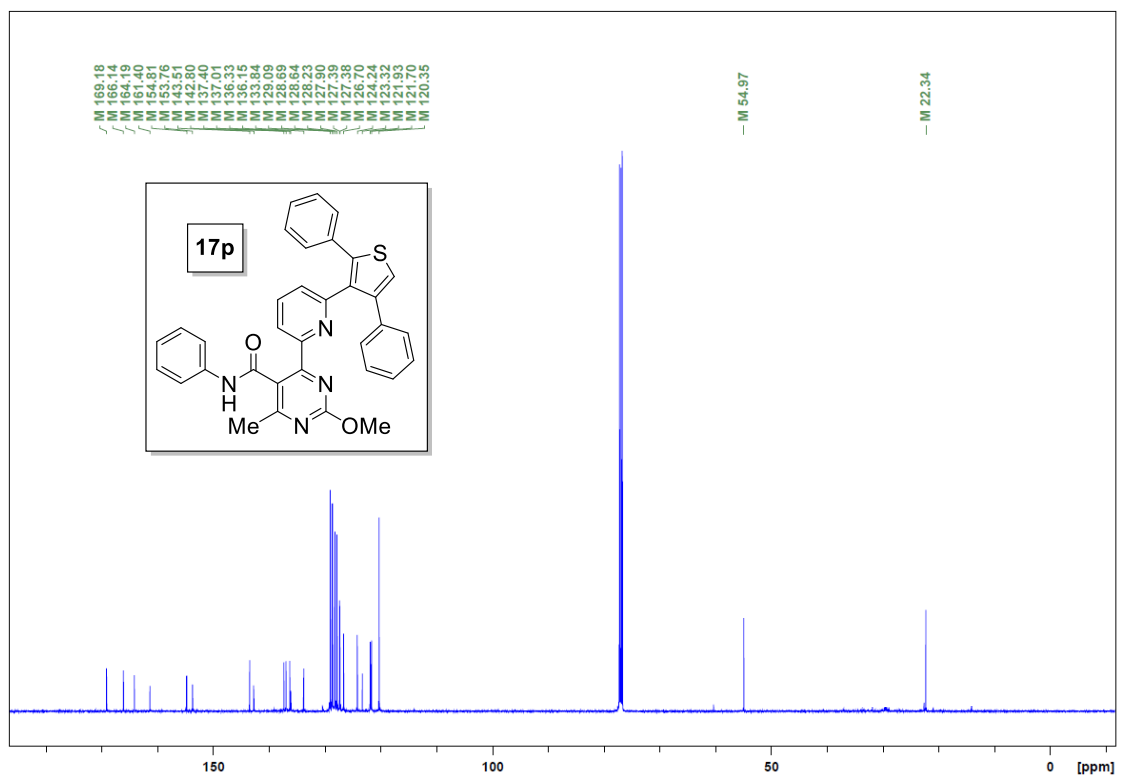
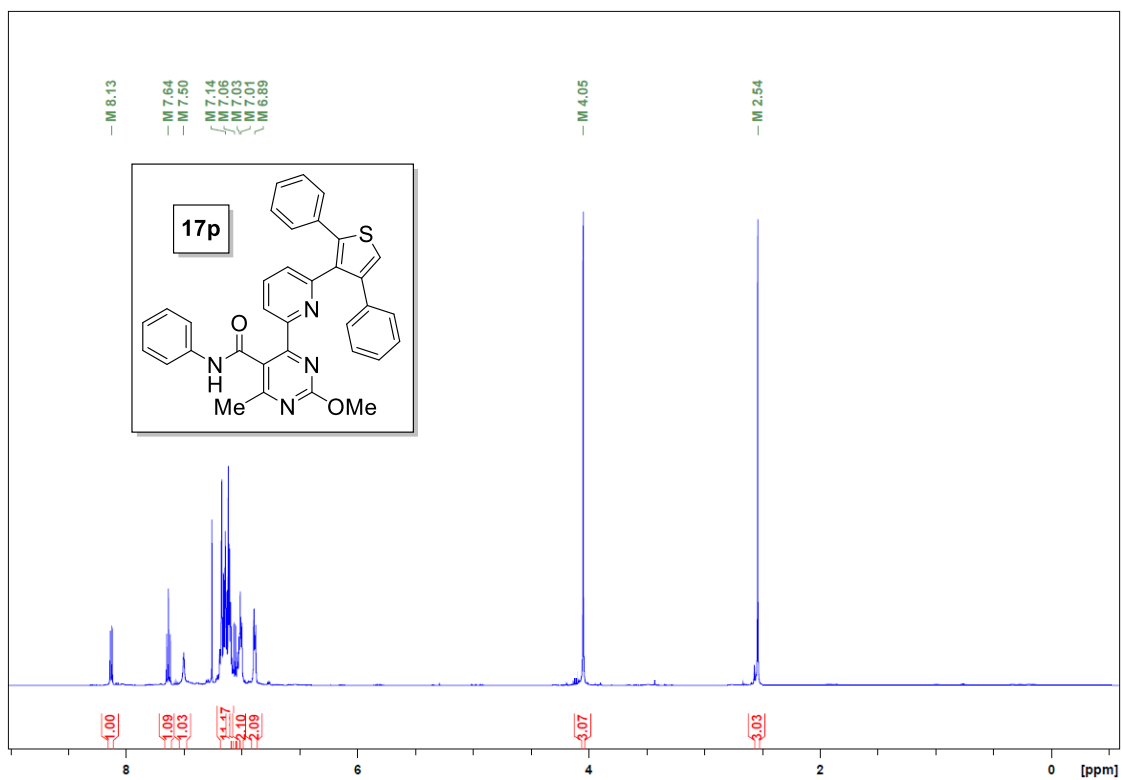


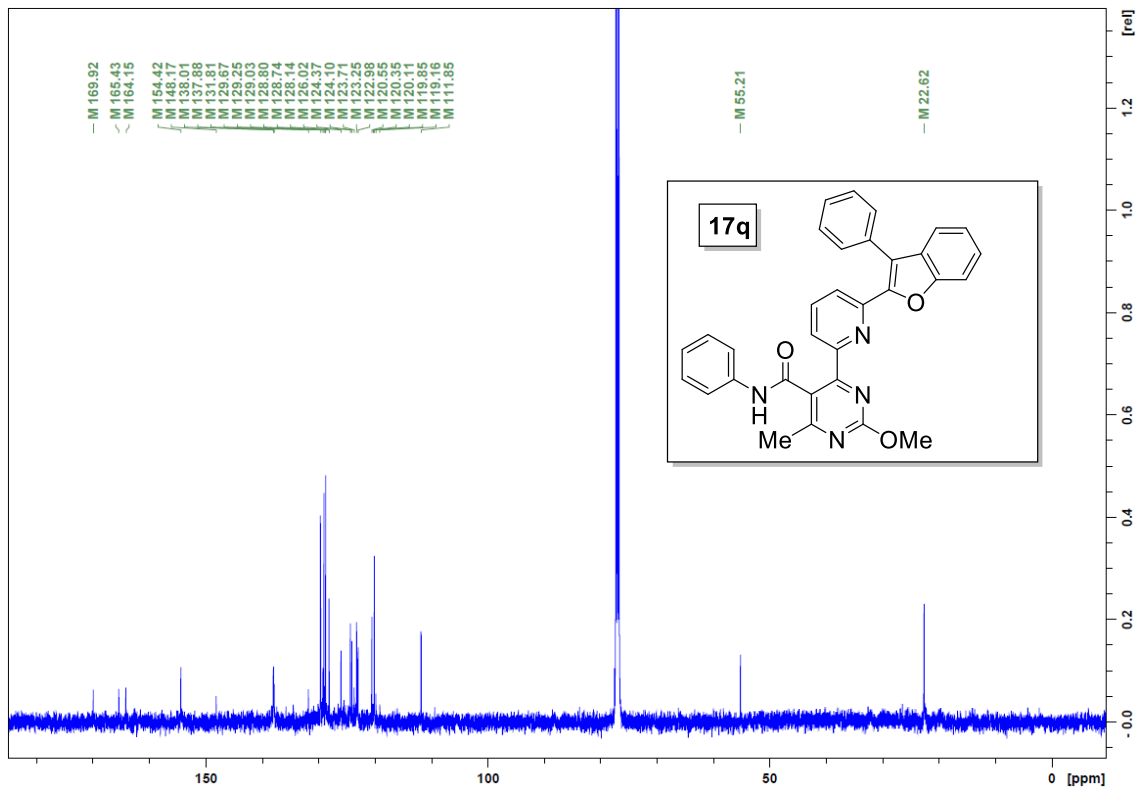
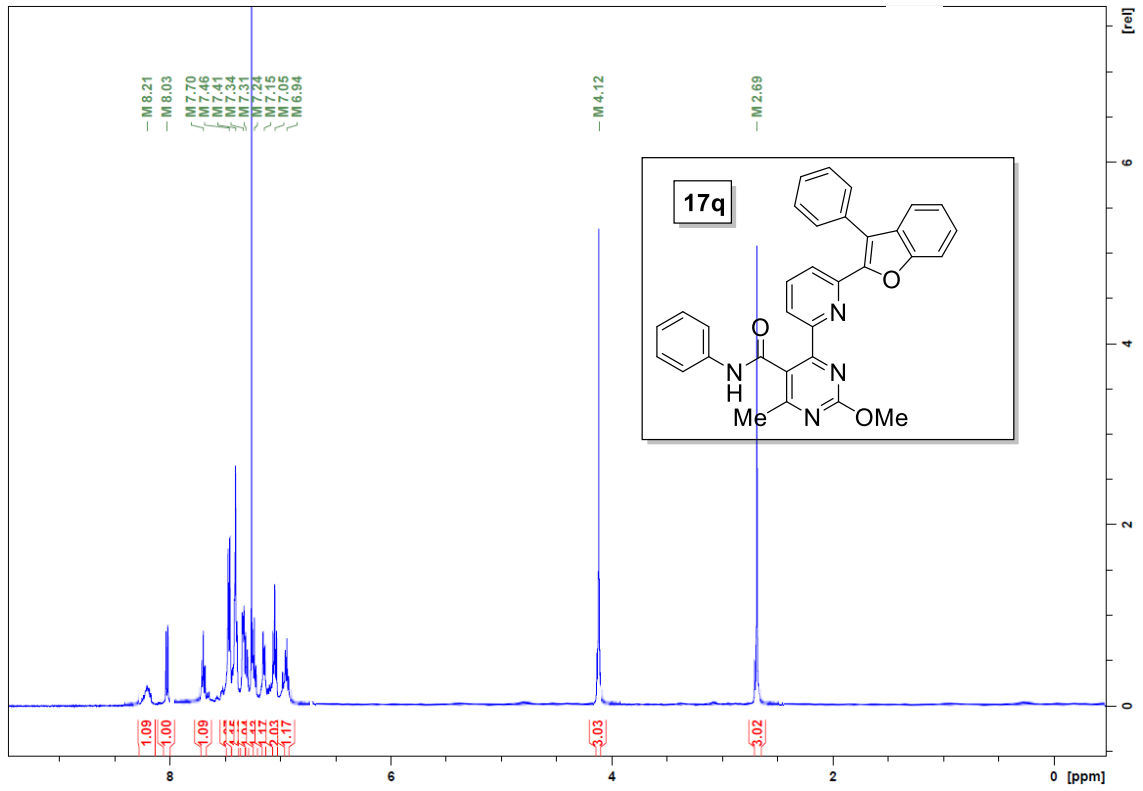


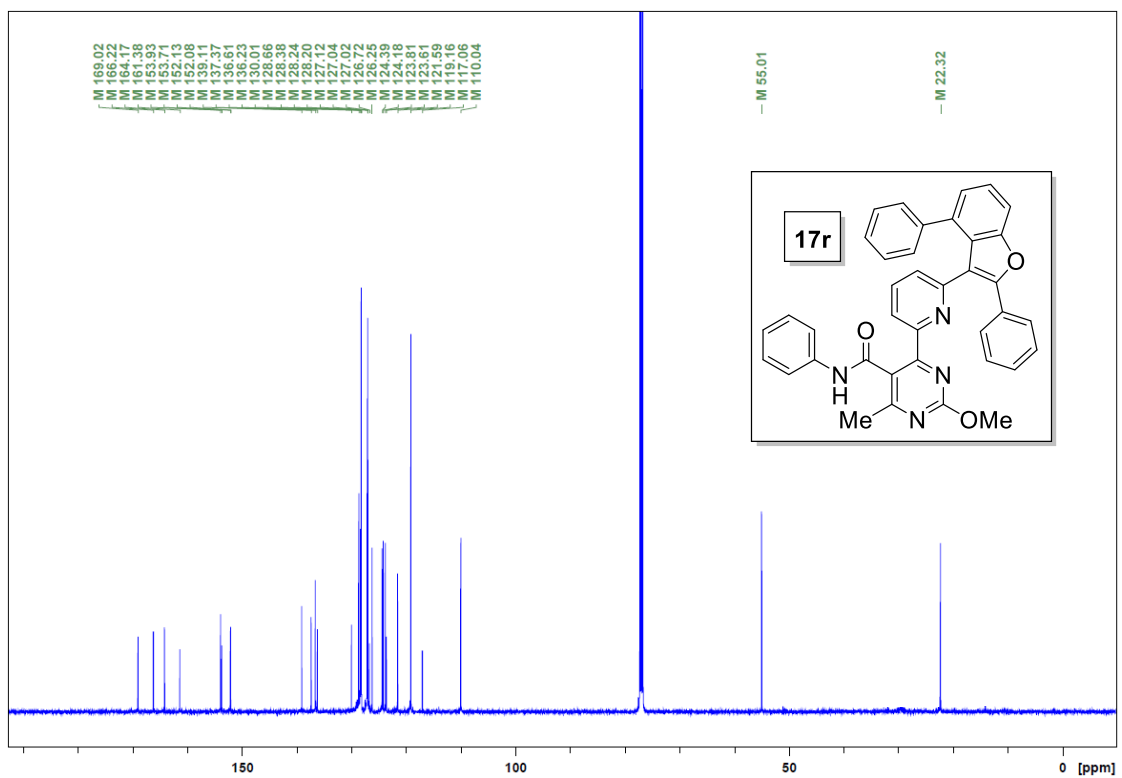
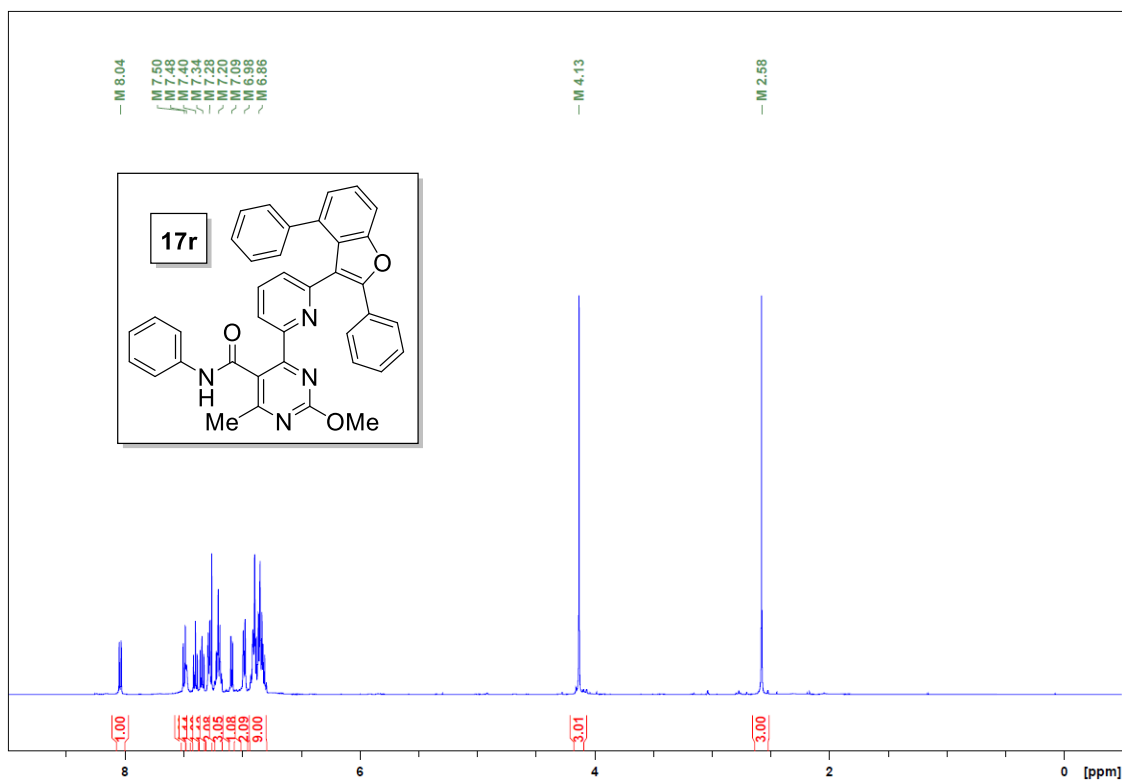


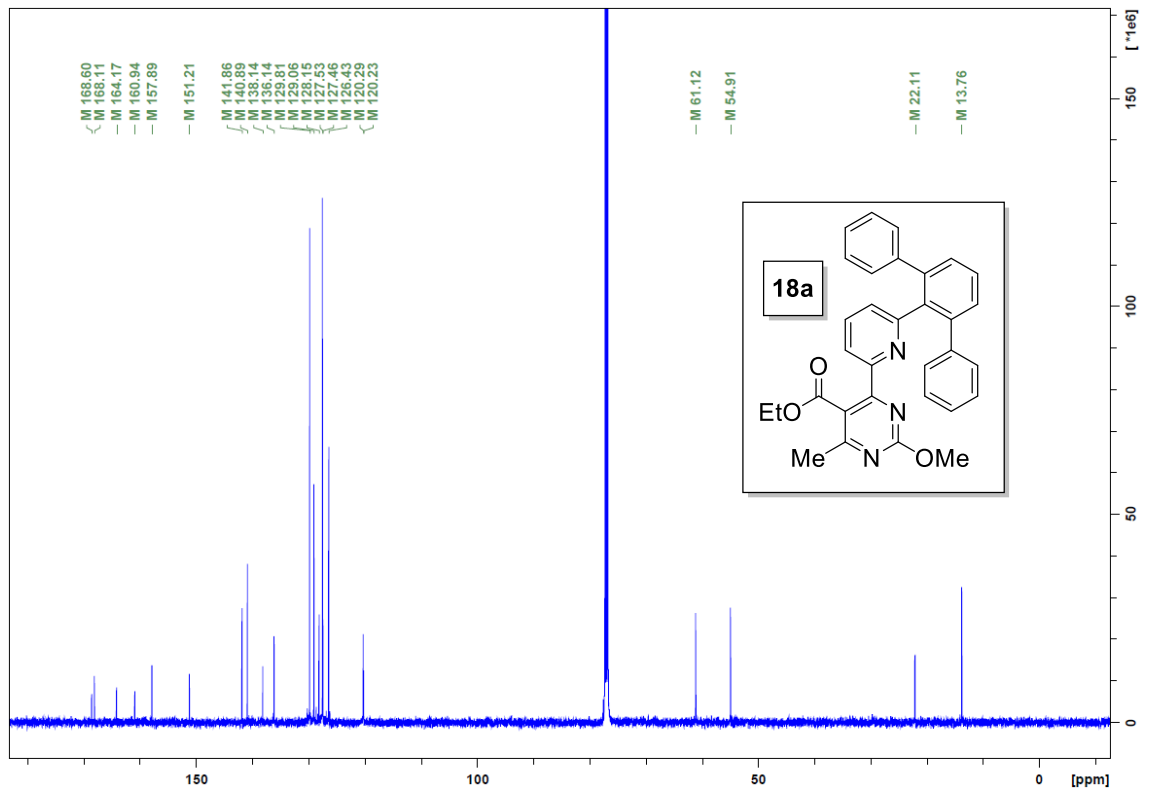
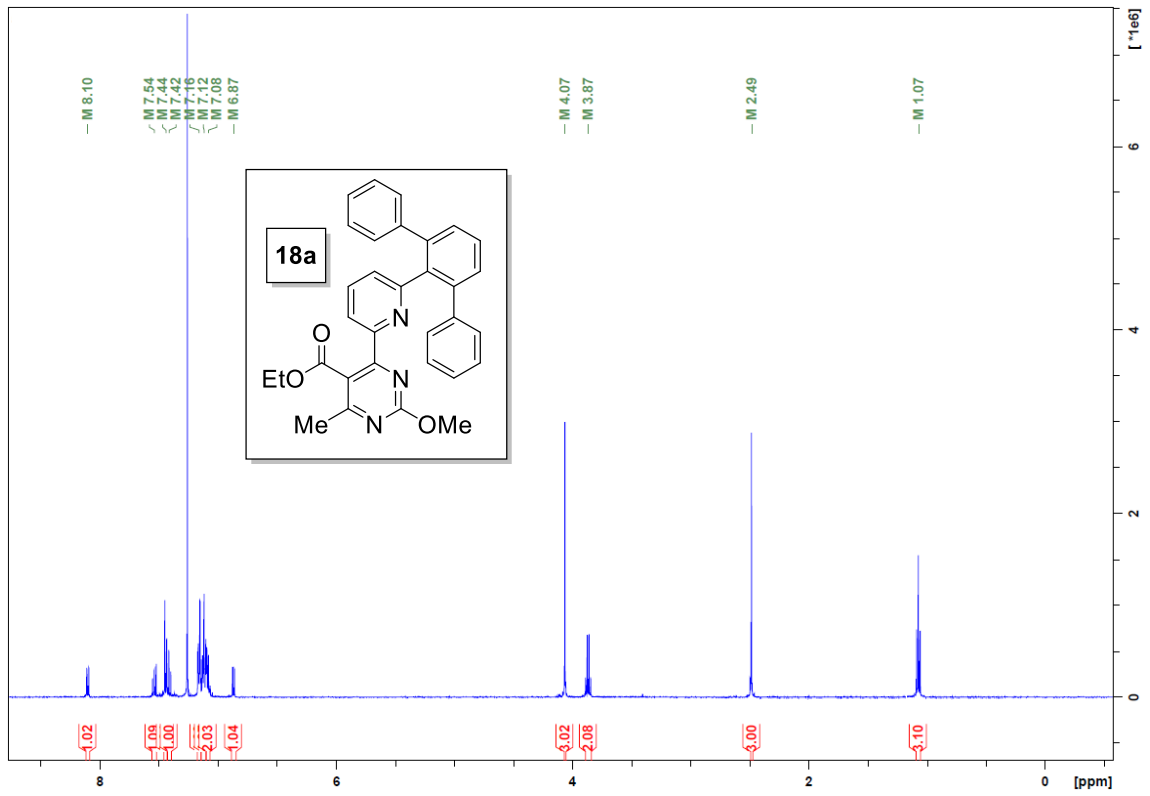


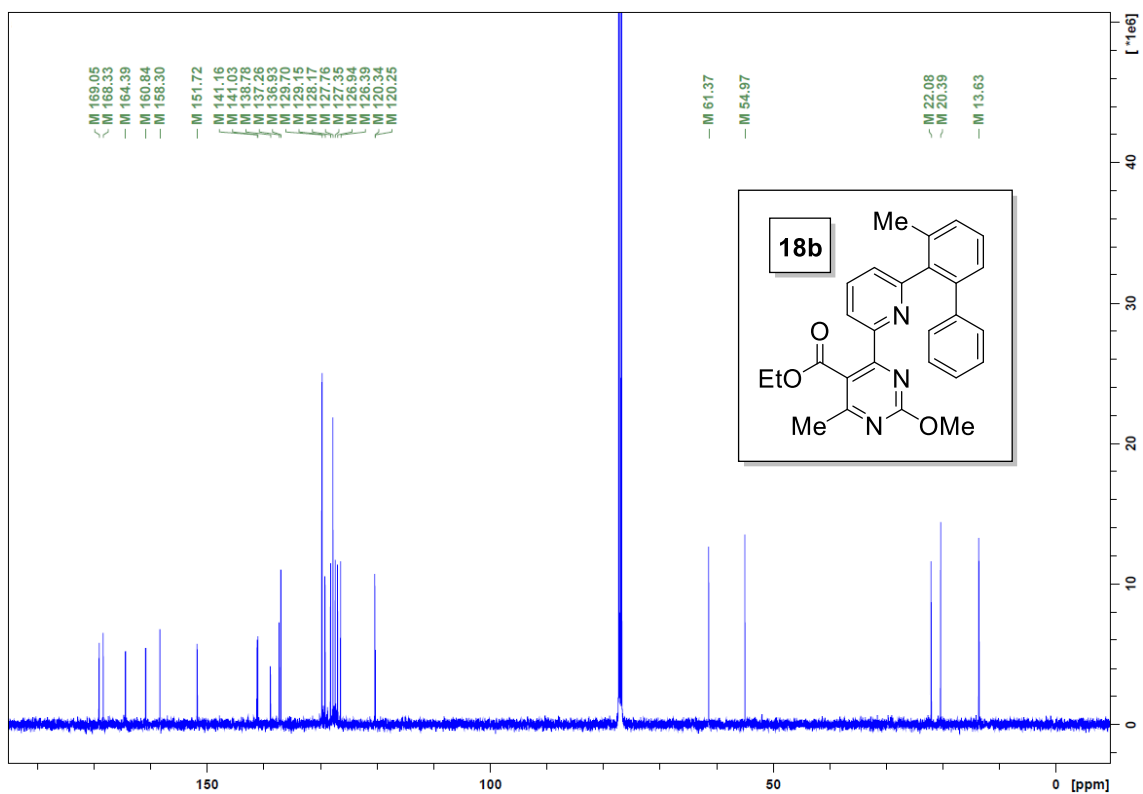
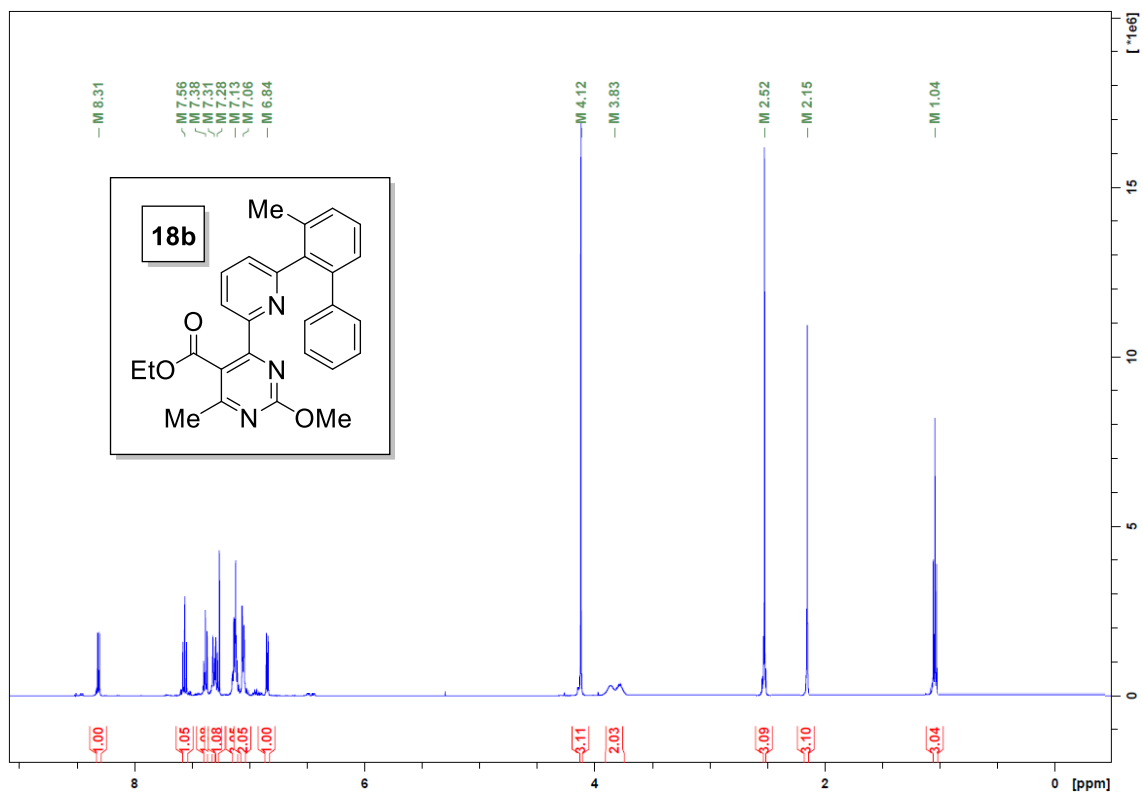


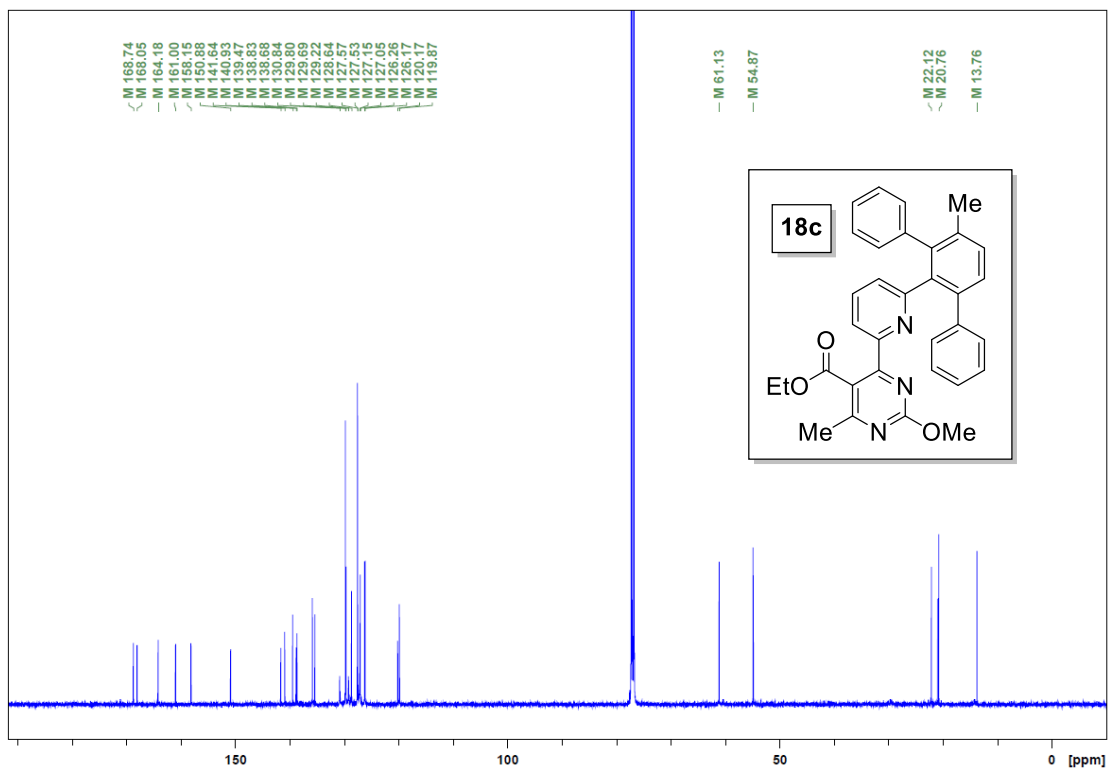
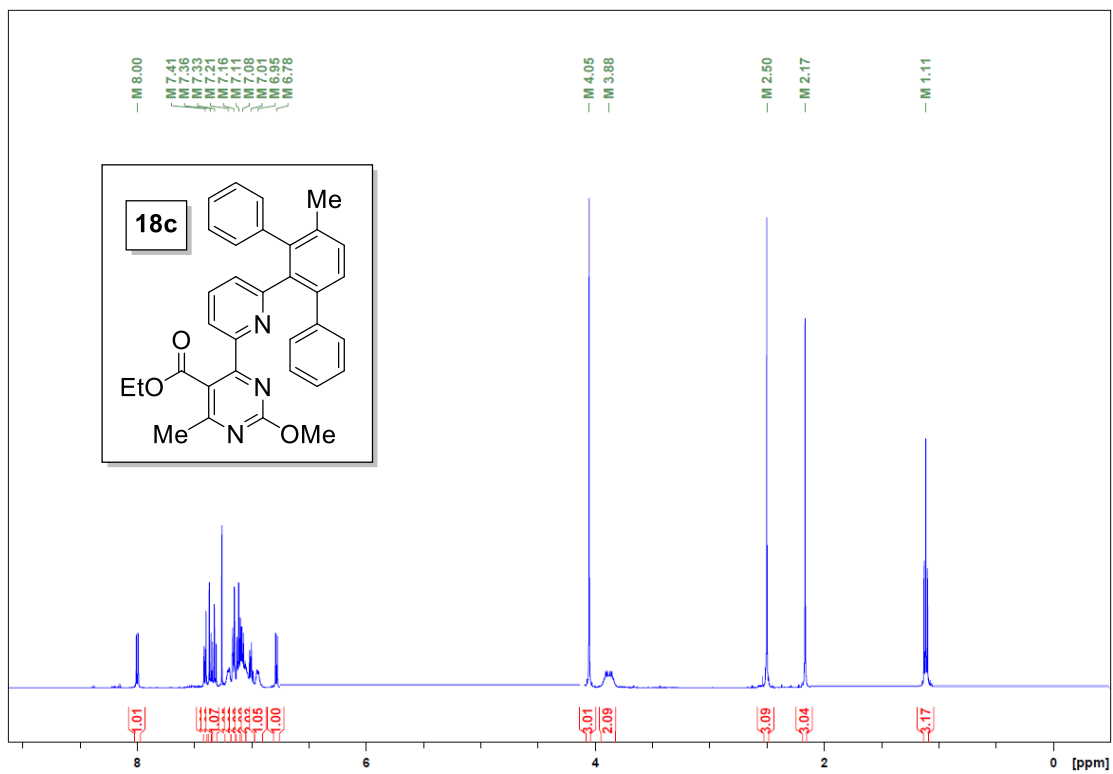


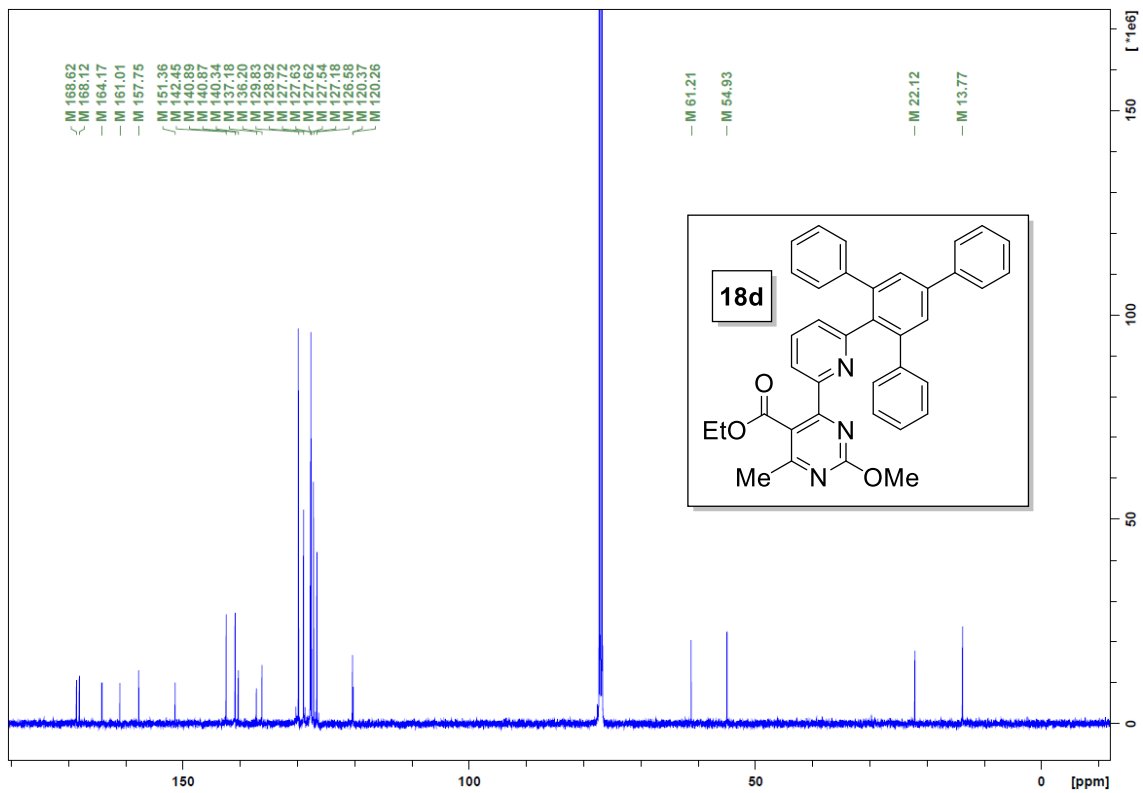
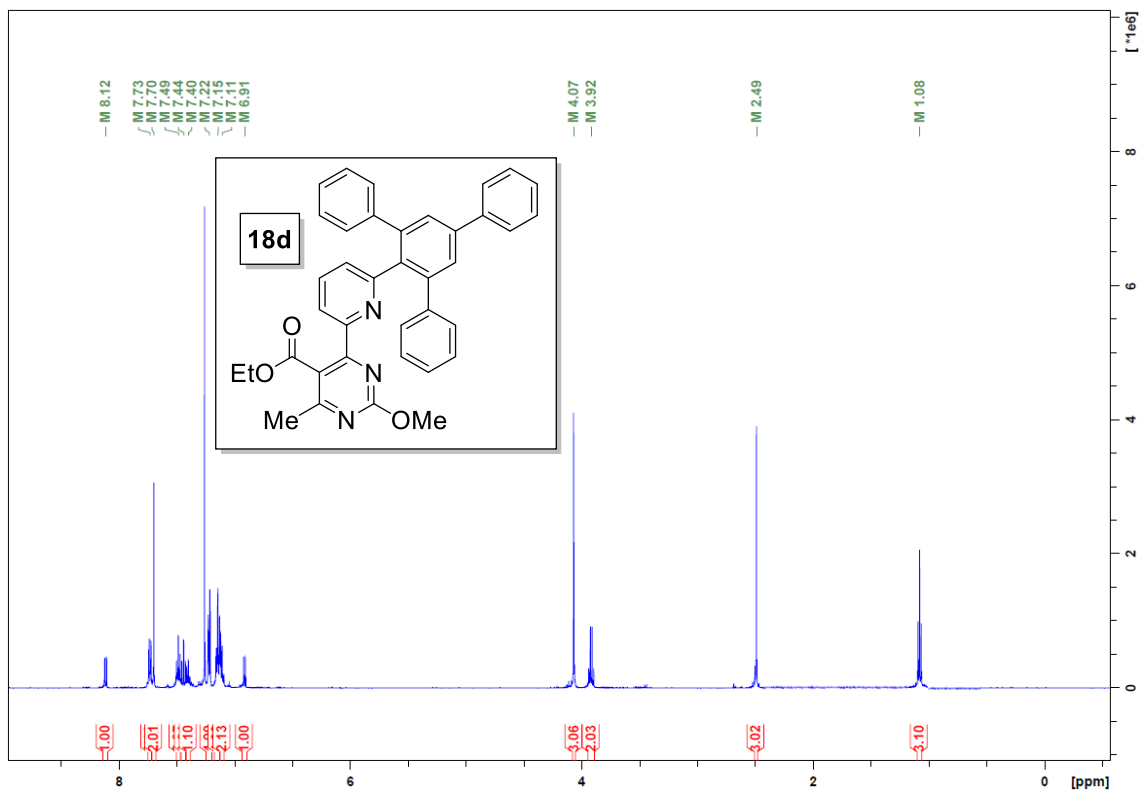


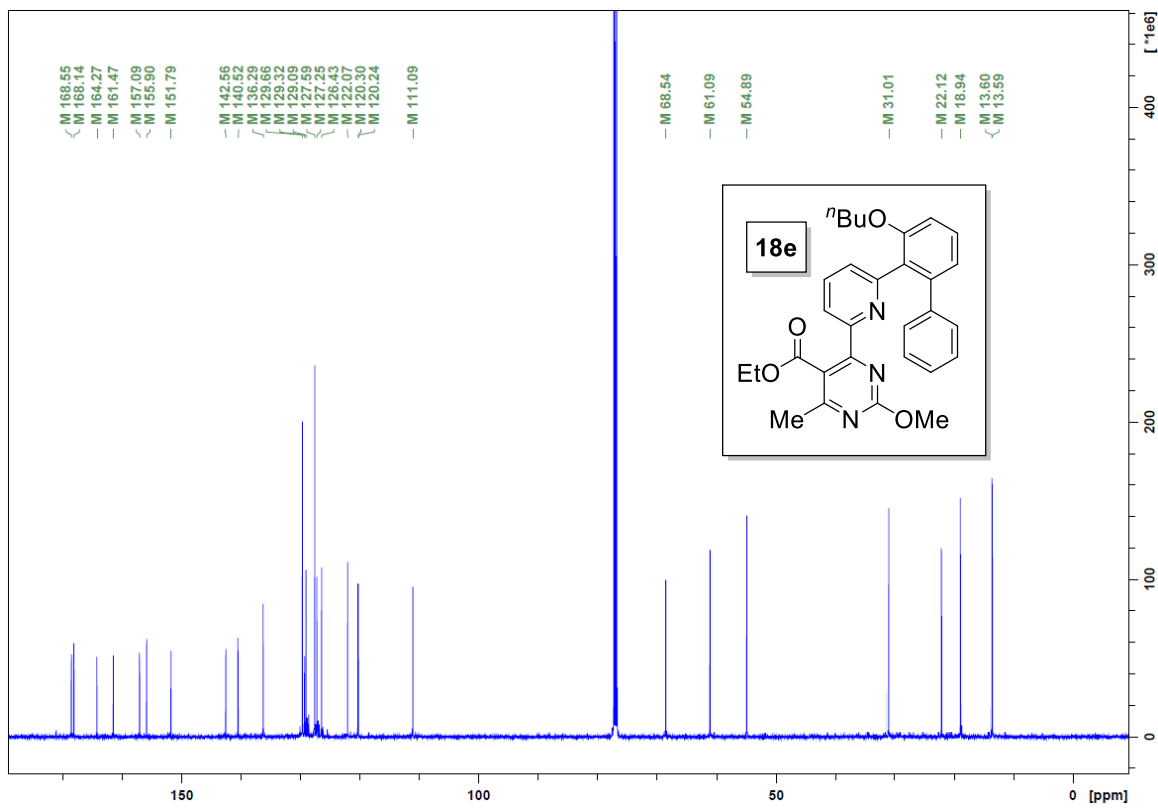
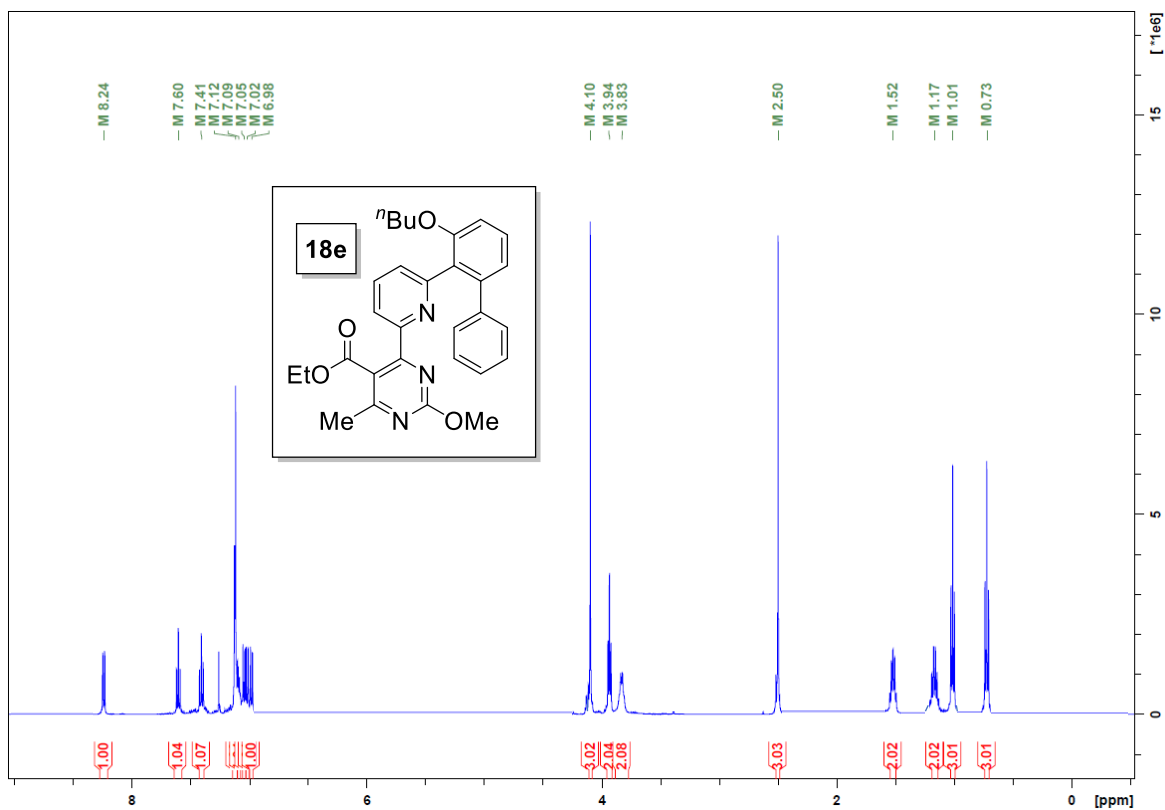


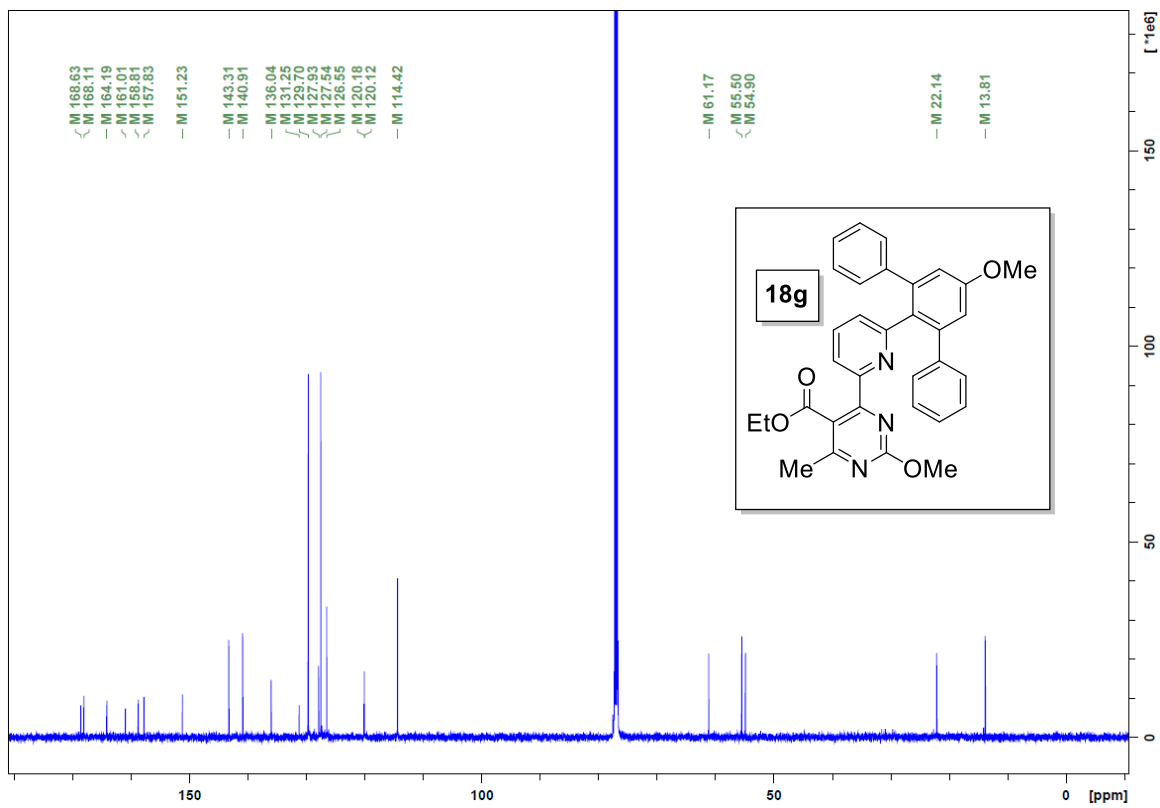
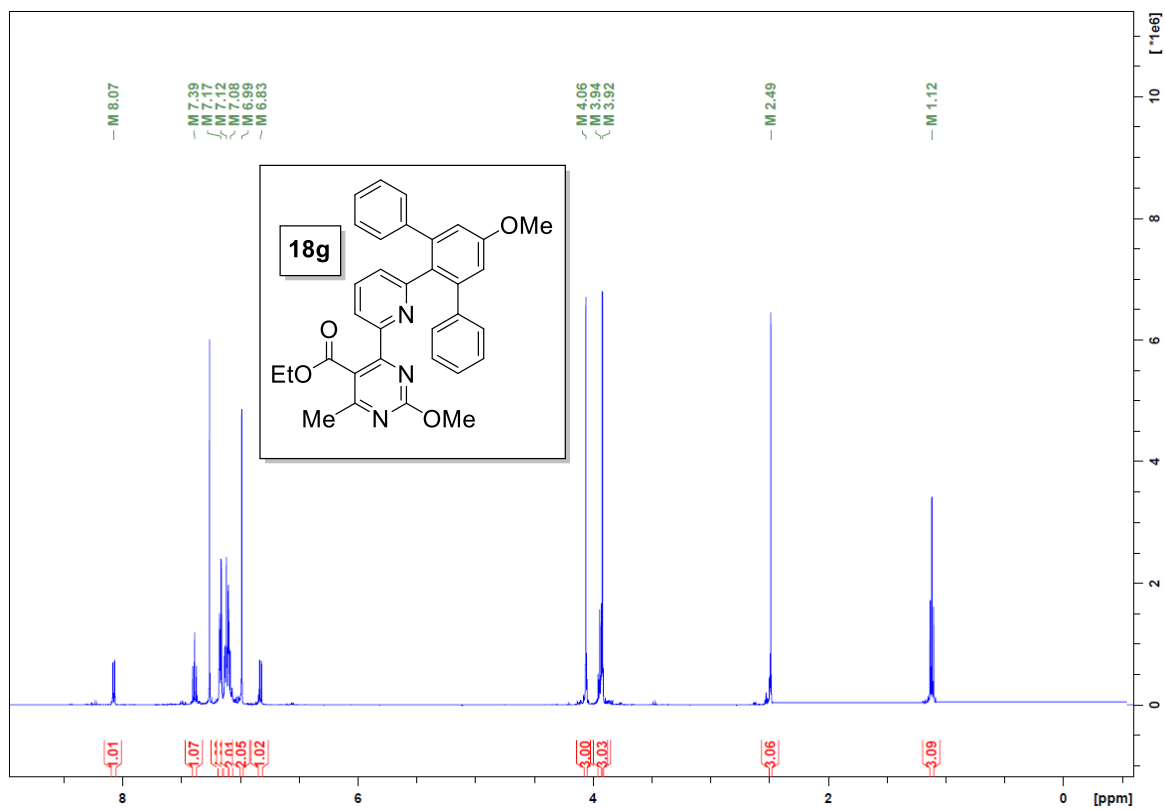


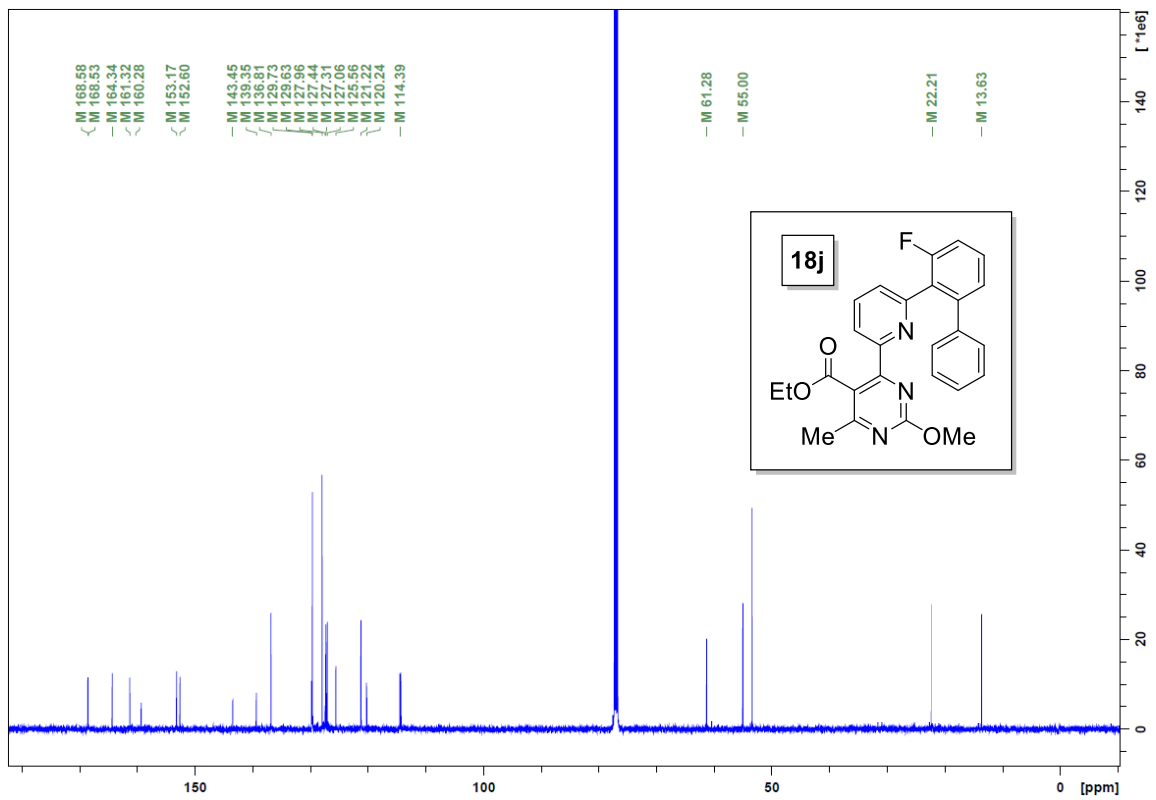
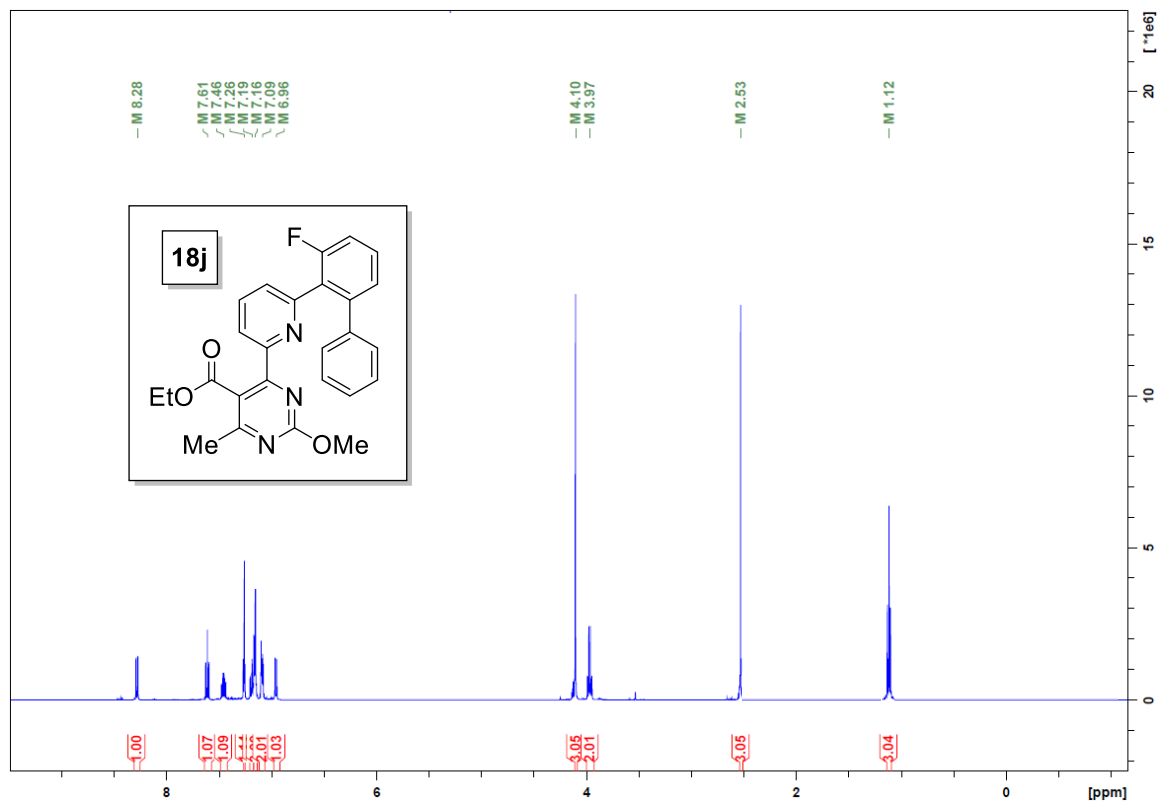


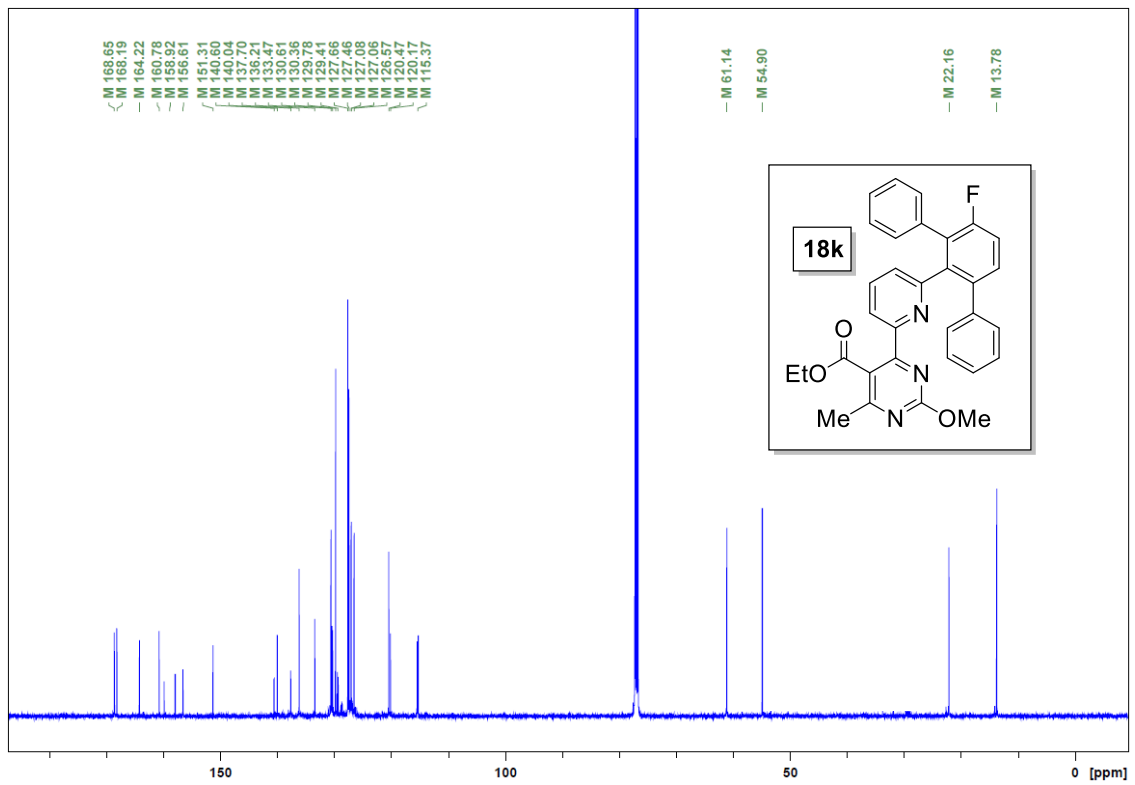
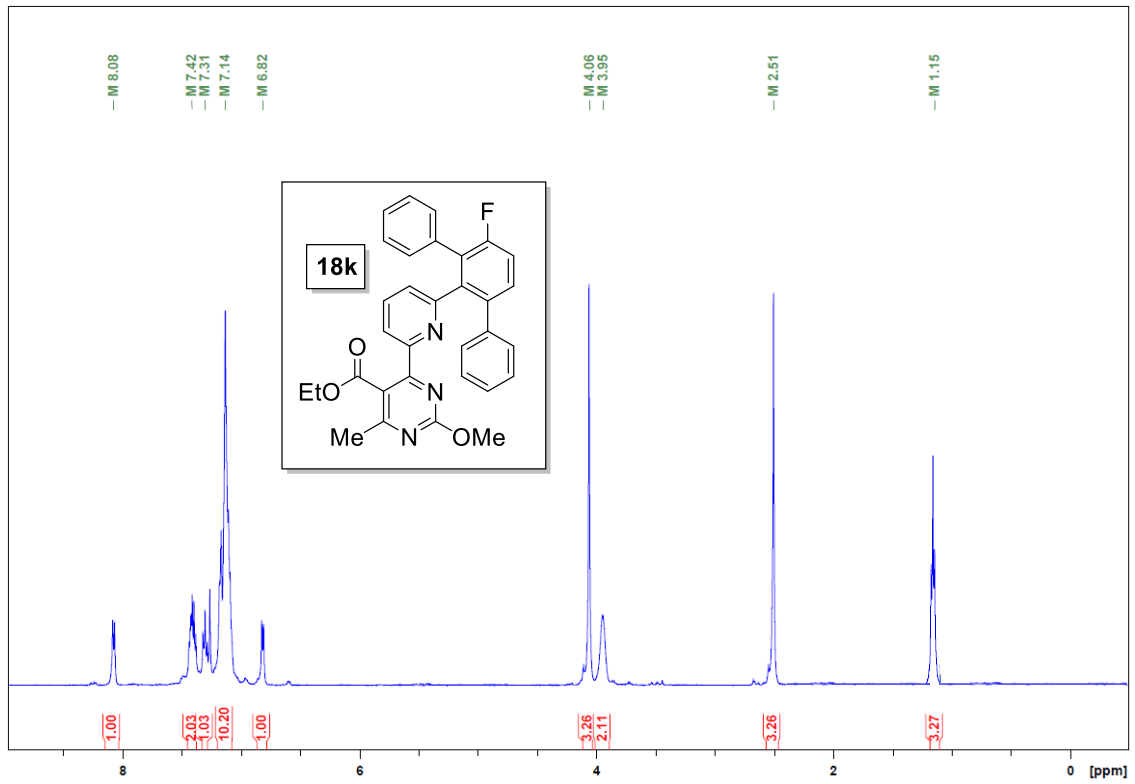


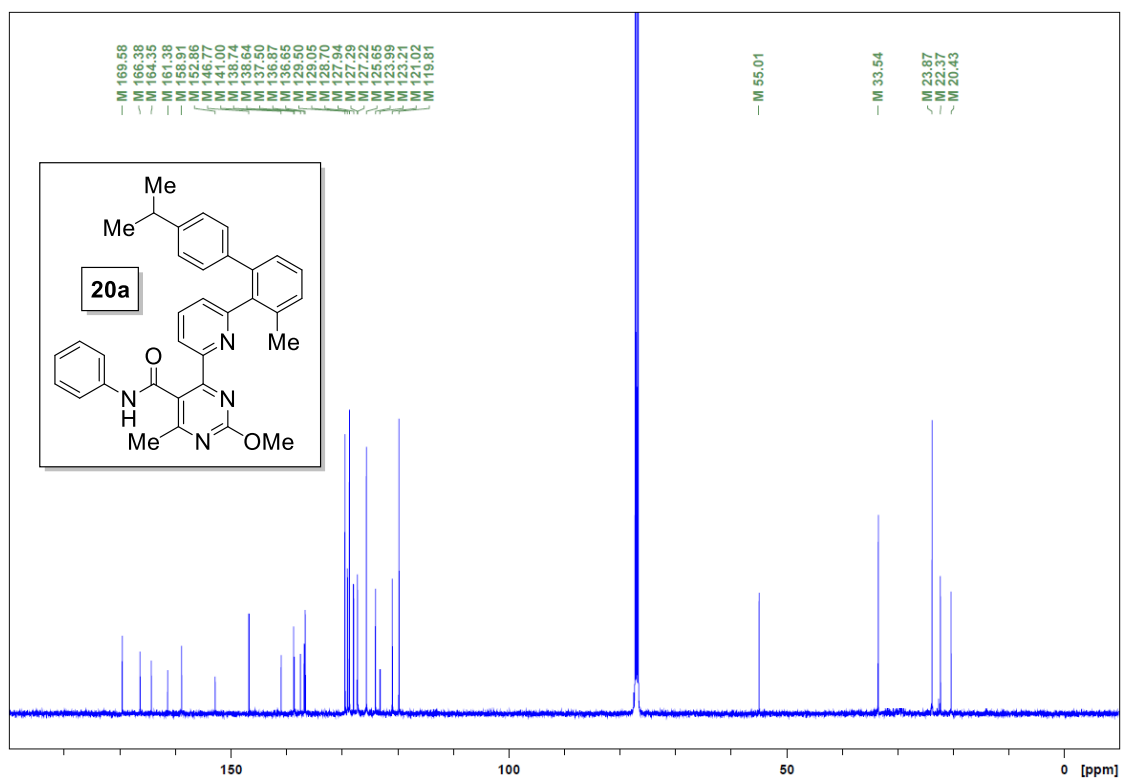
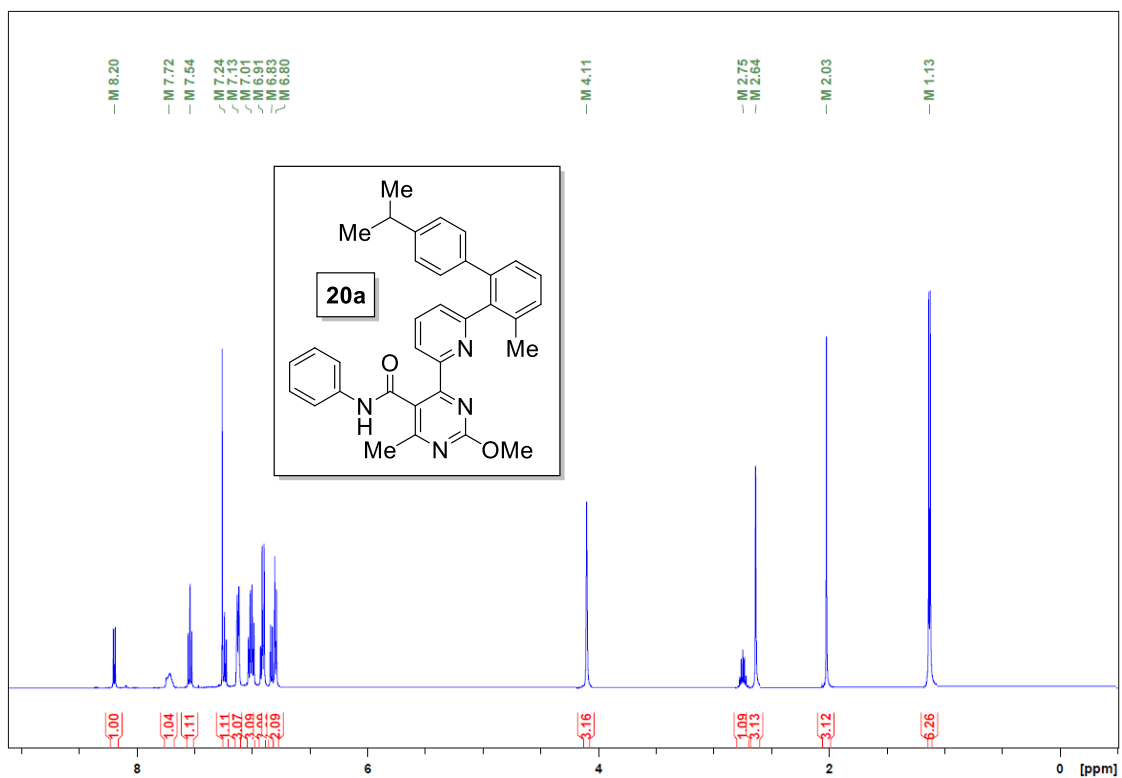


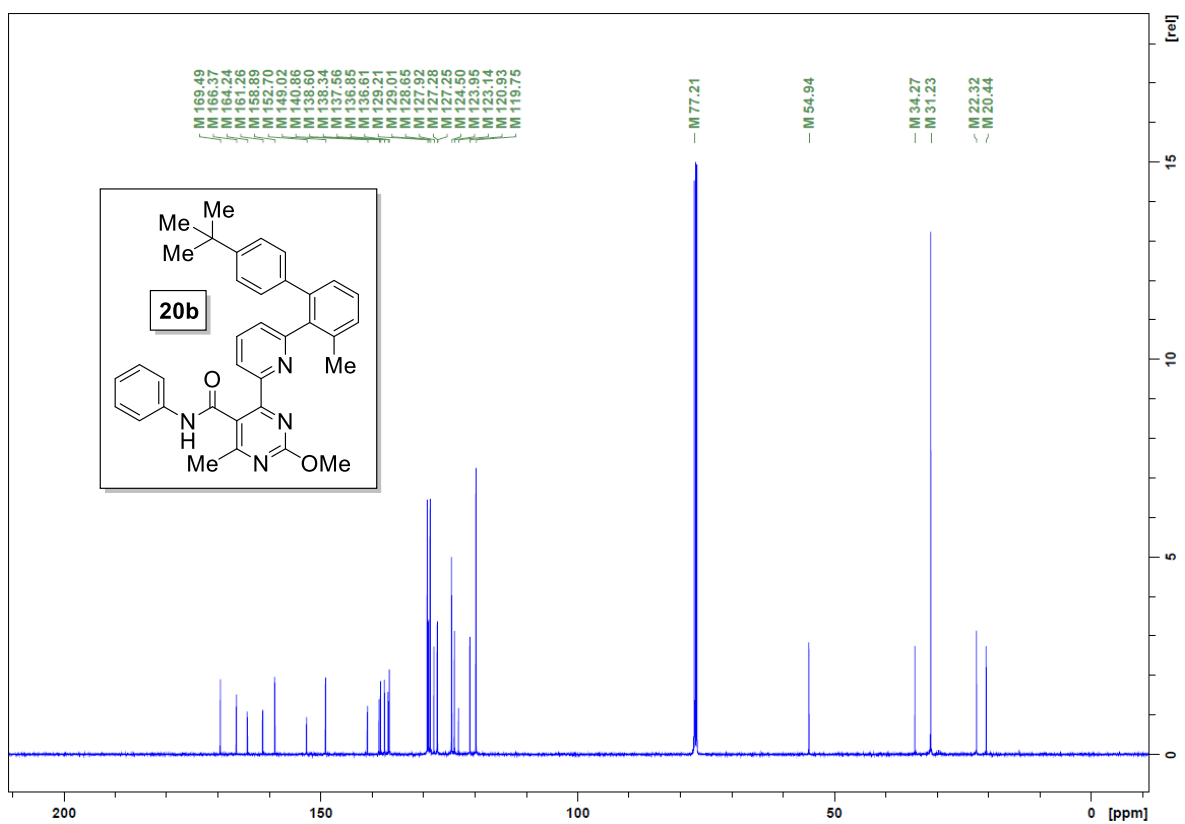
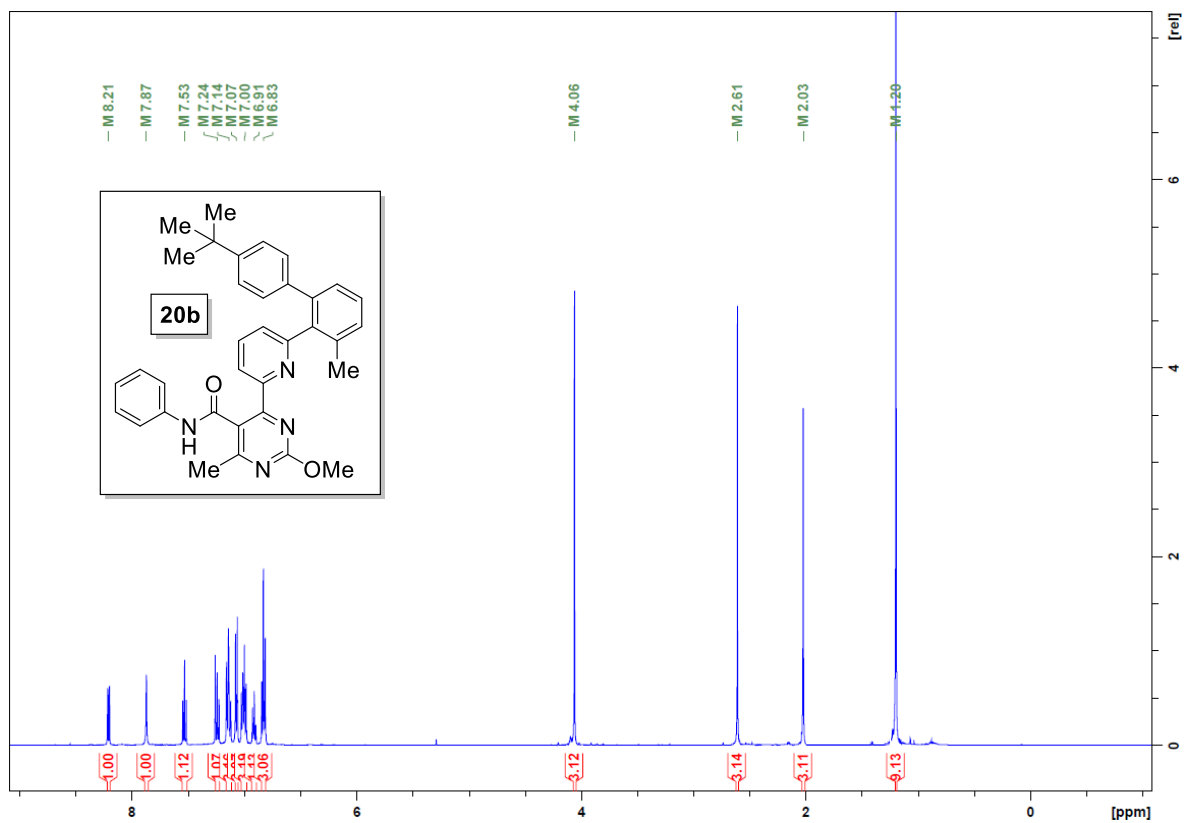


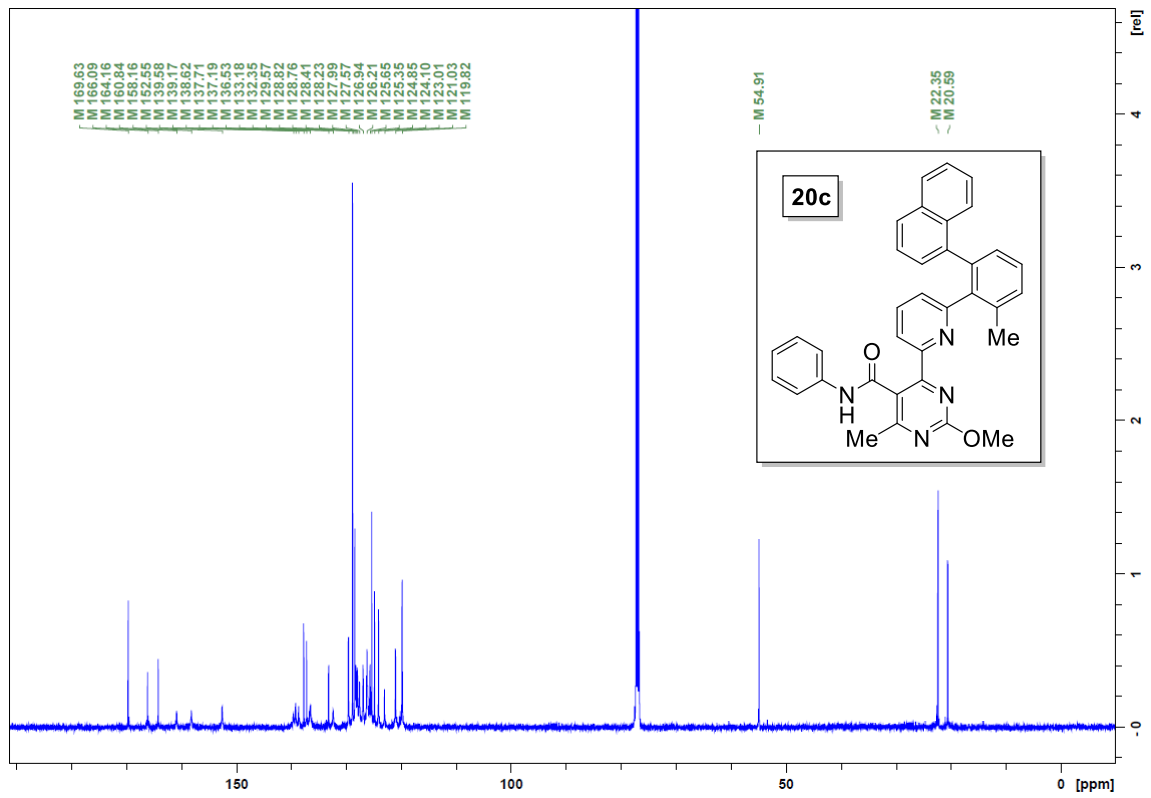
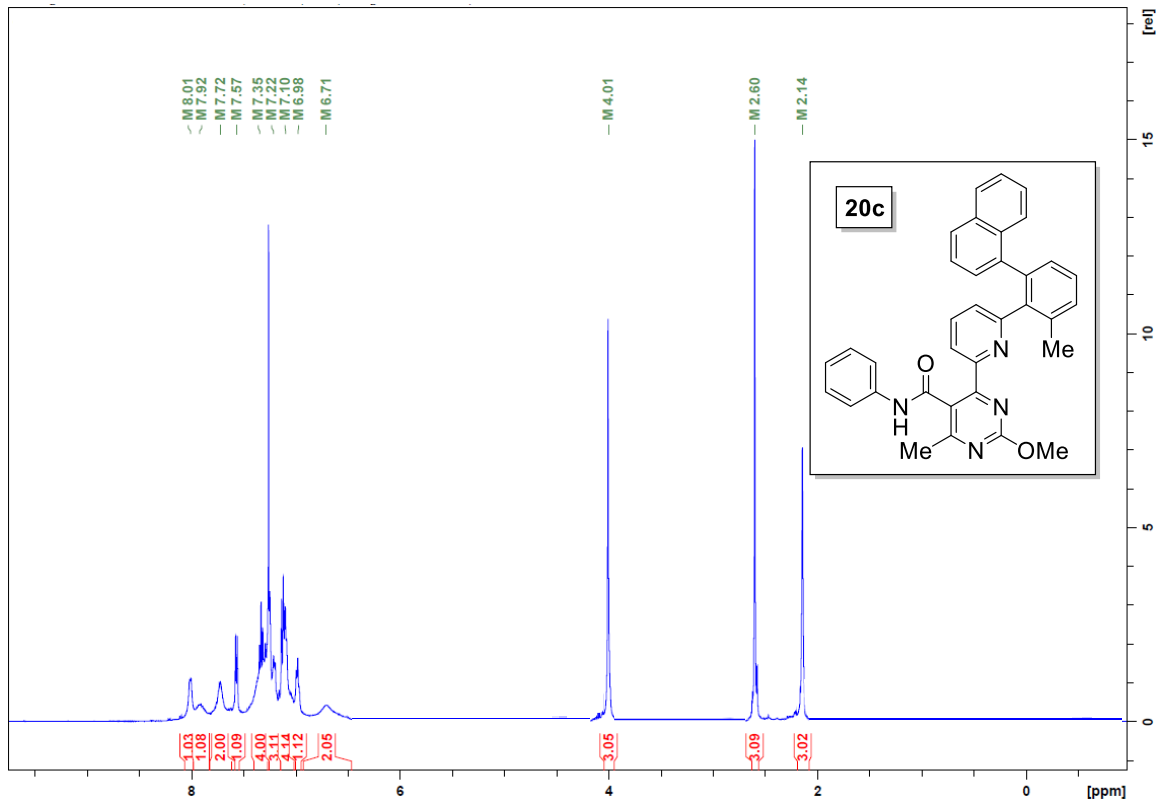


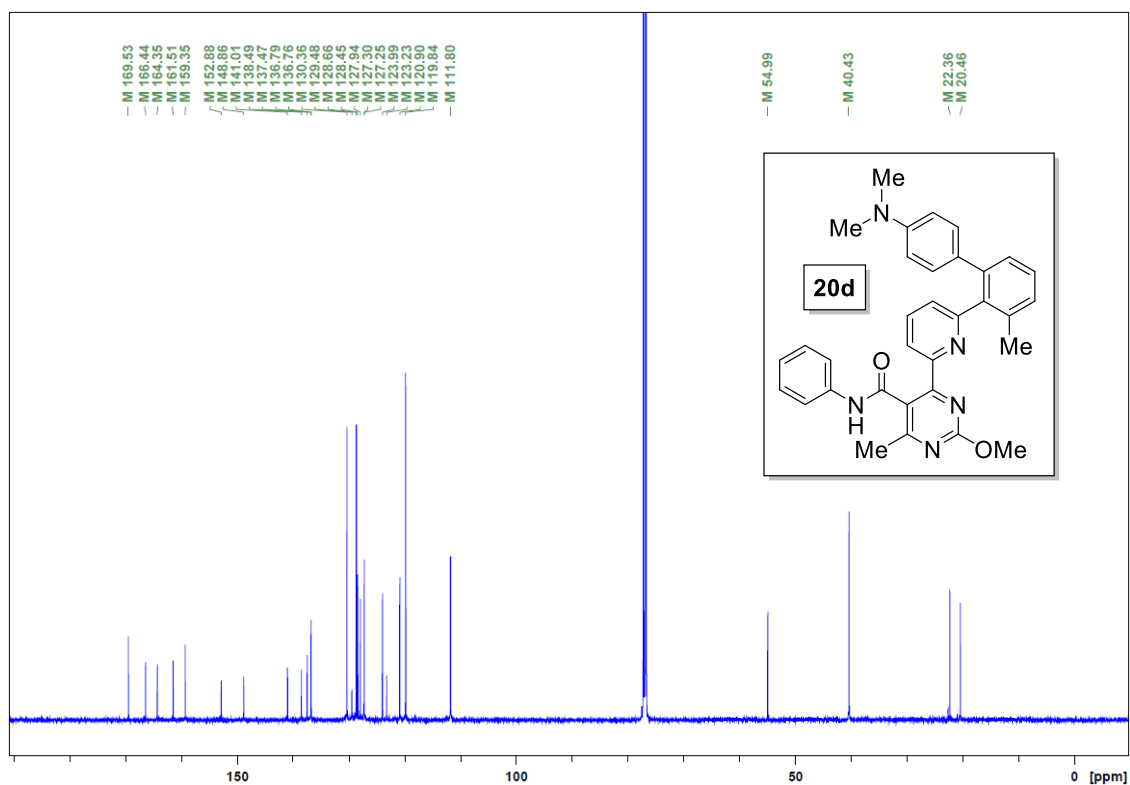
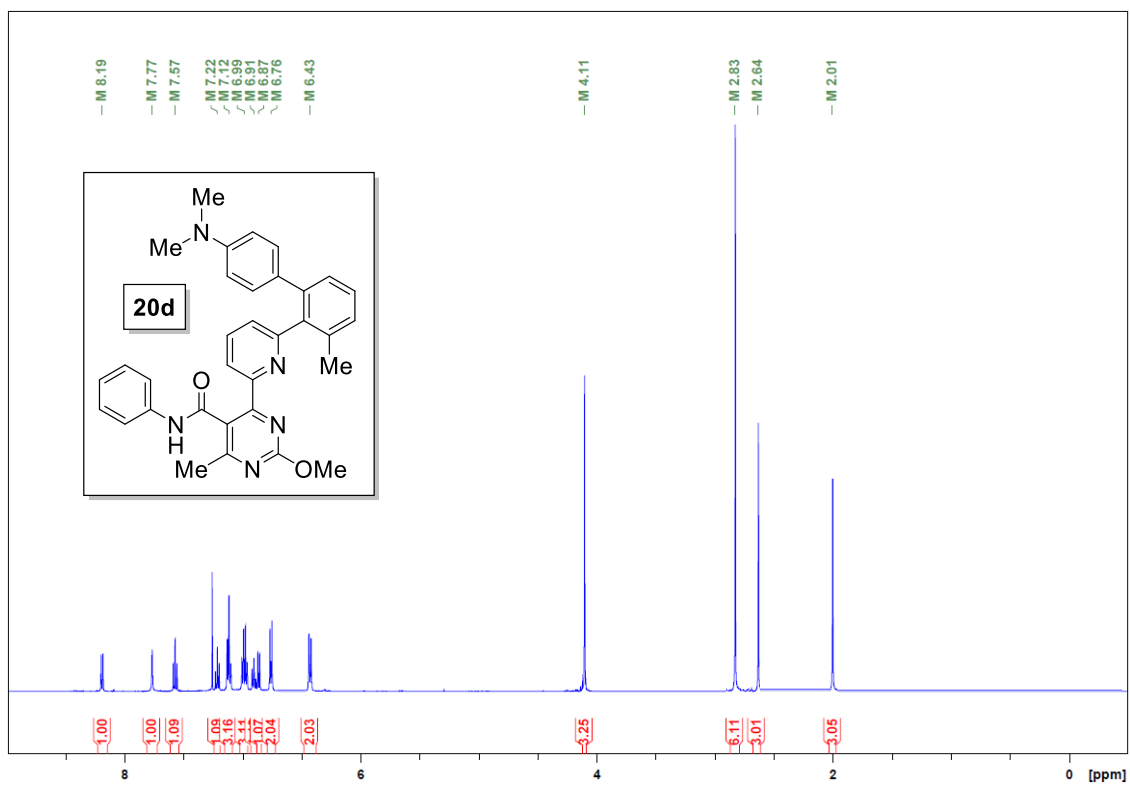


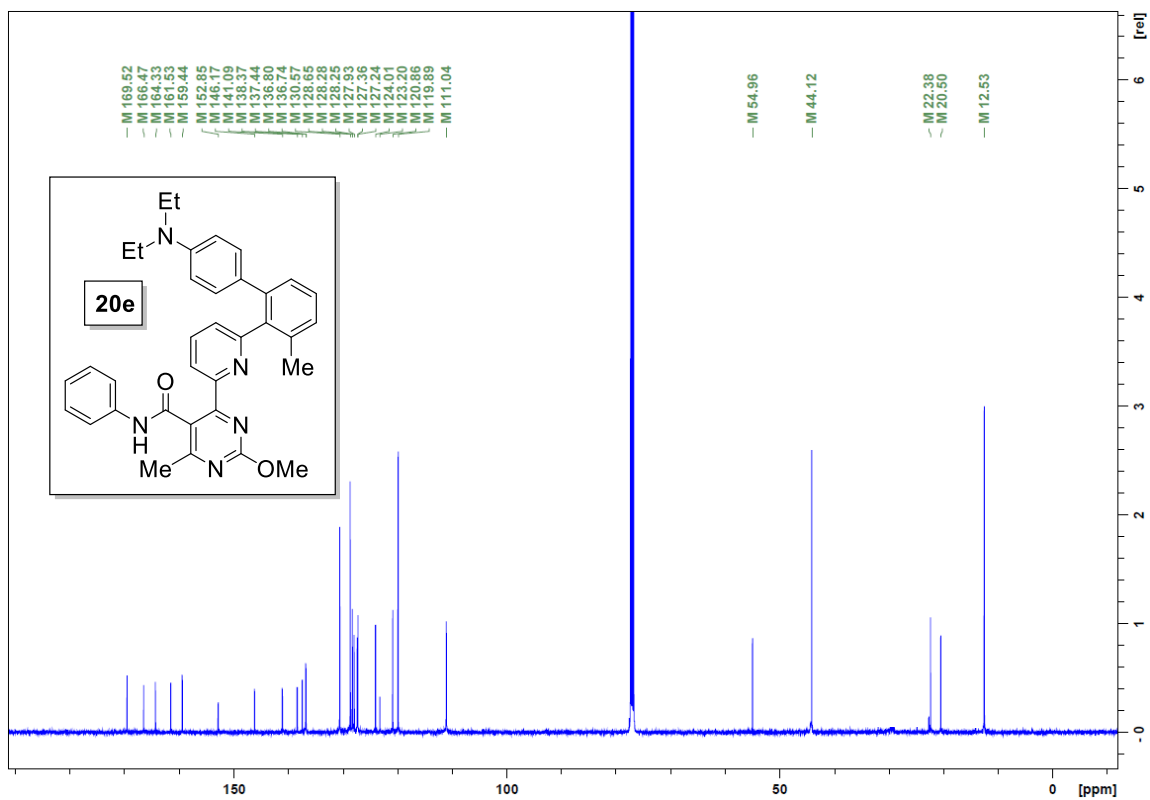
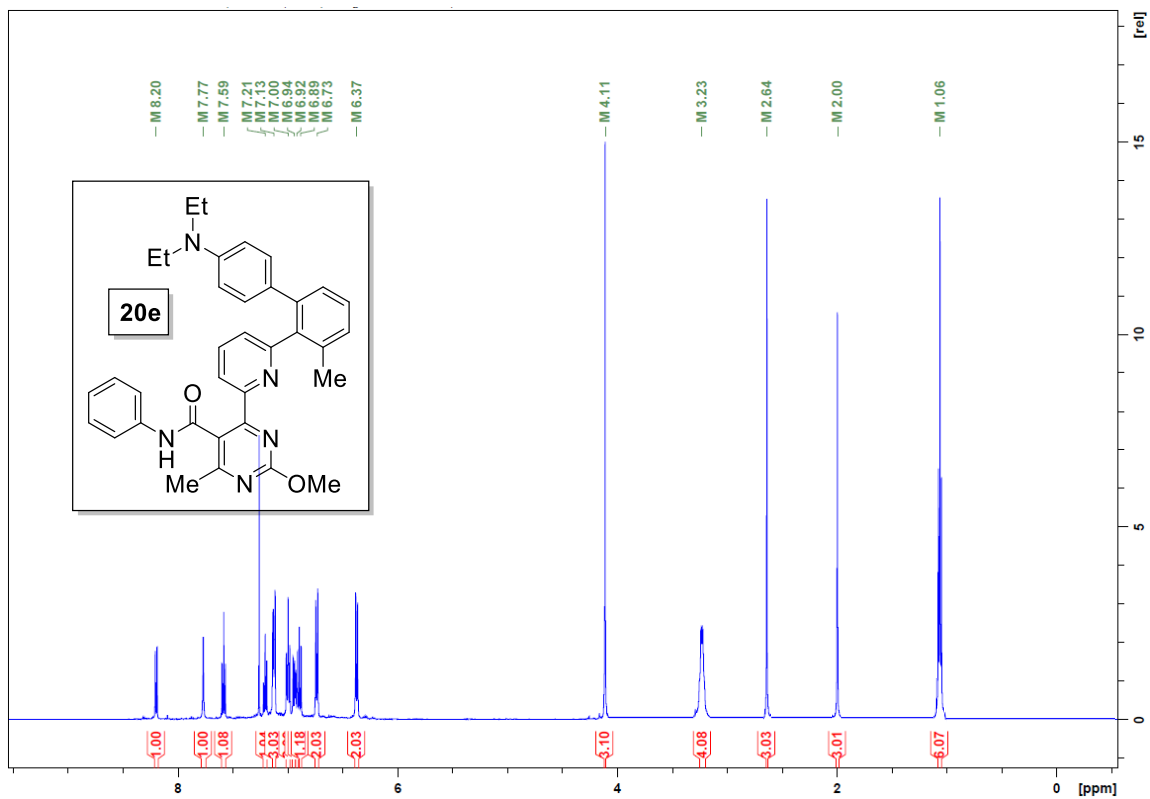


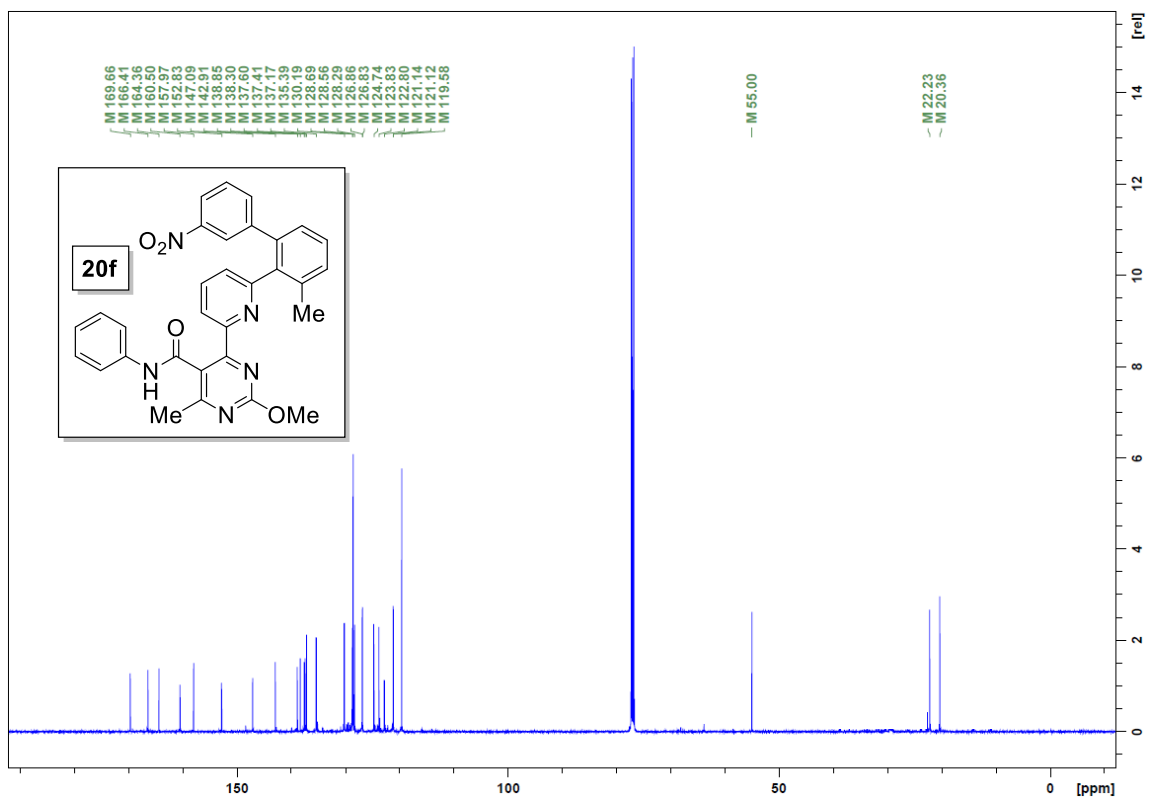
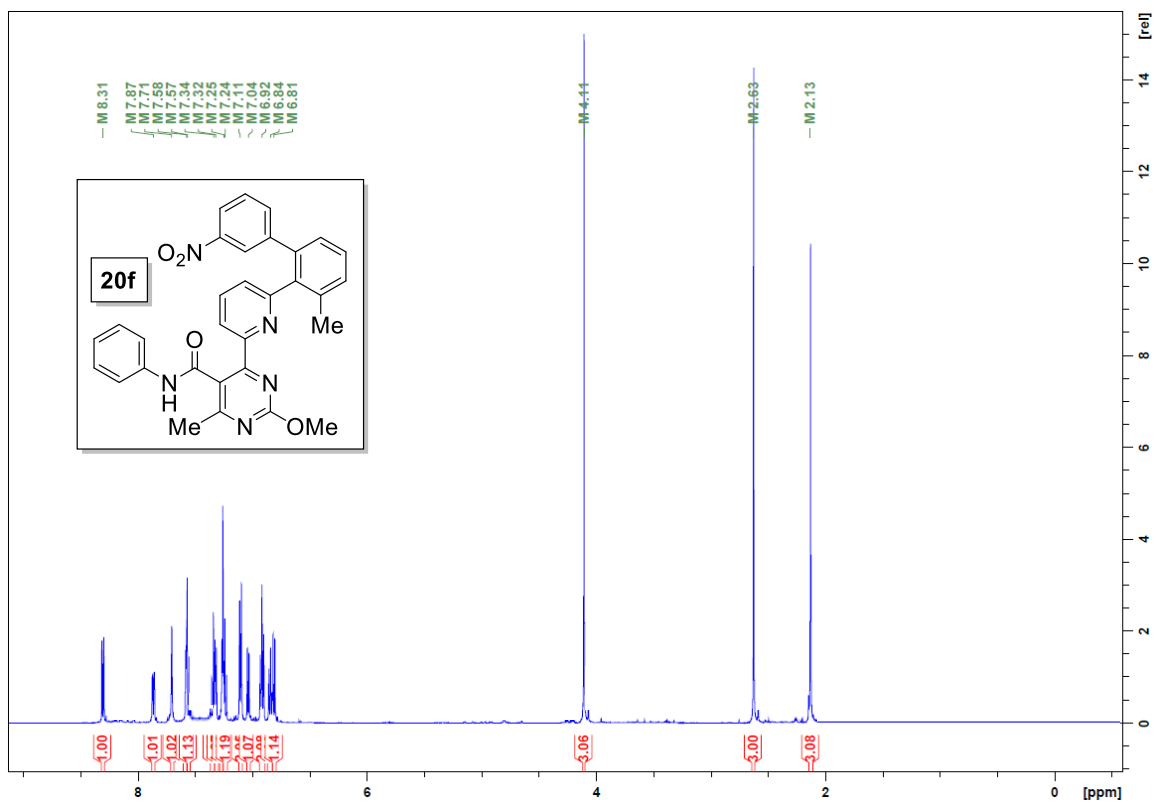


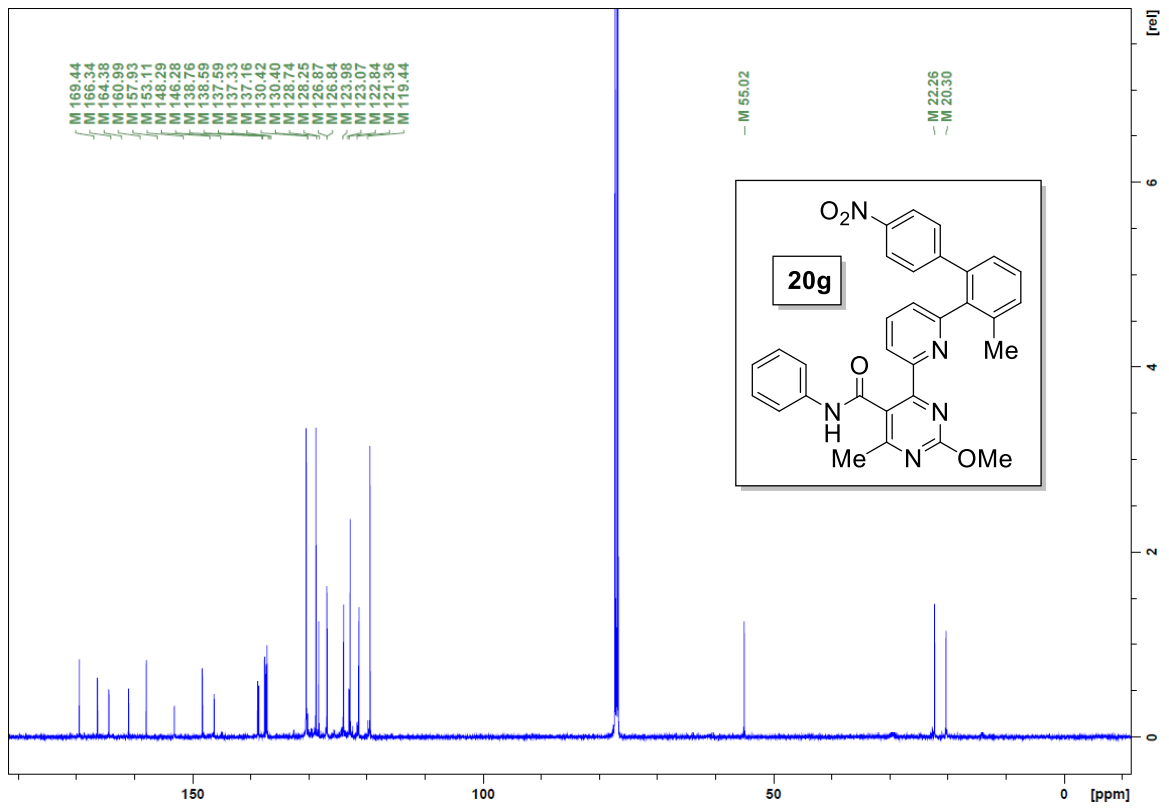
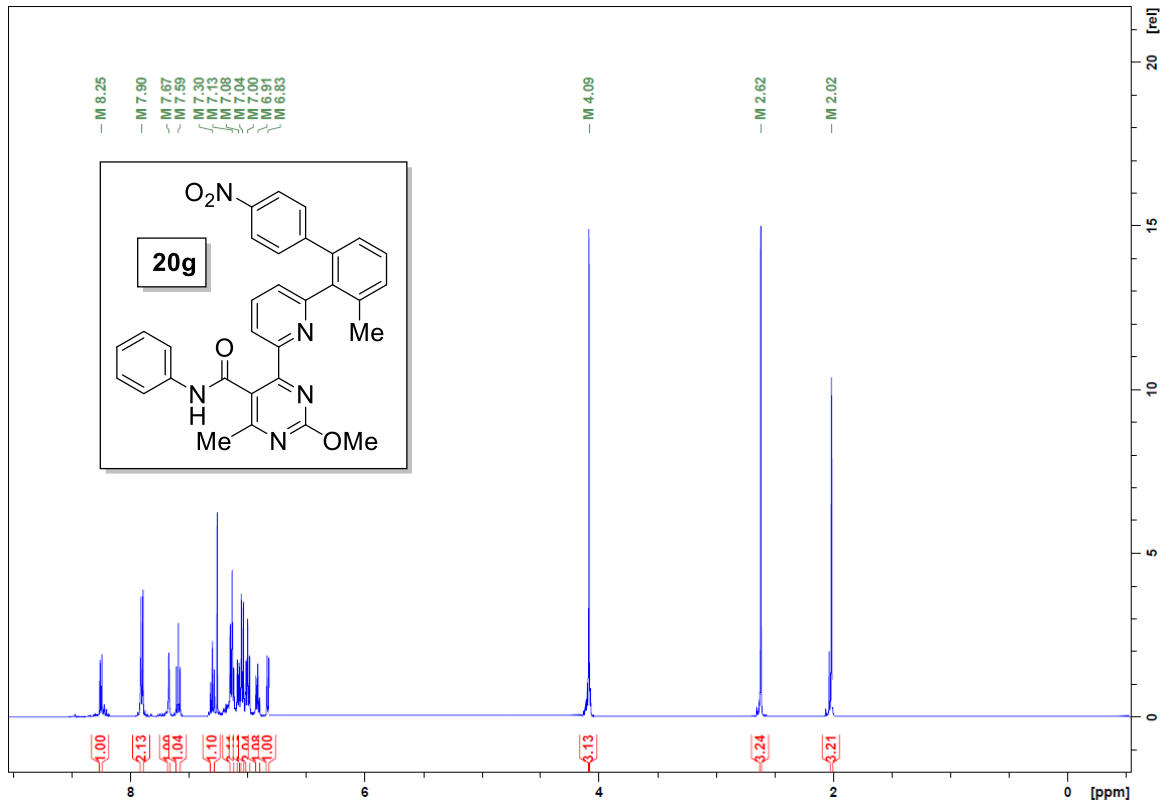


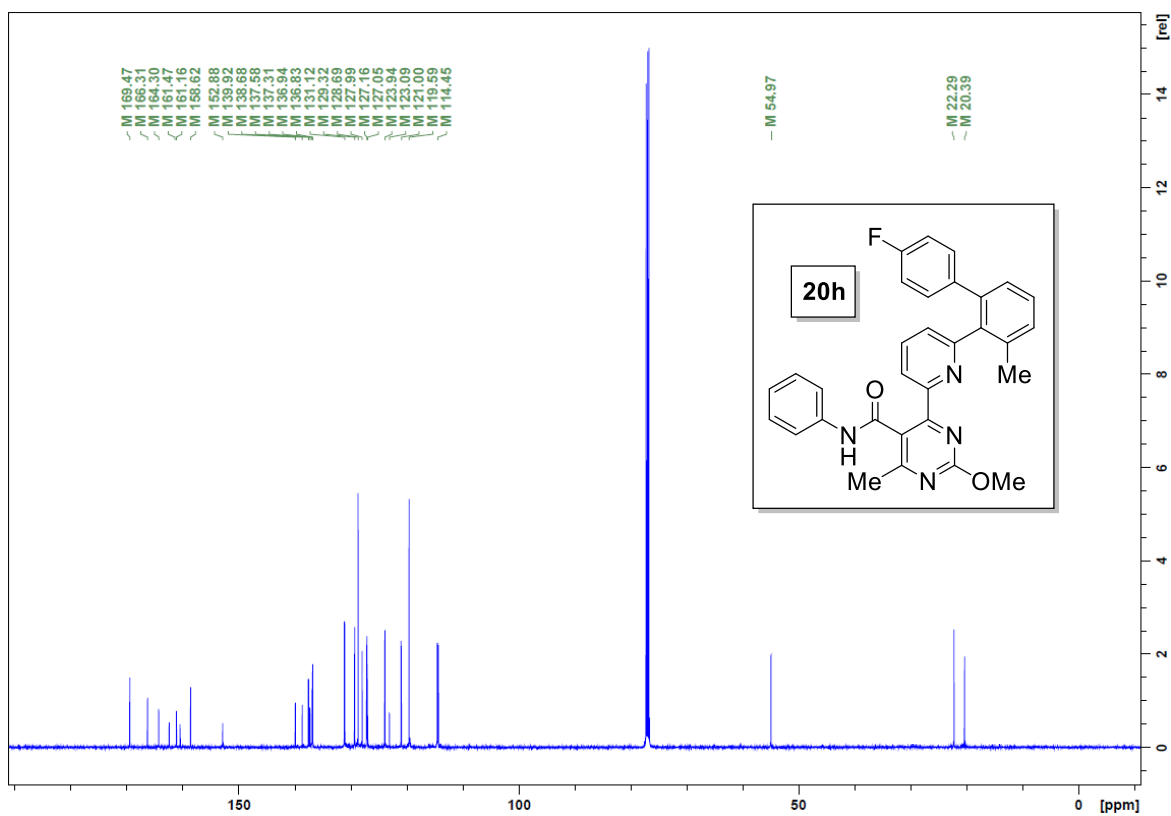
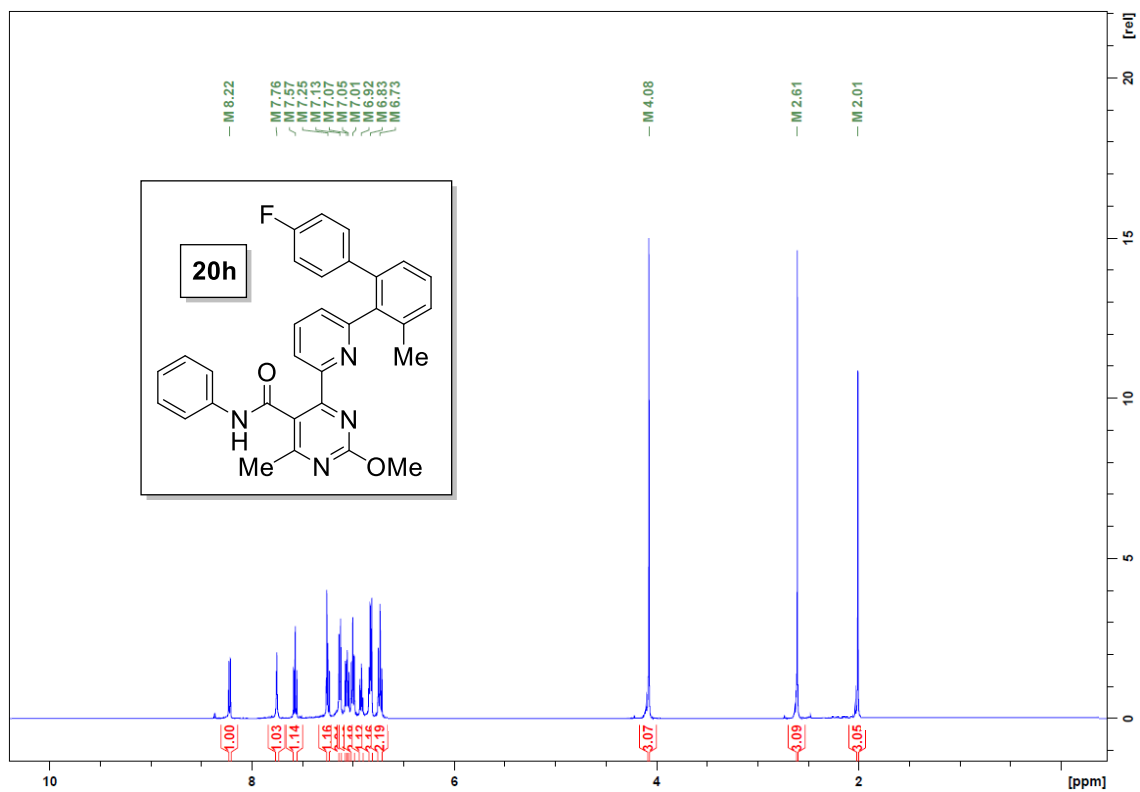


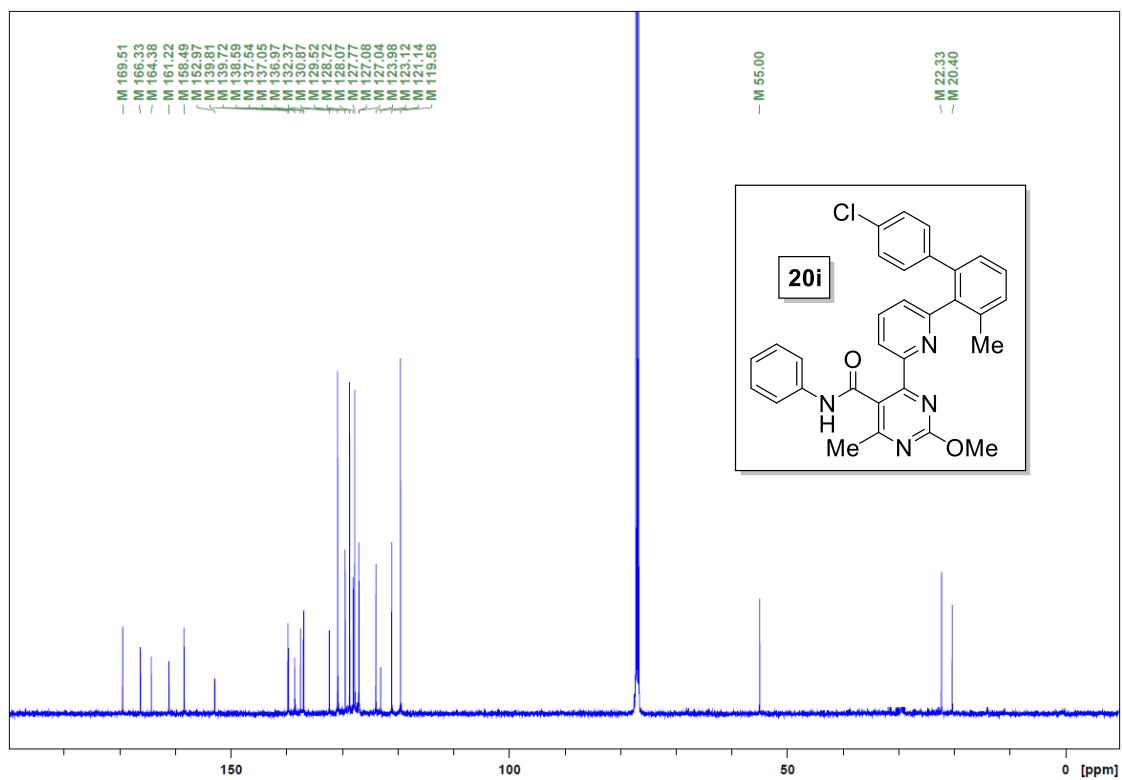
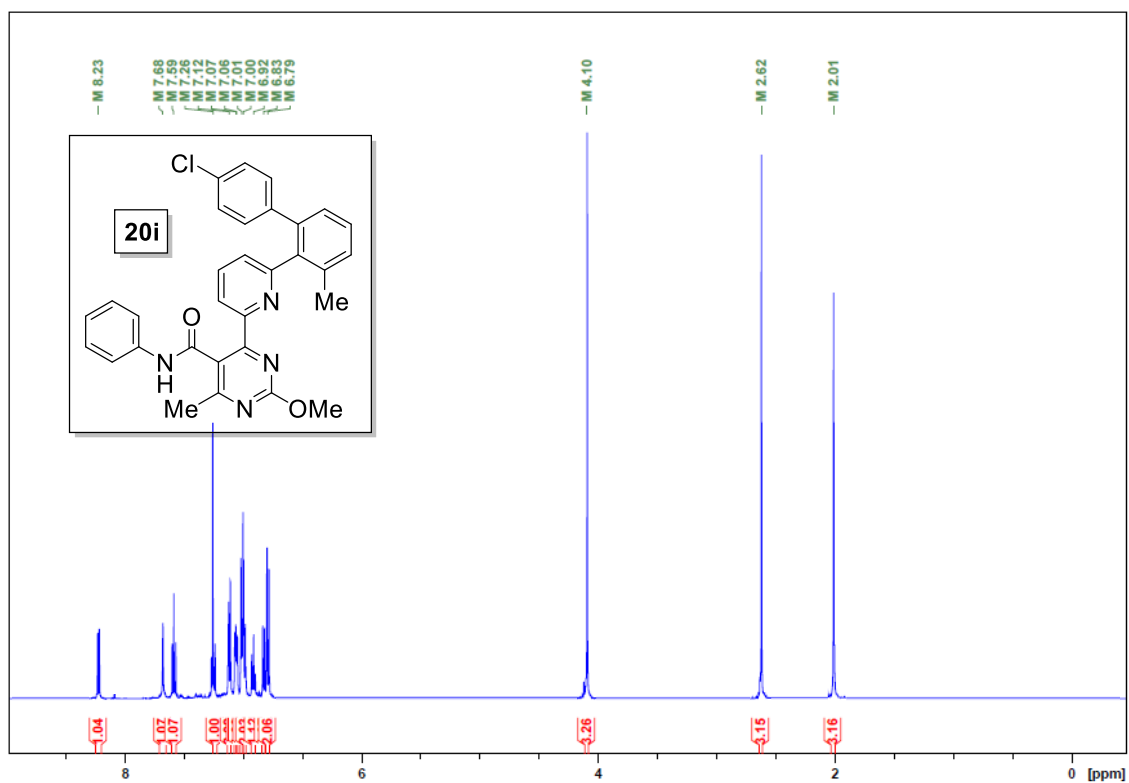


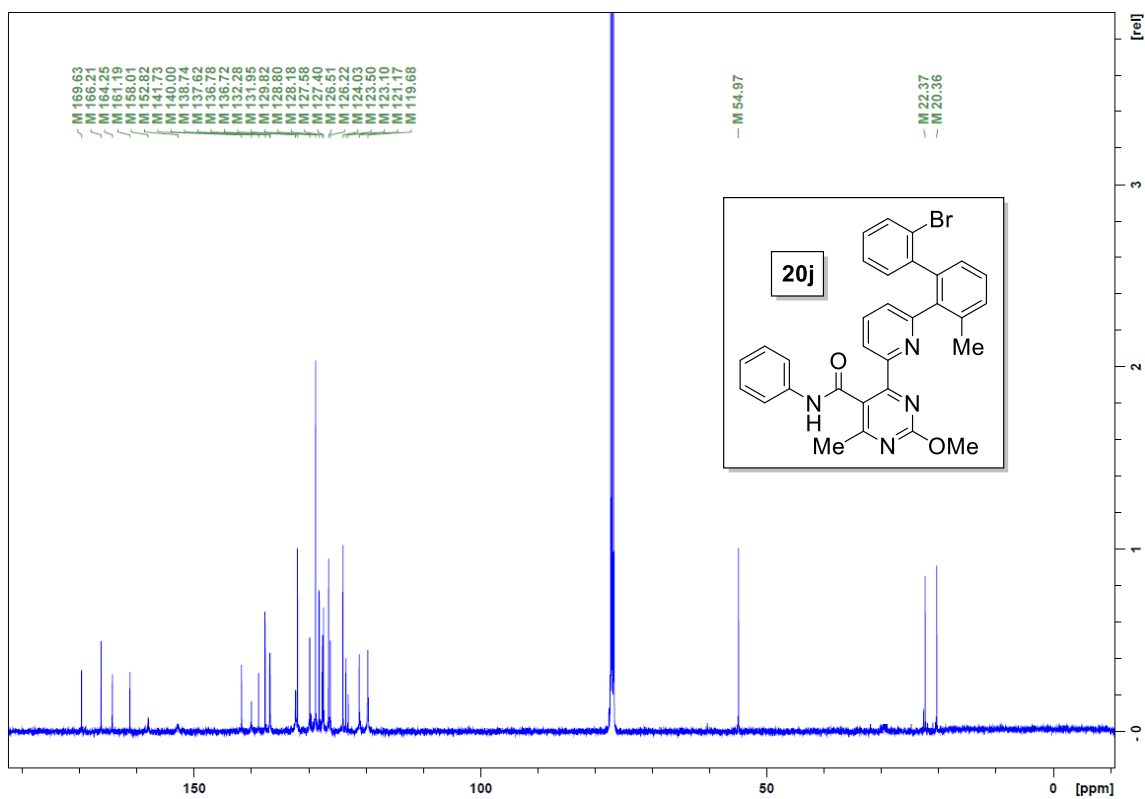
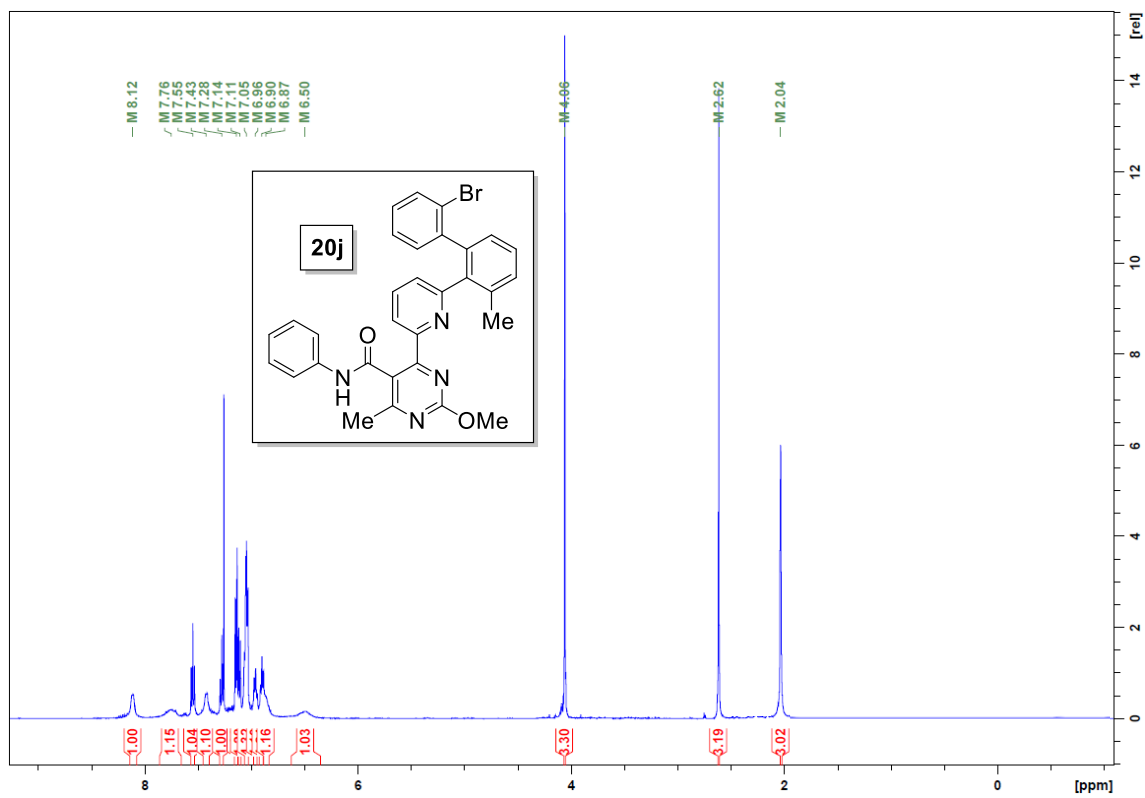


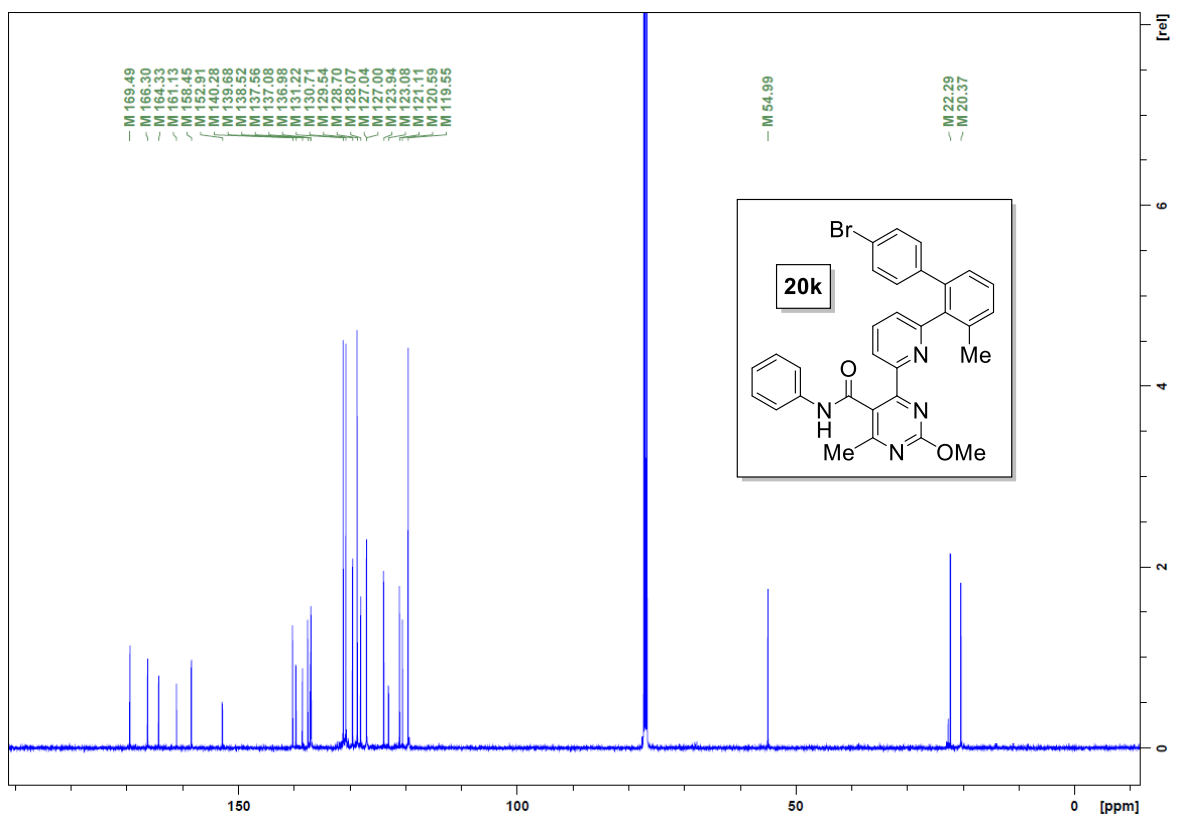
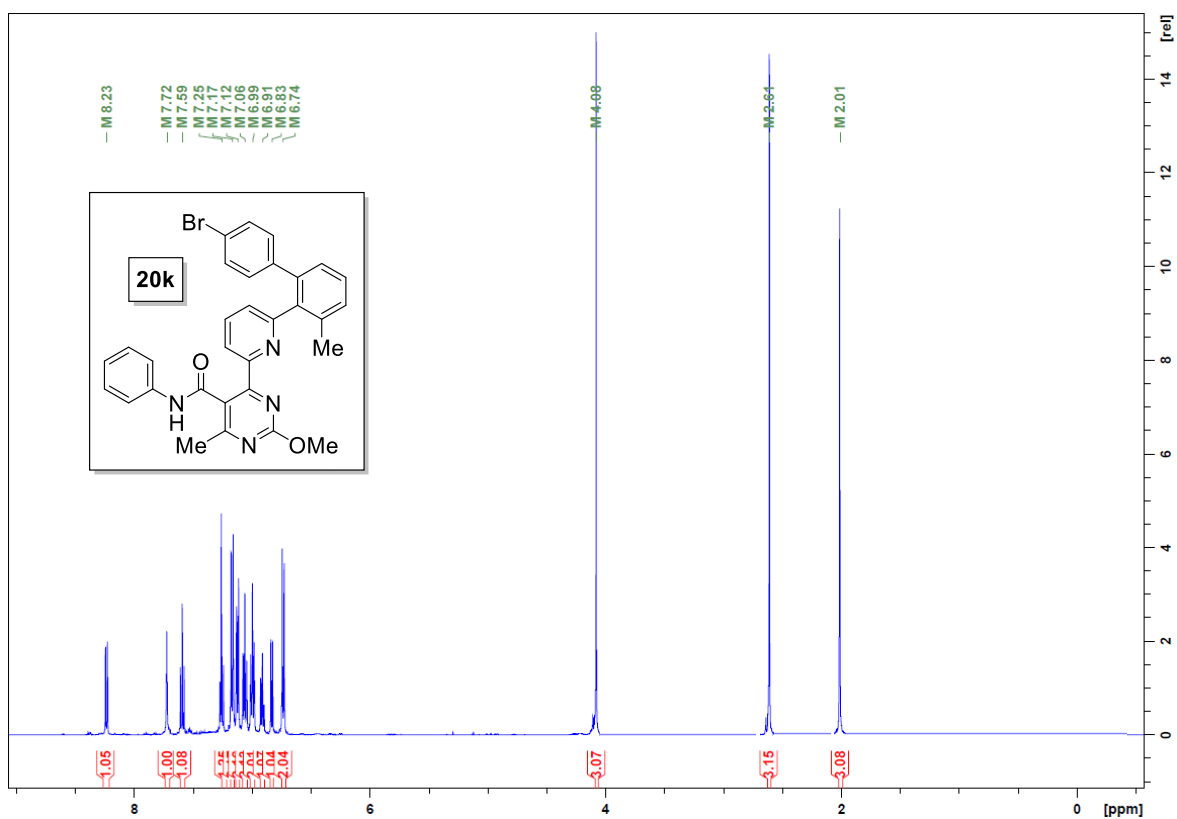


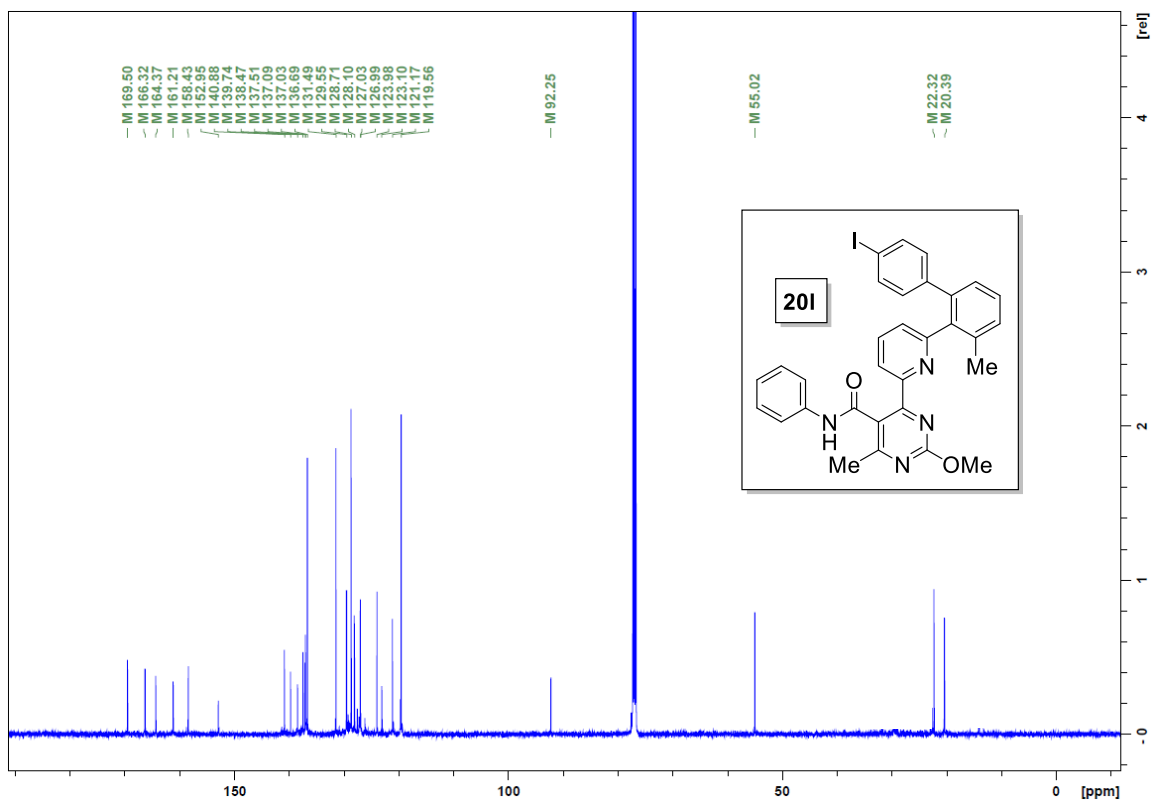
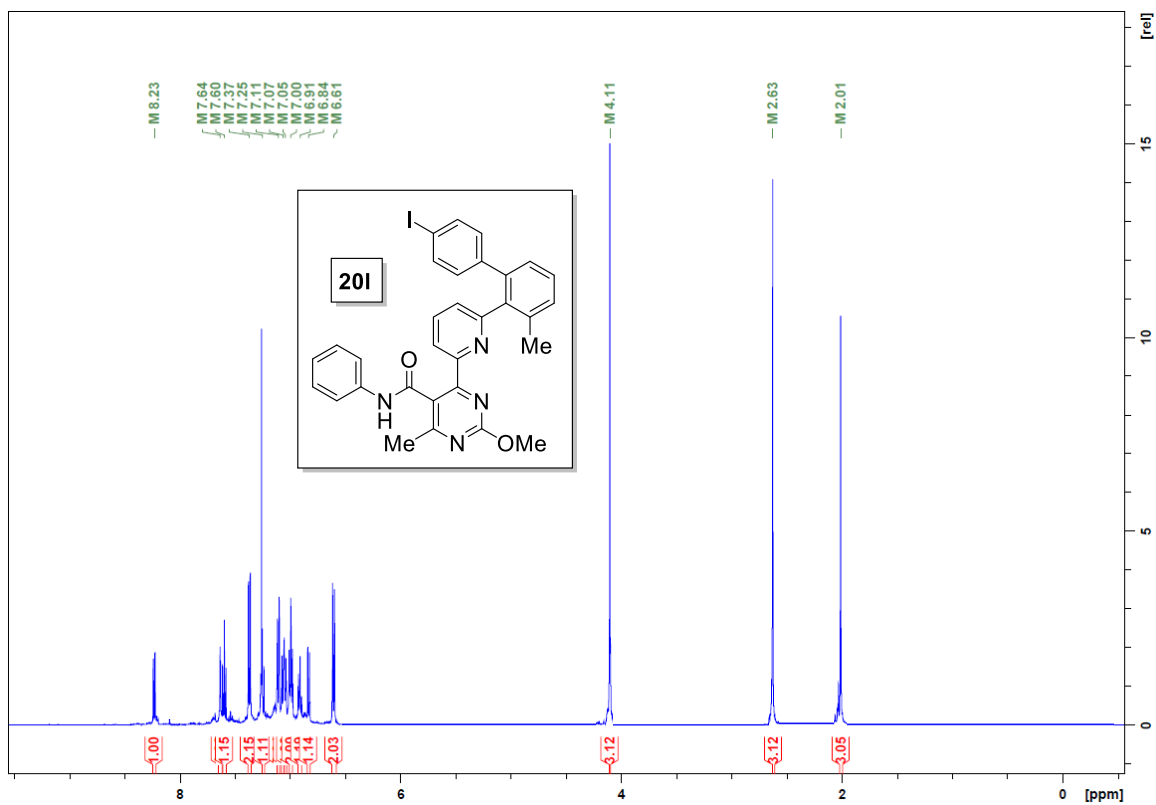


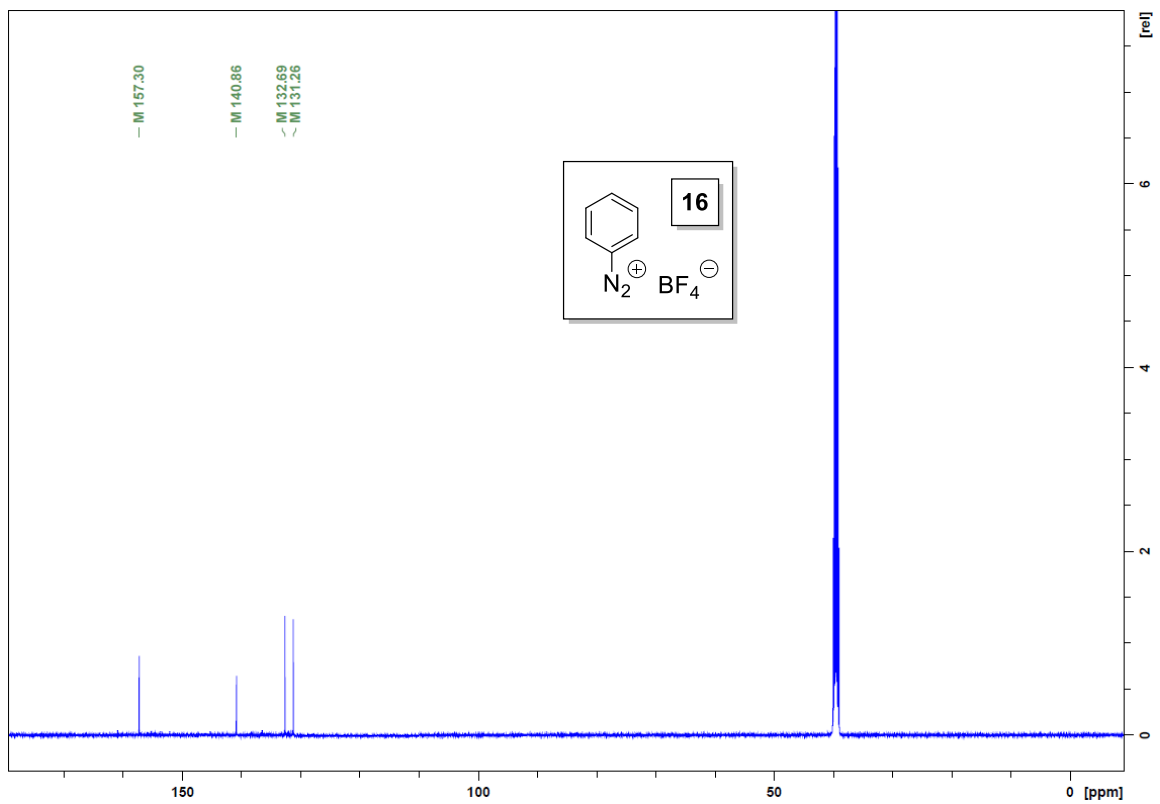
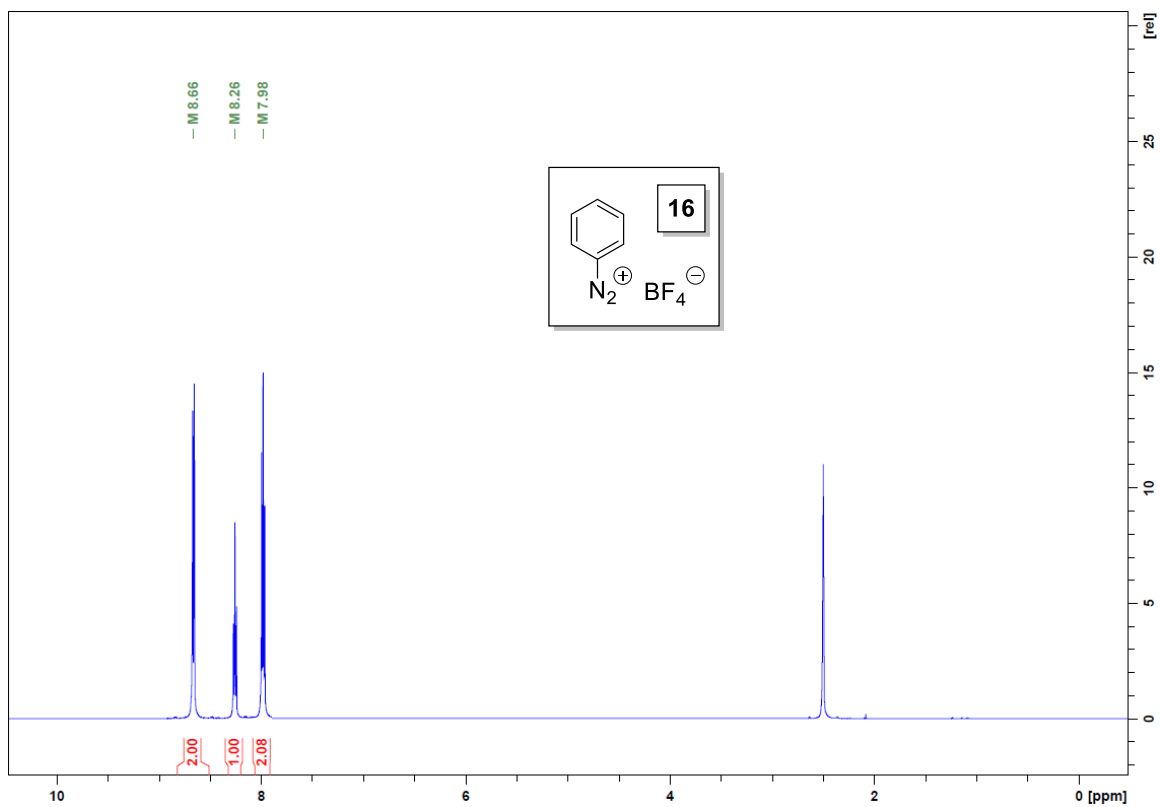


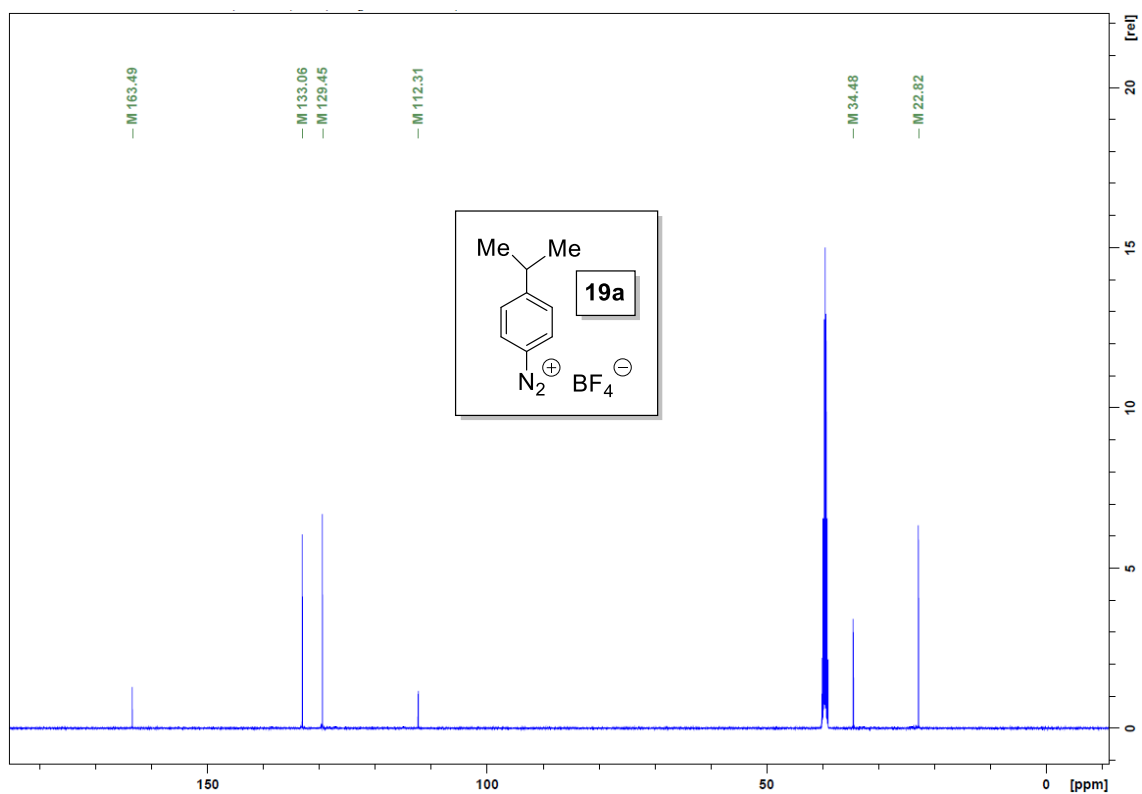
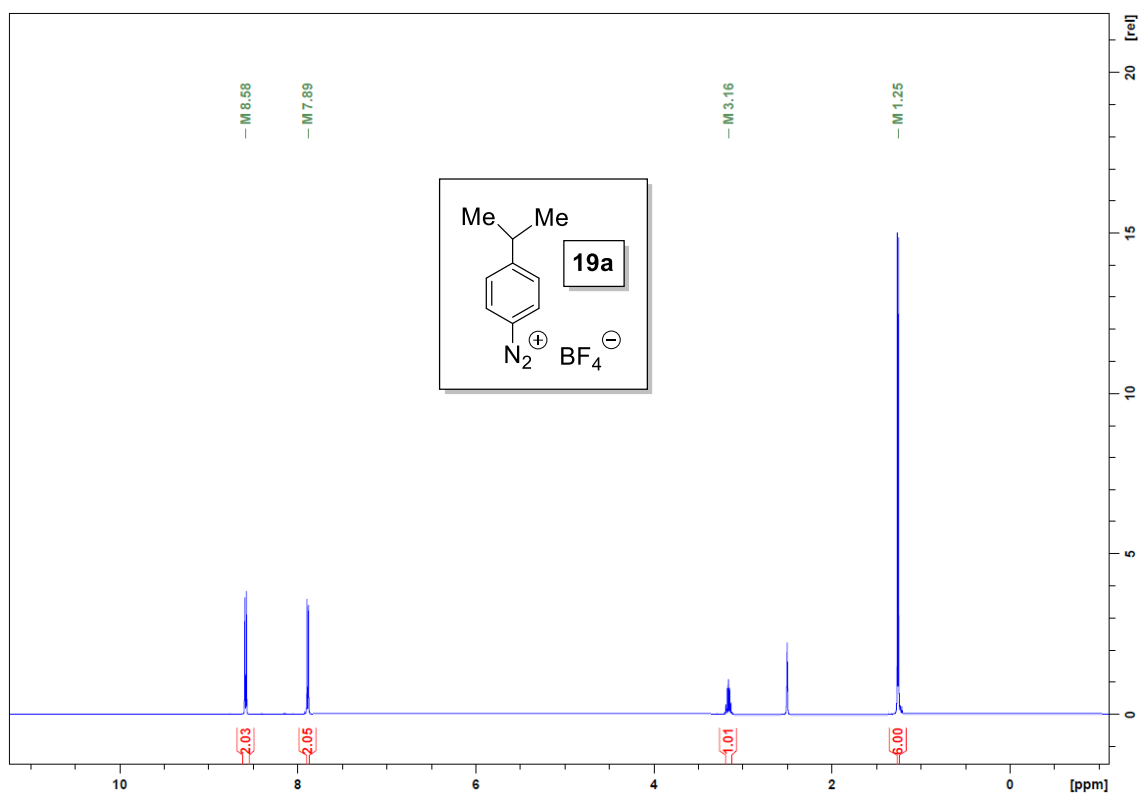


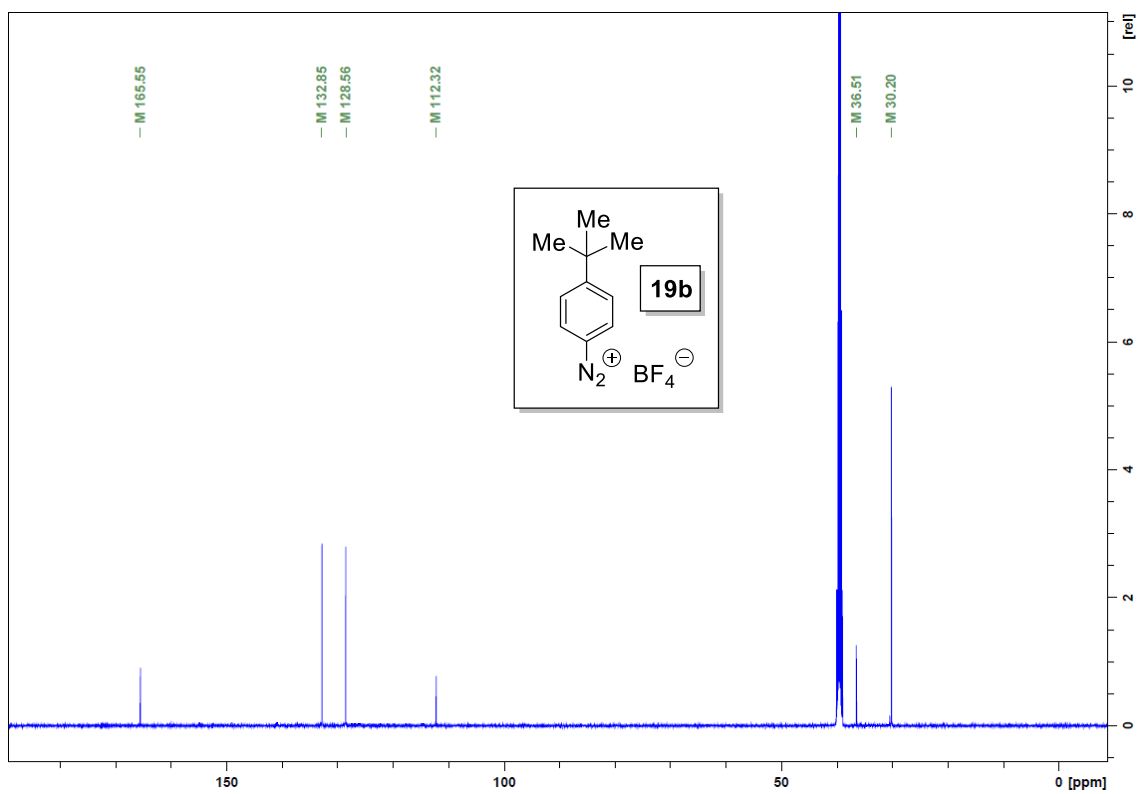
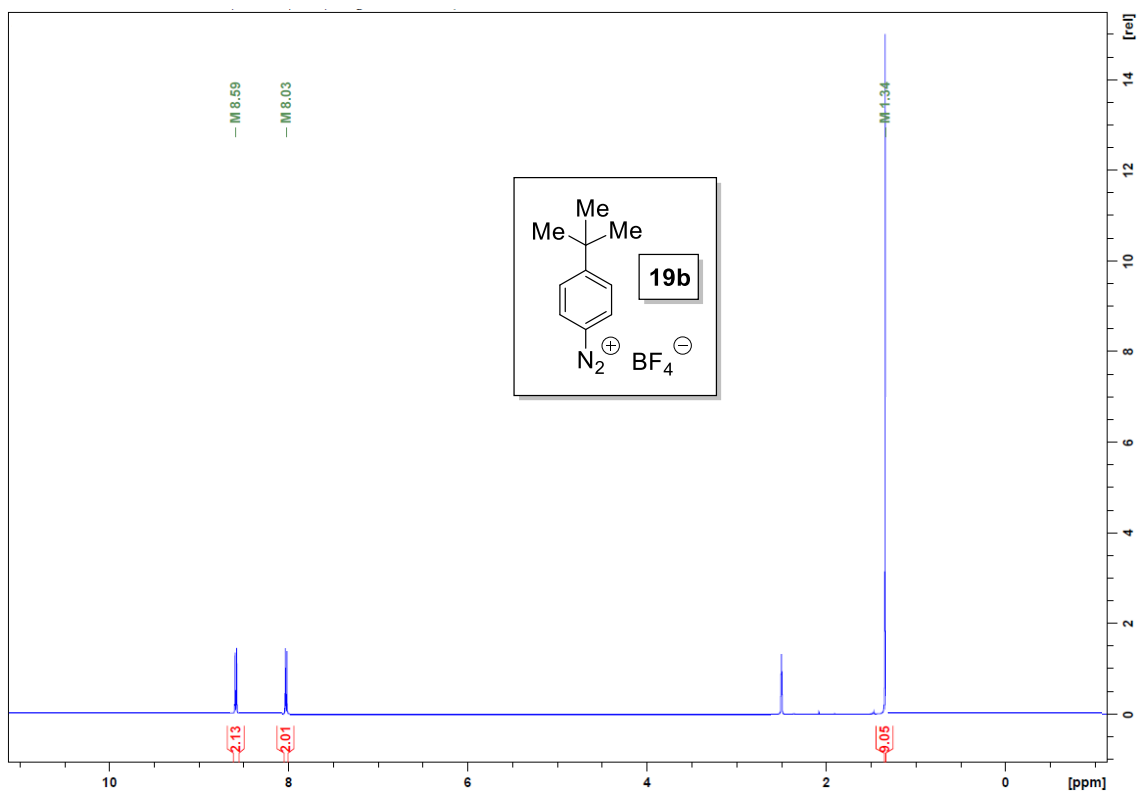


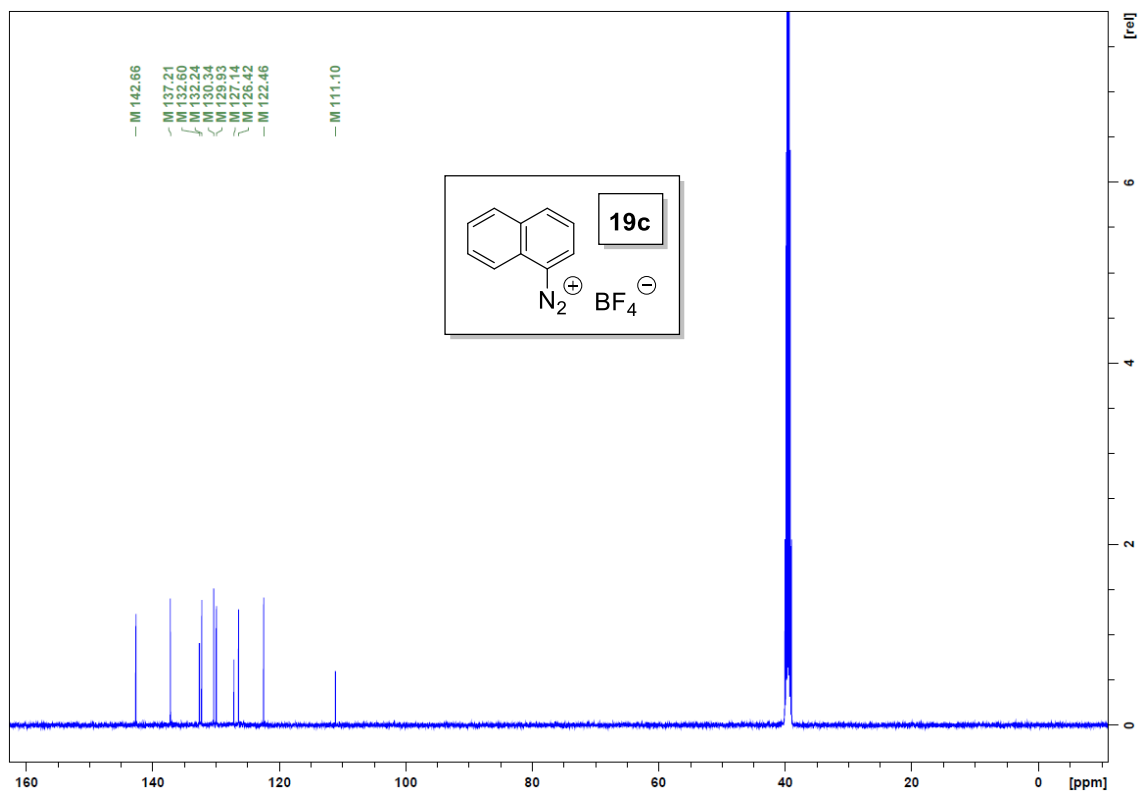
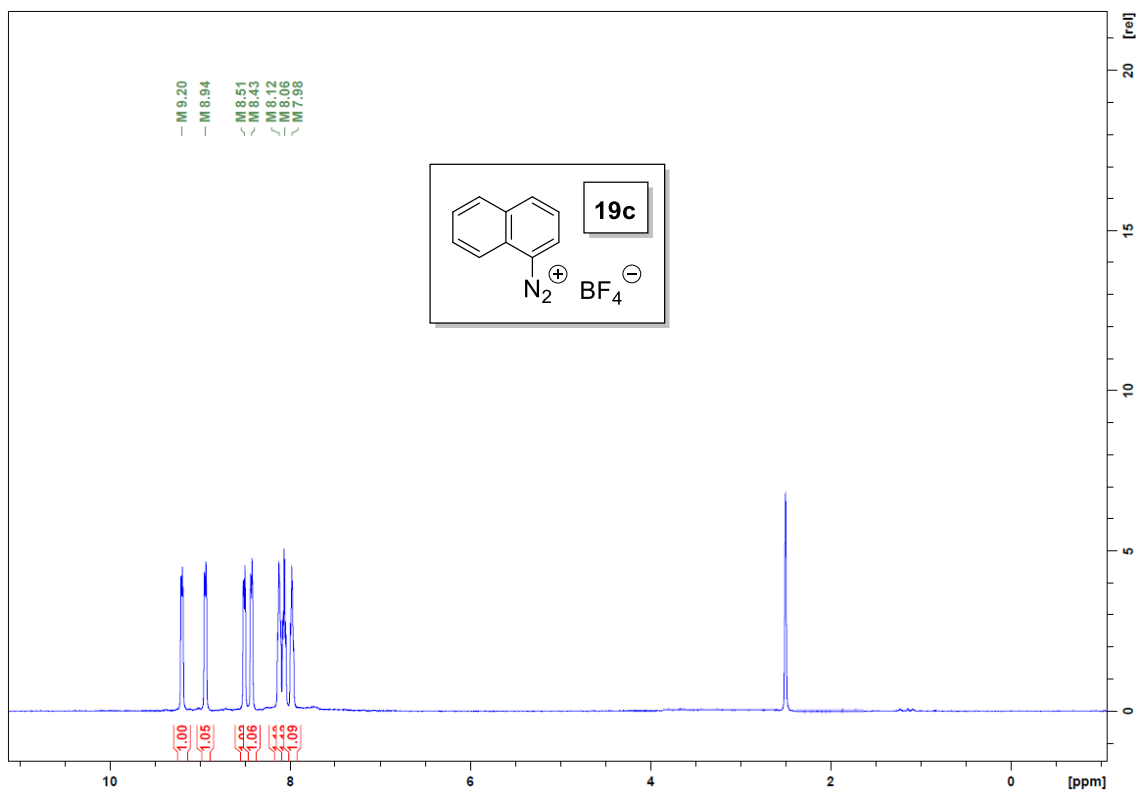


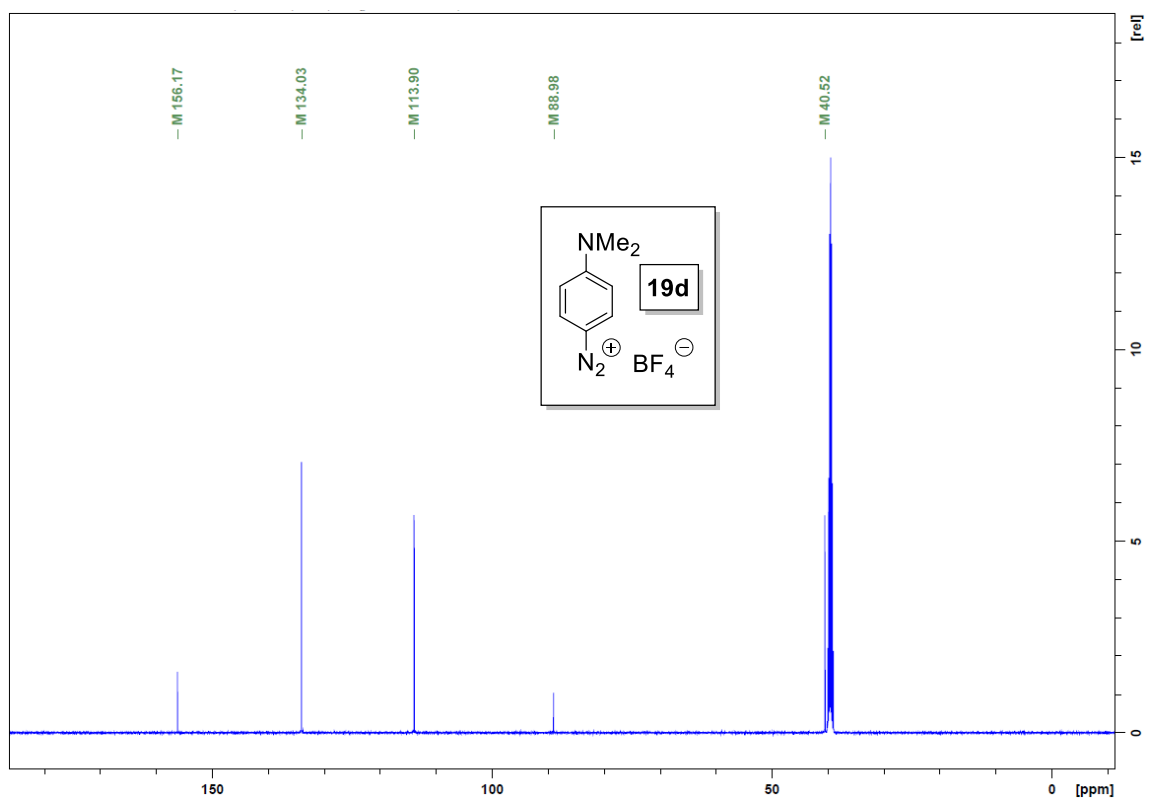
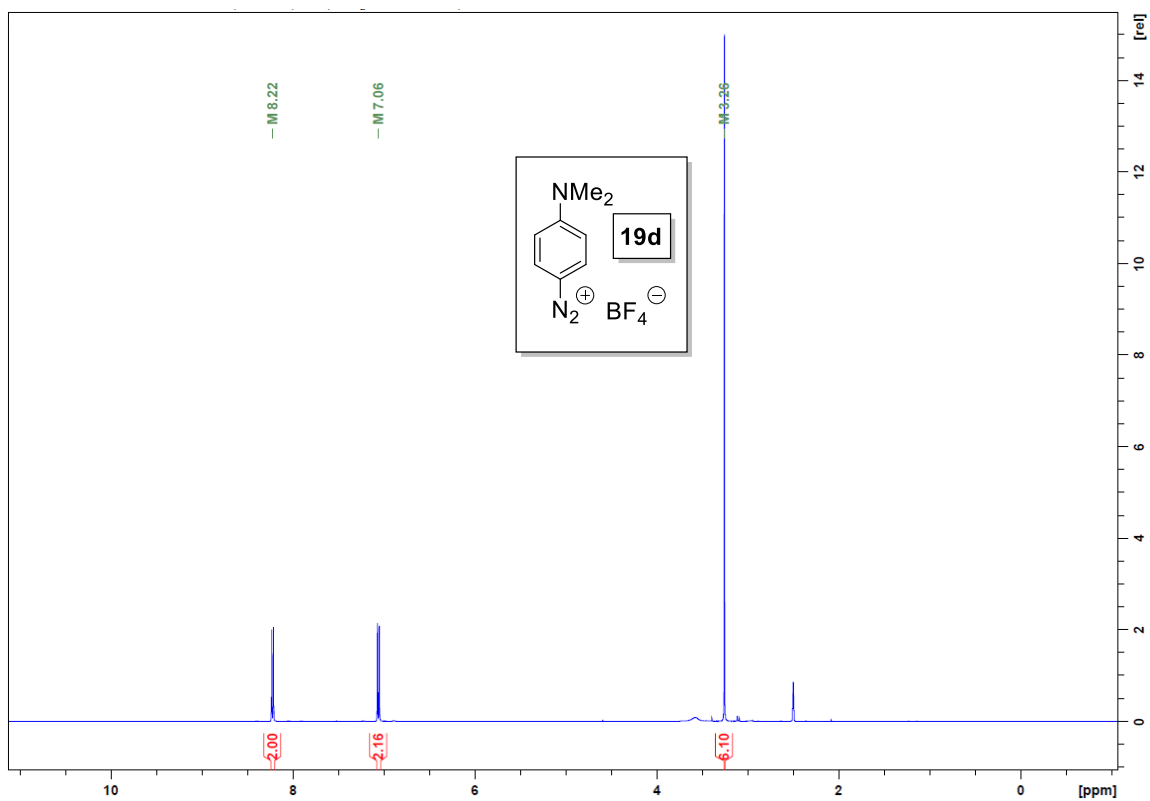


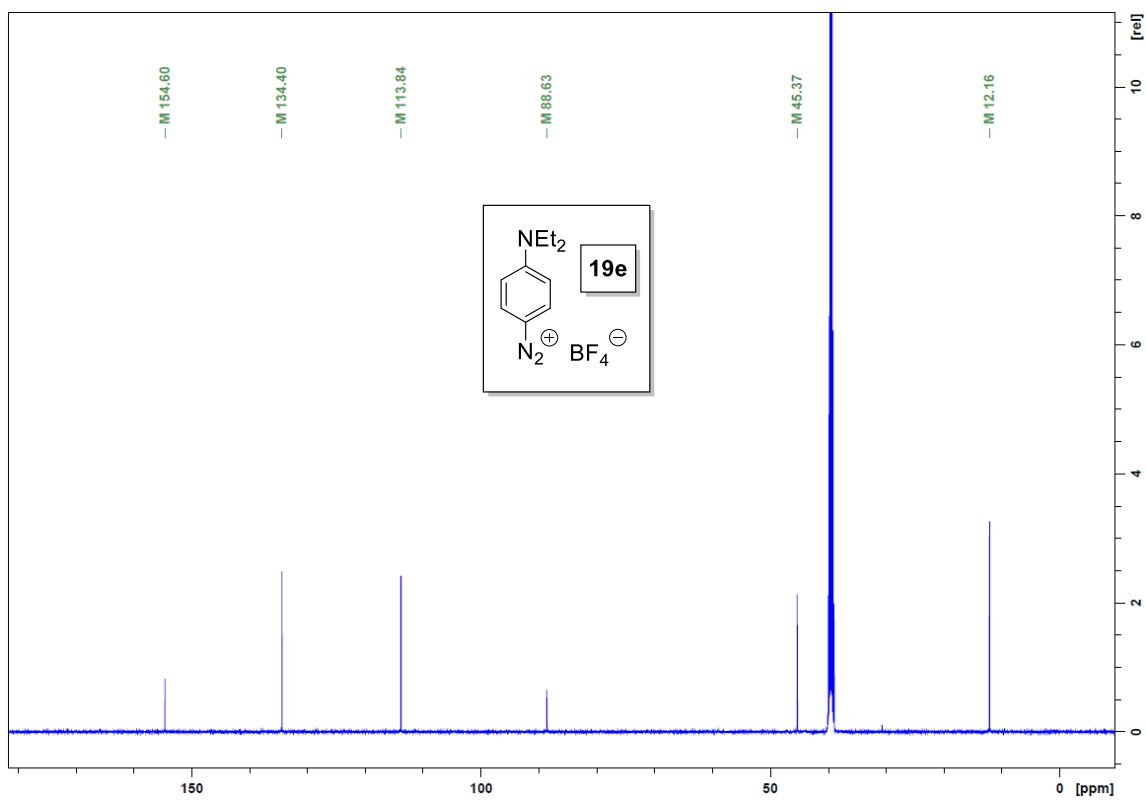
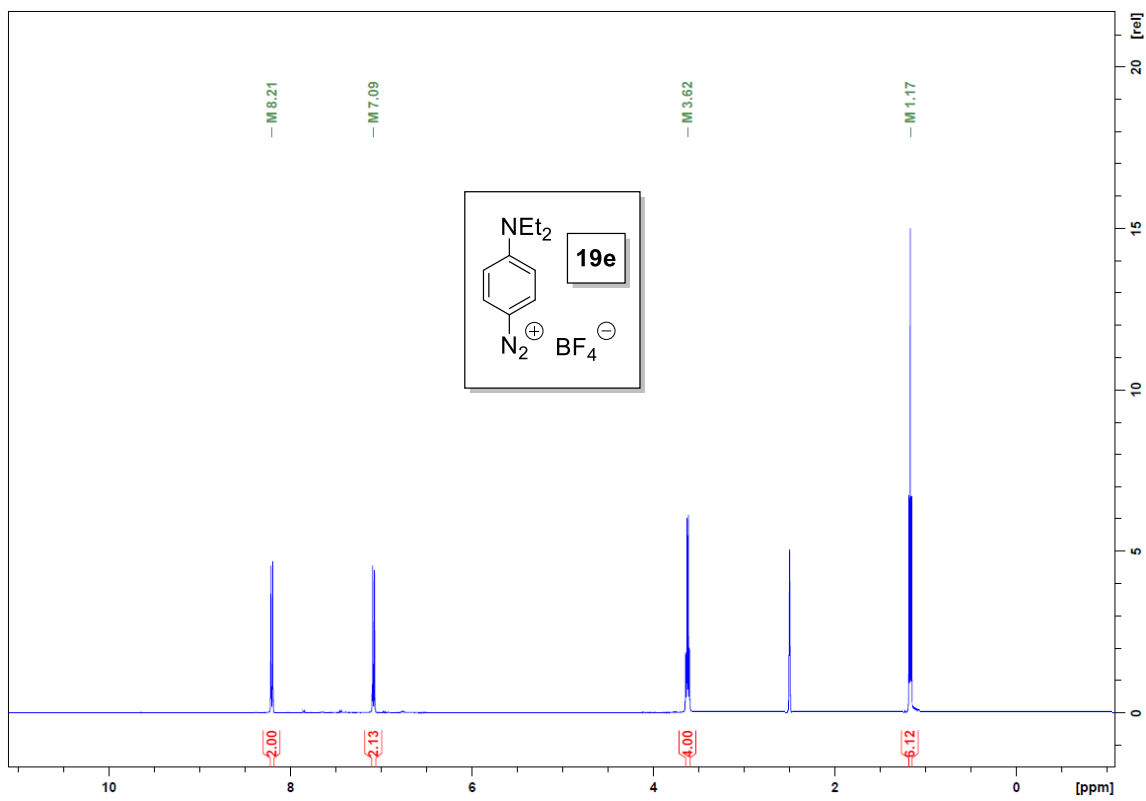


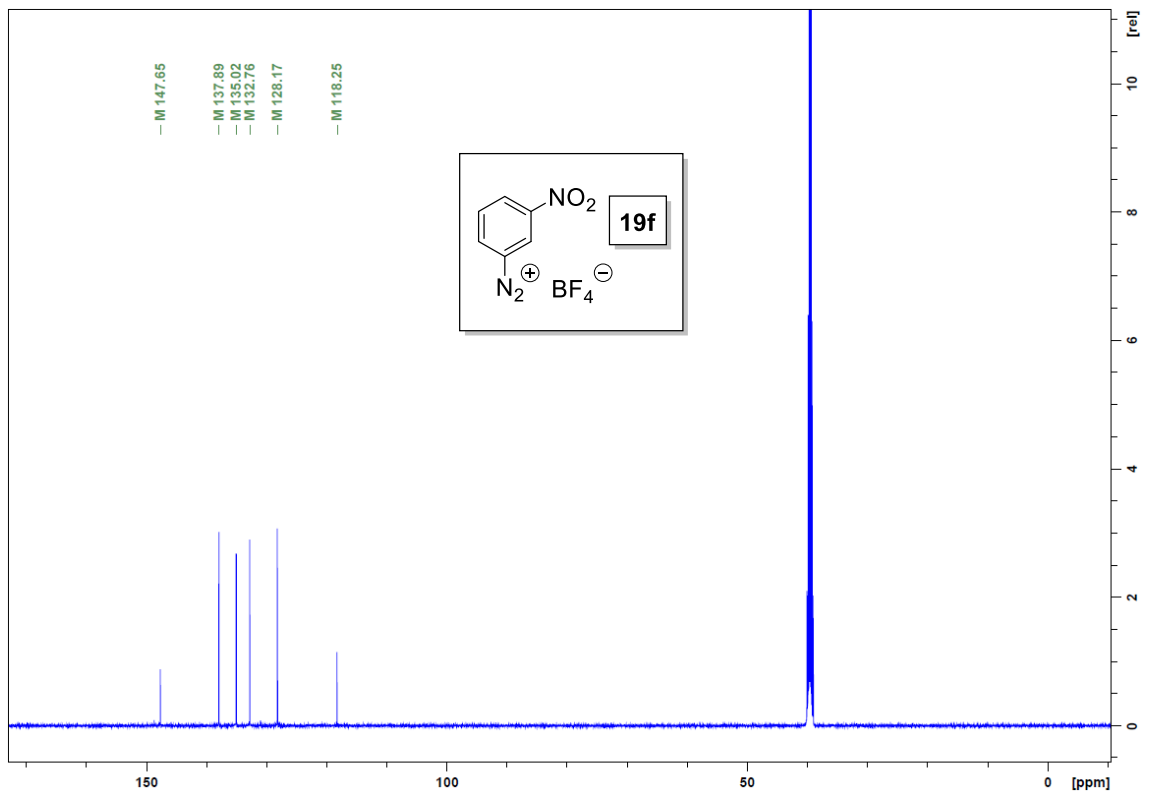
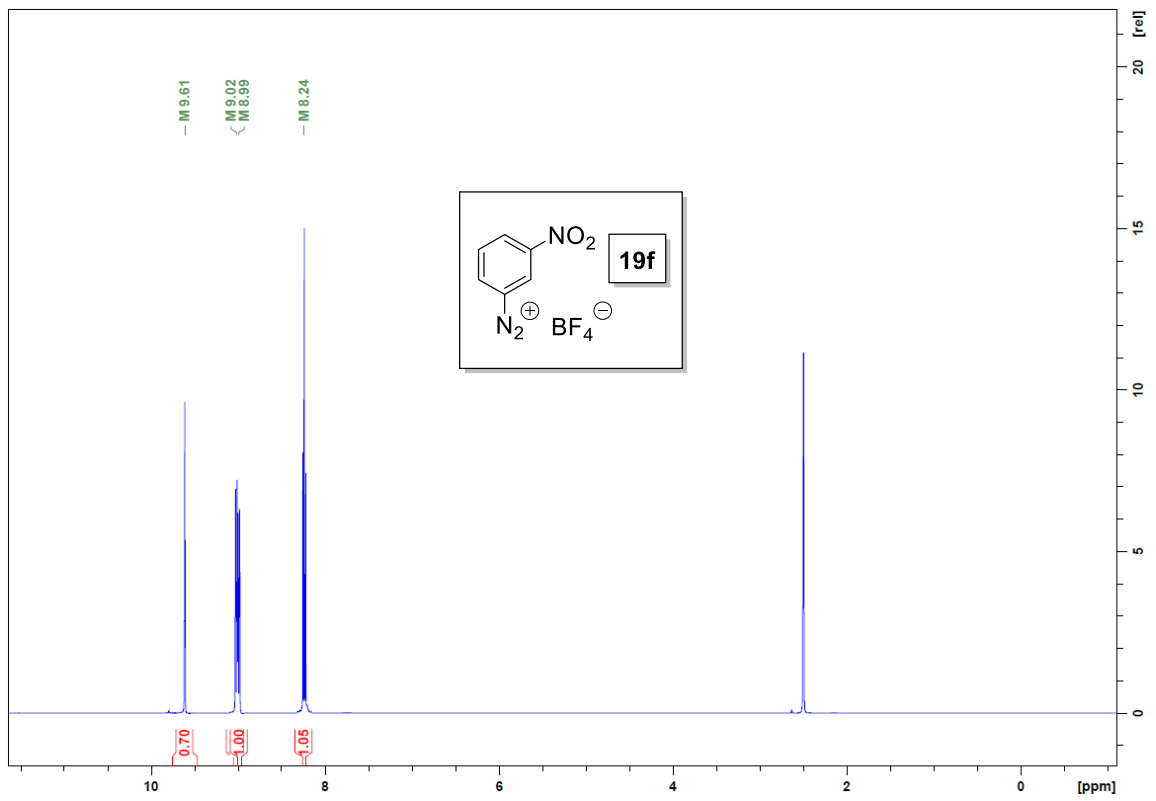


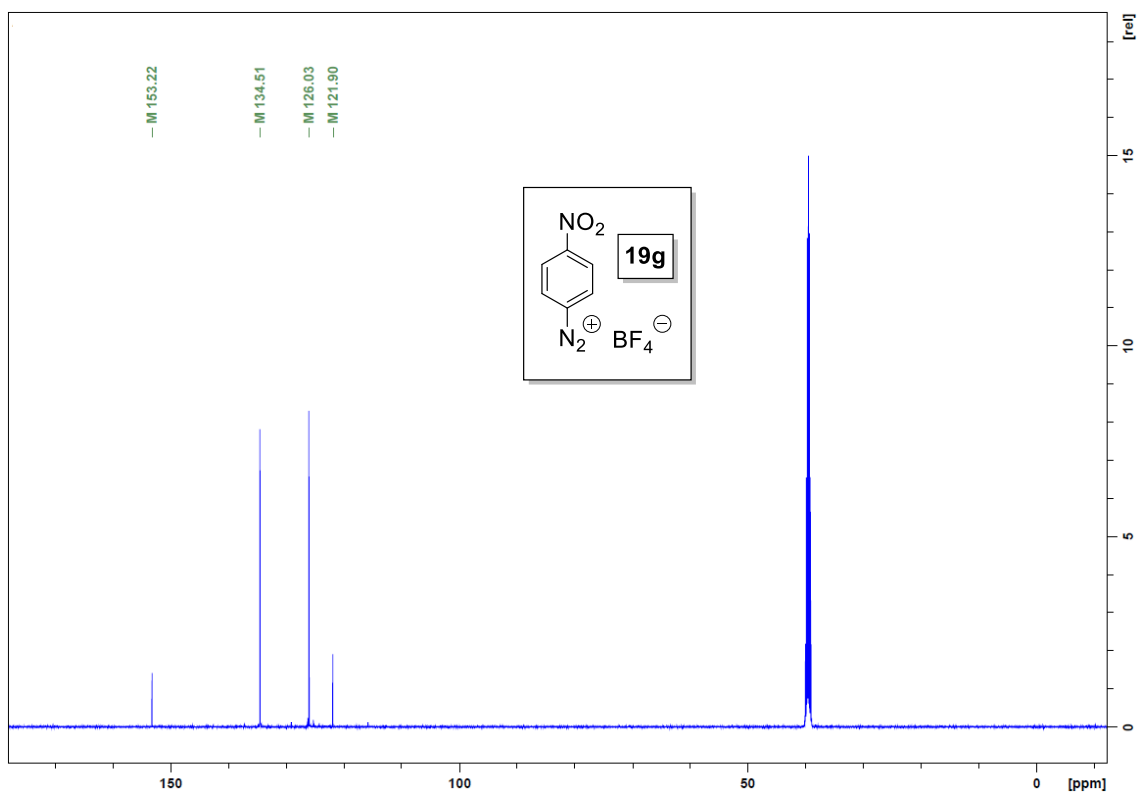
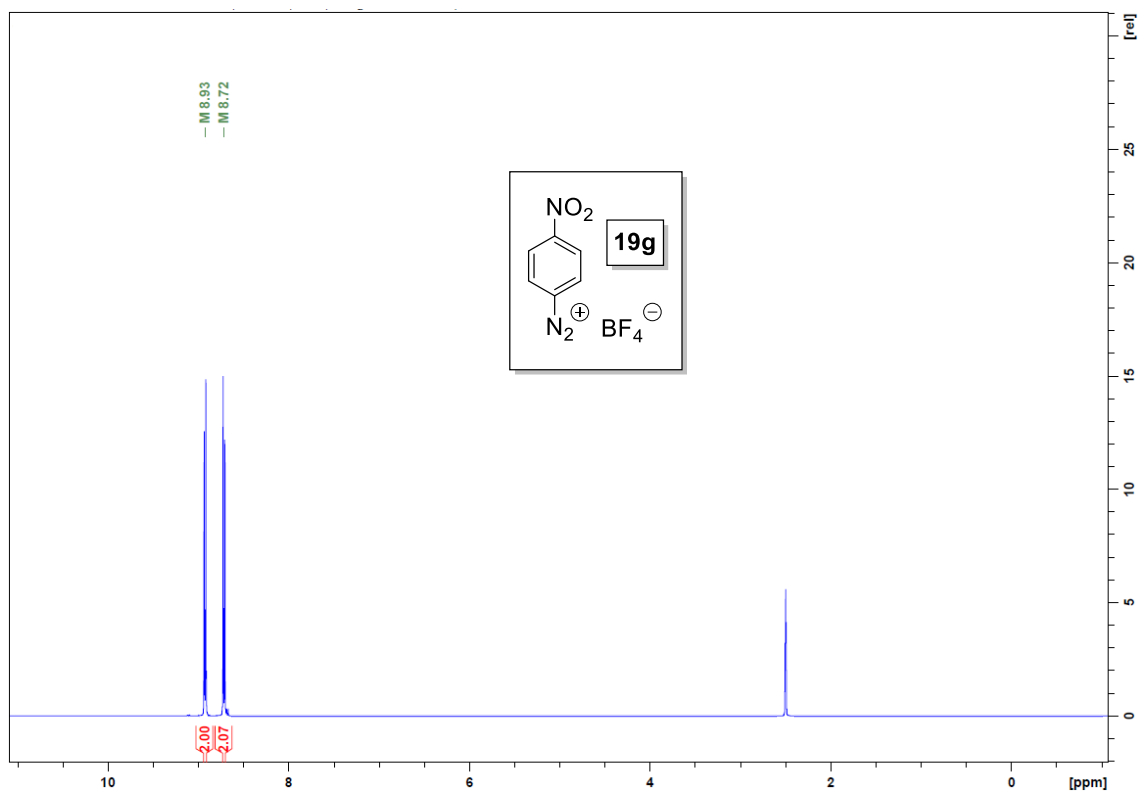


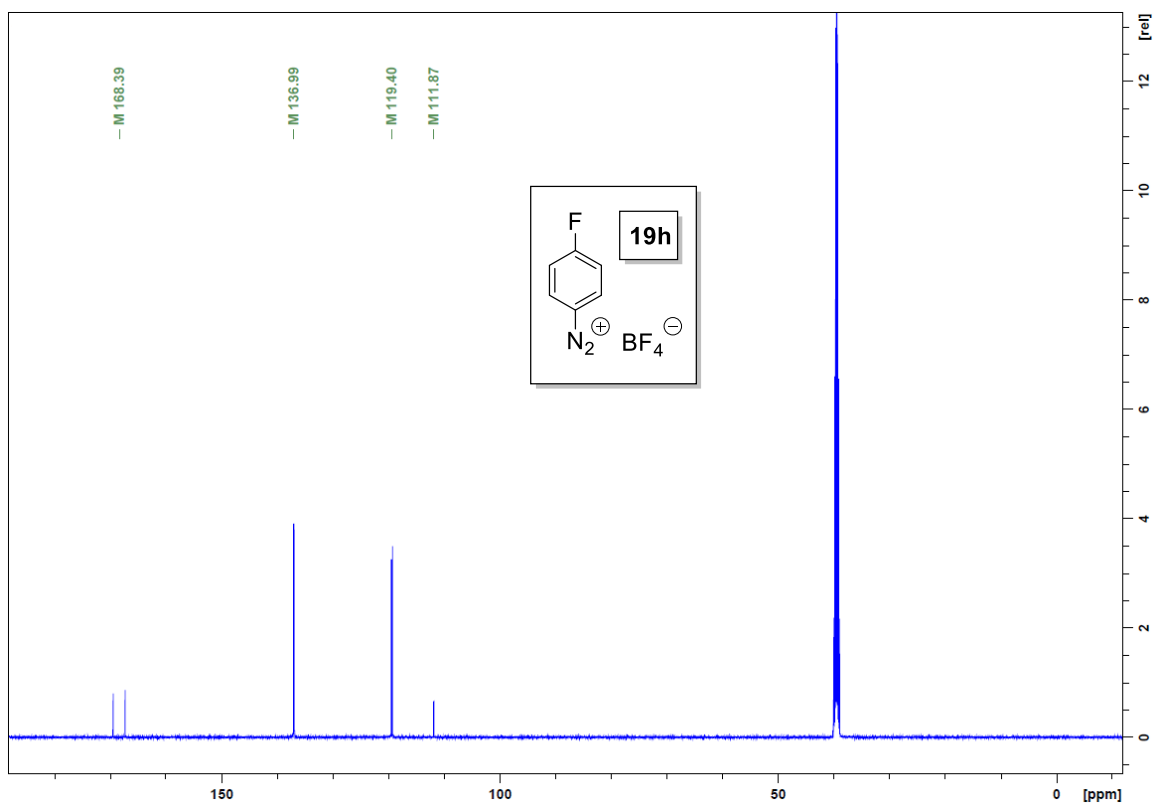
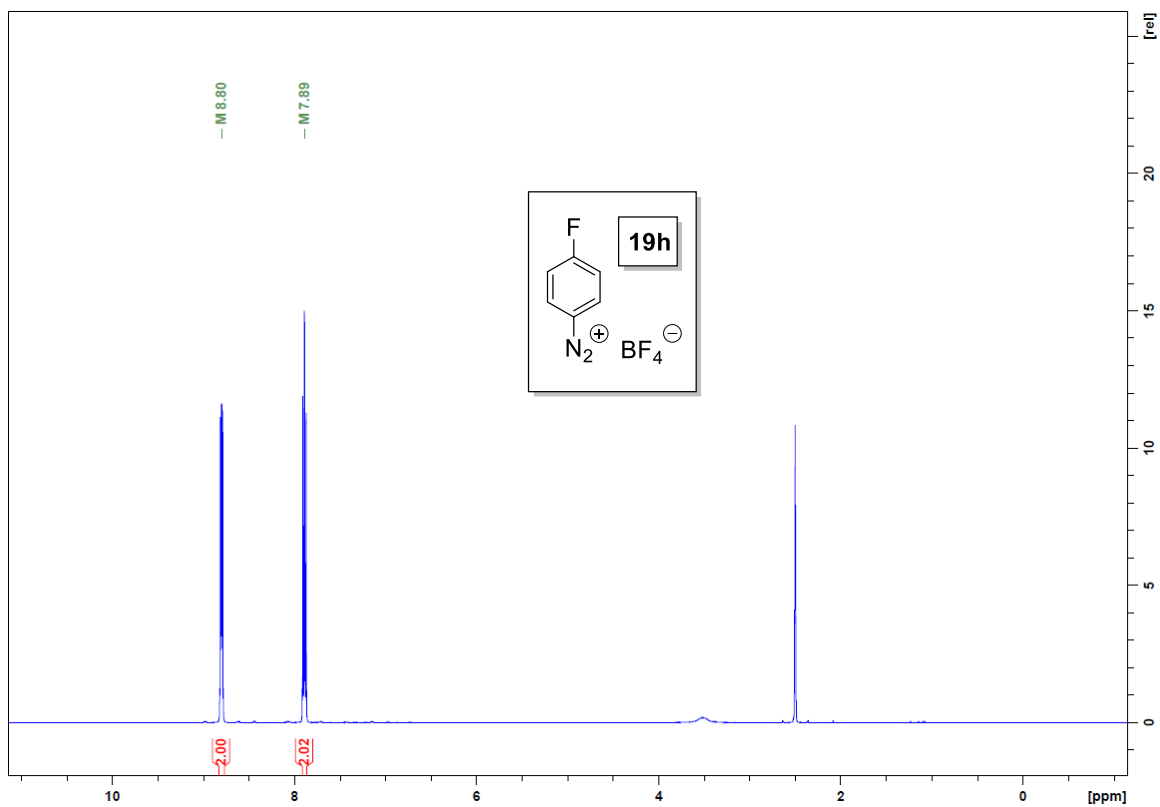


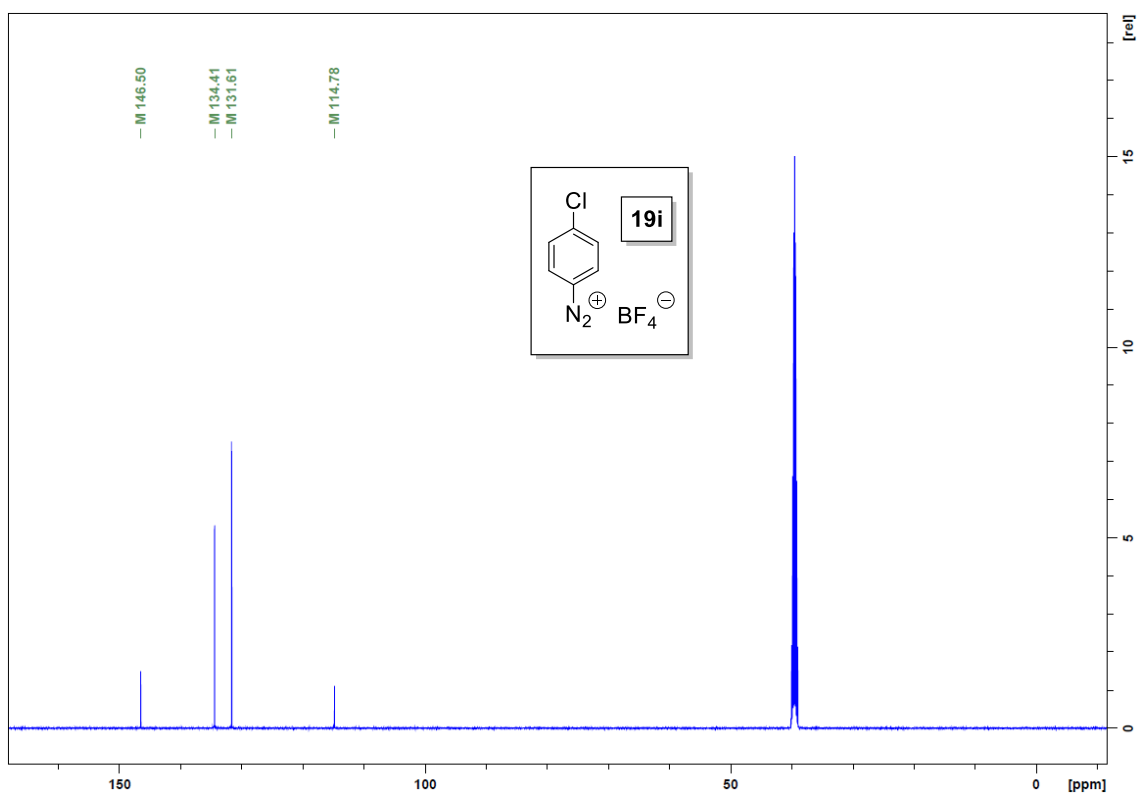
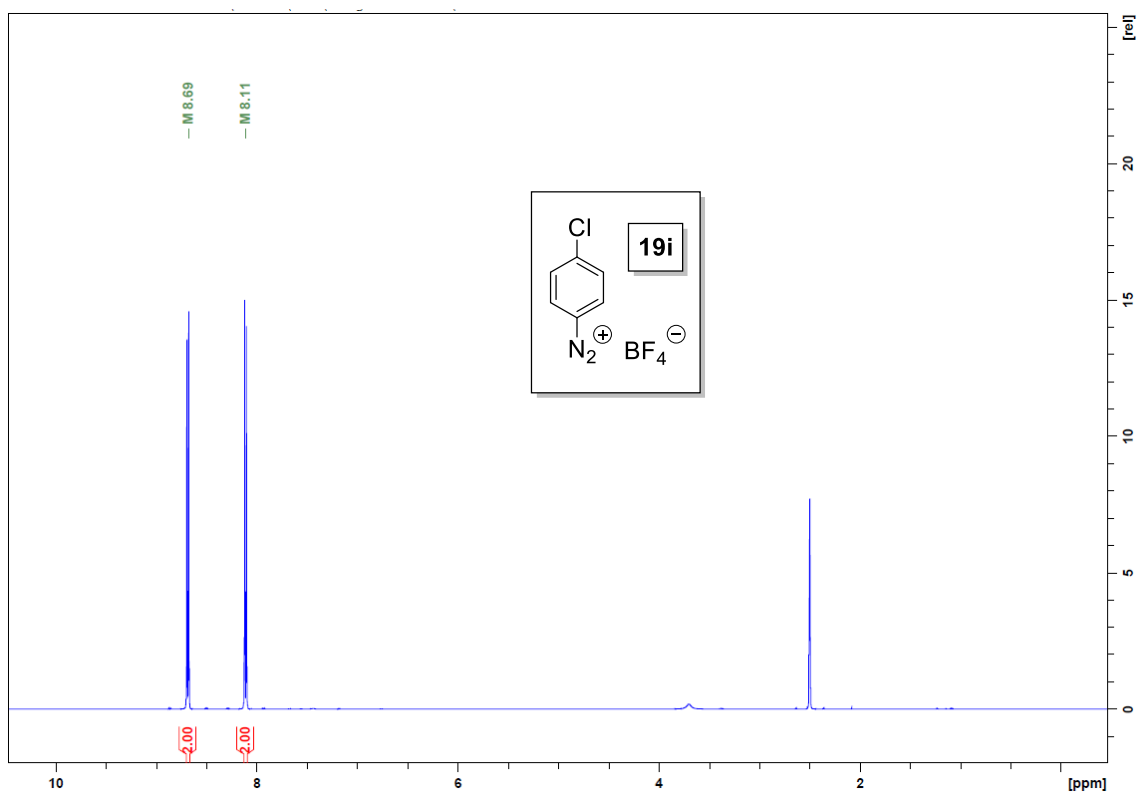


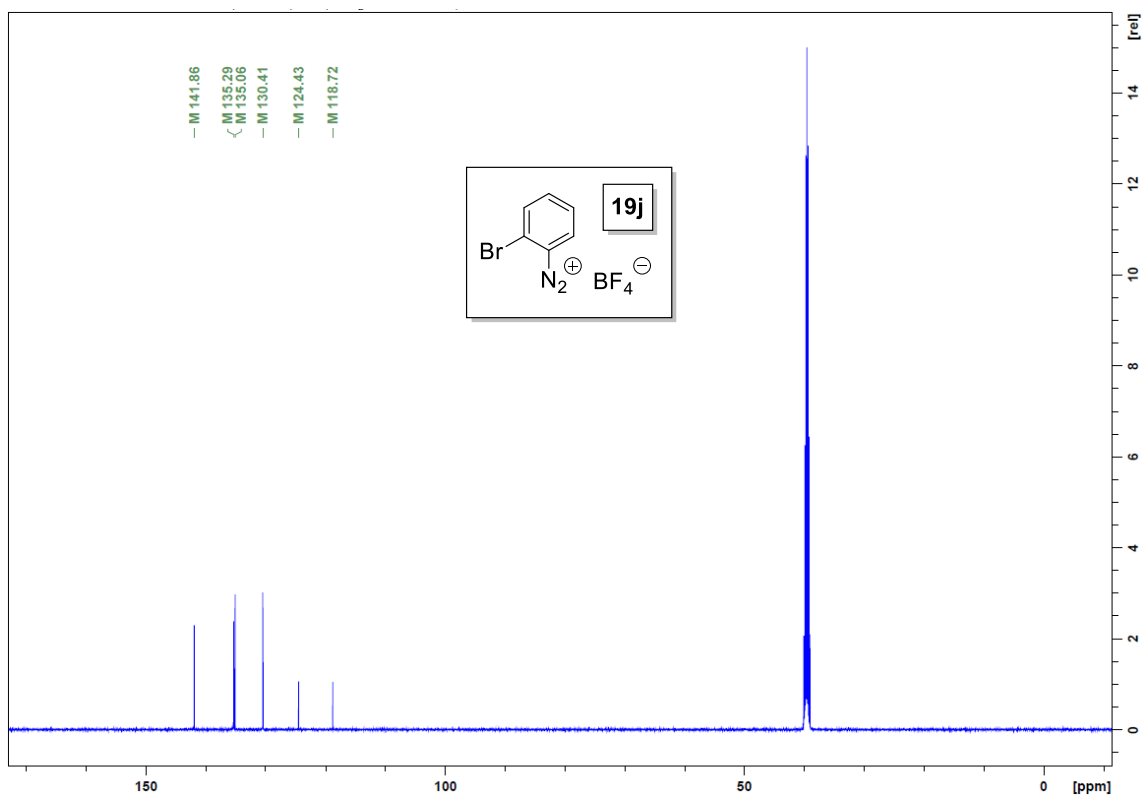
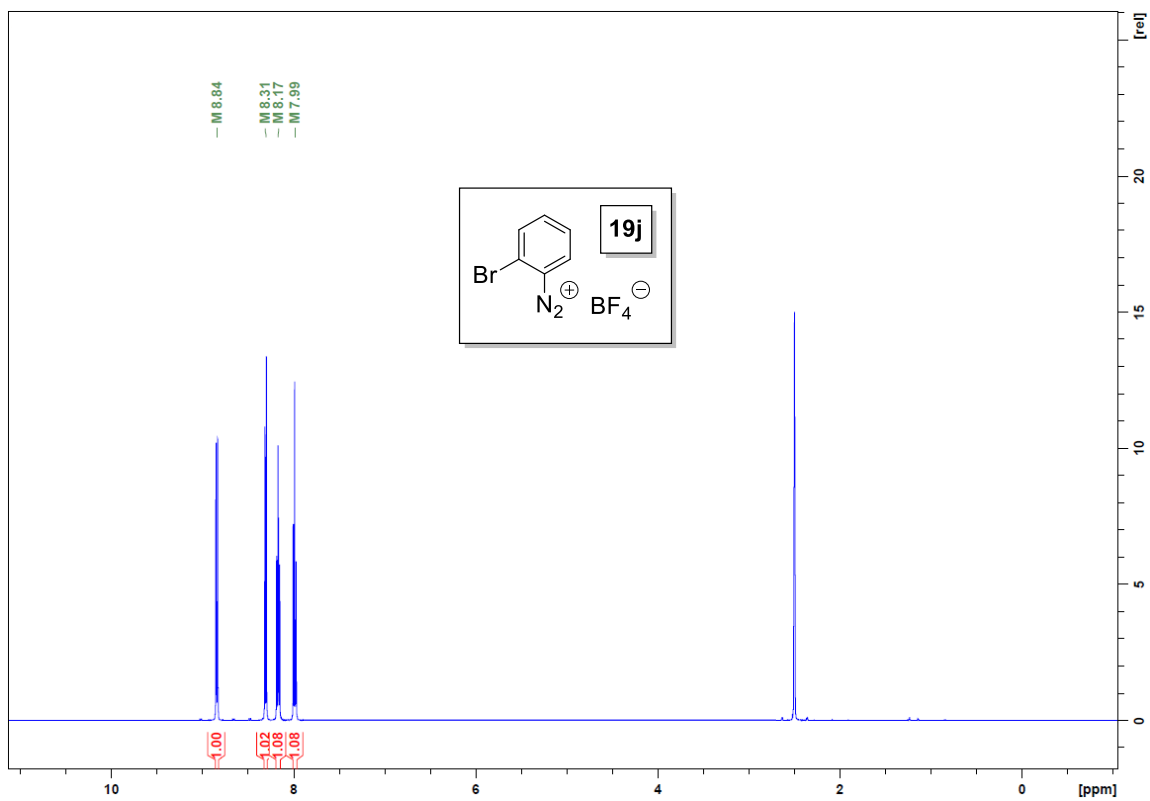


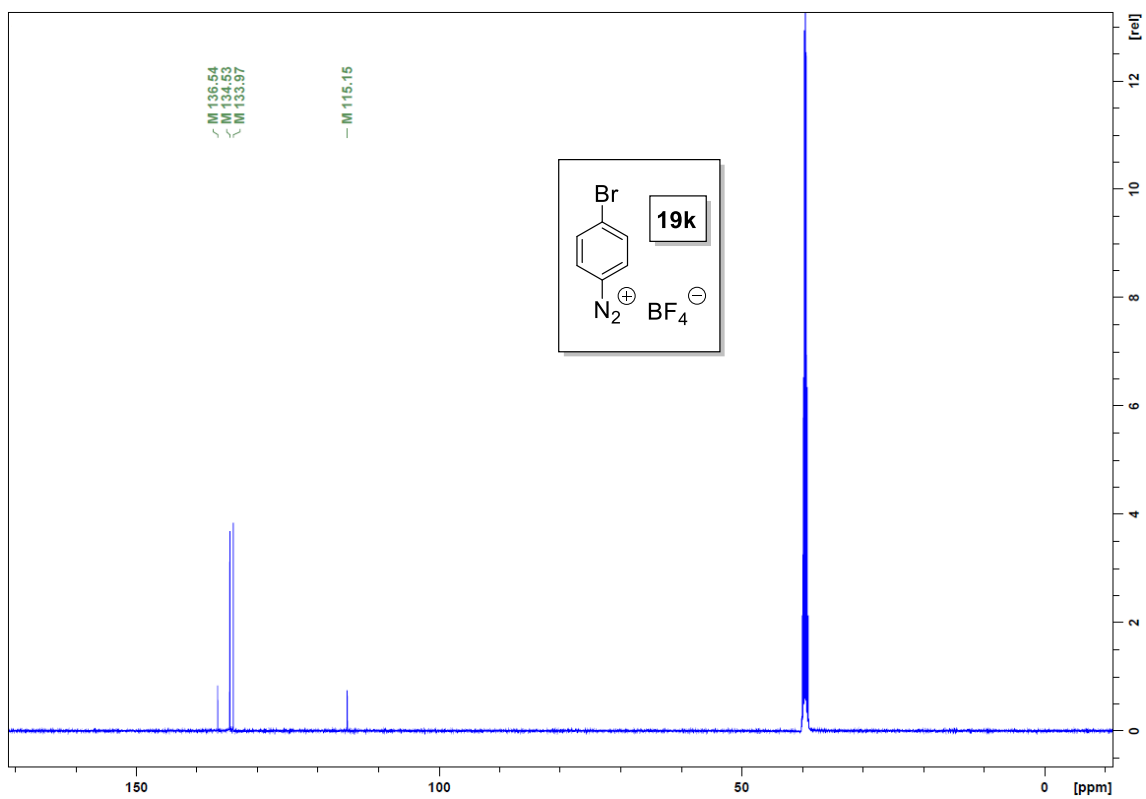
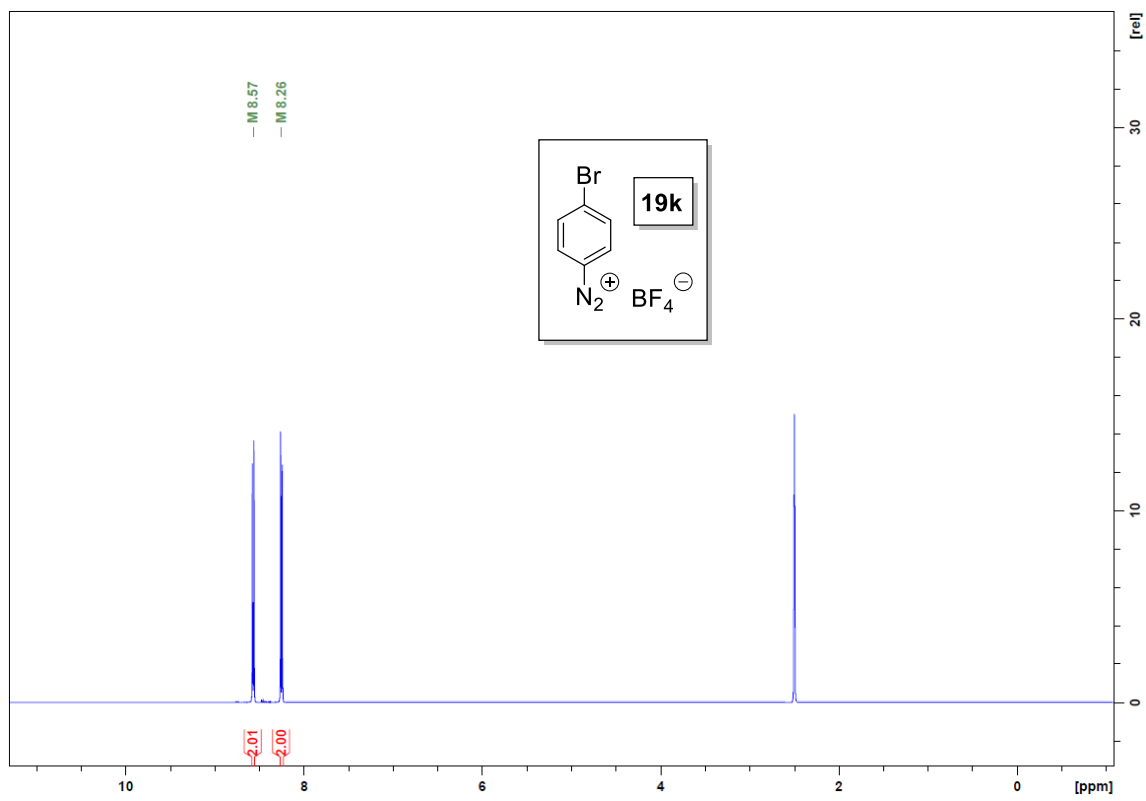


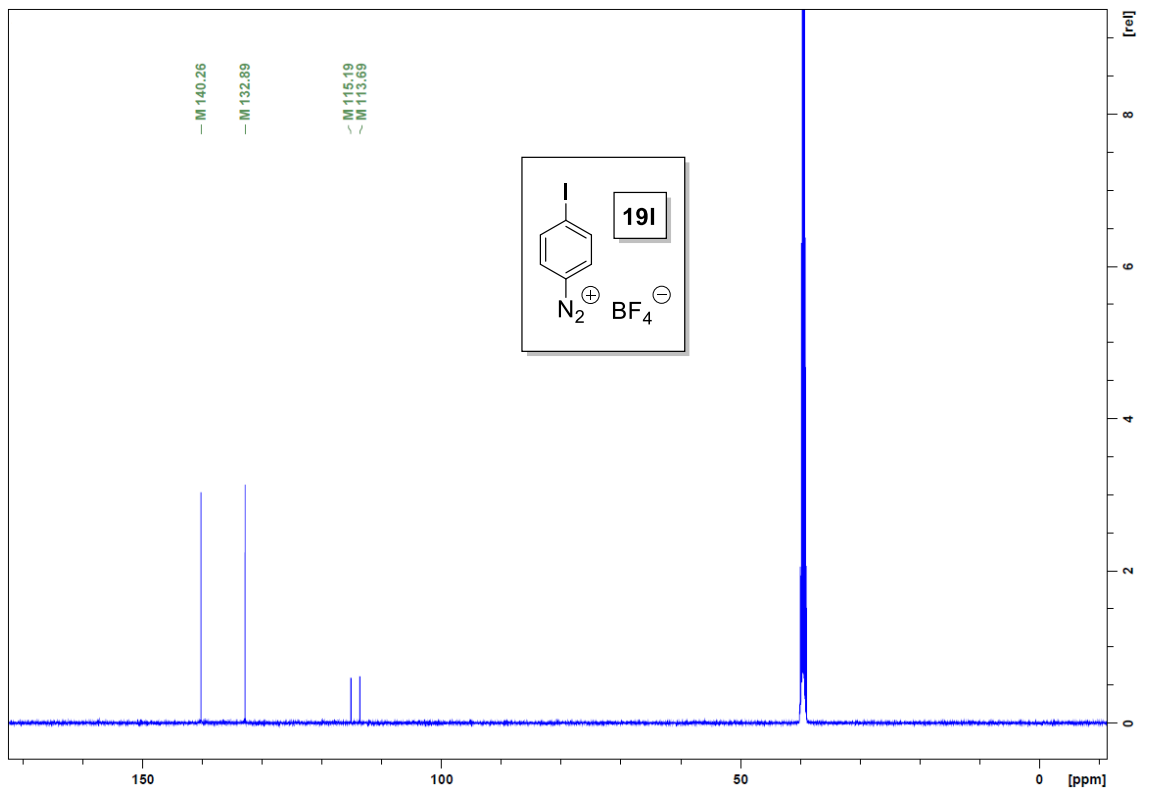
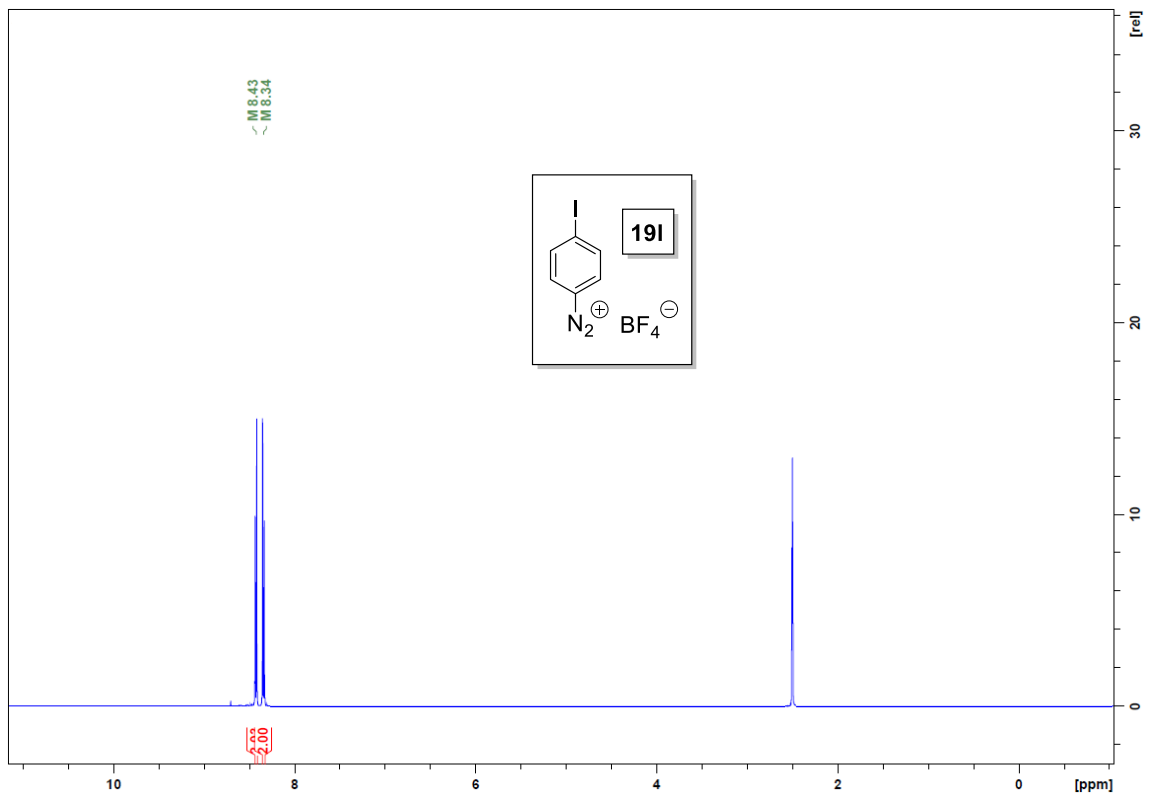












III. Crystal Structures and Single-Crystal X-Ray Diffraction Data

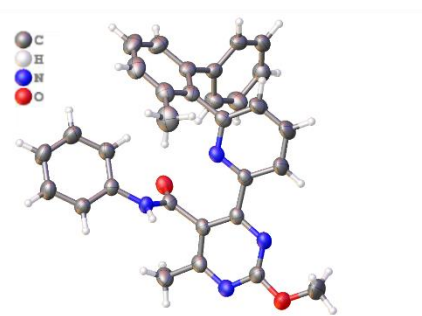


Figure S1. ORTEP drawing of compound **17b**. Thermal ellipsoids were drawn at 50% probability level.

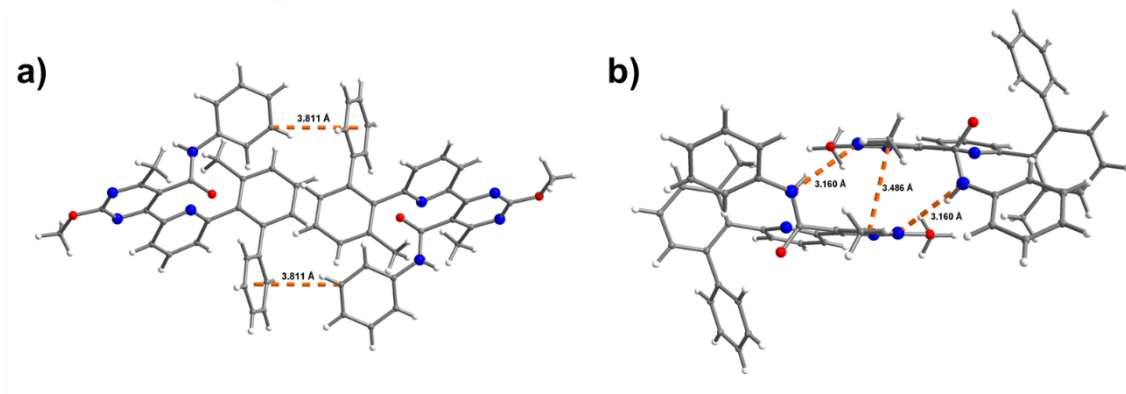


Figure S2. Intermolecular interactions of compound **17b**. Color code: C: grey; H: white; O: red; N: blue.

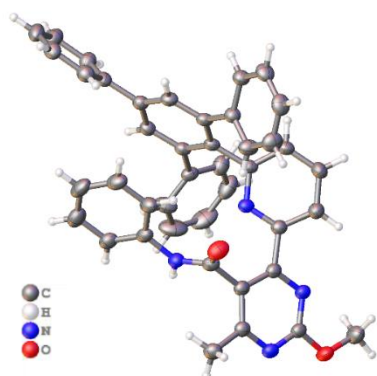


Figure S3. ORTEP drawing of compound **17d**. Thermal ellipsoids were drawn at 50% probability level.

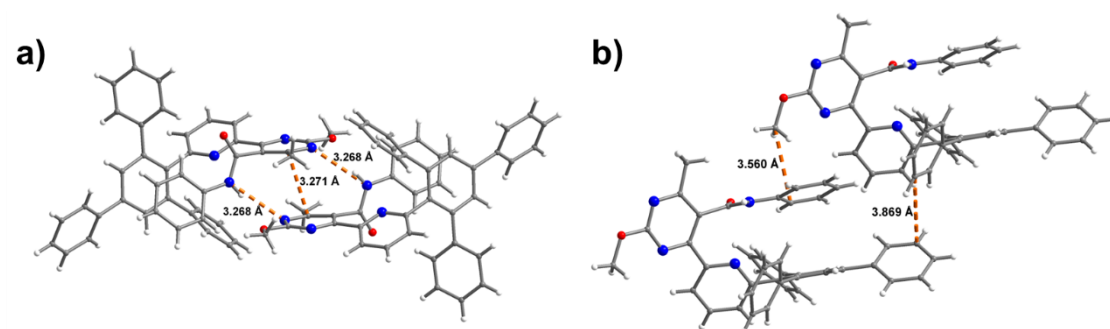


Figure S4. Intermolecular interactions of compound **17d**. Color code: C: grey; H: white; O: red; N: blue.

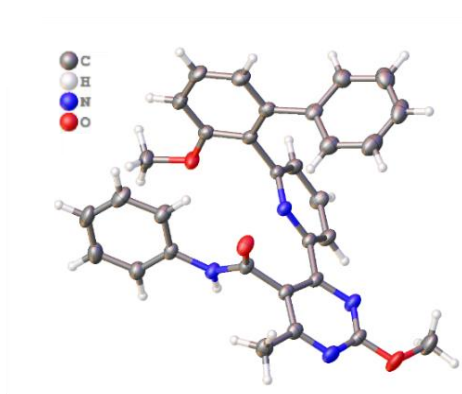


Figure S5. ORTEP drawing of compound **17f**. Thermal ellipsoids were drawn at 50% probability level.

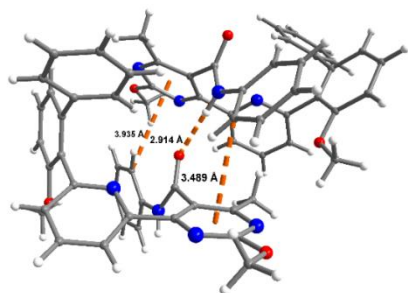


Figure S6. Intermolecular interactions of compound **17f**. Color code: C: grey; H: white; O: red; N: blue.

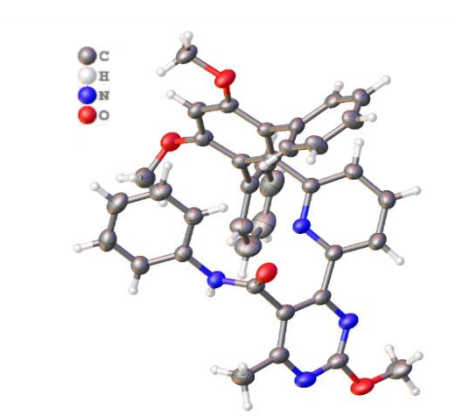


Figure S7. ORTEP drawing of compound **17h**. Thermal ellipsoids were drawn at 50% probability level.

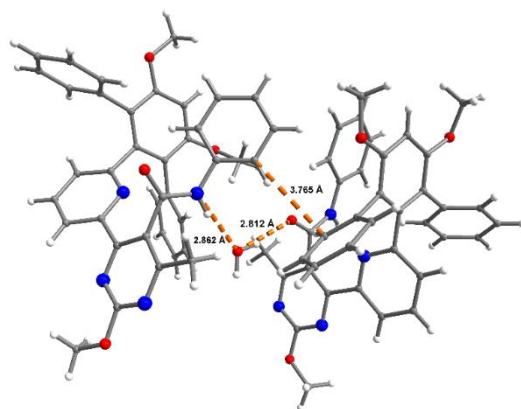


Figure S8. Intermolecular interactions of compound **17h**. Color code: C: grey; H: white; O: red; N: blue.

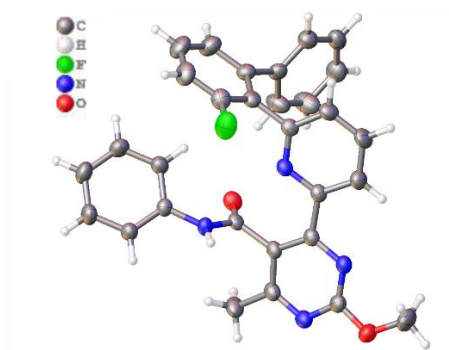


Figure S9. ORTEP drawing of compound **17j**. Thermal ellipsoids were drawn at 50% probability level.

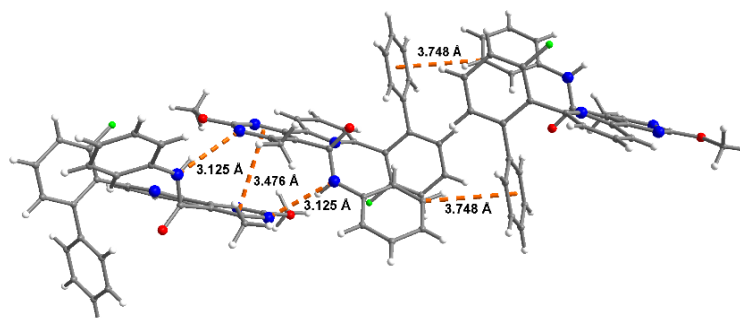


Figure S10. Intermolecular interactions of compound **17j**. Color code: C: grey; H: white; O: red; N: blue; F: light green.

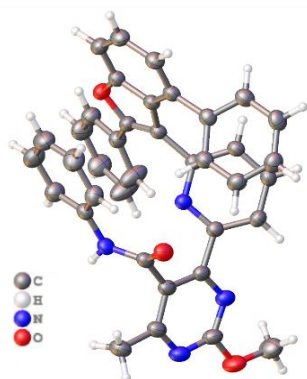


Figure S11. ORTEP drawing of compound **17r**. Thermal ellipsoids were drawn at 50% probability level.

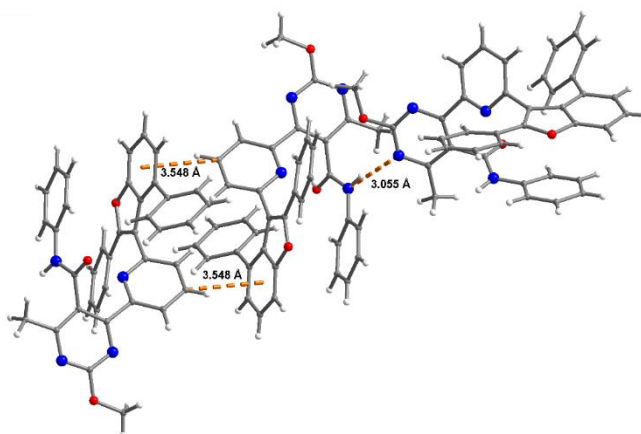


Figure S12. Intermolecular interactions of compound **17r**. Color code: C: grey; H: white; O: red; N: blue.

The asymmetric unit of **23** consists of two neutral molecules (corresponding to different conformers), where the Pd(II) centers adopt a distorted square planar coordination geometry. The coordination sphere of each Pd(II) consists of a tridentate N³C ligand and a terminally ligated Cl⁻. The maximum deviation from coordination planes is 0.03 Å (N3, N20, C33, Cl1) and 0.13 Å (N42, N58, C72, Cl2). The first conformer of **23** is nearly planar, where all 24 non-hydrogen atoms lie on the same plane, however a slight distortion is observed in the second conformer, which can be rationalized by taking into account the relatively high dihedral angle (~17°) between the planes of the benzofuryl moiety and the pyridylpyrimidine moiety. The tridentate ligand's bite angle in the two conformers is 158.3° and 158.5°.

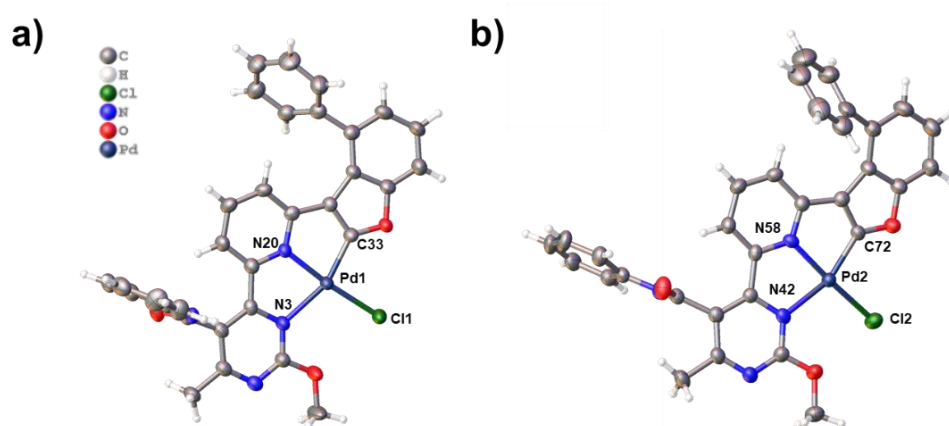


Figure S13. ORTEP drawings of the two conformations of Pd-complex **23** found in the crystal. Thermal ellipsoids were drawn at 50% probability level.

Complex **23** dimers in the asymmetric unit interact through N-H...Cl hydrogen bonds between the terminally ligated Cl⁻ anion and the nitrogen atom of the amide group, π - π stacking between the pyridine ring and the benzofuryl moiety, as well as CH- π T-shaped packing between the benzoylamido group and the benzofuryl moiety.

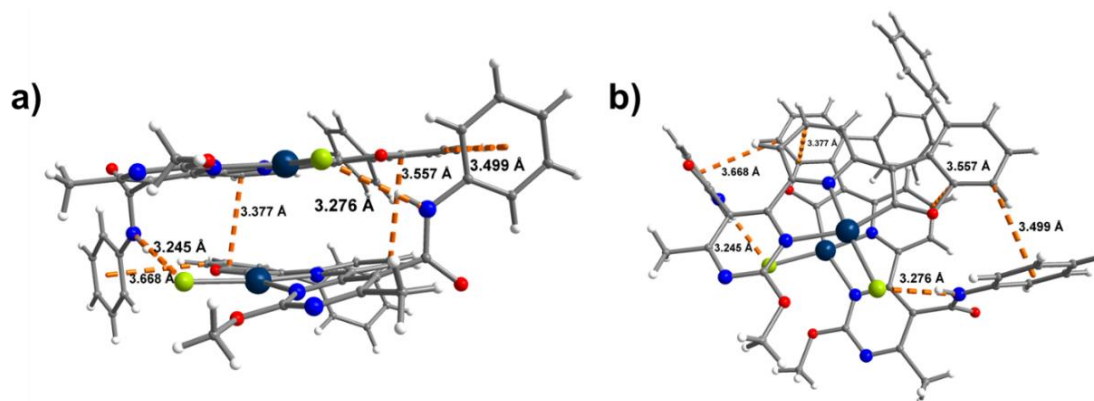


Figure S14. Intermolecular interactions of Pd-complex **23**: a) side view; b) top view. Color code: C: grey; H: white; O: red; N: blue; Cl: lime green; Pd: dark blue.

Table S1. Selected crystal data for compounds **17b**, **17d**, **17f**, **17h**, **17j**, **17r** and Pd-complex **23**.

Identification code	17b	17d.EtOAc^a	17f.DCM^a	17h.½EtOAc.½H₂O^a	17j	17r	23.½DCM^a
Empirical formula (cryst. unit)	C ₃₁ H ₂₆ N ₄ O ₂	C ₄₆ H ₄₀ N ₄ O ₄	C ₃₂ H ₂₈ Cl ₂ N ₄ O ₃	C ₈₀ H ₇₄ N ₈ O ₁₁	C ₃₀ H ₂₃ FN ₄ O ₂	C ₃₈ H ₂₈ N ₄ O ₃	C ₆₅ H ₄₈ Cl ₄ N ₈ O ₆ Pd ₂
Formula weight (cryst. unit)	486.56	712.82	587.48	1323.47	490.52	588.64	1391.71
Temperature (K)	180(1)	180(1)	180(1)	180(1)	180(1)	150(1)	150(1)
Crystal system	monoclinic	triclinic	monoclinic	triclinic	monoclinic	monoclinic	monoclinic
Space group	C2/c	P $\bar{1}$	P21/n	P $\bar{1}$	C2/c	P21/c	P21/c
a (Å)	30.8184(4)	10.1753(2)	14.20645(12)	11.6496(2)	29.7627(4)	10.57556(11)	13.6930(3)
b (Å)	8.96166(12)	10.8280(2)	9.47536(7)	14.1847(2)	9.05888(12)	33.1193(3)	26.2789(5)
c (Å)	18.6116(2)	18.8802(3)	21.65599(18)	22.6036(3)	18.3792(2)	9.47501(10)	16.4539(4)
α , b, c (°)	90, 94.552(2), 90	102.097(2), 99.993(2), 106.014(2)	90, 91.450(1), 90	105.402(1), 90.354(1), 107.050(2)	90, 92.102(2), 90	90, 98.599(1), 90	90, 102.605(2), 90
Volume (Å ³)	5124.01(12)	1894.91(6)	2914.21(4)	3428.40(10)	4952.00(11)	3281.37(6)	5778.0(2)
Z	8	2	4	2	8	4	4
$\rho_{\text{calc}}/\text{cm}^3$	1.261	1	1.339	1.282	1.316	1.192	1.600
μ/mm^{-1}	0.641	0.641	2.331	0.698	0.729	0.614	7.230
F(000)	2048.0	752	1224.0	1396.0	2048.0	1232.0	2808.0
Reflections collected	27427	22574	40637	42543	29030	23004	39464
Independent reflections	4572 [R _{int} = 0.0355, R _{sigma} = 0.0261]	6736 [R _{int} = 0.0266, R _{sigma} = 0.0287]	5191 [R _{int} = 0.0371, R _{sigma} = 0.0226]	12203 [R _{int} = 0.0262, R _{sigma} = 0.0273]	4412 [R _{int} = 0.0350, R _{sigma} = 0.0233]	5857 [R _{int} = 0.0333, R _{sigma} = 0.0303]	10285 [R _{int} = 0.0788, R _{sigma} = 0.0744]
Data/restraints/parameters	4572/0/337	6736/146/547	5191/0/373	12203/91/996	4412/0/336	5857/0/408	10285/55/780
Goodness-of-fit on F ²	1.049	1	1.044	1.060	1.051	1.031	1.053
Final R index values [I > 2 σ (I)]	R ₁ = 0.0373, wR ₂ = 0.0982	R ₁ = 0.0375, wR ₂ = 0.1013	R ₁ = 0.0568, wR ₂ = 0.1529	R ₁ = 0.0392, wR ₂ = 0.1030	R ₁ = 0.0334, wR ₂ = 0.0892	R ₁ = 0.0443, wR ₂ = 0.1296	R ₁ = 0.0549, wR ₂ = 0.1371
Final R index values [all data]	R ₁ = 0.0443, wR ₂ = 0.1017	R ₁ = 0.0427, wR ₂ = 0.1044	R ₁ = 0.0588, wR ₂ = 0.1545	R ₁ = 0.0437, wR ₂ = 0.1058	R ₁ = 0.0375, wR ₂ = 0.0916	R ₁ = 0.0475, wR ₂ = 0.1324	R ₁ = 0.0762, wR ₂ = 0.1477

^aR = $\sum ||F_o| - |F_c|| / \sum |F_o|$, wR = $\{\sum [w(|F_o|^2 - |F_c|^2)^2] / \sum [w(|F_o|^4)]\}^{1/2}$ and ^bw = $1/[\sigma^2(F_o^2) + (mP)^2 + nP]$ where $P = (F_o^2 + 2F_c^2)/3$ and m and n are constants. [^aSolvents co-crystallizing with the compounds.]