Synthesis of 6-Arylpyrimido[4,5-*e*]indolizine-2,4(1*H*,3*H*)-diones

Supporting Information

Contents

Single-crystal X-ray diffraction data

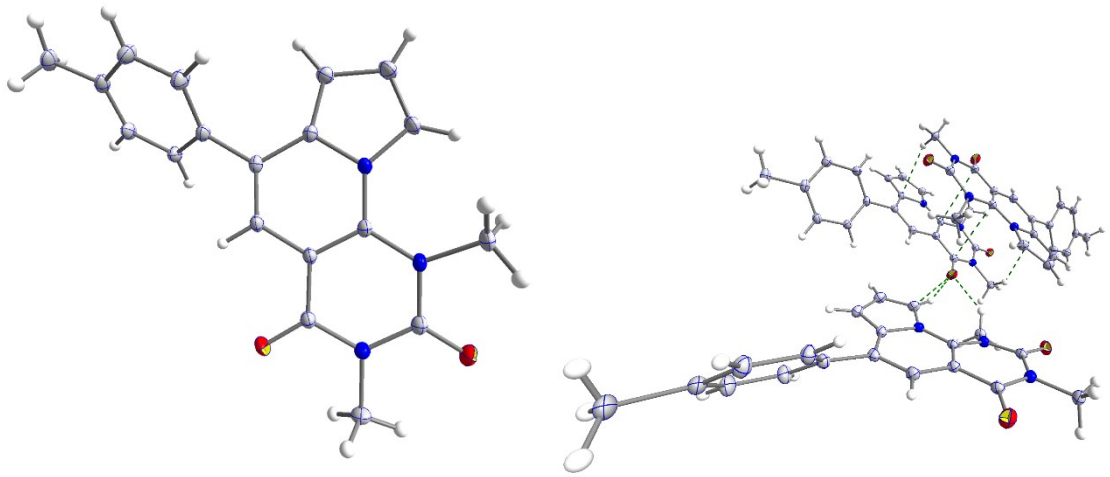


Figure 1. ORTEP of **4a** (left); short contact interactions within the crystal lattice (right). Element colours: carbon (grey), hydrogen (white), oxygen (red) and nitrogen (blue). The thermal ellipsoids are drawn at the 50% probability level.

	4a
Chem. Formula	$C_{19}H_{17}N_3O_2$
Form. Weight [g mol−1]	319.13
Cryst. system	monoclinic
Cryt. descript	block
Space group **(Hall group)**	P 21/n -P 2yn
Color	colourless
a [Å]	14.5685(10)
b [Å]	7.0647(4)
c [Å]	16.3807(11)
α [°]	90
β [°]	116.123(2)
γ [°]	90
V [Å^3]	1513.72(17)
Z	4
N_{ref}	4820
θ [°]	30.996
h,k,l_{max}	21,10,23
Dx [g cm^{-3}]	1.401
μ [mm^{-1}]	0.093
$\lambda_{MoK\alpha}$ [Å]	0.71073
T [K]	123
F(000)	672.0
Npar	220
R	0.0425(4157)
w*R*	0.1265(4820)
S	1.042

Experimental data

A representative method for the preparation of the starting material 1

6-Chloro-uracil (22.9 mmol; 4.00 g) was dissolved in glacial acetic acid (60 ml). After 5 min. acetic anhydride (3 ml) was added. The reaction mixture was stirred for 10 min. Then bromine (1 equiv.; 23.4 mmol; 1.2 ml) was slowly added dropwise. After 1 hour, the reaction was stopped by adding water (25 ml) and cooling to 4°C for 30 minutes. The precipitate was then filtered and dried.

5-Bromo-6-chloro-1,3-dimethyluracil (1). The compound **1** was obtained as a white solid in 52 % yield (3.01 g, 11.9 mmol, R_f = 0.21 heptane/ethyl acetate, 3: 2). ^{1}H NMR (300 MHz, DMSO-d_6) δ = 3.52 (s, 3H), 3.22 (s, 3H). ^{13}C {^{1}H} NMR (75 MHz, DMSO-d_6) δ = 157.7, 149.9, 145.6, 96.6, 35.4, 29.3. HRMS (ESI-TOF): calcd. for $C_6H_7BrClN_2O_2$ $[M+H]^+$ 252.9379, found: 252.9385.

Representative procedure A for the synthesis of 2a-e.

Pyrrole (1.1 equiv.; 343 µmol; 0.03 ml) was dissolved in THF (3 ml) under an inert gas atmosphere and then cooled to -78°C. This was followed by dropwise addition of *n*-BuLi (1 equiv.; 400 µmol; 0.16 mL of a 2.5 mol dm^{-3} solution in hexanes) and stirring for 30 min. Subsequently, **1** (395 µmol; 100 mg) was also dissolved in THF (1 ml) and added dropwise to the reaction mixture. Stirring continued for 6 hours at room temperature. The reaction was monitored by TLC until the reaction was complete. The reaction was stopped by the addition of a saturated NH_4Cl solution (15 mL), the phases separated, and the aqueous layer extracted with dichloromethane (3 x 10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under reduced pressure and purified by column chromatography (heptane/ethyl acetate).

5-Bromo-1,3-dimethyl-6-(1*H*-pyrrol-1-yl)pyrimidine-2,4(1*H*,3*H*)-dione (2a). According to the general procedure A, compound **2a** was obtained as a brown solid in 80 % yield (459 mg, 1.61 mmol, R_f = 0.27 heptane/ethyl acetate, 3: 2); mp: 127–129 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1646 (vs), 1617 (s), 1428 (s), 1386 (s), 1277 (s),1259 (m), 989 (s), 752 (s), 735 (vs). ^{1}H NMR (300 MHz, Chloroform-*d*) δ = 6.79 (dd, *J* = 2, 2 Hz, 2H), 6.58 – 6.42 (m, 2H), 3.54 (s, 3H), 3.15 (s, 3H). ^{13}C {^{1}H} NMR (75 MHz, Chloroform-*d*) δ = 159.2, 150.7, 146.7, 120.6, 112.1, 97.1, 32.9, 29.9 (signals of two carbons are absent, which may relate to signal overlap). MS (EI, 70 eV): *m/z* (%) = 282 (13, M^+), 207 (13), 204 (19), 160 (100), 149 (11), 134 (21). HRMS (EI): calcd. for $C_{10}H_{10}BrN_3O_2$ $[M]^+$ 282.99509, found: 282.99475.

5-Bromo-1,3-dimethyl-6-(1*H*-pyrazol-1-yl)pyrimidine-2,4(1*H*,3*H*)-dione (2b). According to the general procedure A, compound **2b** was obtained as a brown solid in 47 % yield (81.3 mg,

0.285 mmol, R_f = 0.11 heptane/ethyl acetate, 3: 2); mp: 154–156 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1700 (s), 1650 (vs), 1625 (vs), 1454 (s), 1392 (s), 1302 (s), 1020 (s), 984 (s). ^{1}H NMR (500 MHz, Chloroform-*d*) δ = 7.85 (d, *J* = 1.9 Hz, 1H), 7.70 (d, *J* = 2.6 Hz, 1H), 6.55 (dd, *J* = 2.6, 1.9 Hz, 1H), 3.46 (s, 3H), 3.08 (s, 3H). ^{13}C {^{1}H} NMR (126 MHz, Chloroform-*d*) δ = 159.1, 150.5, 145.7, 143.3, 132.0, 108.4, 97.0, 33.1, 30.0. MS (EI, 70 eV): *m*/*z* (%) = 283 (13, M$^+$), 205 (11), 162 (97), 160 (100), 148 (22), 132 (19). HRMS (EI): calcd. for $C_9H_9BrN_4O_2$ [M]$^+$ 283.99034, found: 283.99036.

5-Bromo-6-(1*H*-indol-1-yl)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (2c). According to the general procedure A, compound **2c** was obtained as a brown solid in 62 % yield (81.1 mg, 0.242 mmol, R_f = 0.26 heptane/ethyl acetate, 3: 2); mp: 149–151 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1700 (s), 1650 (vs), 1619 (s), 1430 (s), 1217 (s), 1011 (m), 745 (s), 719 (s). ^{1}H NMR (500 MHz, Chloroform-*d*) δ = 7.71 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.35 – 7.30 (m, 1H), 7.29 – 7.25 (m, 1H), 7.15 (dt, *J* = 8.1, 1.0 Hz, 1H), 7.09 (d, *J* = 3.4 Hz, 1H), 6.82 (d, *J* = 3.3 Hz, 1H), 3.53 (s, 3H), 3.06 (s, 3H). ^{13}C {^{1}H} NMR (126 MHz, Chloroform-*d*) δ = 159.3, 151.0, 145.3, 134.8, 128.7, 125.9, 124.3, 122.2, 121.9, 110.2, 107.0, 98.4, 33.0, 30.0. MS (EI, 70 eV): *m*/*z* (%) = 333 (100, M$^+$), 254 (92), 207 (29), 197 (55), 169 (94), 162 (82). HRMS (EI): calcd. for $C_{14}H_{12}BrN_3O_2$ [M]$^+$ 333.01074, found: 333.01051.

5-Bromo-6-(5-fluoro-1*H*-indol-1-yl)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (2d). According to the general procedure A, compound **2d** was obtained as a brown solid in 63 % yield (457 mg, 1.30 mmol, R_f = 0.19 heptane/ethyl acetate, 3: 2); mp: 149–151 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1708 (m), 1648 (vs), 1615 (s), 1471 (s), 1434 (s), 1238 (s), 1127 (m), 809 (s). ^{1}H NMR (500 MHz, Chloroform-*d*) δ = 7.38 – 7.34 (m, 1H), 7.13 (d, *J* = 3.4 Hz, 1H), 7.08 (d, *J* = 1.5 Hz, 1H), 7.08 – 7.06 (m, 1H), 6.79 (d, *J* = 3.4 Hz, 1H), 3.53 (s, 3H), 3.06 (s, 3H). ^{19}F NMR (282 MHz, Chloroform-*d*) δ = -121.5. ^{13}C {^{1}H} NMR (100 MHz, Chloroform-*d*) δ = 159.2, 159.2 (d, *J* = 238.4 Hz), 150.9, 145.0, 131.3, 129.4 (d, *J* = 10.6 Hz), 127.6, 112.7 (d, *J* = 26.5 Hz), 111.1 (d, *J* = 9.6 Hz), 107.2 (d, *J* = 24.1 Hz), 107.0 (d, *J* = 4.5 Hz), 98.5, 33.0, 30.0. MS (EI, 70 eV): *m*/*z* (%) = 351 (94, M$^+$), 272 (97), 215 (87), 207 (19), 187 (84), 160 (100). HRMS (EI): calcd. for $C_{14}H_{11}BrFN_3O_2$ [M]$^+$ 351.00132, found: 351.00039.

6-(1*H*-Benzo[*d*]imidazol-1-yl)-5-bromo-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (2e). According to the general procedure A, compound **2e** was obtained as a brown solid in 40 % yield (383 mg, 1.08 mmol, R_f = 0.05 heptane/ethyl acetate, 3: 2); mp: 161–163 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1702 (s), 1642 (vs), 1611 (s), 1432 (s), 1277 (s), 1219 (s), 1180 (s), 1011 (s). ^{1}H NMR (500 MHz, Chloroform-*d*) δ = 8.19 (s, 1H), 7.99 – 7.93 (m, 1H), 7.50 – 7.45 (m, 2H), 7.31 – 7.27 (m, 1H), 3.54 (s, 3H), 3.16 (s, 3H). ^{13}C {^{1}H} NMR (126 MHz, Chloroform-*d*) δ = 158.7,

150.6, 142.3, 140.7, 131.7, 126.0, 124.9, 121.3, 110.2, 98.9, 33.2, 30.2 (signal of one carbon is absent, which may relate to signal overlap). MS (EI, 70 eV): *m*/*z* (%) = 334 (97, M^+), 255 (100), 227 (85), 198 (77), 170 (82), 160 (90). HRMS (EI): calcd. for $C_{13}H_{11}BrN_4O_2$ $[M]^+$ 334.00599, found: 334.00551.

Representative procedure B for the synthesis of 3a-i.

A mixture of **2d** (853 µmol; 300 mg), $Pd(PPh_3)_2Cl_2$ (5 mol%; 43 µmol; 30.2 mg), CuI (5 mol%; 45 µmol; 8.6 mg) was dissolved in DMSO (5 ml) and stirred for 5 min. under argon atmosphere. NEt_3 (11 equiv.; 9.33 mmol; 1.3 ml) was added and the reaction mixture was heated to 100 °C. The corresponding arylacetylene (*p*-tolylacetylene, 1.2 equiv.; 1.03 mmol; 0.13 ml) was slowly added dropwise to the reaction mixture and stirred for 6 hours at 100 °C. The reaction was monitored by TLC until the reaction was complete. The reaction was stopped by the addition of a saturated NH_4Cl solution (15 mL), the phases separated, and the aqueous layer extracted with dichloromethane (3 x 20 mL). The combined organic layers were dried over Na_2SO_4, concentrated under reduced pressure and purified by column chromatography (heptane/ethyl acetate).

1,3-Dimethyl-6-(1*H*-pyrrol-1-yl)-5-(*p*-tolylethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (3a). According to the general procedure B, compound **3a** was obtained as a brown solid in 80 % yield (90.2 mg, 0.282 mmol, R_f = 0.22 heptane/ethyl acetate, 3: 2); mp: 175–177 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1704 (s), 1652 (vs), 1574 (s), 1432 (s), 1360 (s), 1007 (s), 836 (s), 748 (s). ^{1}H NMR (500 MHz, Chloroform-*d*) δ = 7.20 – 7.17 (m, 2H), 7.08 – 7.04 (m, 2H), 6.88 – 6.85 (m, 2H), 6.45 – 6.42 (m, 2H), 3.46 (s, 3H), 3.20 (s, 3H), 2.31 (s, 3H). ^{13}C {^{1}H} NMR (126 MHz, Chloroform-*d*) δ = 161.1, 150.8, 149.7, 138.8, 131.5, 129.1, 121.5, 119.7, 111.6, 97.9, 96.5, 78.5, 33.1, 29.1, 21.7 (signals of four carbons are absent, which may relate to signal overlap). MS (EI, 70 eV): *m*/*z* (%) = 319 (100, M^+), 304 (19), 290 (24), 262 (15), 247 (21), 233 (10). HRMS (ESI-TOF): calcd. for $C_{19}H_{18}N_3O_2$ $[M+H]^+$ 320.1399, found: 320.1402.

1,3-Dimethyl-5-(phenylethynyl)-6-(1*H*-pyrrol-1-yl)pyrimidine-2,4(1*H*,3*H*)-dione (3b). According to the general procedure B, compound **3b** was obtained as a brown solid in 85 % yield (276 mg, 0.902 mmol, R_f = 0.21 heptane/ethyl acetate, 3: 2); mp: 124–126 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1710 (s), 1658 (vs), 1615 (s), 1479 (s), 1440 (s), 1256 (s), 1096 (s), 1069 (s). ^{1}H NMR (300 MHz, Chloroform-*d*) δ = 7.28 – 7.23 (m, 5H), 6.87 (dd, *J* = 2 Hz, 2H), 6.43 (dd, *J* = 2 Hz, 2H), 3.44 (s, 3H), 3.18 (s, 3H). ^{13}C {^{1}H} NMR (75 MHz, Chloroform-*d*) δ = 161.0, 150.7, 149.9, 131.5, 128.5, 128.3, 122.8, 121.5, 111.6, 97.6, 96.1, 79.2, 33.1, 29.1 (signals of four carbons are absent, which may relate to signal overlap). MS (EI, 70 eV): *m*/*z* (%) = 305 (100, M^+), 276 (32), 249 (23), 233 (23), 219 (12), 205 (11). HRMS (ESI-TOF): calcd. for $C_{18}H_{16}N_3O_2$ $[M+H]^+$ 306.1242, found: 306.1248.

5-((4-(Dimethylamino)phenyl)ethynyl)-1,3-dimethyl-6-(1*H*-pyrrol-1-yl)pyrimidine-2,4(1*H*,3*H*)-dione (3c). According to the general procedure B, compound **3c** was obtained as a brown solid in 86 % yield (323 mg, 0.928 mmol, R_f = 0.14 heptane/ethyl acetate, 3: 2); mp: 163–165 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1708 (s), 1656 (vs), 1601 (s), 1522 (s), 1481 (s), 1442 (s), 1362 (s), 1333 (s). ^{1}H NMR (500 MHz, Chloroform-*d*) δ = 7.17 – 7.14 (m, 2H), 6.86 (t, *J* = 2.2 Hz, 2H), 6.57 – 6.53 (m, 2H), 6.41 (t, *J* = 2.2 Hz, 2H), 3.44 (s, 3H), 3.16 (s, 3H), 2.94 (s, 6H). ^{13}C {^{1}H} NMR (126 MHz, Chloroform-*d*) δ = 161.2, 150.7, 150.3, 148.5, 132.7, 121.5, 111.7, 111.3, 109.5, 98.6, 97.7, 40.2, 33.0, 29.0 (signals of five carbons are absent, which may relate to signal overlap). MS (EI, 70 eV): *m*/*z* (%) = 348 (84, M$^+$), 333 (30), 262 (100), 207 (19), 183 (96), 152 (19). HRMS (EI): calcd. for $C_{20}H_{20}N_4O_2$ [M]$^+$ 348.15808, found: 348.15709.

5-((4-Fluorophenyl)ethynyl)-1,3-dimethyl-6-(1*H*-pyrrol-1-yl)pyrimidine-2,4(1*H*,3*H*)-dione (3d). According to the general procedure B, compound **3d** was obtained as a brown solid in 68 % yield (231 mg, 0.713 mmol, R_f = 0.22 heptane/ethyl acetate, 3: 2); mp: 154–156 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1712 (s), 1658 (vs), 1506 (s), 1479 (s), 1448 (s), 1215 (s), 1096 (s), 836 (s). ^{1}H NMR (500 MHz, Chloroform-*d*) δ = 7.22 – 7.14 (m, 2H), 6.91 – 6.83 (m, 2H), 6.83 – 6.77 (m, 2H), 6.40 – 6.35 (m, 2H), 3.37 (s, 3H), 3.12 (s, 3H). ^{19}F NMR (471 MHz, Chloroform-*d*) δ = -110.4. ^{13}C {^{1}H} NMR (75 MHz, Chloroform-*d*) δ = 162.7 (d, *J* = 250.9 Hz), 161.0, 150.7, 150.0, 133.4 (d, *J* = 8.4 Hz), 121.5, 118.9 (d, *J* = 3.5 Hz), 115.6 (d, *J* = 22.2 Hz), 111.6, 97.5, 95.0, 78.9 (d, *J* = 1.5 Hz), 33.1, 29.1 (signals of four carbons are absent, which may relate to signal overlap). MS (EI, 70 eV): *m*/*z* (%) = 323 (100, M$^+$), 294 (35), 267 (28), 251 (27), 238 (14), 223 (13). HRMS (ESI-TOF): calcd. for $C_{18}H_{15}FN_3O_2$ [M+H]$^+$ 324.1148, found: 324.1143.

1,3-Dimethyl-6-(1*H*-pyrrol-1-yl)-5-((4-(trifluoromethyl)phenyl)ethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (3e). According to the general procedure B, compound **3e** was obtained as a brown solid in 92 % yield (363 mg, 0.973 mmol, R_f = 0.20 heptane/ethyl acetate, 3: 2); mp: 168–170 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1708 (s), 1660 (vs), 1642 (s), 1483 (s), 1444 (s), 1327 (vs), 1102 (vs), 1063 (vs). ^{1}H NMR (300 MHz, Chloroform-*d*) δ = 7.50 (d, *J* = 8 Hz, 2H), 7.39 – 7.33 (m, 2H), 6.88 (dd, *J* = 2 Hz, 2H), 6.45 (dd, *J* = 3 Hz, 2H), 3.45 (s, 3H), 3.22 (s, 3H). ^{19}F NMR (282 MHz, Chloroform-*d*) δ = -62.9. ^{13}C {^{1}H} NMR (75 MHz, Chloroform-*d*) δ = 160.9, 150.8, 150.6, 131.7, 130.1 (q, *J* = 32 Hz), 126.6 (d, *J* = 1 Hz), 125.2 (q, *J* = 4 Hz), 124.0 (q, *J* = 272 Hz), 121.5, 111.8, 97.0, 94.6, 81.8, 33.2, 29.1 (signals of four carbons are absent, which may relate to signal overlap). MS (EI, 70 eV): *m*/*z* (%) = 373 (100, M$^+$), 354 (11), 344 (30), 316 (28), 301 (22), 288 (13). HRMS (ESI-TOF): calcd. for $C_{19}H_{15}F_3N_3O_2$ [M+H]$^+$ 374.1116, found: 374.1110.

1,3-Dimethyl-6-(1*H*-pyrrol-1-yl)-5-(thiophen-3-ylethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (3f). According to the general procedure B, compound **3f** was obtained as a brown solid in 86 % yield (236 mg, 0.759 mmol, R_f = 0.20 heptane/ethyl acetate, 3: 2); mp: 116–118 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1708 (s), 1656 (vs), 1609 (s), 1481 (s), 1446 (s), 1372 (m), 1256 (m), 780 (s). ^{1}H NMR (500 MHz, Chloroform-*d*) δ = 7.32 (dd, *J* = 3.0, 1.2 Hz, 1H), 7.19 (dd, *J* = 5.0, 3.0 Hz, 1H), 6.96 (dd, *J* = 5.0, 1.1 Hz, 1H), 6.86 (dd, *J* = 2.2 Hz, 2H), 6.42 (dd, *J* = 2.2 Hz, 2H), 3.43 (s, 3H), 3.18 (s, 3H). ^{13}C {^{1}H} NMR (75 MHz, Chloroform-*d*) δ = 161.0, 150.7, 149.8, 129.7, 129.1, 125.3, 121.8, 121.4, 111.6, 97.6, 91.4, 78.7, 33.1, 29.0 (signals of two carbons are absent, which may relate to signal overlap). MS (EI, 70 eV): *m*/*z* (%) = 311 (100, M$^+$), 296 (10), 282 (26), 252 (20), 239 (21), 227 (20). HRMS (EI): calcd. for $C_{16}H_{13}N_3O_2S$ [M]$^+$ 311.07230, found: 311.07164.

6-(1*H*-Indol-1-yl)-1,3-dimethyl-5-(*p*-tolylethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (3g). According to the general procedure B, compound **3g** was obtained as a brown solid in 98 % yield (273 mg, 0.739 mmol, R_f = 0.23 heptane/ethyl acetate, 3: 2); mp: 185–186 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1710 (s), 1660 (vs), 1619 (s), 1477 (s), 1438 (s), 1331 (s), 1215 (s), 743 (vs). ^{1}H NMR (500 MHz, Chloroform-*d*) δ = 7.72 – 7.68 (m, 1H), 7.31 – 7.21 (m, 4H), 6.96 – 6.92 (m, 2H), 6.85 – 6.82 (m, 2H), 6.80 (dd, *J* = 3.4, 0.9 Hz, 1H), 3.49 (s, 3H), 3.17 (s, 3H), 2.24 (s, 3H). ^{13}C {^{1}H} NMR (126 MHz, Chloroform-*d*) δ = 161.2, 151.0, 148.3, 138.7, 135.4, 131.3, 128.9, 128.9, 127.0, 124.0, 122.0, 121.7, 119.4, 111.2, 106.6, 98.8, 97.6, 78.6, 33.1, 29.1, 21.6 (signals of two carbons are absent, which may relate to signal overlap). MS (EI, 70 eV): *m*/*z* (%) = 368 (100, M$^+$), 168 (18), 153 (9). HRMS (EI): calcd. for $C_{23}H_{18}N_3O_2$ [M]$^+$ 368.13935, found: 368.13903.

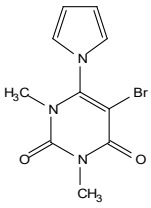
6-(5-Fluoro-1*H*-indol-1-yl)-1,3-dimethyl-5-(*p*-tolylethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (3h). According to the general procedure B, compound **3h** was obtained as a brown solid in 86 % yield (282 mg, 729 µmol, R_f = 0.20 heptane/ethyl acetate, 3: 2); mp: 159–161 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1656 (vs), 1613 (s), 1467 (s), 1440 (vs), 1228 (s), 1207 (s), 1123 (s). ^{1}H NMR (300 MHz, Chloroform-*d*) δ = 7.36 (dd, *J* = 9, 3 Hz, 1H), 7.27 (d, *J* = 4 Hz, 1H), 7.17 (dd, *J* = 9, 4 Hz, 1H), 7.05 (td, *J* = 9, 3 Hz, 1H), 7.00 – 6.94 (m, 2H), 6.89 – 6.84 (m, 2H), 6.78 (dd, *J* = 3, 1 Hz, 1H), 3.49 (s, 3H), 3.18 (s, 3H), 2.26 (s, 3H). ^{19}F NMR (282 MHz, Chloroform-*d*) δ = -121.9. ^{13}C {^{1}H} NMR (75 MHz, Chloroform-*d*) δ = 161.0, 159.1 (d, *J* = 238 Hz), 150.9, 147.9, 138.9, 131.9, 131.3, 129.5 (d, *J* = 10 Hz), 129.0, 128.6, 119.3, 112.3 (d, *J* = 26 Hz), 111.9 (d, *J* = 10 Hz), 106.9 (d, *J* = 24 Hz), 106.5 (d, *J* = 4 Hz), 99.0, 97.8, 78.3, 33.1, 29.2, 21.6 (signals of two carbons are absent, which may relate to signal overlap). MS (EI, 70 eV): *m*/*z* (%) = 387 (40, M$^+$), 168 (23), 153 (12), 134 (4), 126 (5). HRMS (ESI-TOF): calcd. for $C_{23}H_{19}FN_3O_2$ [M+H]$^+$ 388.1461, found: 388.1459.

6-(1*H*-Benzo[*d*]imidazol-1-yl)-1,3-dimethyl-5-(*p*-tolylethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (3i). According to the general procedure B, compound **3i** was obtained as a brown solid in 75 % yield (251 mg, 678 µmol, R_f = 0.05 heptane/ethyl acetate, 3: 2); mp: 248–250 °C. IR (ATR): $\tilde{\nu}$ [cm^{-1}] = 1662 (vs), 1623 (m), 1444 (vs), 1353 (m), 1337 (m), 1273 (m), 1211 (m). ^{1}H NMR (250 MHz, DMSO-d_6) δ = 10.8 (s, 1H), 10.2 – 10.1 (m, 1H), 10.0 – 9.9 (m, 1H), 9.7 – 9.6 (m, 2H), 9.3 (d, J = 8.0 Hz, 2H), 9.0 – 9.0 (m, 2H), 5.6 (s, 3H), 5.4 (s, 3H), 4.5 (s, 3H). ^{13}C {^{1}H} NMR (63 MHz, DMSO-d_6) δ = 160.3, 150.2, 146.8, 142.8, 142.7, 138.7, 132.6, 130.4, 129.2, 124.4, 123.4, 120.1, 118.5, 111.6, 97.5, 95.4, 79.3, 32.5, 28.6, 20.9 (signals of two carbons are absent, which may relate to signal overlap). MS (EI, 70 eV): *m*/*z* (%) = 370 (36, M$^+$), 196 (5), 167 (22), 153 (10). HRMS (ESI-TOF): calcd. for $C_{22}H_{19}N_4O_2$ [M+H]$^+$ 371.1508, found: 371.1508.

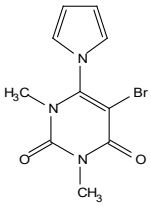
1H, 13C, 19F NMR spectra

5-Bromo-1,3-dimethyl-6-(1*H*-pyrrol-1-yl)pyrimidine-2,4(1*H*,3*H*)-dione (2a)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	287.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1225.3
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

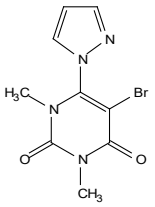


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Experiment	1D
5	Number of Scans	1024
6	Receiver Gain	2050.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1457.9
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

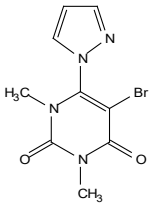


5-Bromo-1,3-dimethyl-6-(1*H*-pyrazol-1-yl)pyrimidine-2,4(1*H*,3*H*)-dione (2b)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	101.0
7	Relaxation Delay	1.0000
8	Pulse Width	8.0000
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1924.3
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

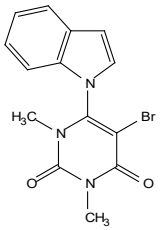


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zgpg30
4	Experiment	1D
5	Number of Scans	1024
6	Receiver Gain	101.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	125.77
10	Spectral Width	30120.5
11	Lowest Frequency	-2474.3
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

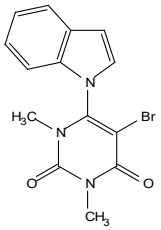


5-Bromo-6-(1*H*-indol-1-yl)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (2c)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	101.0
7	Relaxation Delay	1.0000
8	Pulse Width	8.0000
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1924.1
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

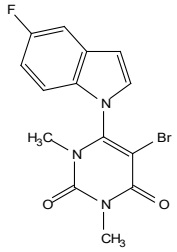


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zgpg30
4	Experiment	1D
5	Number of Scans	1024
6	Receiver Gain	101.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	125.77
10	Spectral Width	30120.5
11	Lowest Frequency	-2471.4
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

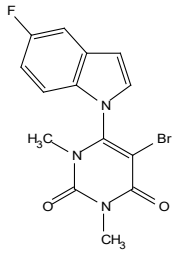


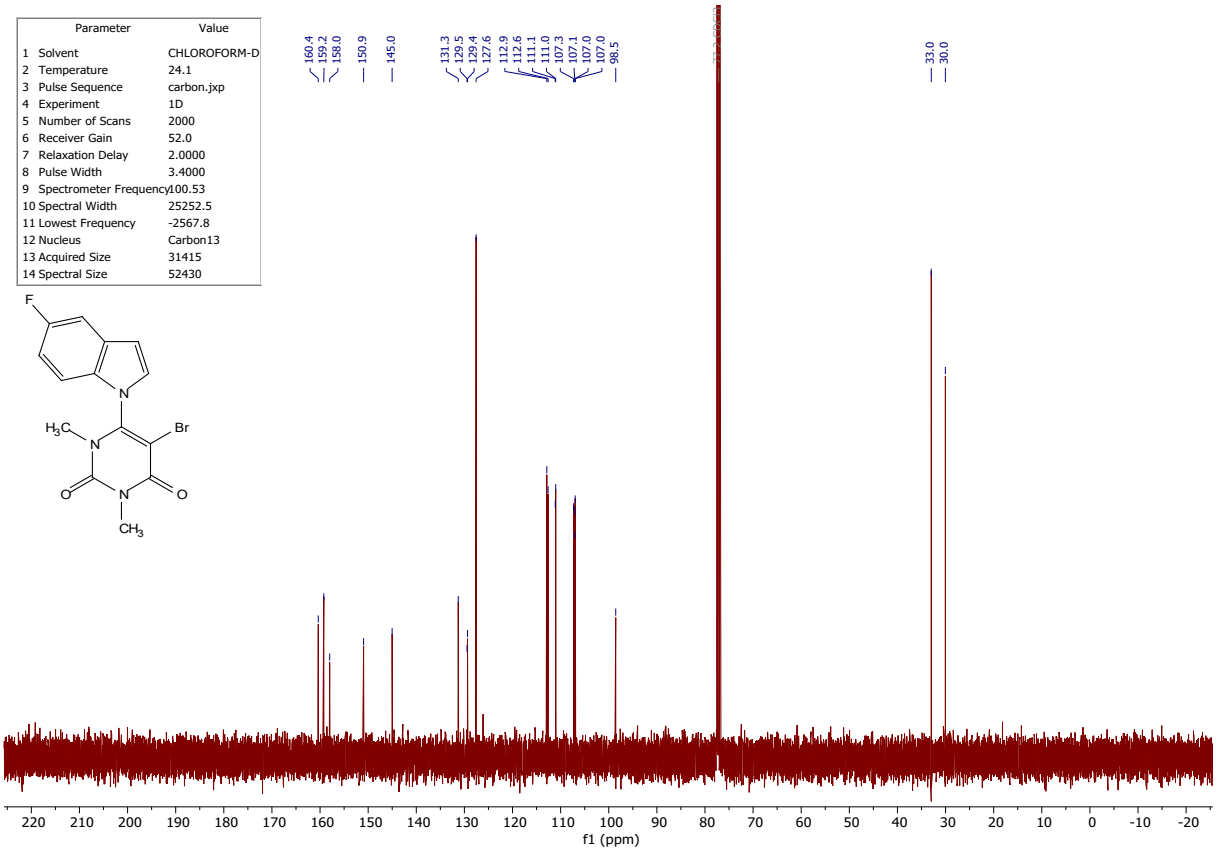
5-Bromo-6-(5-fluoro-1*H*-indol-1-yl)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (2d)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	101.0
7	Relaxation Delay	1.0000
8	Pulse Width	8.0000
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1924.0
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



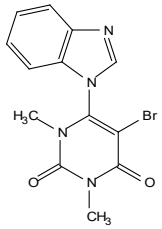
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgig
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	101.0
7	Relaxation Delay	1.0000
8	Pulse Width	12.0000
9	Spectrometer Frequency	470.55
10	Spectral Width	113636.4
11	Lowest Frequency	-103877.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072



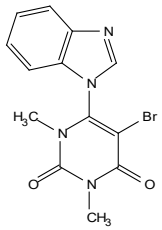

Parameter Value
1 Solvent CHLOROFORM-D
2 Temperature 24.1
3 Pulse Sequence carbon.jxp
4 Experiment 1D
5 Number of Scans 2000
6 Receiver Gain 52.0
7 Relaxation Delay 2.0000
8 Pulse Width 3.4000
9 Spectrometer Frequency 100.53
10 Spectral Width 25252.5
11 Lowest Frequency -2567.8
12 Nucleus Carbon13
13 Acquired Size 31415
14 Spectral Size 52430
160.4
159.2
158.0
150.9
145.0
131.3
129.5
129.4
127.6
112.9
112.6
111.1
111.0
107.3
107.1
107.0
107.0
96.5
33.0
30.0
F
N
H3C
N
Br
O
N
O
CH3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

6-(1*H*-Benzo[*d*]imidazol-1-yl)-5-bromo-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (2e).

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	8
6	Receiver Gain	101.0
7	Relaxation Delay	1.0000
8	Pulse Width	8.0000
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1924.0
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

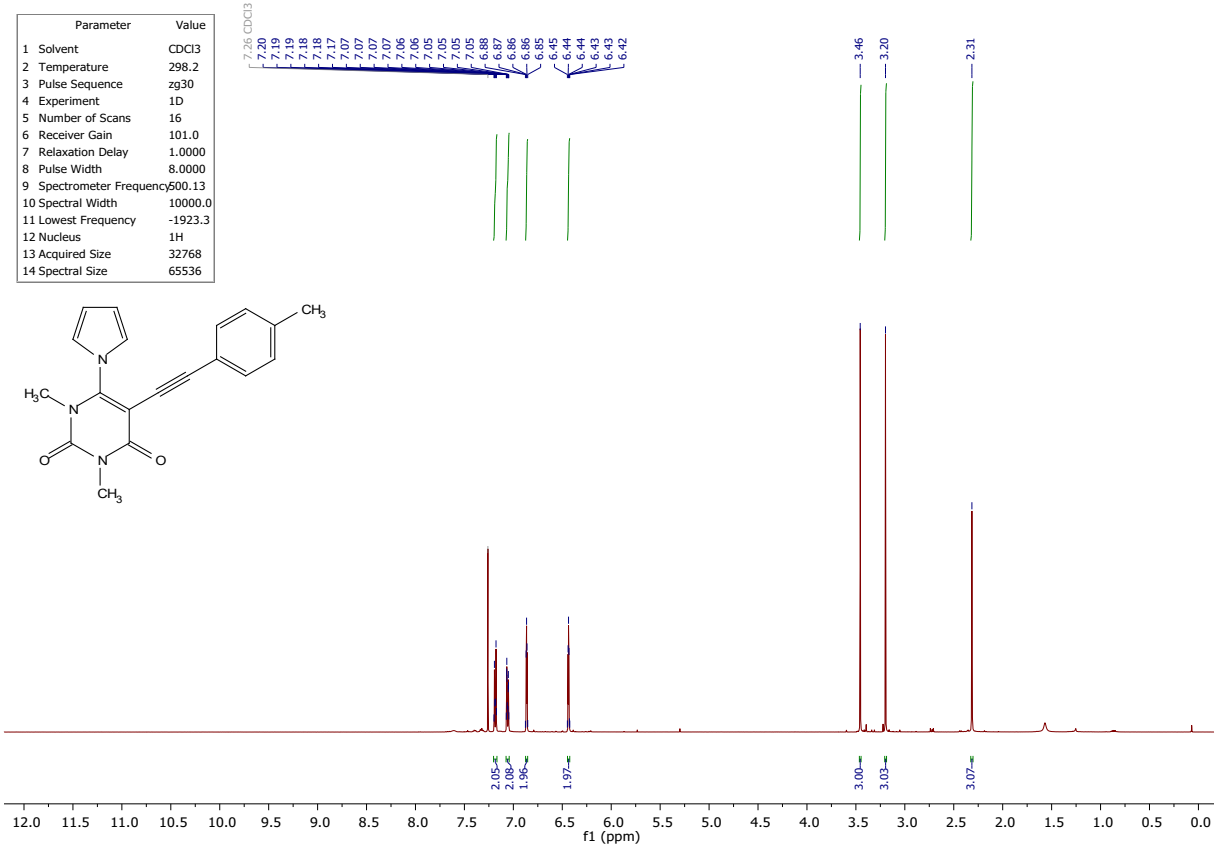


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Experiment	1D
5	Number of Scans	512
6	Receiver Gain	101.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	125.77
10	Spectral Width	30120.5
11	Lowest Frequency	-2484.5
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

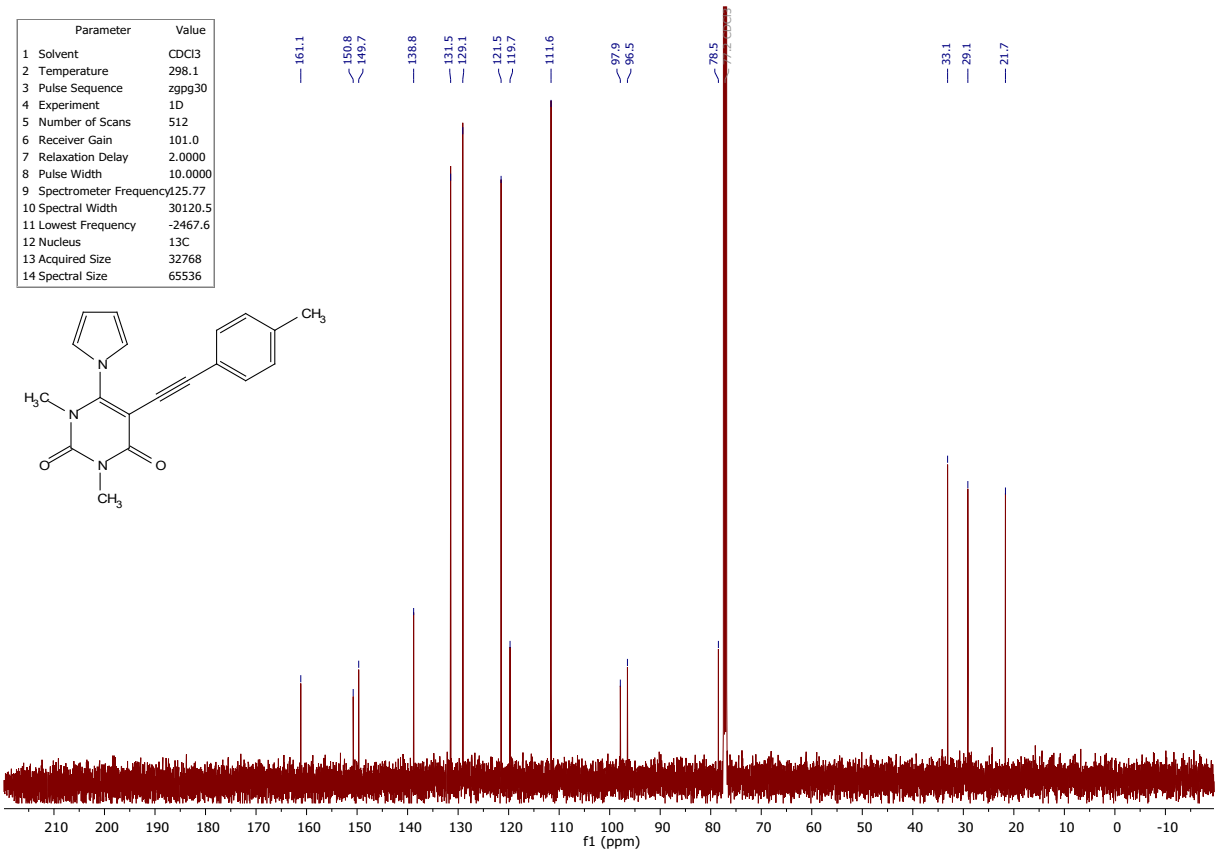


1,3-Dimethyl-6-(1*H*-pyrrol-1-yl)-5-(*p*-tolylethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (3a)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	101.0
7	Relaxation Delay	1.0000
8	Pulse Width	8.0000
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1923.3
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

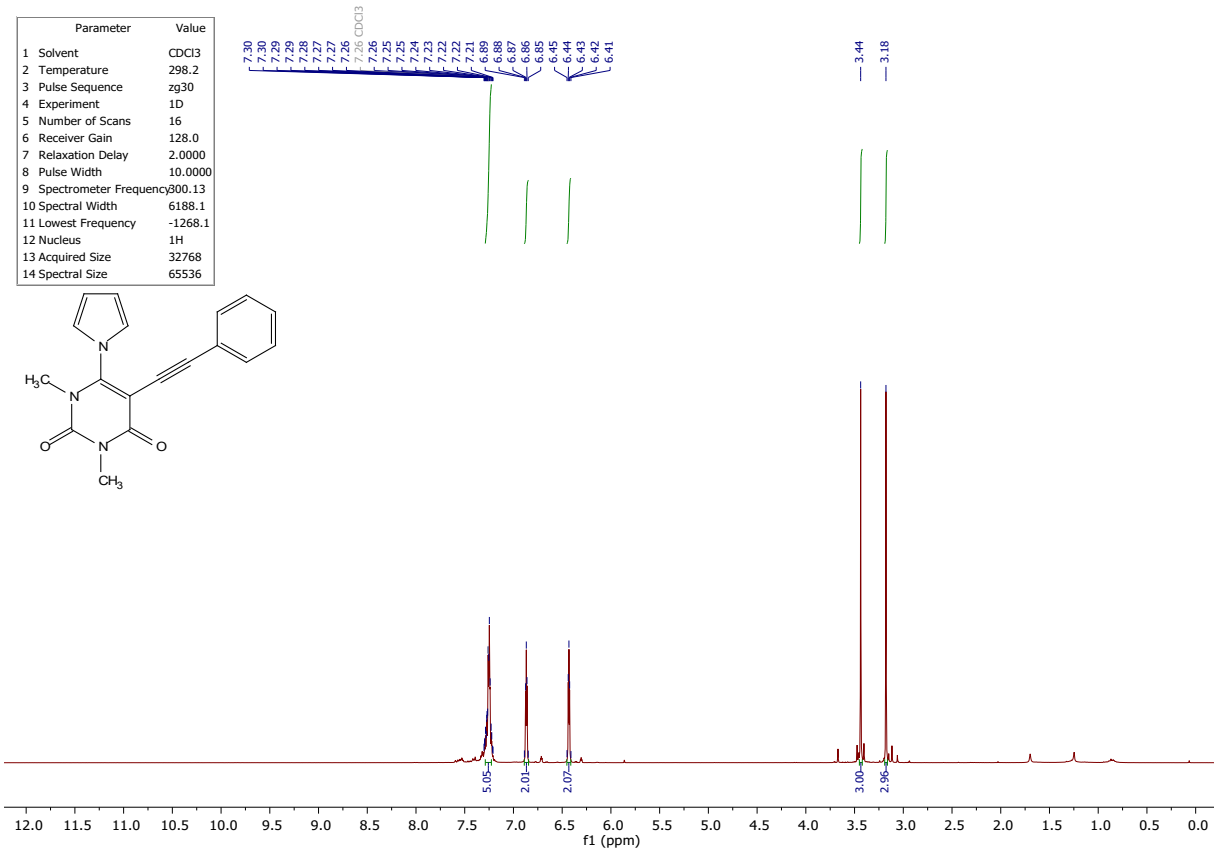


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zgpg30
4	Experiment	1D
5	Number of Scans	512
6	Receiver Gain	101.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	125.77
10	Spectral Width	30120.5
11	Lowest Frequency	-2467.6
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

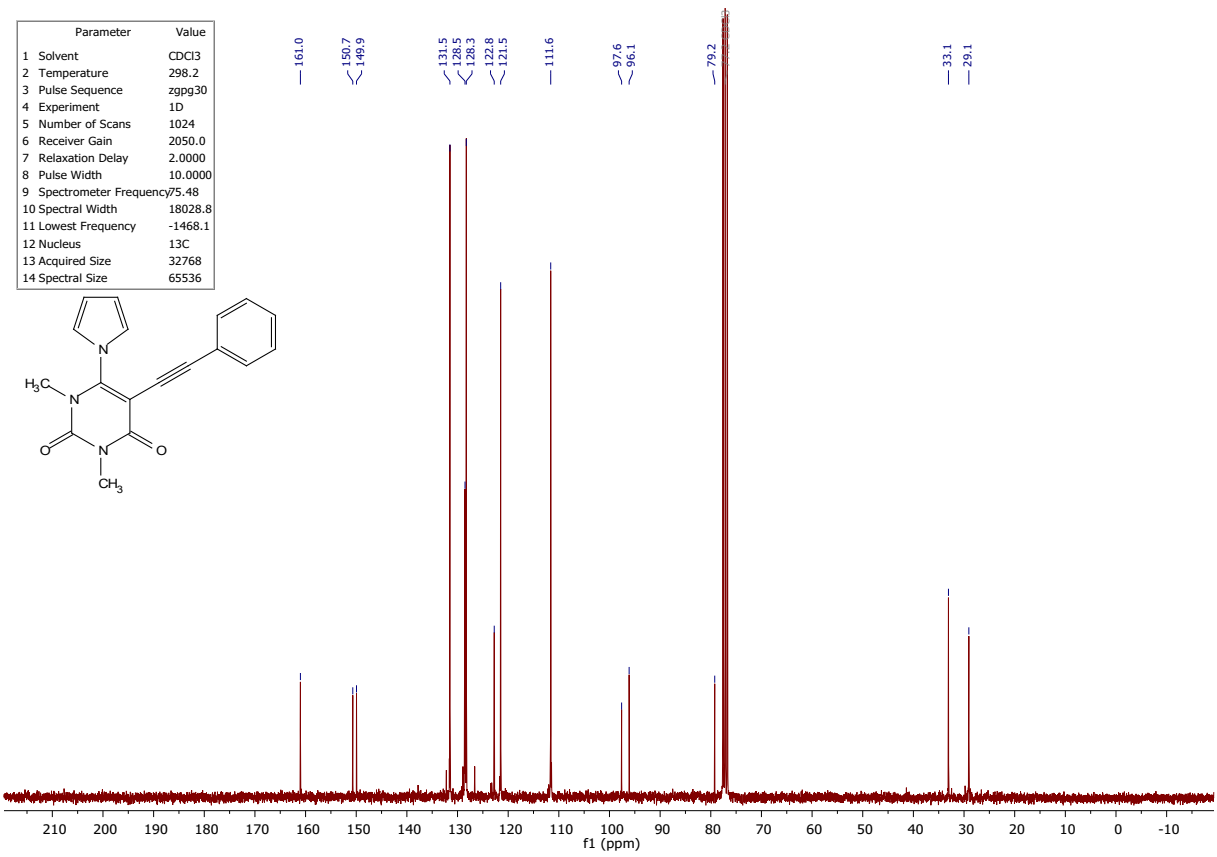


1,3-Dimethyl-5-(phenylethynyl)-6-(1*H*-pyrrol-1-yl)pyrimidine-2,4(1*H*,3*H*)-dione (3b)

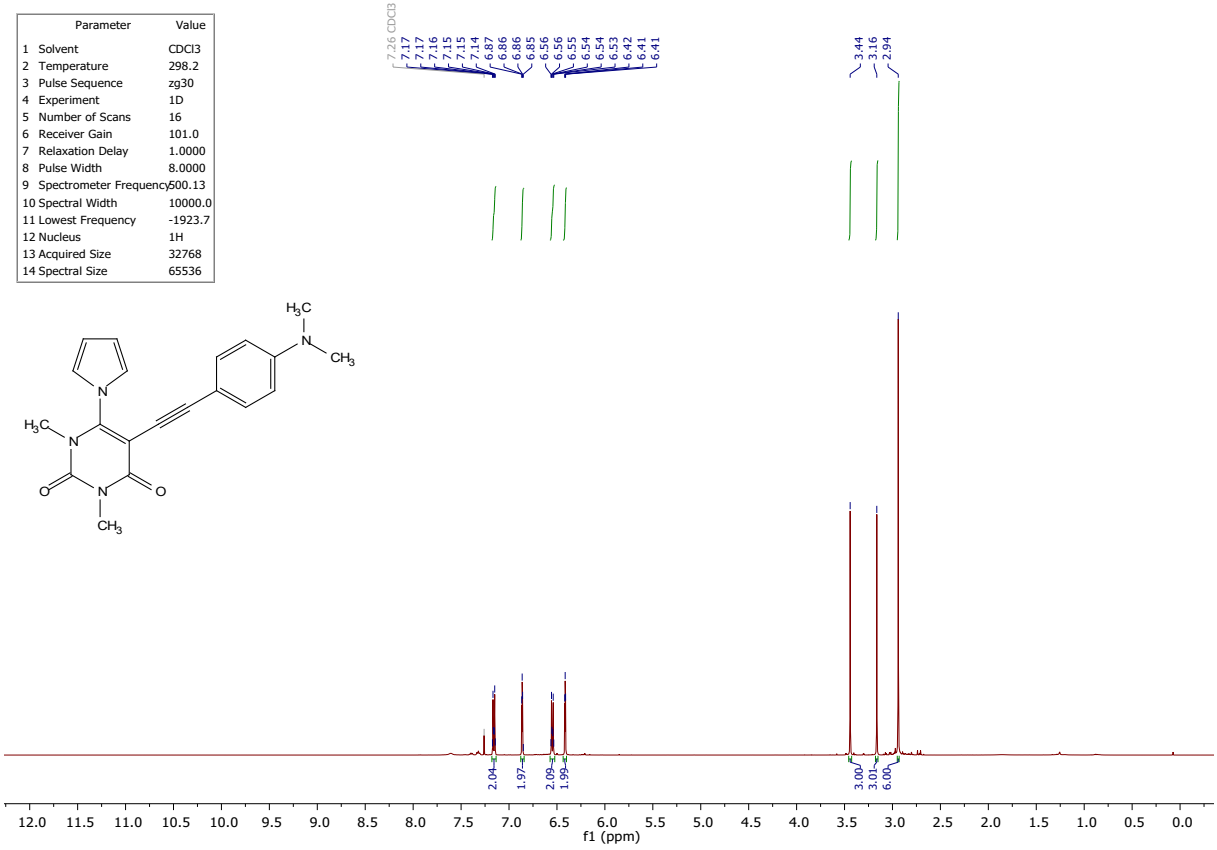
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	128.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1268.1
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

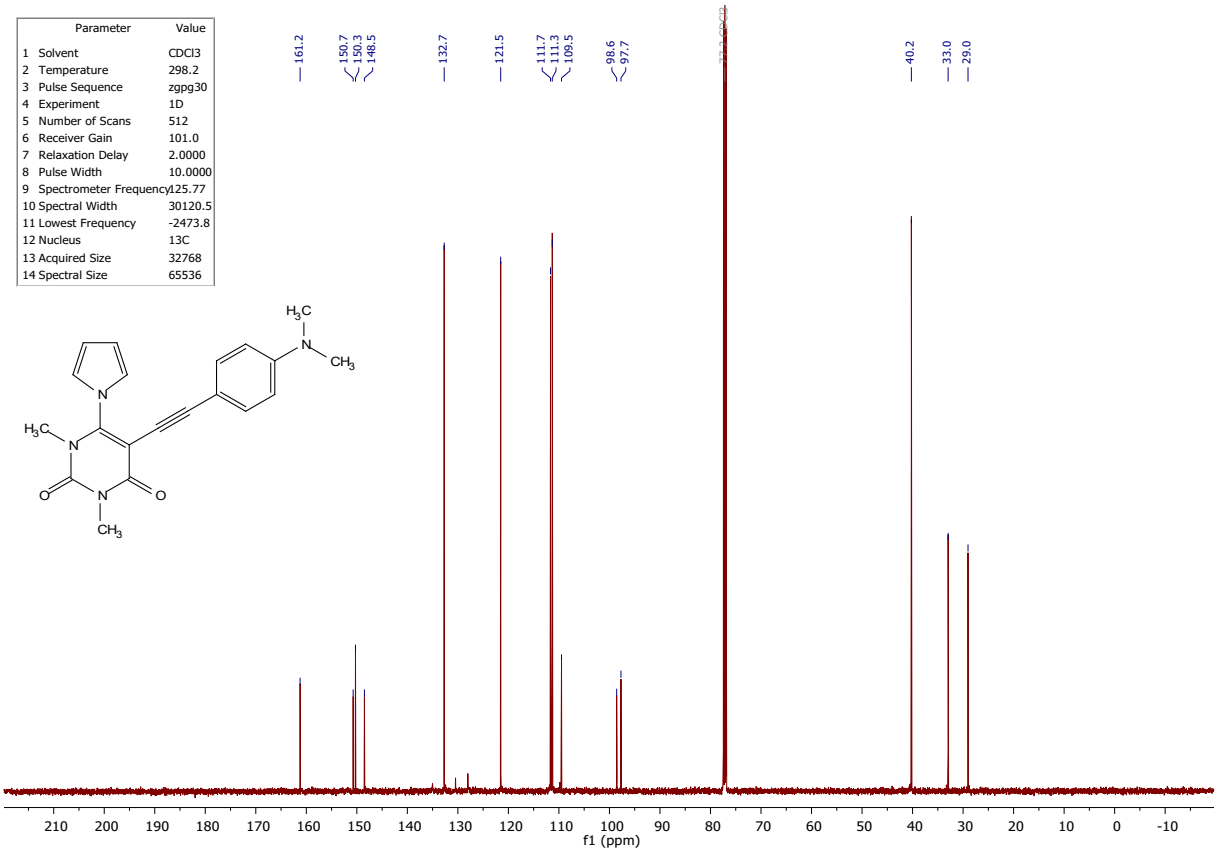


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Experiment	1D
5	Number of Scans	1024
6	Receiver Gain	2050.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1468.1
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536



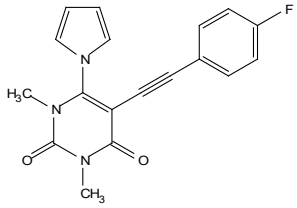
5-((4-(Dimethylamino)phenyl)ethynyl)-1,3-dimethyl-6-(1*H*-pyrrol-1-yl)pyrimidine-2,4(1*H*,3*H*)-dione (3c)



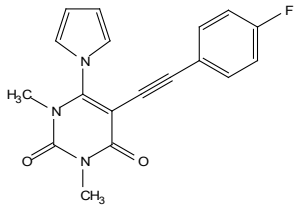


5-((4-Fluorophenyl)ethynyl)-1,3-dimethyl-6-(1*H*-pyrrol-1-yl)pyrimidine-2,4(1*H*,3*H*)-dione (3d)

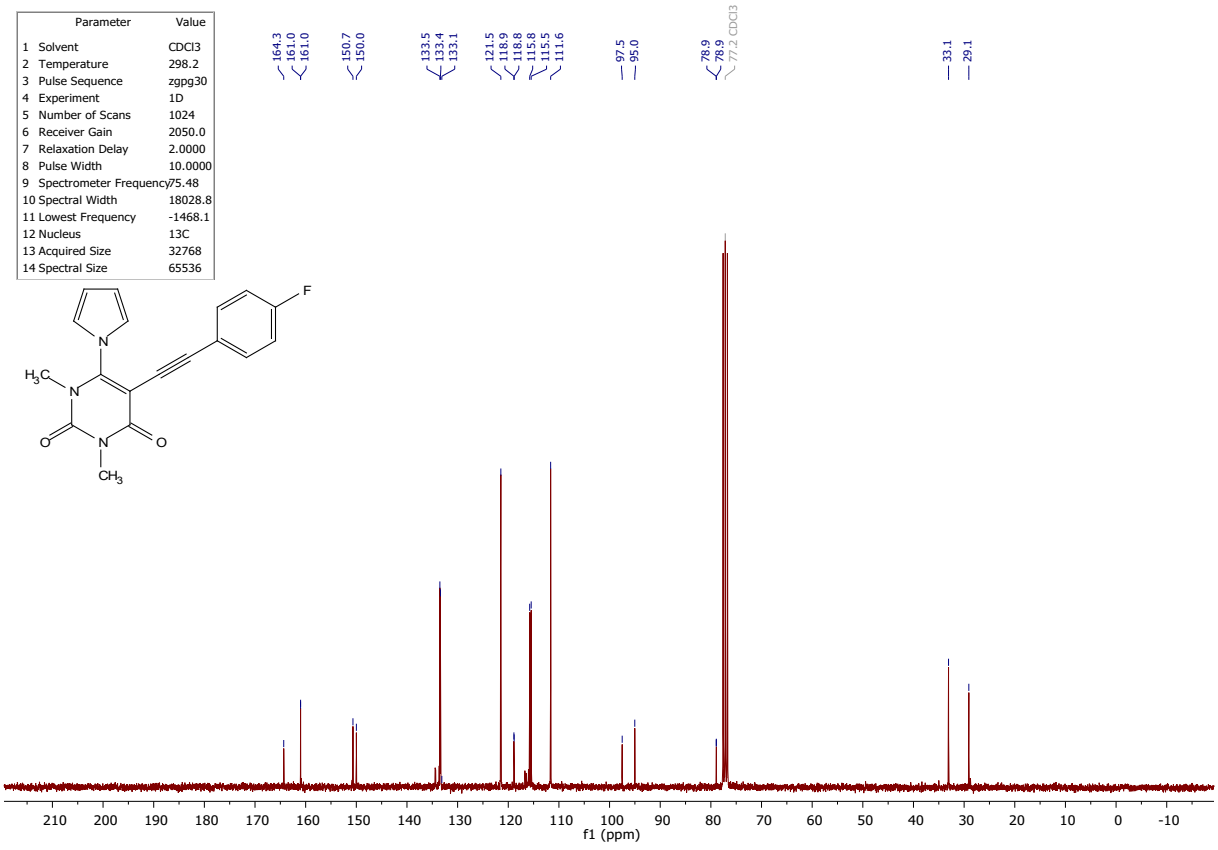
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	101.0
7	Relaxation Delay	1.0000
8	Pulse Width	8.0000
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1957.8
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.3
3	Pulse Sequence	zgig
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	101.0
7	Relaxation Delay	1.0000
8	Pulse Width	12.0000
9	Spectrometer Frequency	470.55
10	Spectral Width	113636.4
11	Lowest Frequency	-103877.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072

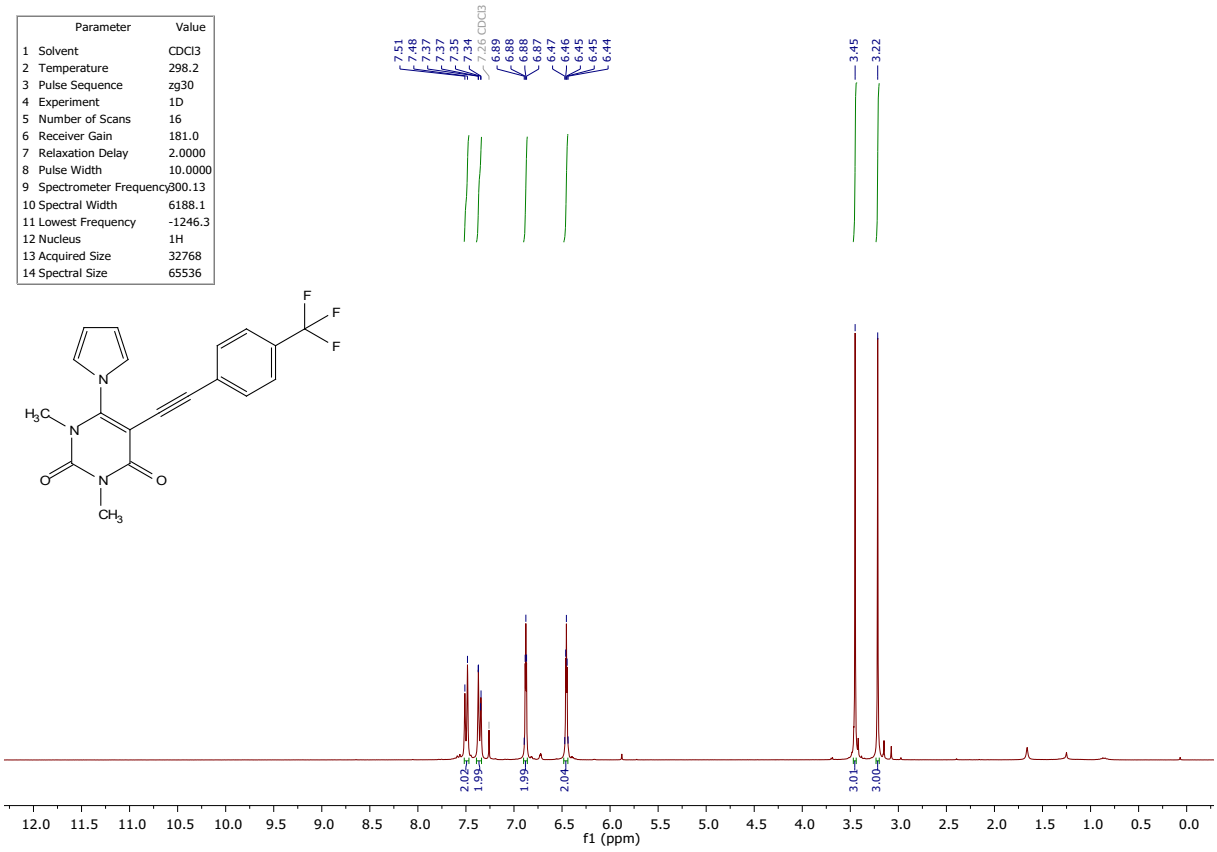


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Experiment	1D
5	Number of Scans	1024
6	Receiver Gain	2050.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1468.1
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

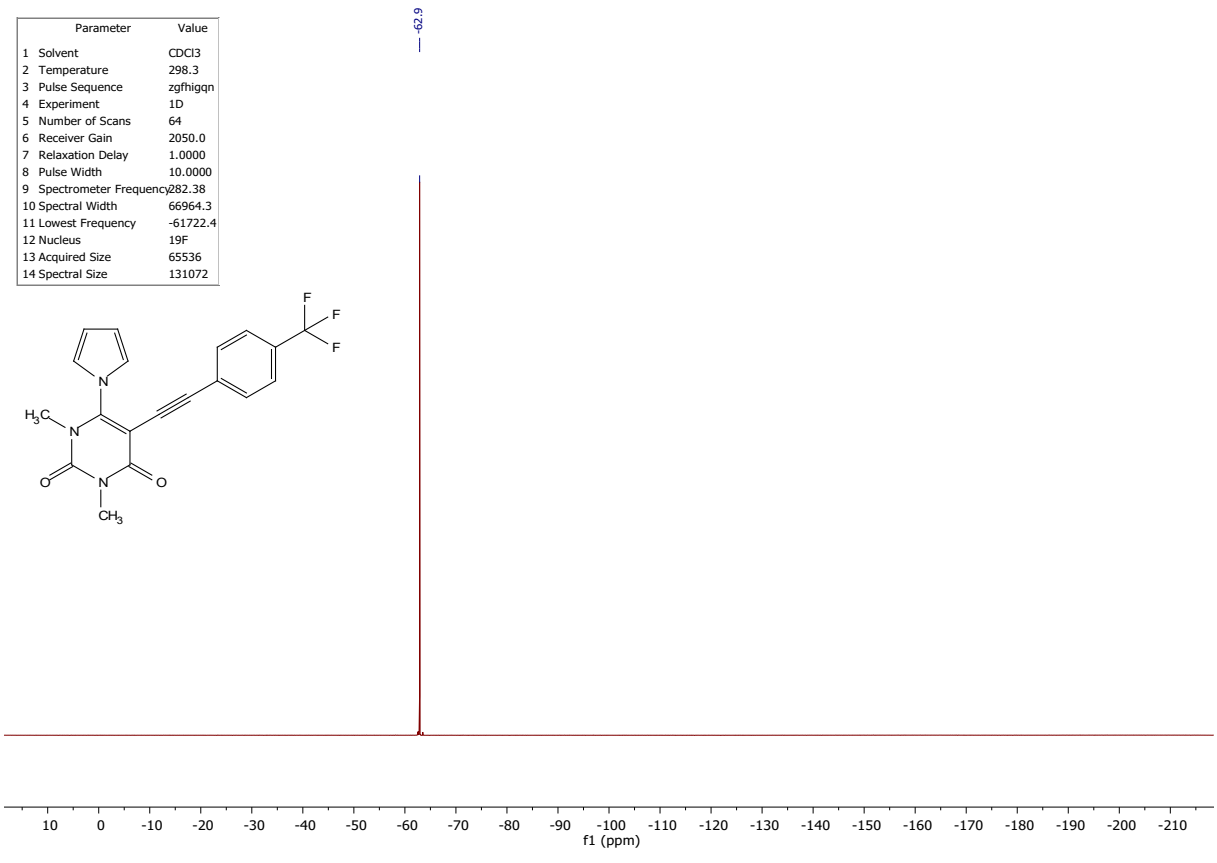


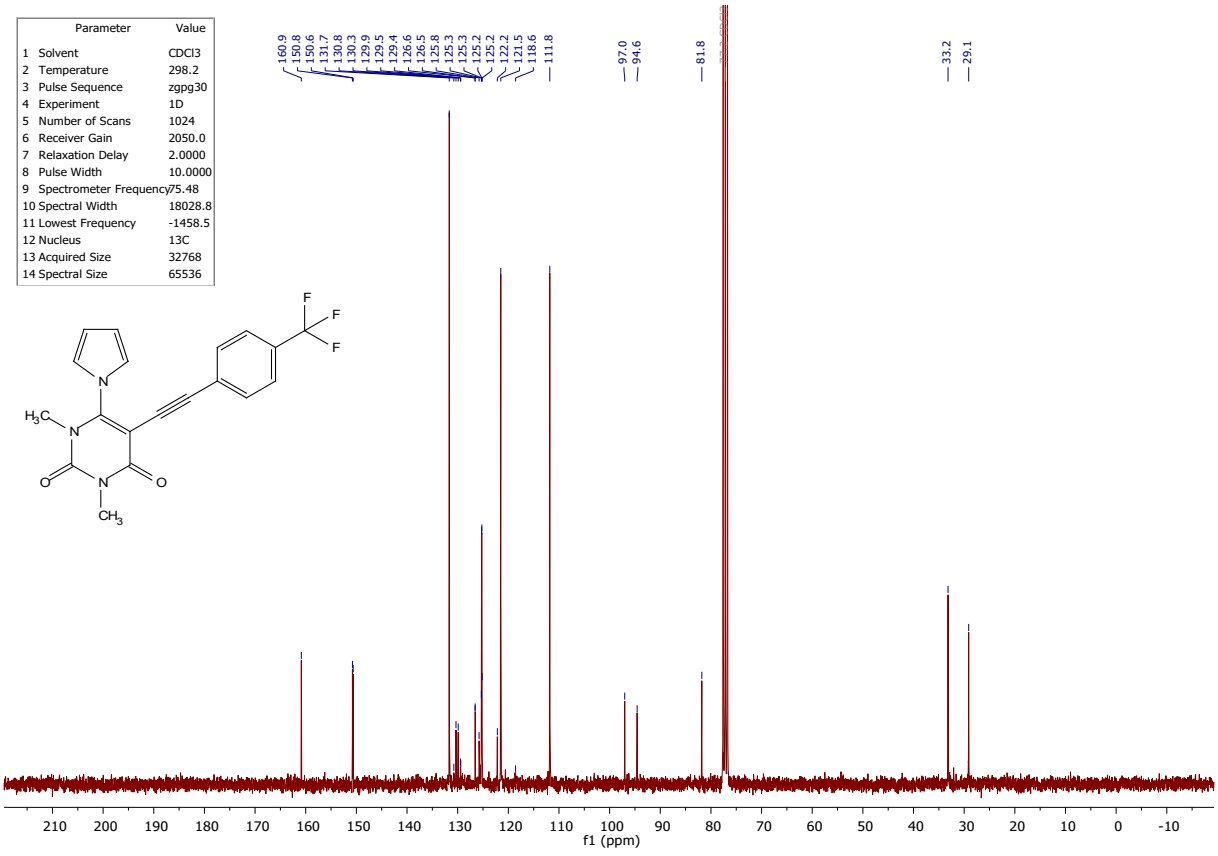
1,3-Dimethyl-6-(1*H*-pyrrol-1-yl)-5-((4-(trifluoromethyl)phenyl)ethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (3e)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	181.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.3
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

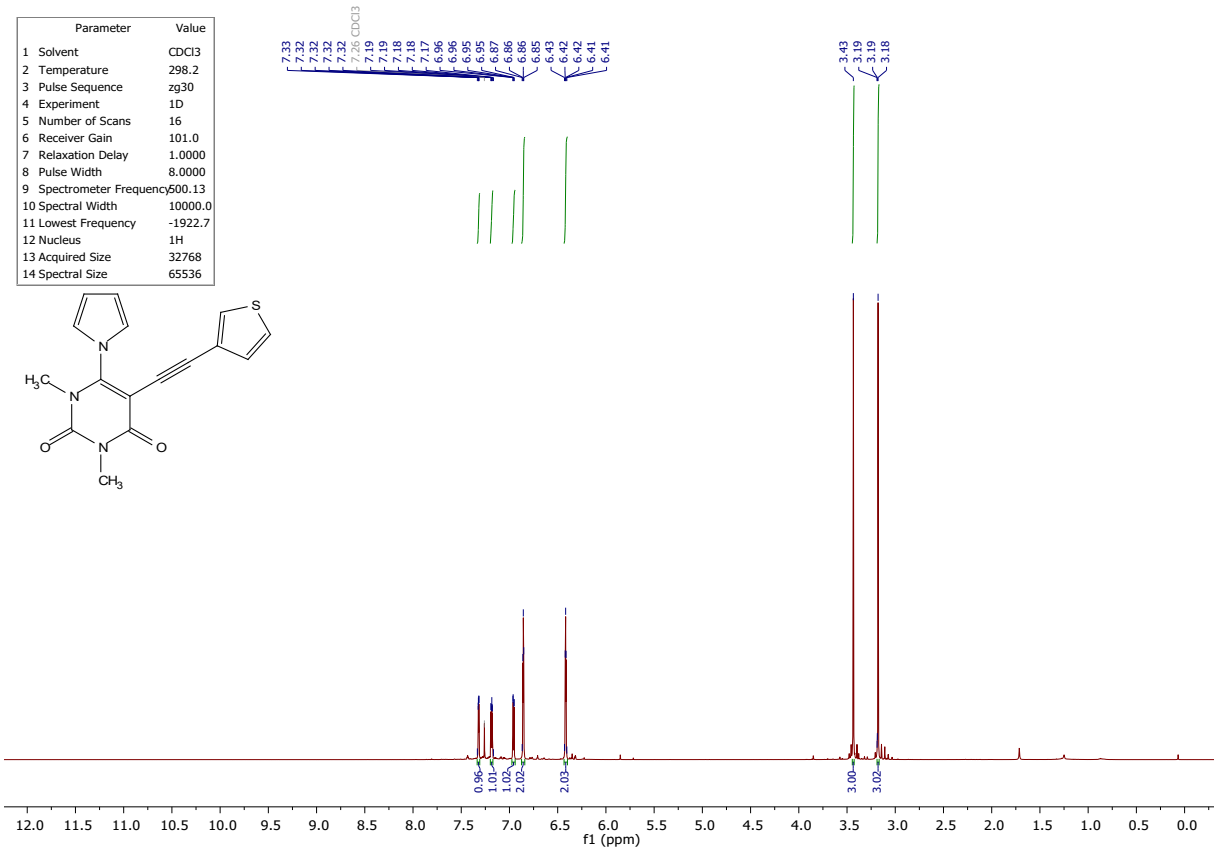


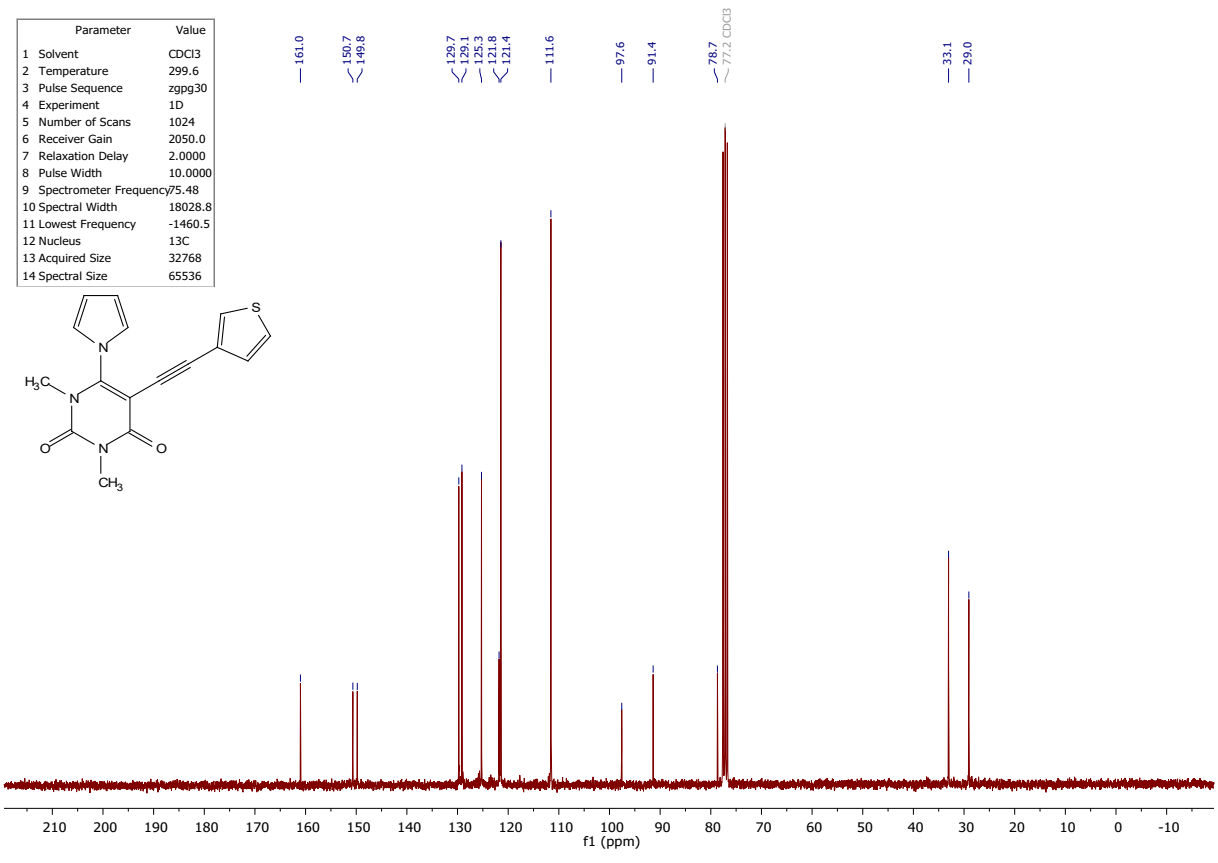
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.3
3	Pulse Sequence	zgfhigqn
4	Experiment	1D
5	Number of Scans	64
6	Receiver Gain	2050.0
7	Relaxation Delay	1.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	282.38
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072




Parameter Value
1 Solvent CDCl3
2 Temperature 298.2
3 Pulse Sequence zgpg30
4 Experiment 1D
5 Number of Scans 1024
6 Receiver Gain 2050.0
7 Relaxation Delay 2.0000
8 Pulse Width 10.0000
9 Spectrometer Frequency 75.48
10 Spectral Width 18028.8
11 Lowest Frequency -1458.5
12 Nucleus 13C
13 Acquired Size 32768
14 Spectral Size 65536
160.9
150.8
150.6
131.7
130.8
130.3
129.9
129.5
129.4
126.6
126.5
125.8
125.3
125.3
125.2
125.2
122.2
121.5
118.6
111.8
97.0
94.6
81.8
33.2
29.1
F
F
F
N
H3C
N
O
N
O
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

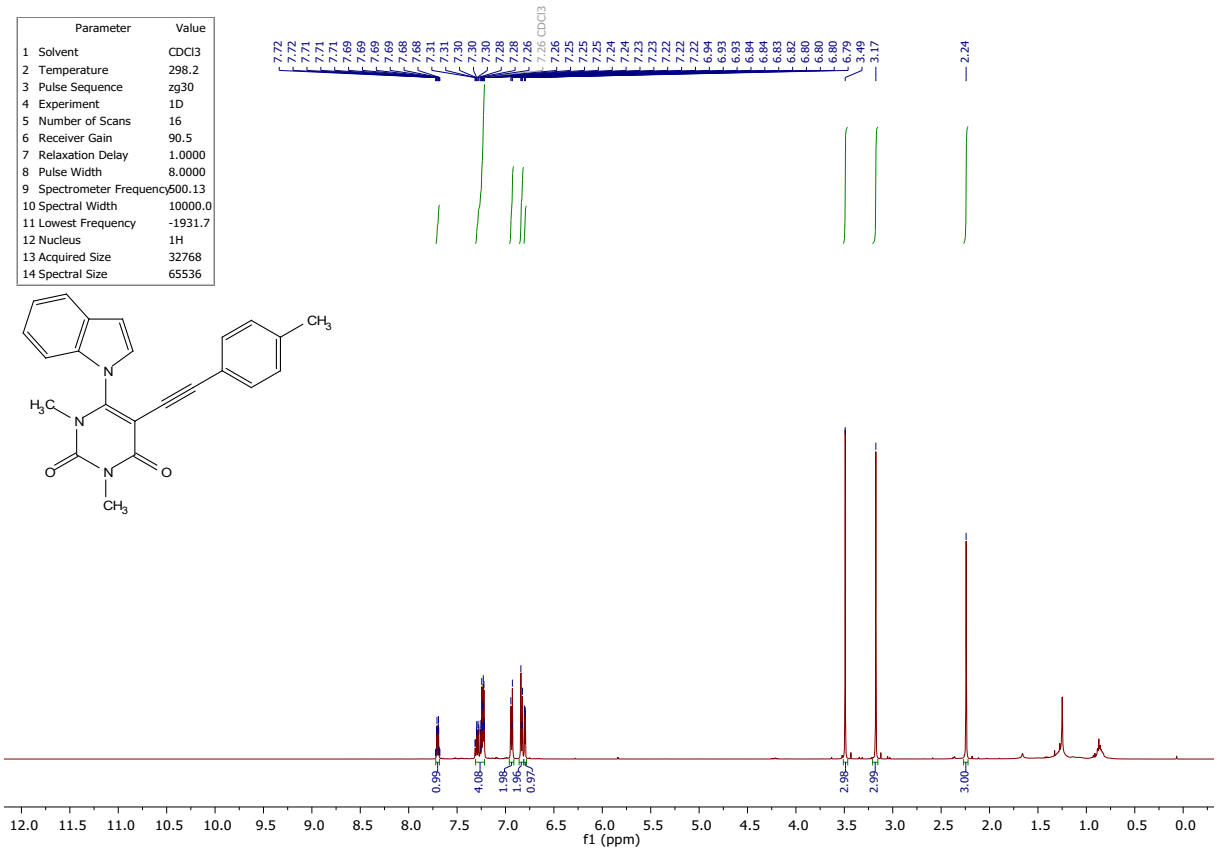
1,3-Dimethyl-6-(1*H*-pyrrol-1-yl)-5-(thiophen-3-ylethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (3f)



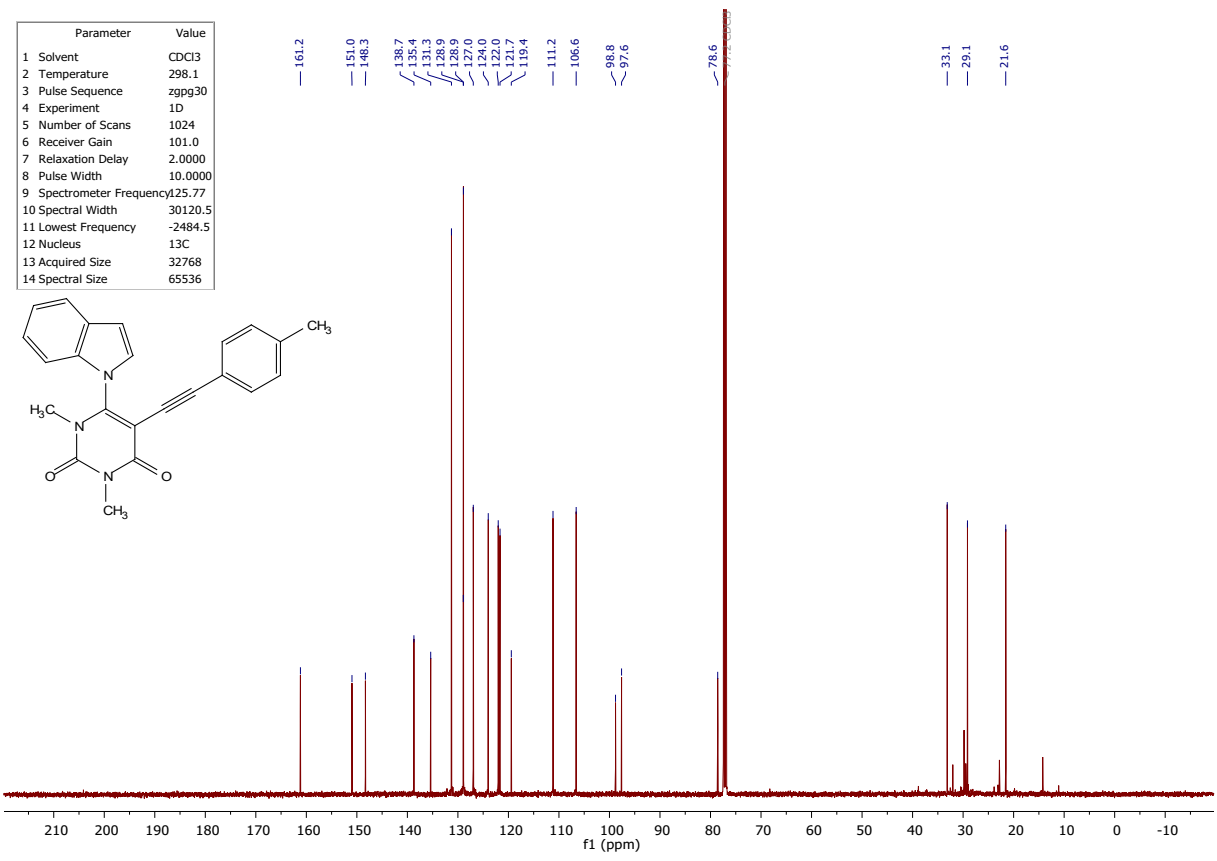


6-(1*H*-Indol-1-yl)-1,3-dimethyl-5-(*p*-tolylethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (3g)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	90.5
7	Relaxation Delay	1.0000
8	Pulse Width	8.0000
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1931.7
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

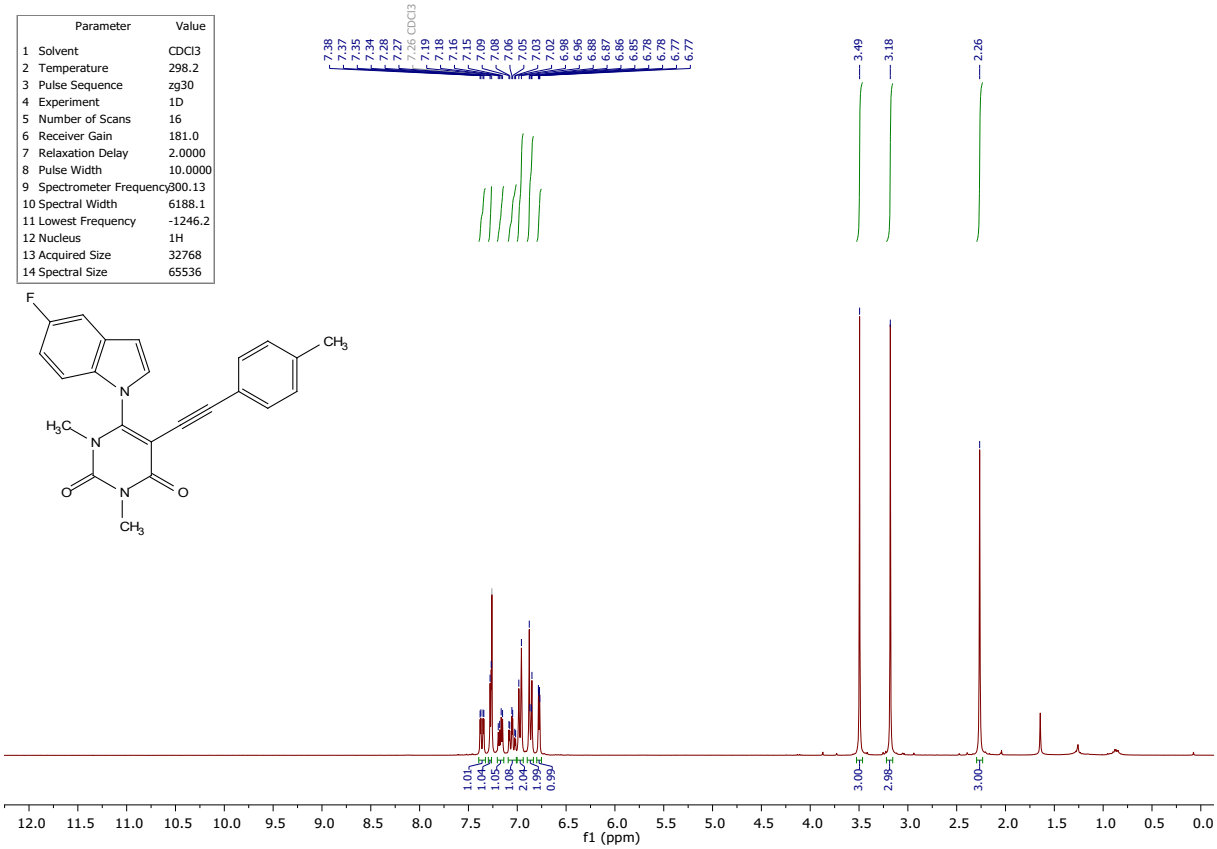


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zgpg30
4	Experiment	1D
5	Number of Scans	1024
6	Receiver Gain	101.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	125.77
10	Spectral Width	30120.5
11	Lowest Frequency	-2484.5
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

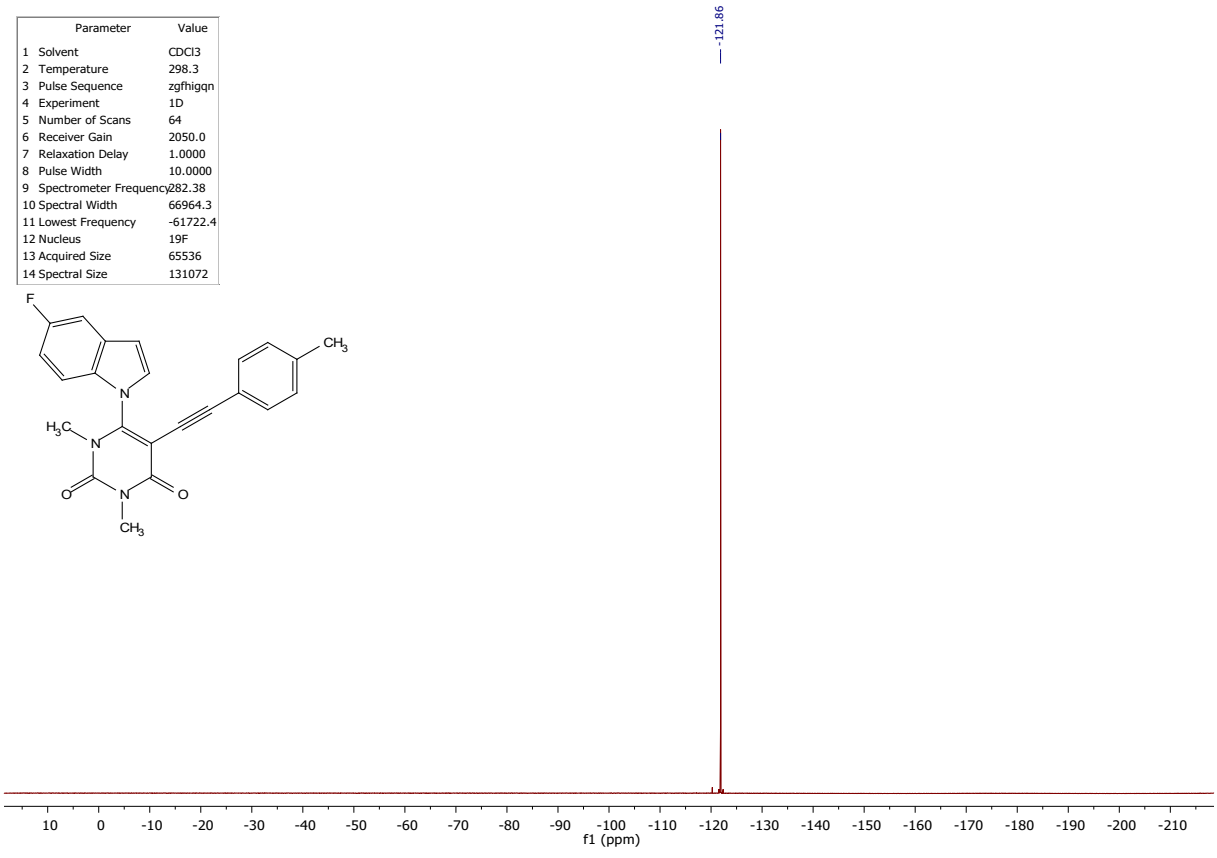


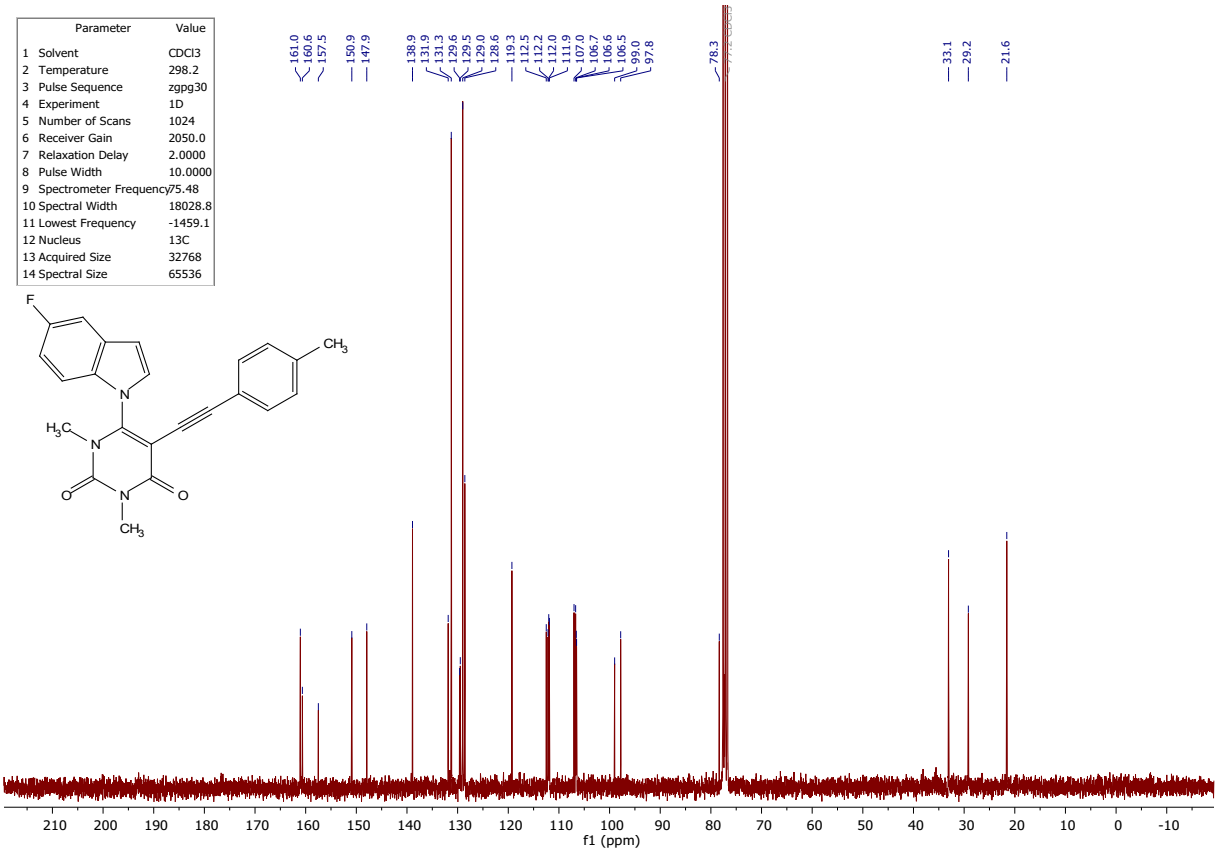
6-(5-Fluoro-1*H*-indol-1-yl)-1,3-dimethyl-5-(*p*-tolylethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (3h).

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	181.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.2
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

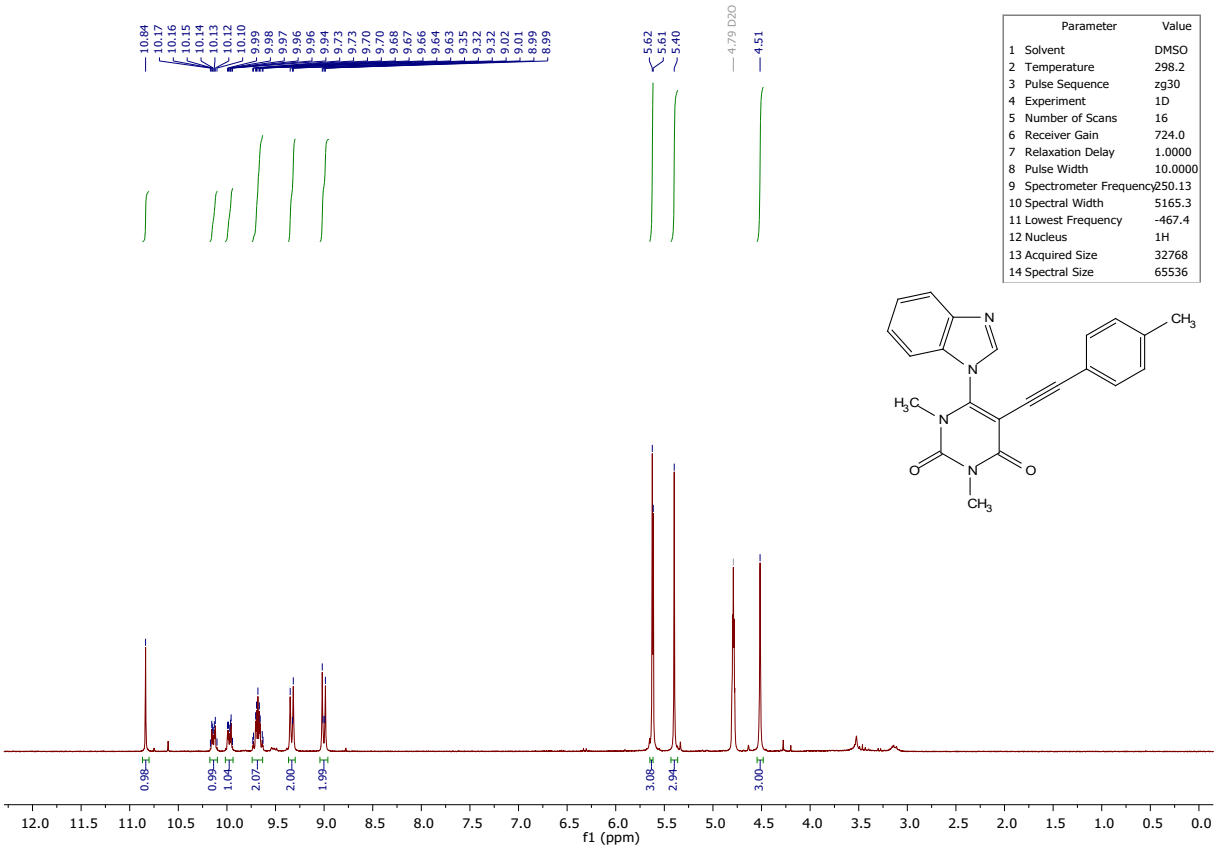


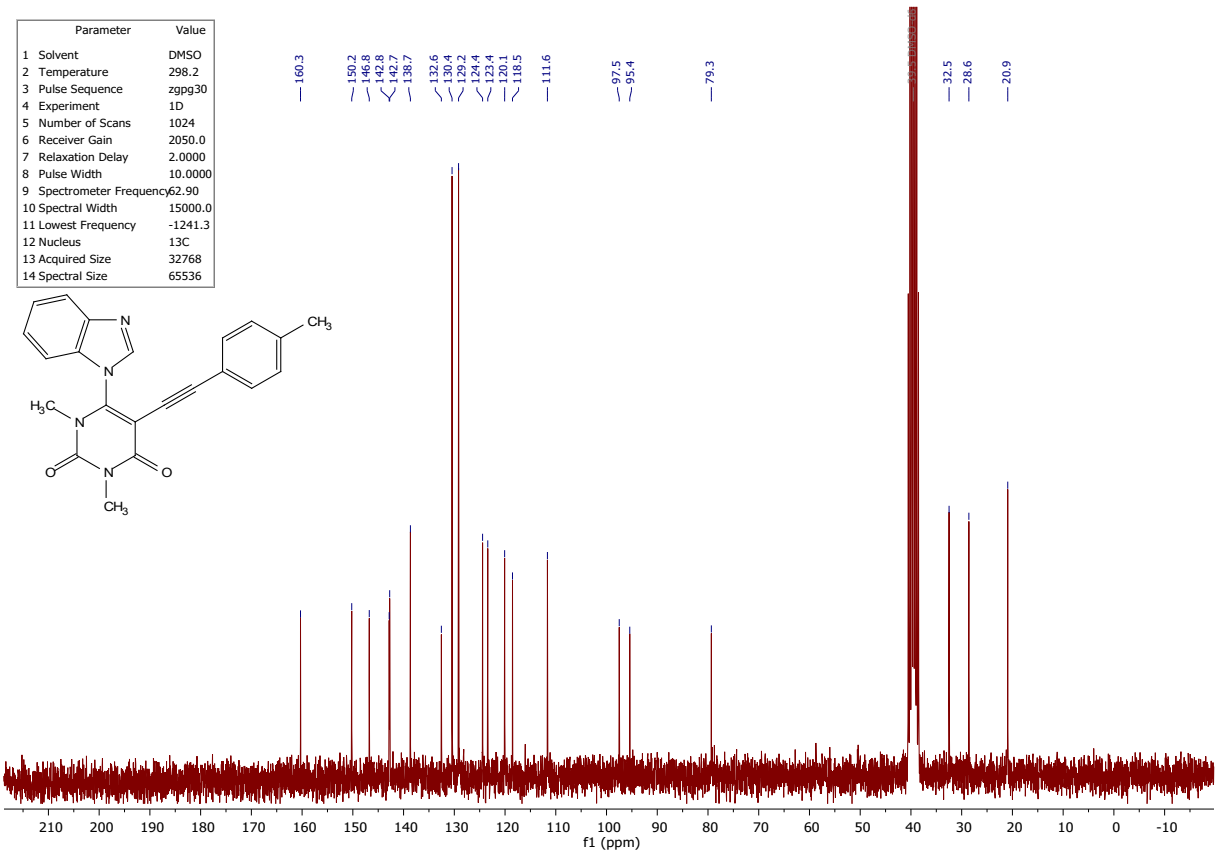
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.3
3	Pulse Sequence	zgfhigqn
4	Experiment	1D
5	Number of Scans	64
6	Receiver Gain	2050.0
7	Relaxation Delay	1.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	282.38
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072



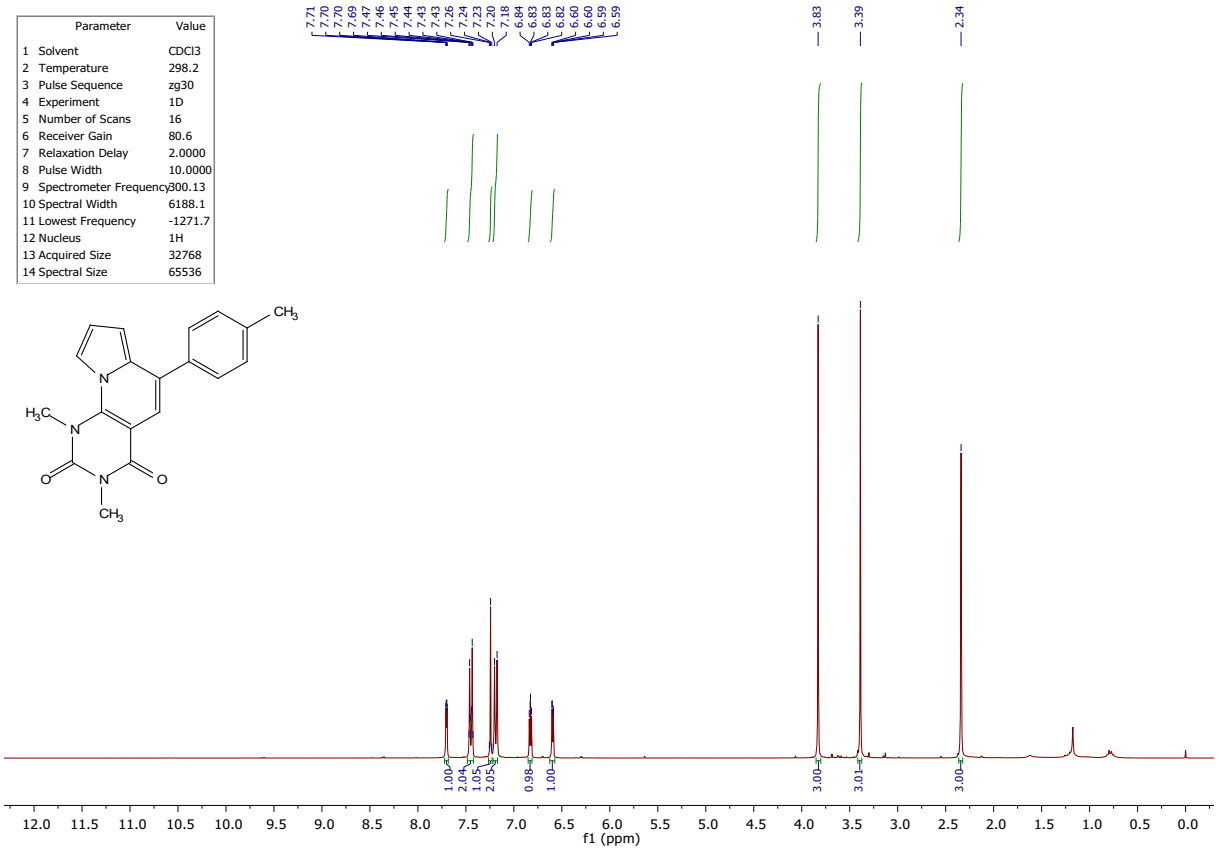

Parameter Value
1 Solvent CDCl3
2 Temperature 298.2
3 Pulse Sequence zgpg30
4 Experiment 1D
5 Number of Scans 1024
6 Receiver Gain 2050.0
7 Relaxation Delay 2.0000
8 Pulse Width 10.0000
9 Spectrometer Frequency 75.48
10 Spectral Width 18028.8
11 Lowest Frequency -1459.1
12 Nucleus 13C
13 Acquired Size 32768
14 Spectral Size 65536
161.0
160.6
157.5
150.9
147.9
138.9
131.9
131.3
129.6
129.5
129.0
128.6
119.3
112.5
112.2
112.0
111.9
107.0
106.7
106.6
106.5
99.0
97.8
78.3
33.1
29.2
21.6
F
N
CH3
H3C
N
O
N
O
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

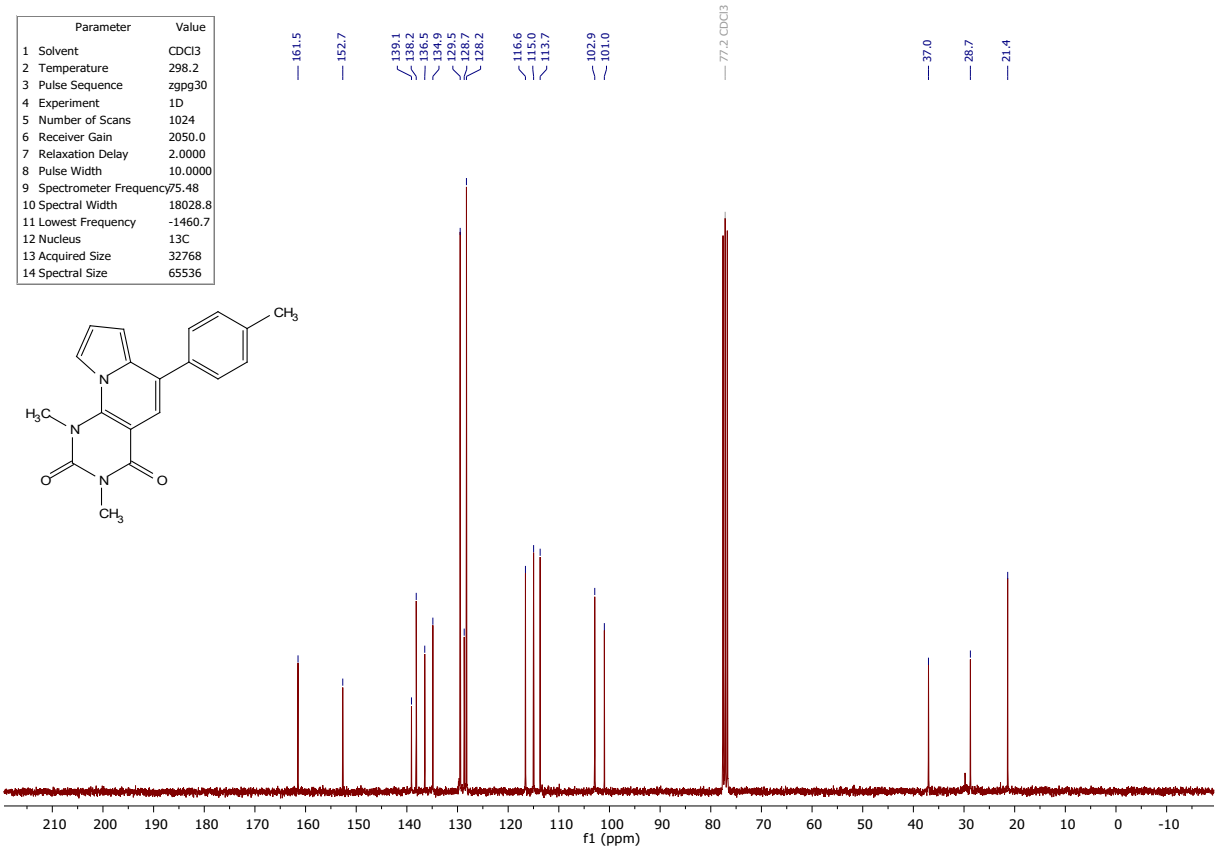
6-(1*H*-Benzo[*d*]imidazol-1-yl)-1,3-dimethyl-5-(*p*-tolylethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (3i)



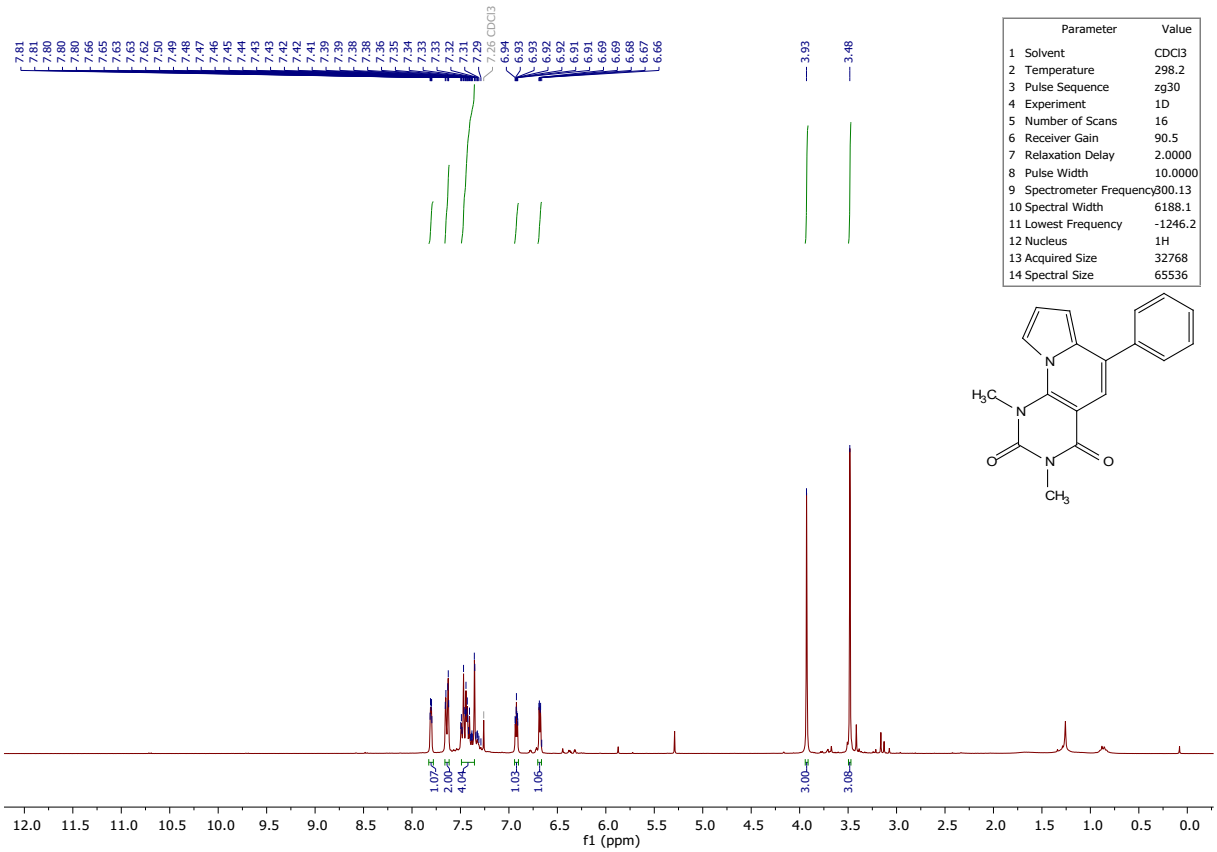


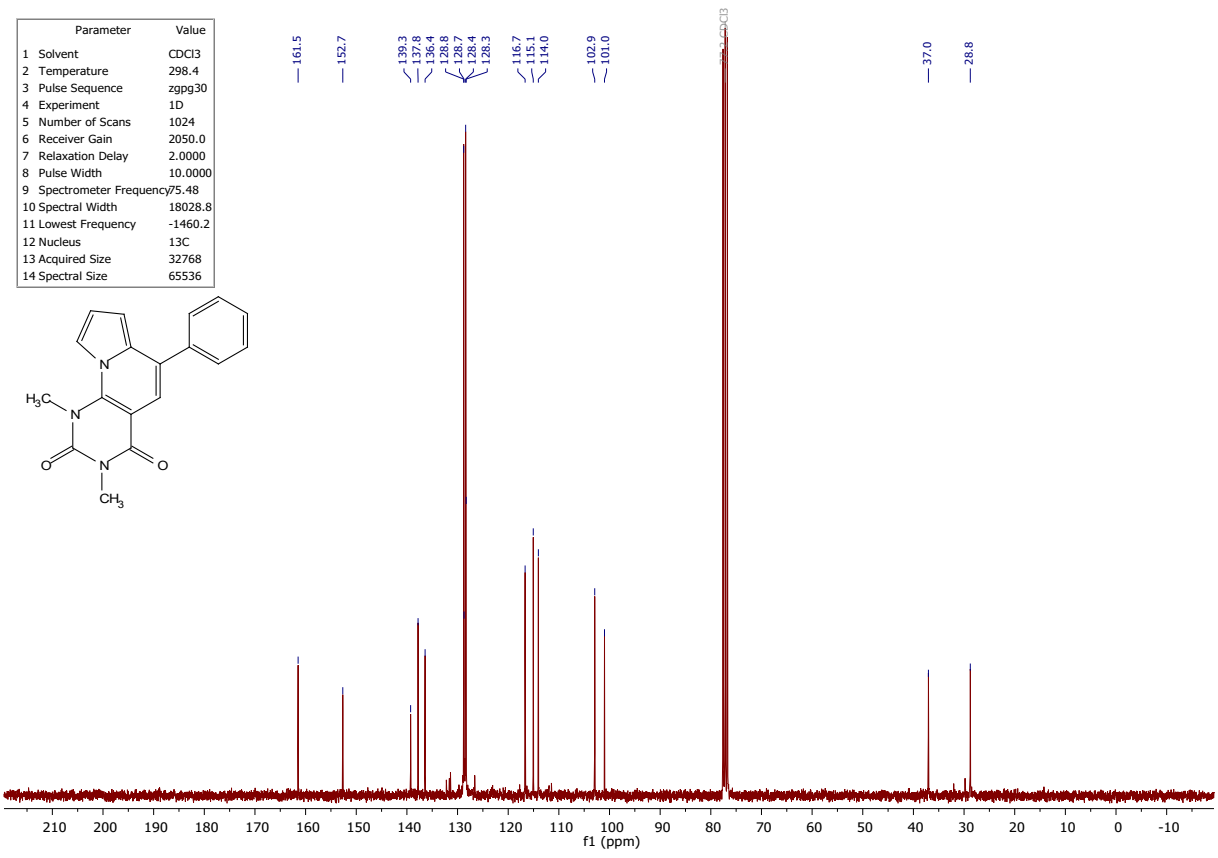
1,3-dimethyl-6-(p-tolyl)pyrimido[4,5-e]indolizine-2,4(1H,3H)-dione (4a)





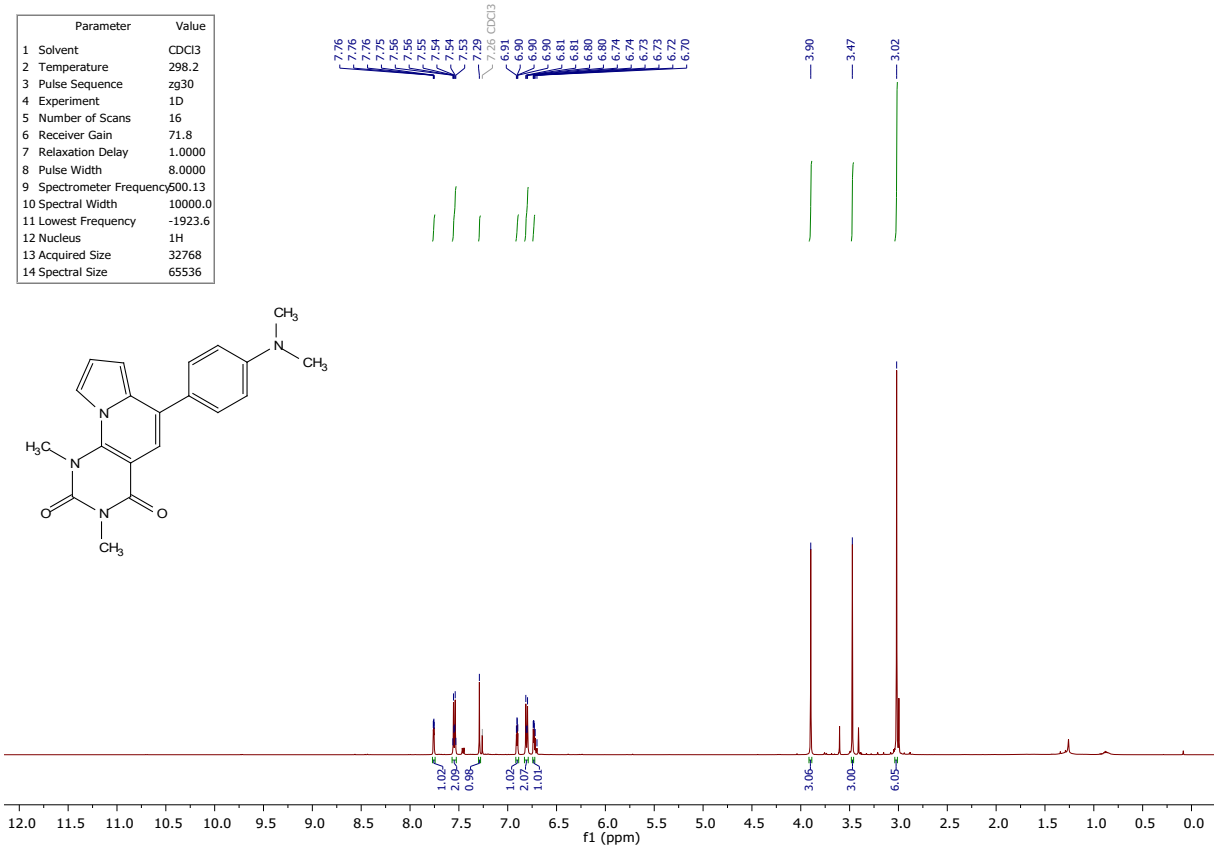
1,3-Dimethyl-6-phenylpyrimido[4,5-*e*]indolizine-2,4(1*H*,3*H*)-dione (4b)



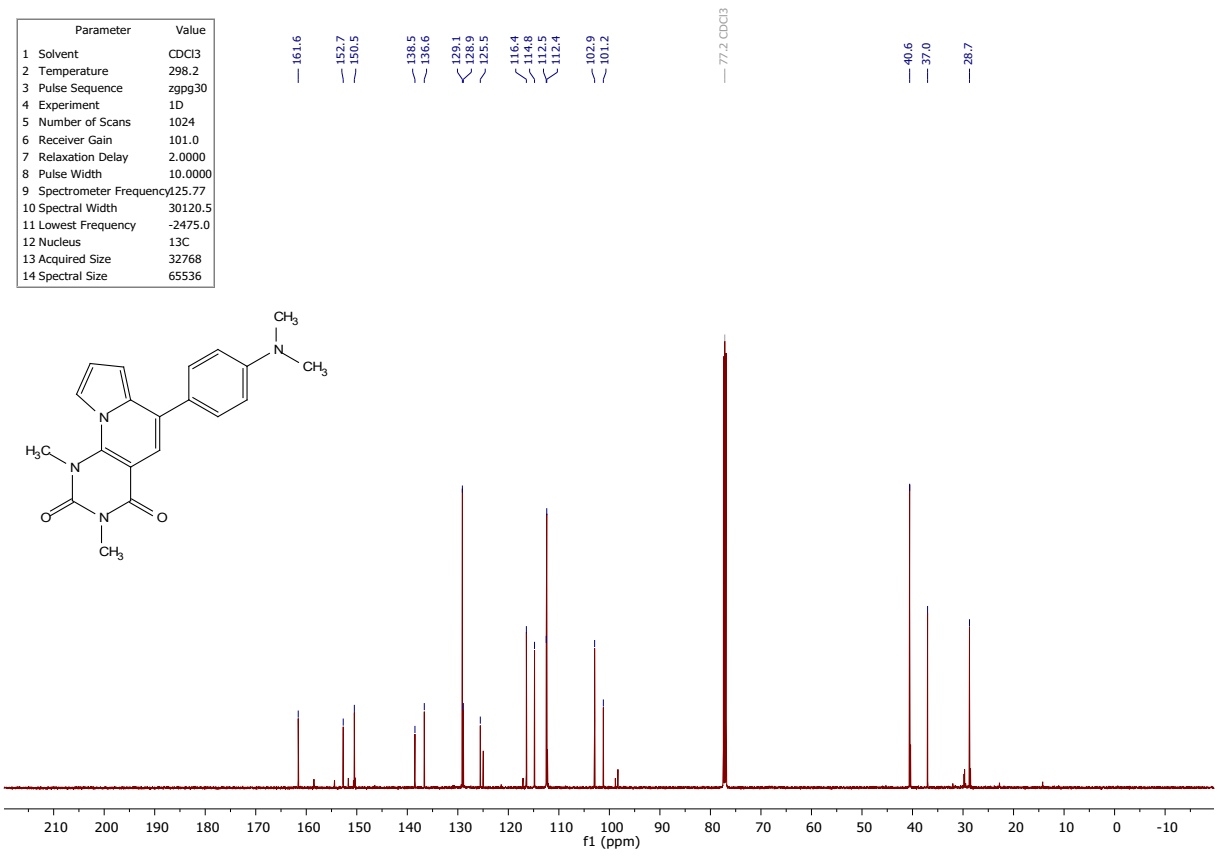


6-(4-(Dimethylamino)phenyl)-1,3-dimethylpyrimido[4,5-*e*]indolizine-2,4(1*H*,3*H*)-dione (4c)

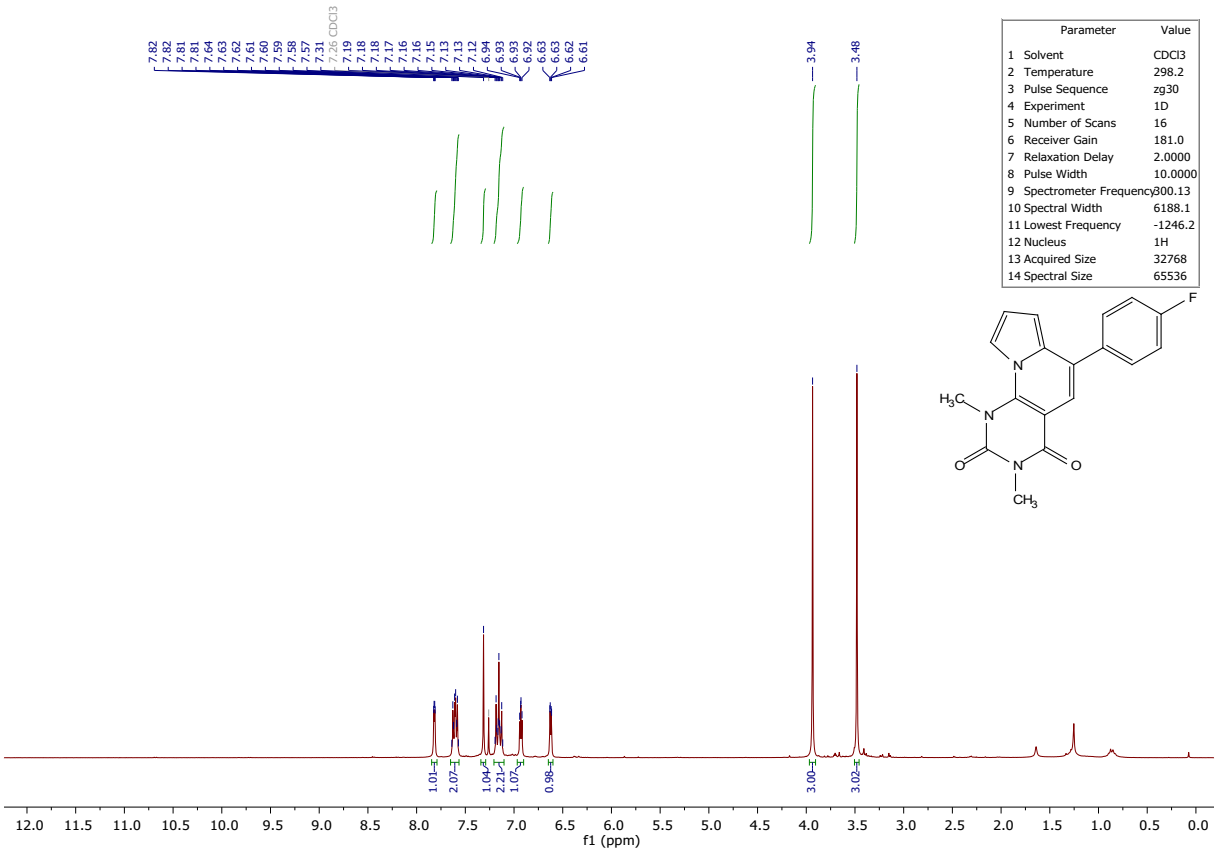
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	71.8
7	Relaxation Delay	1.0000
8	Pulse Width	8.0000
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1923.6
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

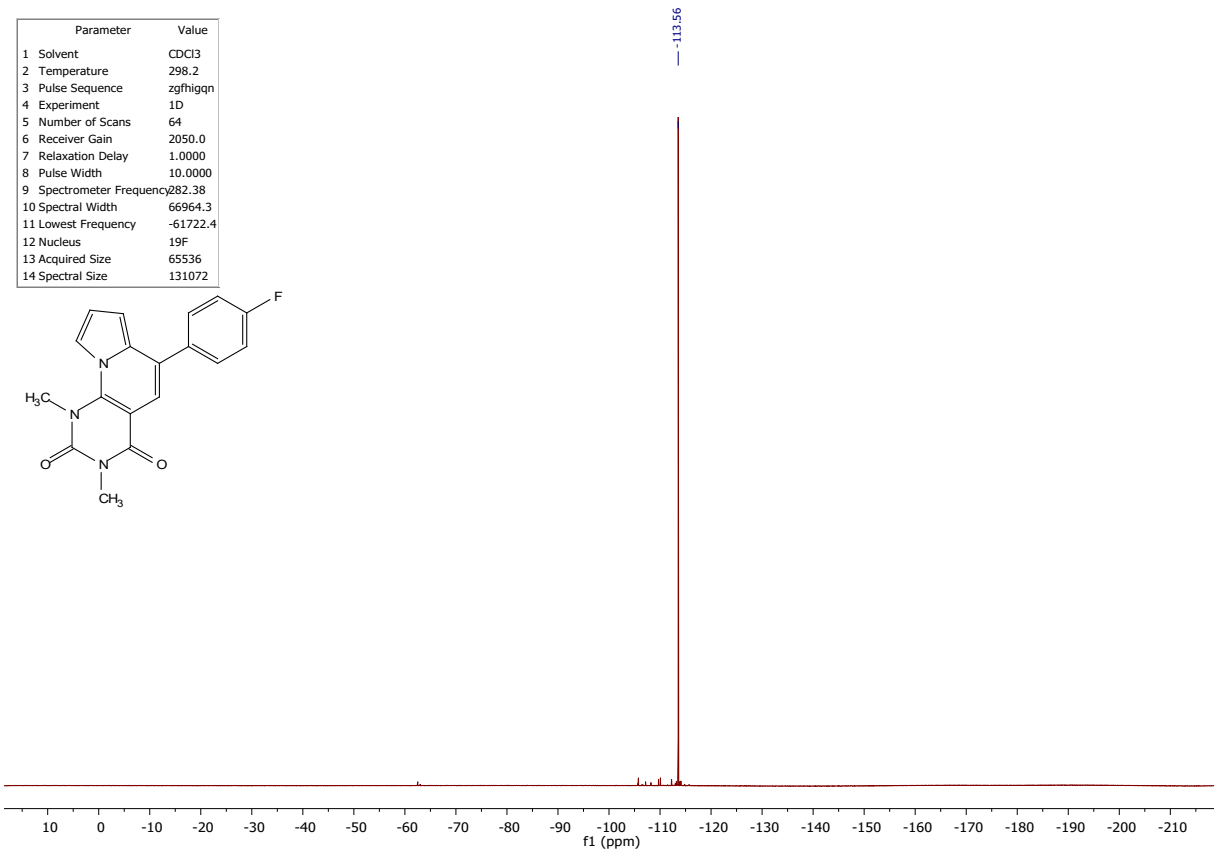


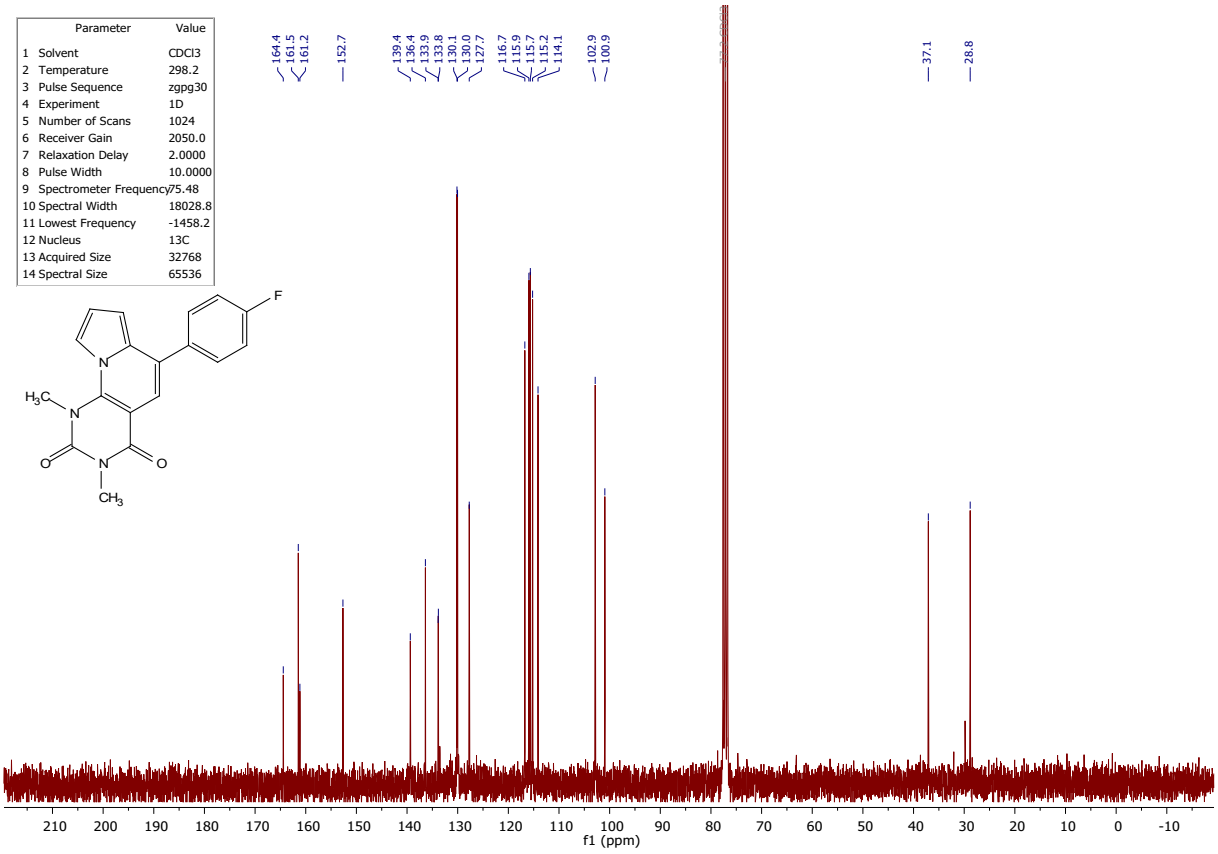
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Experiment	1D
5	Number of Scans	1024
6	Receiver Gain	101.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	125.77
10	Spectral Width	30120.5
11	Lowest Frequency	-2475.0
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536



6-(4-Fluorophenyl)-1,3-dimethylpyrimido[4,5-e]indolizine-2,4(1*H*,3*H*)-dione (4d)

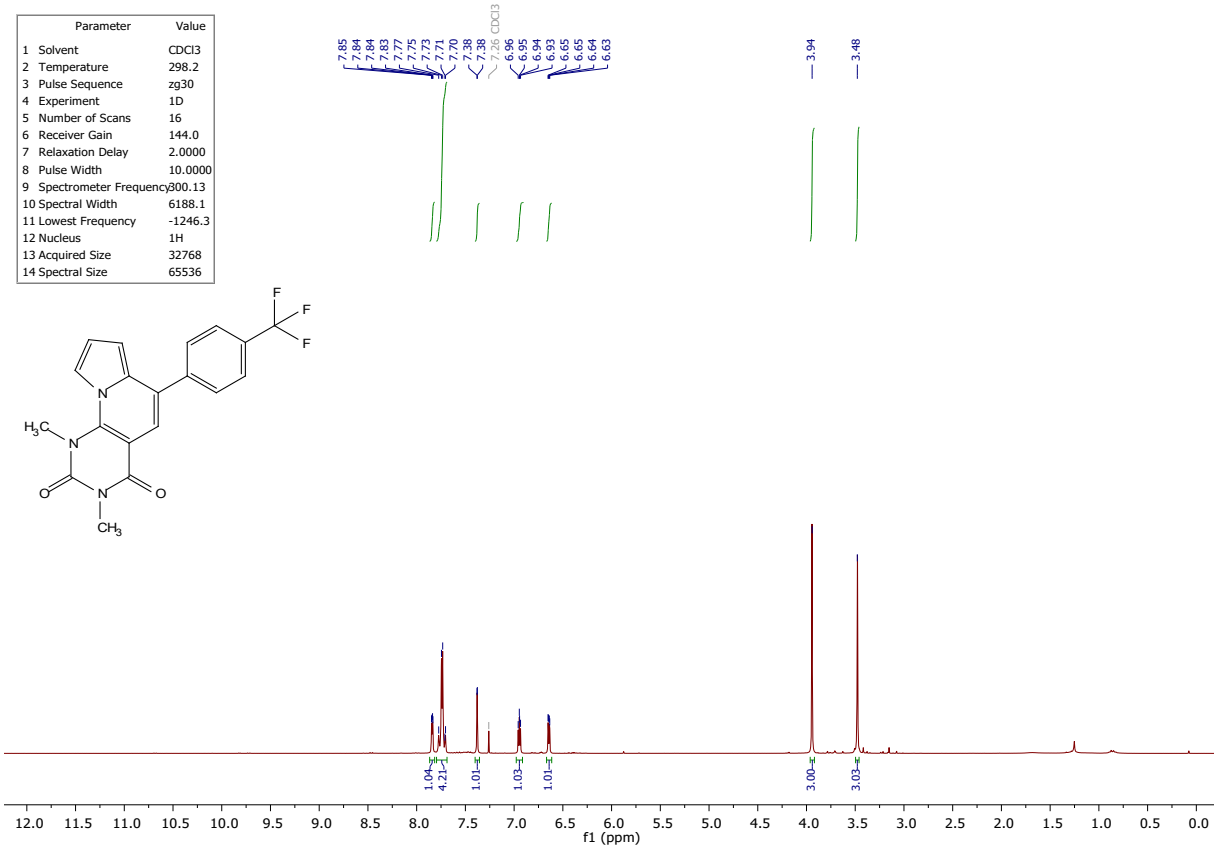




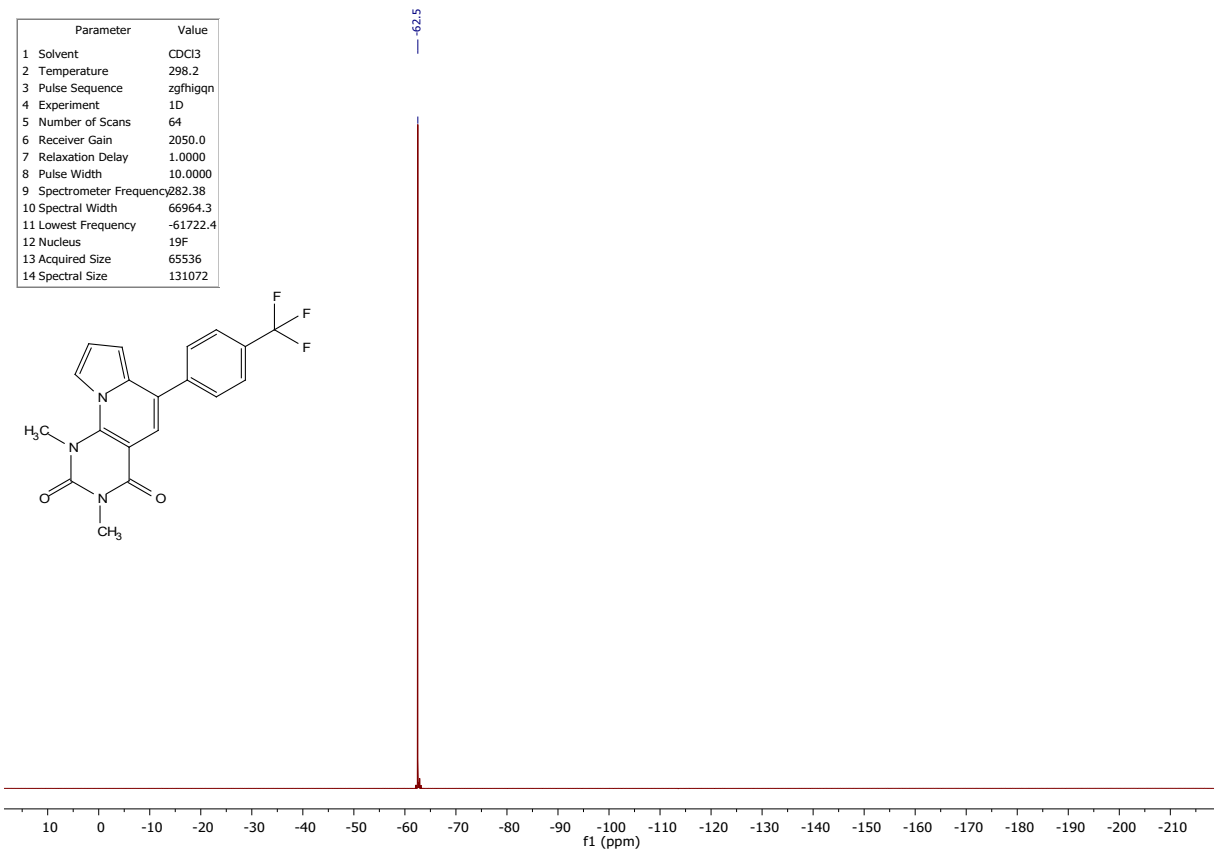

Parameter Value
1 Solvent CDCl3
2 Temperature 298.2
3 Pulse Sequence zgpg30
4 Experiment 1D
5 Number of Scans 1024
6 Receiver Gain 2050.0
7 Relaxation Delay 2.0000
8 Pulse Width 10.0000
9 Spectrometer Frequency 75.48
10 Spectral Width 18028.8
11 Lowest Frequency -1458.2
12 Nucleus 13C
13 Acquired Size 32768
14 Spectral Size 65536
164.4
161.5
161.2
152.7
139.4
136.4
133.9
133.8
130.1
130.0
127.7
116.7
115.9
115.7
115.2
114.1
102.9
100.9
37.1
28.8
F
N
H3C
N
O
O
N
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

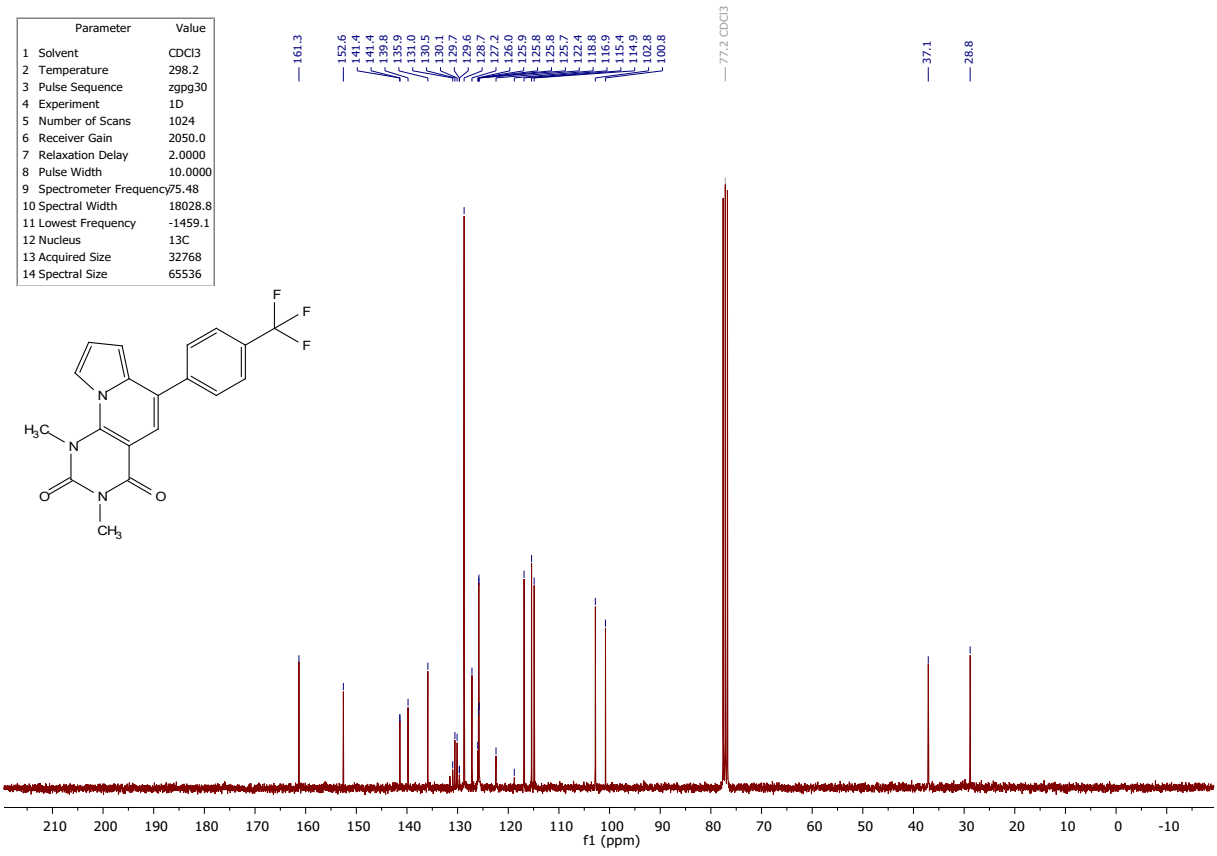
1,3-Dimethyl-6-(4-(trifluoromethyl)phenyl)pyrimido[4,5-*e*]indolizine-2,4(1*H*,3*H*)-dione (4e)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	144.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.3
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



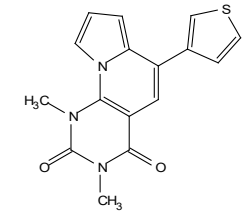
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgfhigqn
4	Experiment	1D
5	Number of Scans	64
6	Receiver Gain	2050.0
7	Relaxation Delay	1.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	282.38
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072



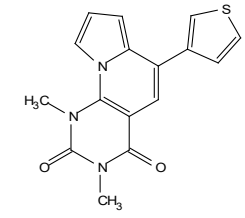

Parameter Value
1 Solvent CDCl3
2 Temperature 298.2
3 Pulse Sequence zgpg30
4 Experiment 1D
5 Number of Scans 1024
6 Receiver Gain 2050.0
7 Relaxation Delay 2.0000
8 Pulse Width 10.0000
9 Spectrometer Frequency 75.48
10 Spectral Width 18028.8
11 Lowest Frequency -1459.1
12 Nucleus 13C
13 Acquired Size 32768
14 Spectral Size 65536
161.3
152.6
141.4
141.4
139.8
135.9
131.0
130.5
130.1
129.7
129.6
128.7
127.2
126.0
125.9
125.8
125.8
125.7
122.4
118.8
116.9
115.4
114.9
102.8
100.8
77.2 CDCl3
37.1
28.8
F
F
F
N
N
H3C
O
N
O
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

1,3-Dimethyl-6-(thiophen-3-yl)pyrimido[4,5-e]indolizine-2,4(1*H*,3*H*)-dione (4f)

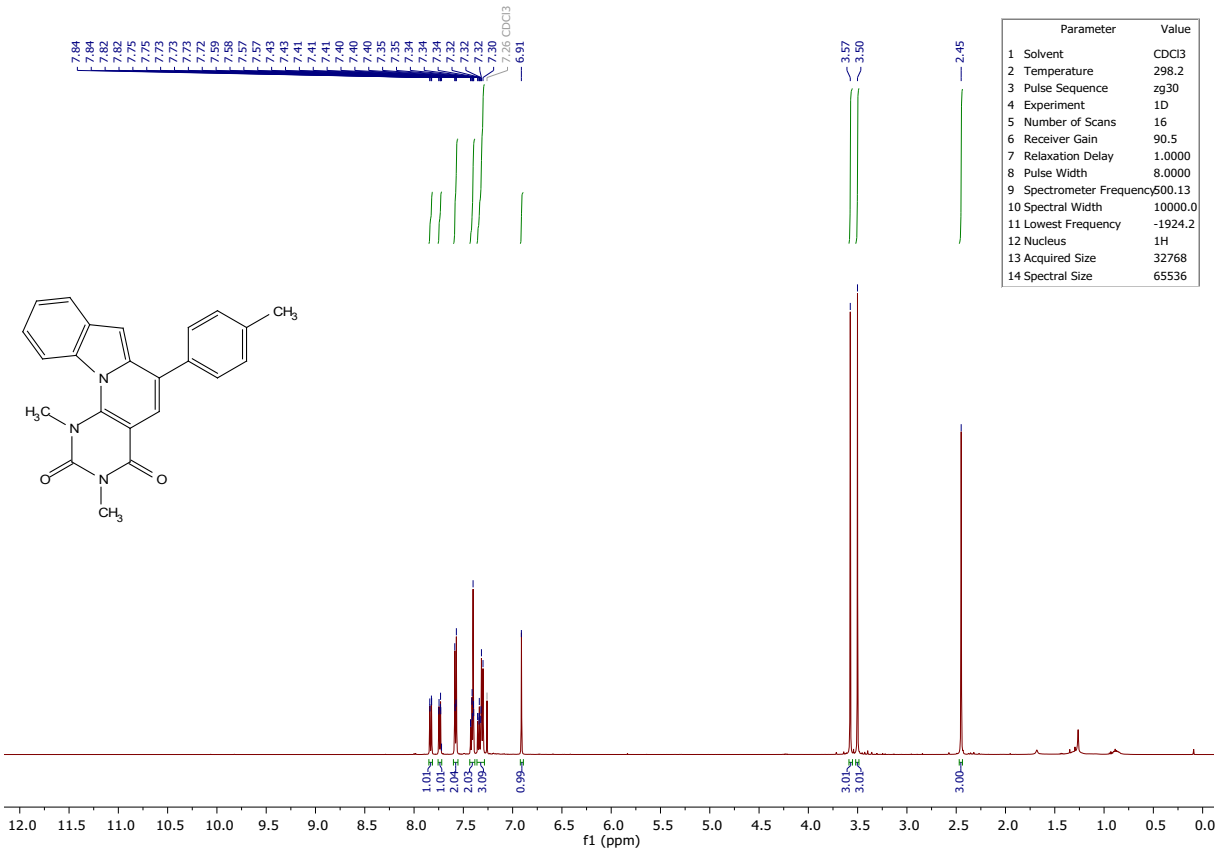
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	181.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.4
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

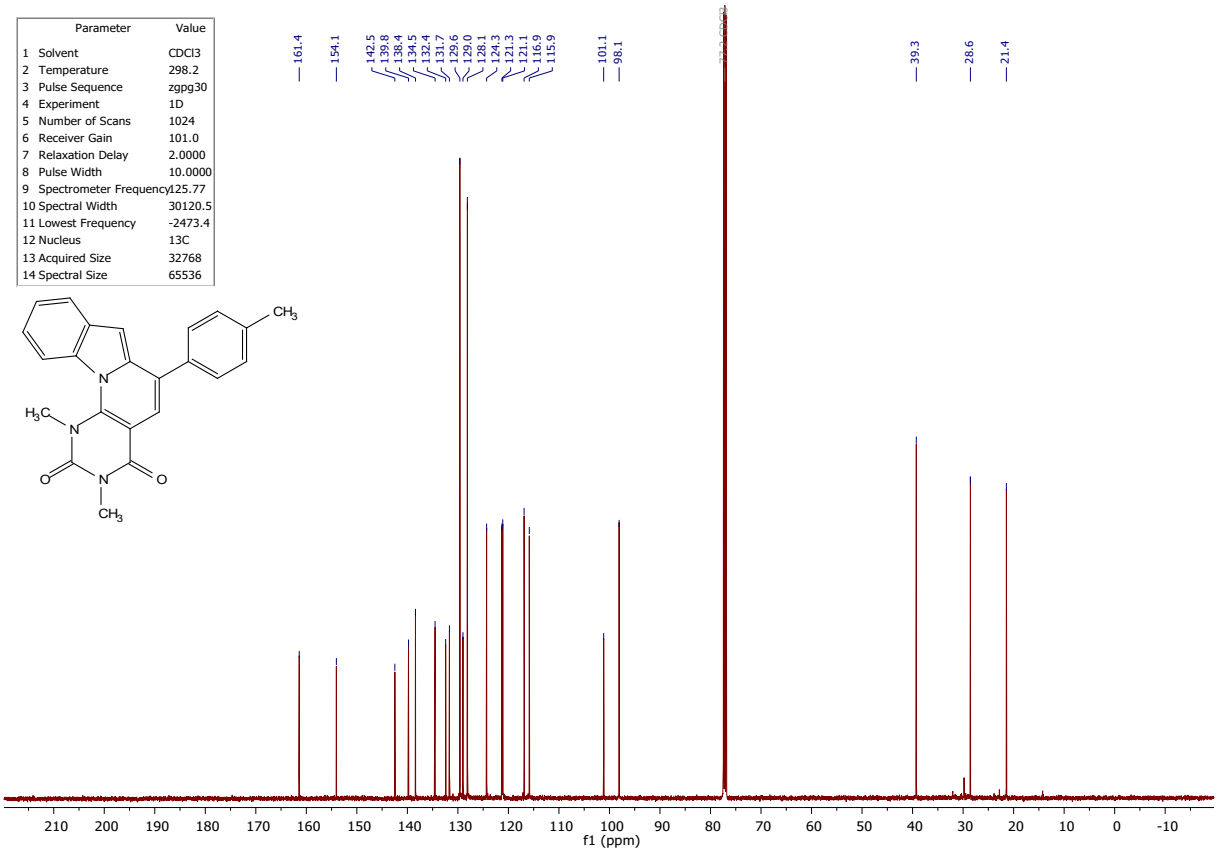


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.8
3	Pulse Sequence	zgpg30
4	Experiment	1D
5	Number of Scans	1024
6	Receiver Gain	2050.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1459.5
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536



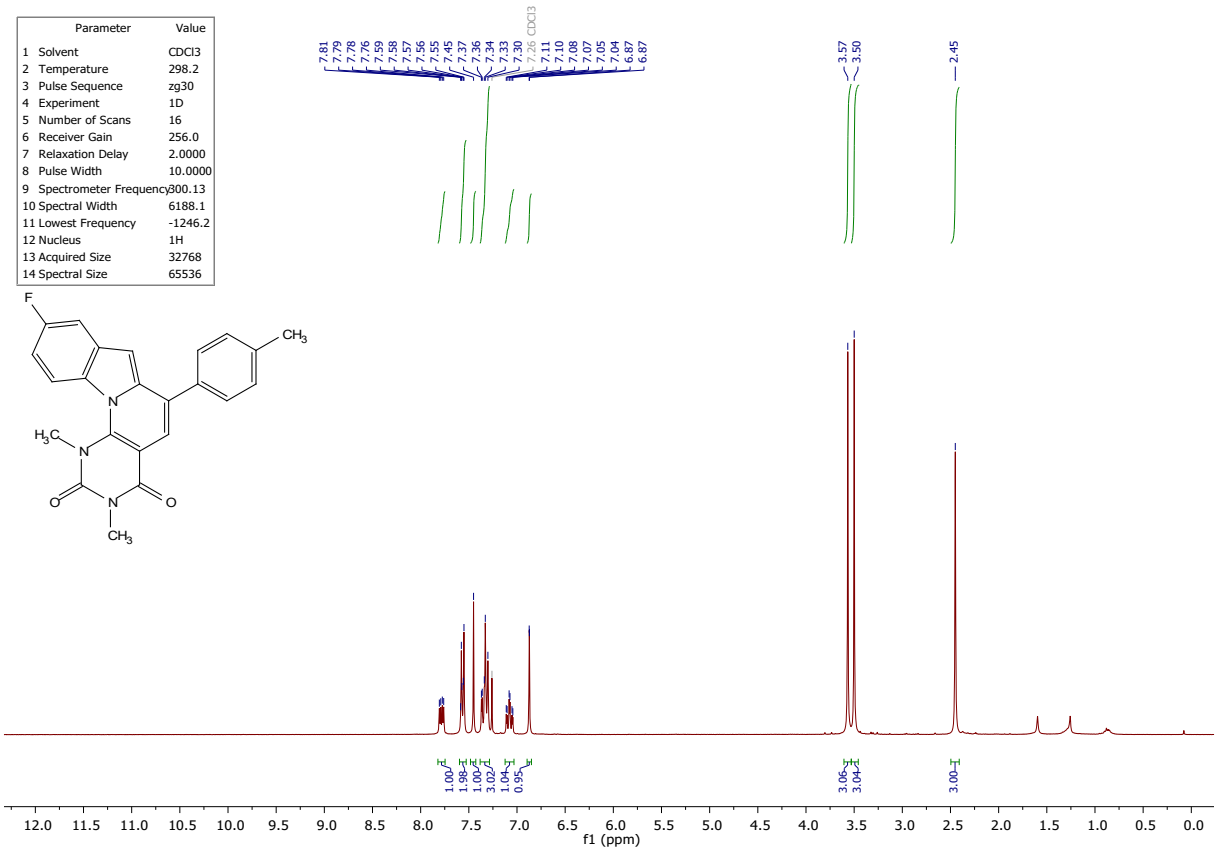
1,3-Dimethyl-6-(*p*-tolyl)pyrimido[5',4':5,6]pyrido[1,2-*a*]indole-2,4(1*H*,3*H*)-dione (4g)



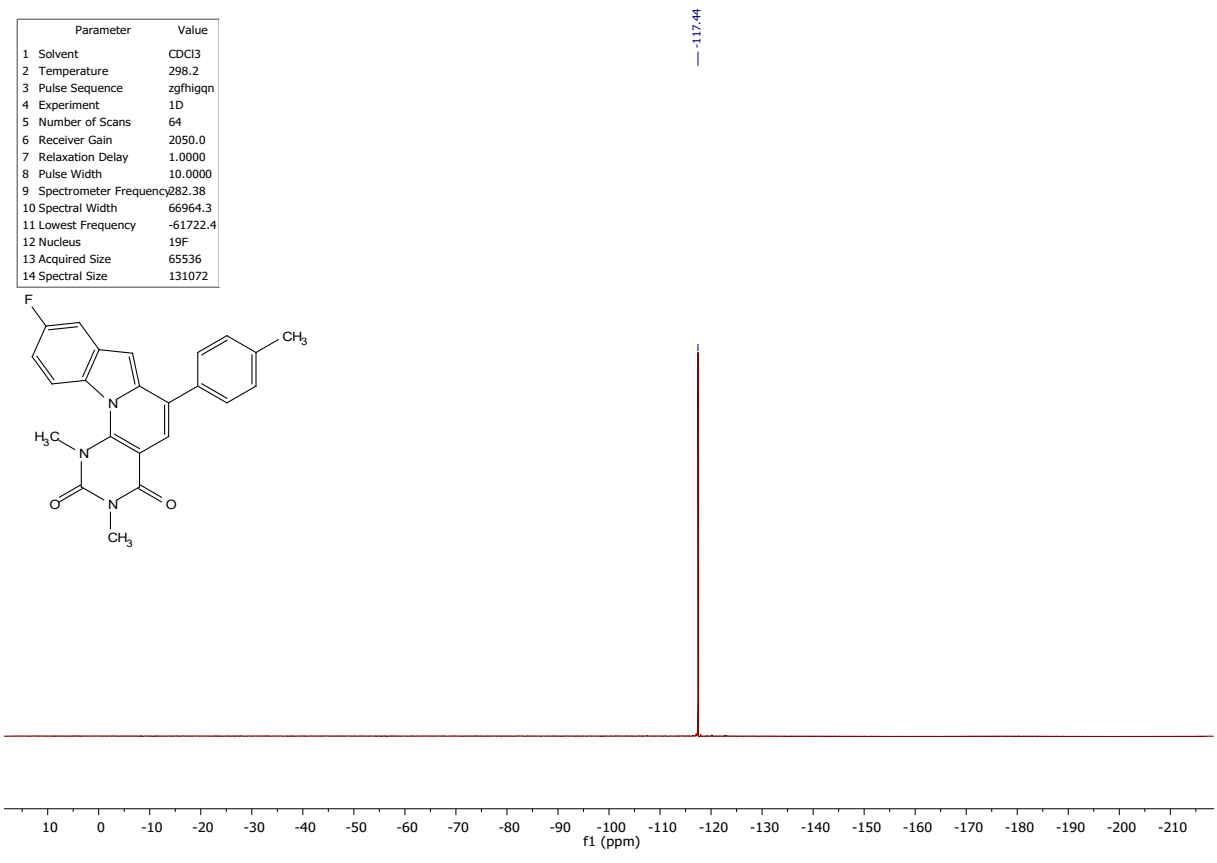


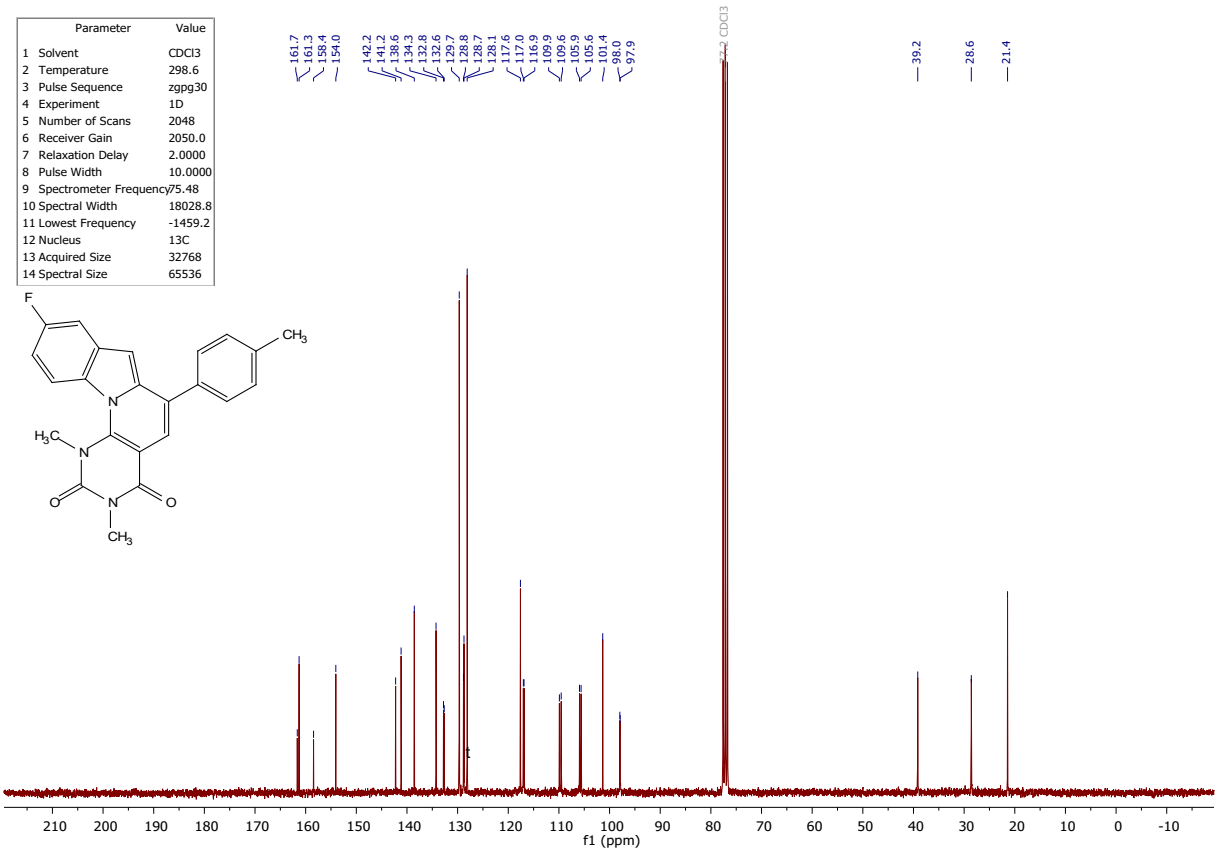
9-Fluoro-1,3-dimethyl-6-(*p*-tolyl)pyrimido[5',4':5,6]pyrido[1,2-*a*]indole-2,4(1*H*,3*H*)-dione (4h)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Number of Scans	16
6	Receiver Gain	256.0
7	Relaxation Delay	2.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.2
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgfhigqn
4	Experiment	1D
5	Number of Scans	64
6	Receiver Gain	2050.0
7	Relaxation Delay	1.0000
8	Pulse Width	10.0000
9	Spectrometer Frequency	282.38
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072




Parameter Value
1 Solvent CDCl3
2 Temperature 298.6
3 Pulse Sequence zgpg30
4 Experiment 1D
5 Number of Scans 2048
6 Receiver Gain 2050.0
7 Relaxation Delay 2.0000
8 Pulse Width 10.0000
9 Spectrometer Frequency 75.48
10 Spectral Width 18028.8
11 Lowest Frequency -1459.2
12 Nucleus 13C
13 Acquired Size 32768
14 Spectral Size 65536
161.7
161.3
158.4
154.0
142.2
141.2
138.6
134.3
132.8
132.6
129.7
128.8
128.7
128.1
117.6
117.0
116.9
109.9
109.6
105.9
105.6
101.4
98.0
97.9
77.2 CDCl3
39.2
28.6
21.4
F
CH3
H3C
N
O
O
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)