Supporting Information for

Stereoselective synthesis of medicinally relevant furo[2,3-*d*]pyrimidine framework by thermal rearrangement of spirocyclic barbiturates

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1. Materials

All melting points were measured with a Gallenkamp melting point apparatus and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded with Bruker AM-300 and Bruker Avance II 300 spectrometers at ambient temperature in DMSO-d_6 solutions using Me_4Si as internal standard. IR spectra were registered with a Bruker FT-IR spectrometer in KBr pellets. Mass-spectra (EI = 70 eV) were obtained directly with a Finningan MAT INCOS 50 spectrometer. DMSO was dried with CaH_2 and then distilled under vacuum. However, it was shown that water does not have an adverse effect on the cyclopropane rearrangement so it could be used without additional purification. All other solvents were purchased and were used without prior purification. The spirocyclic barbiturates **1** or **2** have all been prepared as was reported.[1]

2. General procedure for the thermal rearrangement of spirocyclopropylbarbiturates 1 or 2 to the 5,6-dihydrofuro[2,3-*d*]pyrimidines 3, 4 in DMSO

A suspension of spirocyclic barbiturates **1** or **2** (1 mmol) in 0.5 mL of DMSO in 25 mL round-bottom flask was rapidly heated to 100 ºC and stirred for 30 minutes. Then, the reaction mixture was allowed to cool down to room temperature and 10 mL of water was added. The precipitate was filtered off, washed with water (2 × 5 mL) and dried under reduced pressure. Crude product **3** or **4** was recrystallized from ethyl acetate-hexane mixture.

3. General procedure for the thermal rearrangement of spirocyclopropylbarbiturates 1 or 2 to the 5,6-dihydrofuro[2,3-*d*]pyrimidines 3, 4 in ionic liquid

A suspension of spirocyclic barbiturates **1** or **2** (1 mmol) in 1 mmol (0.27 g) of [BMim]BF_4 in 25 mL round-bottom flask was rapidly heated to 100 ºC and stirred for 30 minutes. Then, the reaction mixture was allowed to cool to *ca.* 60 °C, 15 mL of warm water was added and the mixture left to cool to ambient temperature whereupon the furo[2,3-*d*]pyrimidine products crystallised out. The precipitated solid was collected by filtration and washed with cold water ((2 × 7 mL)) to afford the desired product **3** or **4** with a high purity. The ionic liquid was recovered by removing the water under reduced pressure and could be reused at least five times without any appreciable decrease in yield

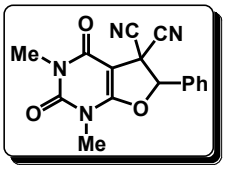
4. X-ray experiment and crystal data for 4a

Single crystals of $C_{17}H_{15}N_3O_5$ (**4a**) were crystallized from acetone/hexane mix (1:1). A suitable crystal was selected and mounted on a glass needle on a Bruker SMART 1000 CCD diffractometer. The crystal was kept at 100 K during data collection. Using Olex2,[2] the structure was solved with the olex2.solve[3] structure solution program using Charge Flipping and refined with the ShelXL[4] refinement package using Least Squares minimization.

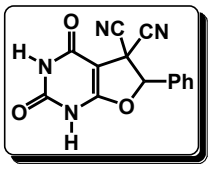
Crystal Data for $C_{17}H_{15}N_3O_5$ (*M* =341.32 g/mol): orthorhombic, space group Fdd2 (no. 43), *a* = 26.589(4) Å, *b* = 32.239(5) Å, *c* = 7.3315(12) Å, *V* = 6284.5(17) Å^3, *Z* = 16, *T* = 100.0 K, μ(MoKα) = 0.108 mm^{-1}, *Dcalc* = 1.443 g/cm^3, 17890 reflections measured (3.972° ≤ 2θ ≤ 60.136°), 4565 unique (R_{int} = 0.0725, R_{sigma} = 0.0769) which were used in all calculations. The final R_1 was 0.0725 (I > 2σ(I)) and wR_2 was 0.1737 (all data).

The structure was deposited with CSD (deposition number CCDC 1423220).

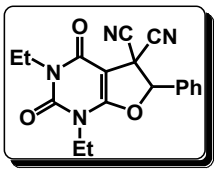
5. Compounds characterized



1,3-dimethyl-2,4-dioxo-6-phenyl-1,2,3,4-tetrahydrofuro[2,3-*d*]pyrimidine-5,5(6*H*)-dicarbonitrile (3a). White solid. Yield: 0.205 g (66%). M.p. 272–273 °C. IR (KBr): 3430, 2975, 2257, 1726, 1670, 1536, 1206, 947, 763, 711 cm^{-1}.^{1}H NMR (300 MHz, DMSO-d_6): 3.21 (s, 3 H, CH_3), 3.30 (s, 3 H, CH_3), 6.96 (s, 1 H, CH), 7.57–7.65 (m, 5 H, Ph). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 27.7, 29.9, 42.9, 81.0, 90.3, 110.9, 112.9, 126.7 (2 C), 129.1 (2 C), 130.9, 132.0, 150.4, 157.3, 163.8. MS: *m/z* (%) = 309 (6, [M$^+$]), 308 (49, [M$^+$]), 281 (12), 251 (42), 223 (14), 195 (35), 194 (70), 166 (73), 117 (87), 91 (100), 56 (45). Anal Calcd for $C_{16}H_{12}N_4O_3$ (308.09): C, 62.33; H, 3.92; N, 18.17. Found: C, 62.23; H, 4.01; N, 18.11.

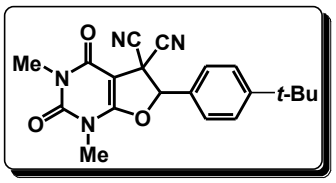


2,4-dioxo-6-phenyl-1,2,3,4-tetrahydrofuro[2,3-*d*]pyrimidine-5,5(6*H*)-dicarbonitrile (3b). White solid. Yield: 0.146 g (52%); mp 295 °C. IR (KBr): 3448, 3222, 3058, 2257, 1735, 1649, 1568, 1399, 1278, 948, 750 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): 6.87 (s, 1 H, CH), 7.52–7.65 (m, 5 H, Ph), 11.31 (s, 1H, NH), 13.00 (br. s, 1H, NH). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 41.8, 81.2, 90.4, 111.2, 113.1, 126.6 (2 C), 129.1 (2 C), 130.8, 132.1, 150.3, 158.9, 165.6. MS: *m/z* (%) = 281 (5, [M$^+$]), 280 (62, [M$^+$]), 253 (46), 238 (8), 237 (10), 210 (26), 194 (60), 166 (61), 105 (81), 77 (100). Anal Calcd for $C_{14}H_8N_4O_3$ (280.06): C, 60.00; H, 2.88; N, 19.99. Found: C, 59.94; H, 2.96; N, 19.94.

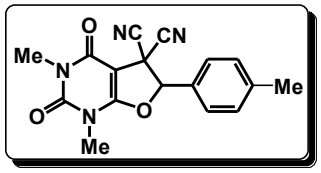


1,3-Diethyl-2,4-dioxo-6-phenyl-1,2,3,4-tetrahydrofuro[2,3-*d*]pyrimidine-5,5(6*H*)-dicarbonitrile (3c). White solid. Yield: 0.205 g (61%). M.p. 188–189 °C. IR (KBr): 3429, 2987, 2259, 1716, 1669, 1521, 1453, 1237, 965, 769 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): 1.15 (t, *J* = 7.0 Hz, 3 H, CH_3), 1.24 (t, *J* = 7.0 Hz 3 H, CH_3),

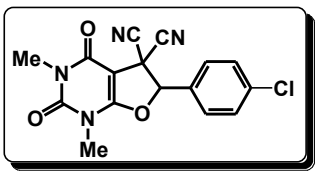
3.82 – 3.90 (m, 4 H, CH_2), 6.93 (s, 1 H, CH), 7.57–7.65 (m, 5 H, Ph). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 12.8, 13.2, 36.1 (2 C), 42.8, 81.3, 90.5, 111.0, 112.9, 126.7 (2 C), 129.1 (2 C), 130.9, 131.9, 150.0, 156.9, 163.5. MS: *m/z* (%) = 337 (11, [M^+]), 336 (51, [M^+]), 309 (5), 265 (21), 236 (13), 194 (100), 166 (35), 98 (40), 73 (73), 57 (84). Anal Calcd for $C_{18}H_{16}N_4O_3$ (336.12): C, 64.28; H, 4.79; N, 16.66. Found: C, 64.21; H, 4.83; N, 16.59.



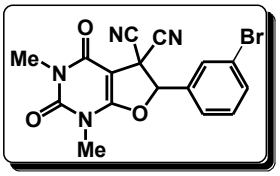
6-(4-*tert*-butylphenyl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydrofuro [2,3-*d*]pyrimidine-5,5(6*H*)-dicarbonitrile (3d). White solid. Yield: 0.212 g (58%). M.p. 209–210 °C. IR (KBr): 2968, 2261, 1726, 1663, 1537, 1527, 1254, 1196, 993, 765 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): 1.31 (s, 9H, CH_3), 3.21 (s, 3 H, CH_3), 3.29 (s, 3 H, CH_3), 6.89 (s, 1 H, CH), 7.55–7.65 (m, 4 H, Ar). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 27.7, 29.8, 30.9 (3 C), 42.8, 81.1, 90.5, 111.0, 112.9, 125.8 (2 C), 126.7 (2 C), 128.8, 132.0, 150.4, 157.3, 163.8. MS: *m/z* (%) = 365 (5, [M^+]), 364 (88, [M^+]), 350 (32), 349 (100), 322 (13), 298 (14), 292 (54), 251 (8), 250 (9), 117 (21). Anal Calcd for $C_{20}H_{20}N_4O_3$ (364.15): C, 65.92; H, 5.53; N, 15.38. Found: C, 65.86; H, 5.61; N, 15.47.



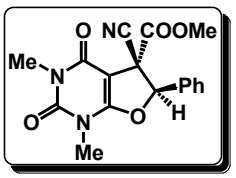
1,3-Dimethyl-6-(4-methylphenyl)-2,4-dioxo-1,2,3,4-tetrahydrofuro [2,3-*d*]pyrimidine-5,5(6*H*)-dicarbonitrile (3e). White solid. Yield: 0.213 g (66%). M.p. 247–248 °C. IR (KBr): 3433, 2956, 2260, 2246, 1725, 1668, 1533, 1438, 1199, 979, 950, 764 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): 2.37 (s, 3 H, CH_3), 3.21 (s, 3 H, CH_3), 3.29 (s, 3 H, CH_3), 6.90 (s, 1 H, CH), 7.36 (d, *J* = 7.4 Hz, 2 H, Ar), 7.54 (d, *J* = 7.4 Hz, 2 H, Ar). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 20.9, 27.7, 29.9, 42.9, 81.0, 90.5, 111.0, 113.0, 126.7 (2 C), 129.0, 129.6 (2 C), 140.7, 150.4, 157.3, 163.8. MS: *m/z* (%) = 322 (72, [M^+]), 295 (32), 265 (26), 238 (17), 208 (100), 180 (75), 117 (55), 91 (45), 73 (37), 57 (28). Anal Calcd for $C_{17}H_{14}N_4O_3$ (322.11): C, 63.35; H, 4.38; N, 17.38. Found: C, 63.27; H, 4.46; N, 17.42.



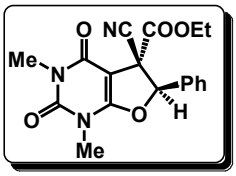
6-(4-Chlorophenyl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydrofuro[2,3-*d*]pyrimidine-5,5(6*H*)-dicarbonitrile (3f). White solid. Yield: 0.172 g (50%). M.p. 289 °C. IR (KBr): 3431, 2960, 2260, 2245, 1720, 1657, 1538, 1203, 1092, 990, 765 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): 3.21 (s, 3 H, CH_3), 3.29 (s, 3 H, CH_3), 7.00 (s, 1 H, CH), 7.63 (d, *J* = 8.4 Hz, 2 H, Ar), 7.71 (d, *J* = 8.4 Hz, 2 H, Ar). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 27.7, 30.0, 42.8, 80.9, 89.5, 110.9, 112.8, 128.8 (2 C), 129.1 (2 C), 131.1, 135.6, 150.4, 157.2, 163.8. MS: *m/z* (%) = 344 (12, [M^+]), 343 (15, [M^+]), 342 (34, [M^+]), 317 (19), 315 (47), 285 (15), 228 (46), 200 (50), 165 (78), 117 (100), 91 (72), 56 (37). Anal Calcd for $C_{16}H_{11}ClN_4O_3$ (342.05): C, 56.07; H, 3.23; Cl, 10.34; N, 16.35. Found: C, 55.09; H, 3.31; Cl, 10.40; N, 16.29.



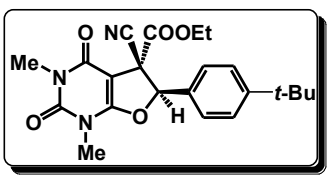
6-(3-Bromophenyl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydrofuro[2,3-*d*]pyrimidine-5,5(6*H*)-dicarbonitrile (3g). Yellowish solid. Yield: 0.239 g (62%). M.p. 248–249 °C. IR (KBr): 3426, 3069, 2260, 1726, 1660, 1537, 1434, 1200, 950, 763 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): 3.21 (s, 3 H, CH_3), 3.29 (s, 3 H, CH_3), 6.97 (s, 1 H, CH), 7.52 (t, J = 7.6 Hz, 1 H, Ar), 7.68 (d, J = 7.6 Hz, 1 H, Ar), 7.77 (d, J = 7.6 Hz, 1 H, Ar), 7.98 (s, 1 H, Ar). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 27.7, 29.9, 42.9, 80.8, 89.1, 110.9, 112.7, 122.2, 126.0, 129.6, 131.2, 133.8, 134.5, 150.4, 157.2, 163.8. MS: *m/z* (%) = 388 (6, $[M^+]$), 386 (6, $[M^+]$), 331 (30), 329 (13), 307 (65), 274 (21), 272 (27), 165 (40), 145 (43), 117 (100), 91 (72), 56 (32). Anal Calcd for $C_{16}H_{11}BrN_4O_3$ (386.00): C, 49.63; H, 2.86; Br, 20.67; N, 14.47. Found: C, 49.65; H, 2.80; Br, 20.60; N, 14.51.



Methyl (5*R,6*R**)-5-cyano-1,3-dimethyl-2,4-dioxo-6-phenyl-1,2,3,4,5,6-hexahydrofuro[2,3-*d*]pyrimidine-5-carboxylate (4a).** White solid. Yield: 0.202 g (59%). M.p. 218 °C. IR (KBr): 3435, 2953, 2246, 1717, 1665, 1530, 1434, 1256, 1203, 728 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): 3.18 (s, 3 H, CH_3), 3.30 (s, 3 H, CH_3), 3.89 (s, 3 H, CH_3), 6.56 (s, 1 H, CH), 7.40-7.55 (m, 5 H, Ph). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 27.6, 29.8, 54.7, 56.2, 84.7, 90.7, 114.0, 126.6 (2 C), 128.7 (2 C), 130.1, 133.6, 150.6, 157.5, 163.3, 166.1. MS: *m/z* (%) = 342 (3, $[M^+]$), 341 (9, $[M^+]$), 283 (35), 282 (100), 225 (17), 197 (19), 169 (32), 168 (45), 140 (66), 91 (50), 77 (46), 57 (68). Anal Calcd for $C_{17}H_{15}N_3O_5$ (341.10): C, 59.82; H, 4.43; N, 12.31. Found: C, 59.76; H, 4.50; N, 12.29.

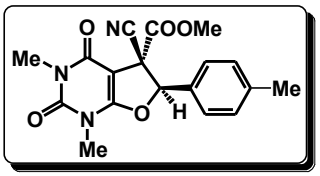


Ethyl (5*R,6*R**)-5-cyano-1,3-dimethyl-2,4-dioxo-6-phenyl-1,2,3,4,5,6-hexahydrofuro[2,3-*d*]pyrimidine-5-carboxylate (4b).** White solid. Yield: 0.182 g (51%). M.p. 121 °C. IR (KBr): 2988, 2243, 1746, 1716, 1670, 1527, 1246, 1202, 918, 725 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): 1.28 (t, J = 7.0 Hz, 3 H, CH_3), 3.18 (s, 3 H, CH_3), 3.31 (s, 3 H, CH_3), 4.36 (dq, J_1 = 7.0 Hz, J_2 = 1.8 Hz, 2 H, CH_2), 6.53 (s, 1 H, CH), 7.49-7.54 (m, 5 H, Ph). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 13.8, 27.6, 29.8, 56.3, 63.9, 84.9, 90.8, 114.1, 126.6 (2 C), 128.7 (2 C), 130.1, 133.5, 150.6, 157.5, 163.2, 165.5. MS: *m/z* (%) = 356 (4, $[M^+]$), 355 (26, $[M^+]$), 283 (98), 297 (63), 282 (100), 225 (25), 197 (15), 169 (27), 168 (86), 140 (52), 91 (37). Anal Calcd for $C_{18}H_{17}N_3O_5$ (355.12): C, 60.84; H, 4.82; N, 11.83. Found: C, 60.78; H, 4.90; N, 11.76.

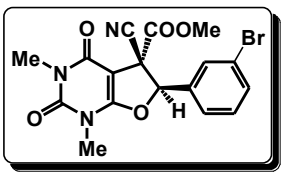


Ethyl (5*R,6*R**)-6-(4-*tert*-butylphenyl)-5-cyano-1,3-dimethyl-2,4-dioxo-1,2,3,4,5,6-hexahydrofuro[2,3-*d*]pyrimidine-5-carboxylate (4c).** White solid. Yield: 0.227 g (55%). M.p. 164 °C. IR (KBr): 3413, 2962, 2248, 1739, 1711, 1668, 1520, 1249, 1202, 934, 769 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): 1.25-1.35 (m, 12 H, CH_3), 3.18 (s, 3 H, CH_3), 3.30 (s, 3 H, CH_3), 4.34 (q, J = 7.0 Hz, 2 H, CH_2), 6.46 (s, 1 H, CH), 7.45 (d, J = 8.4 Hz, 2 H, Ar), 7.52 (d, J = 8.4 Hz, 2 H, Ar). ^{13}C NMR (75

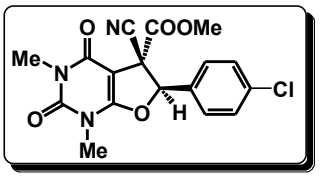
MHz, DMSO-d_6): δ = 13.8, 27.6, 29.8, 30.9 (3 C), 34.5, 56.2, 63.8, 85.0, 91.0, 114.2, 125.4 (2 C), 126.7 (2 C), 130.4, 150.6, 152.8, 157.5, 163.2, 165.5. MS: *m/z* (%) = 412 (5, [M^+]), 411 (34, [M^+]), 396 (6), 366 (6), 338 (100), 300 (16), 283 (9), 279 (10), 209 (14), 138 (6), 135 (21). Anal Calcd for $C_{22}H_{25}N_3O_5$ (411.18): C, 64.22; H, 6.12; N, 10.21. Found: C, 64.15; H, 6.20; N, 10.19.



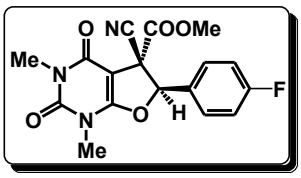
Methyl (5*R,6*R**)-5-cyano-1,3-dimethyl-6-(4-methylphenyl)-2,4-dioxo-1,2,3,4,5,6-hexahydrofuro[2,3-*d*]pyrimidine-5-carboxylate (4d).** White solid. Yield: 0.249 g (70%). M.p. 183–184 °C. IR (KBr): 2964, 2246, 1752, 1714, 1665, 1524, 1255, 1202, 937, 766 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): 2.36 (s, 3 H, CH_3), 3.17 (s, 3 H, CH_3), 3.31 (s, 3 H, CH_3), 3.87 (s, 3 H, CH_3), 6.50 (s, 1 H, CH), 7.30 (d, *J* = 8.0 Hz, 2 H, Ar), 7.43 (d, *J* = 8.0 Hz, 2 H, Ar). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 20.9, 27.6, 29.8, 54.7, 56.3, 84.7, 90.8, 114.1, 126.6 (2 C), 129.2 (2 C), 130.7, 139.8, 150.6, 157.5, 163.3, 166.1. MS: *m/z* (%) = 355 (12, [M^+]), 296 (100), 211 (10), 138 (11), 182 (22), 154 (8), 91 (21). Anal Calcd for $C_{18}H_{17}N_3O_5$ (355.12): C, 60.84; H, 4.82; N, 11.83. Found: C, 60.74; H, 4.94; N, 11.72.



Methyl (5*R,6*R**)-6-(3-bromophenyl)-5-cyano-1,3-dimethyl-2,4-dioxo-1,2,3,4,5,6-hexahydrofuro[2,3-*d*]pyrimidine-5-carboxylate (4e).** Yellowish solid. Yield: 0.306 g (73%). M.p. 184–185 °C. IR (KBr): 3434, 2957, 2244, 1755, 1721, 1709, 1678, 1658, 1528, 1264, 1199, 766 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): 3.17 (s, 3 H, CH_3), 3.31 (s, 3 H, CH_3), 3.88 (s, 3 H, CH_3), 6.58 (s, 1 H, CH), 7.47 (t, *J* = 7.9 Hz, 1 H, Ar), 7.57 (d, *J* = 7.9 Hz, 1 H, Ar), 7.71 (d, *J* = 7.9 Hz, 1 H, Ar), 7.86 (s, 1 H, Ar). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 27.7, 29.9, 54.7, 56.2, 84.5, 89.4, 114.0, 121.9, 125.9, 129.5, 130.9, 133.1, 136.3, 150.6, 157.5, 163.3, 165.9. MS: *m/z* (%) = 420 (5, [M^+]), 418 (4, [M^+]), 362 (90), 360 (100), 248 (13), 246 (14), 167 (29), 139 (17), 91 (13). Anal Calcd for $C_{17}H_{14}BrN_3O_5$ (419.01): C, 48.59; H, 3.36; Br, 19.02; N, 10.00. Found: C, 48.48; H, 3.42; Br, 19.95; N, 9.91.



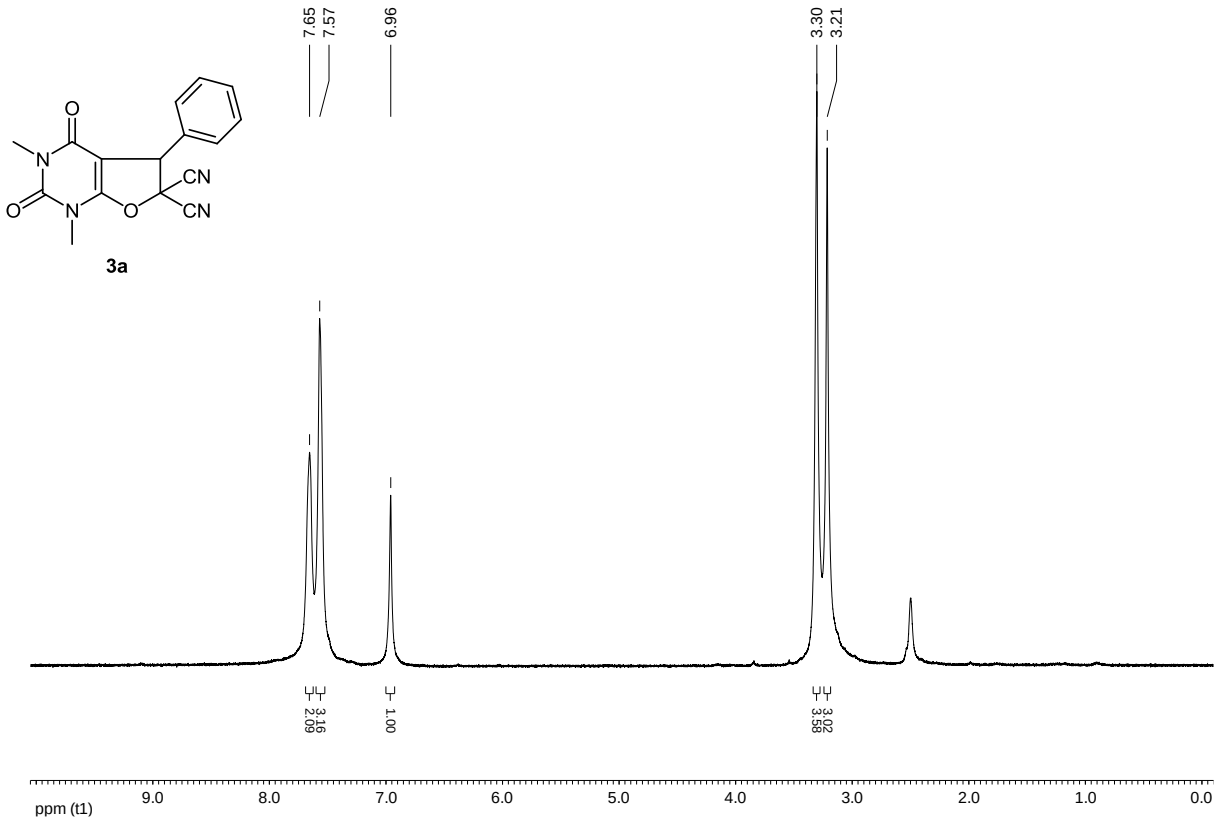
Ethyl (5*R,6*R**)-6-(4-chlorophenyl)-5-cyano-1,3-dimethyl-2,4-dioxo-1,2,3,4,5,6-hexahydrofuro[2,3-*d*]pyrimidine-5-carboxylate (4f).** White solid. Yield: 0.293 g (75%). M.p. 154 °C. IR (KBr): 3435, 2988, 2244, 1748, 1722, 1672, 1523, 1254, 1198, 1018, 762 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): 1.28 (t, *J* = 7 Hz, 3 H, CH_3), 3.17 (s, 3 H, CH_3), 3.31 (s, 3 H, CH_3), 4.33 (q, *J* = 7 Hz, 2 H, CH_2), 6.57 (s, 1 H, CH), 7.55-7.70 (m, 4 H, Ar). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 13.8, 27.6, 29.8, 56.3, 63.9, 84.6, 89.9, 114.0, 128.7 (2 C), 128.8 (2 C), 132.7, 134.9, 150.6, 157.4, 163.2, 165.3. MS: *m/z* (%) = 389 (4, [M^+]), 318 (37), 317 (24), 316 (100), 204 (7), 176 (8), 174 (10), 91 (9). Anal Calcd for $C_{18}H_{16}ClN_3O_5$ (389.08): C, 55.46; H, 4.14; Cl, 9.10; N, 10.78. Found: C, 55.00; H, 4.22; Cl, 9.01; N, 10.85.

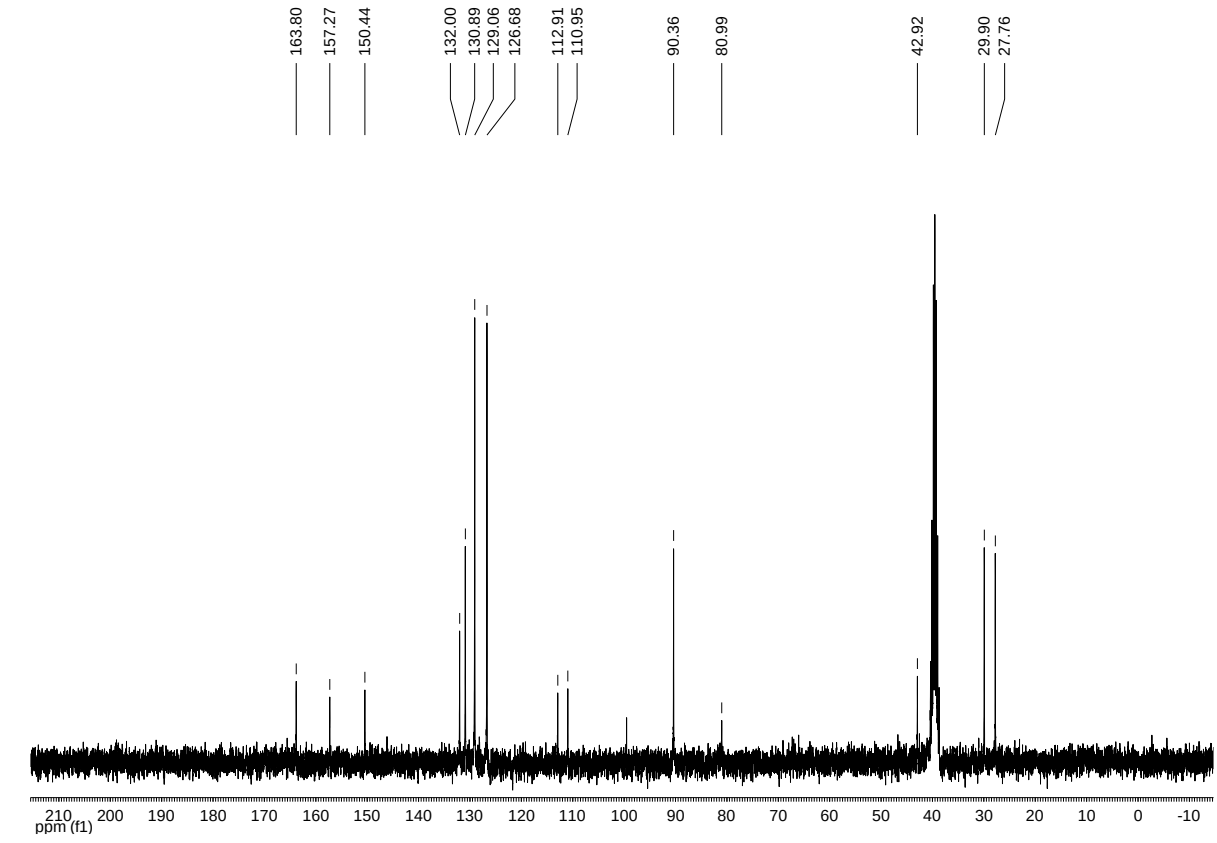


Methyl (5*R,6*R**)-6-cyano-5-(4-fluorophenyl)-1,3-dimethyl-2,4-dioxo-1,2,3,4,5,6-hexahydrofuro[2,3-*d*]pyrimidine-6-carboxylate (4g).** White solid. Yield: 0.202 g (56%). M.p. 227 °C. IR (KBr): 3414, 2963, 2243, 1754, 1718, 1664, 1525, 1435, 1255, 929, 764 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): 3.17 (s, 3 H, CH_3), 3.31 (s, 3 H, CH_3), 3.88 (s, 3 H, CH_3), 6.59 (s, 1 H, CH), 7.35 (t, J = 8.79 Hz, 2 H, Ar), 7.60-7.70 (m, 2 H, Ar). ^{13}C NMR (75 MHz, DMSO-d_6): δ = 27.6, 29.8, 54.7, 56.3, 84.5, 89.9, 114.1, 115.7 (d, J = 21.9 Hz, 2 C), 129.3 (d, J = 8.7 Hz, 2 C), 130.1, 150.6, 157.5, 163.0 (d, J = 247.4 Hz), 163.3, 166.0. MS: *m/z* (%) = 359 (6, $[M^+]$), 301 (18), 300 (100), 187 (8), 186 (21), 156 (47), 123 (12), 95 (10), 91 (19). Anal Calcd for $C_{17}H_{14}FN_3O_5$ (359.09): C, 56.83; H, 3.93; F, 5.29; N, 11.69. Found: C, 56.73; H, 4.03; F, 5.19; N, 11.74.

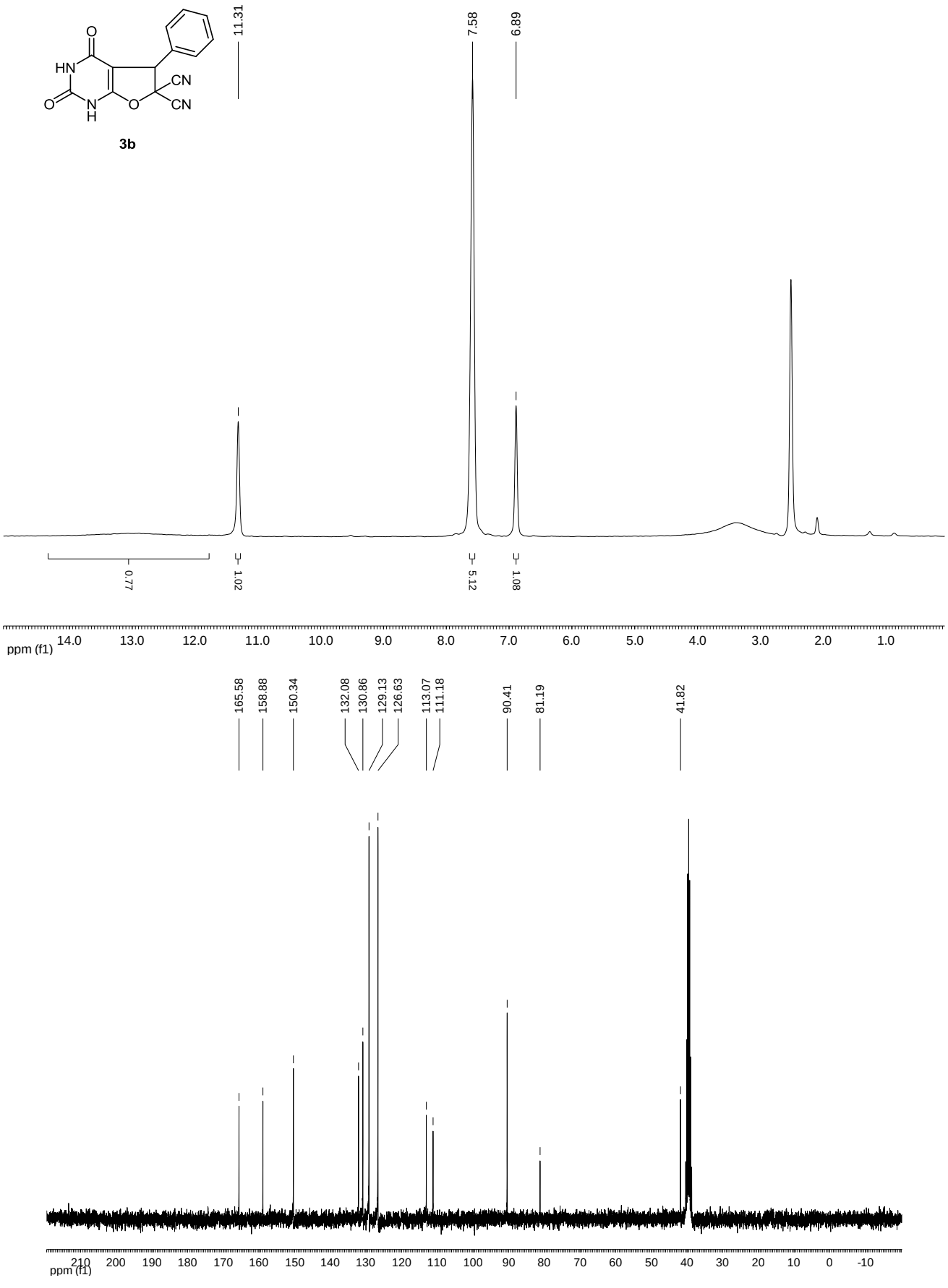
6. ^{1}H and ^{13}C – NMR data for the new compounds

^{1}H and ^{13}C – NMR of compound **3a**:

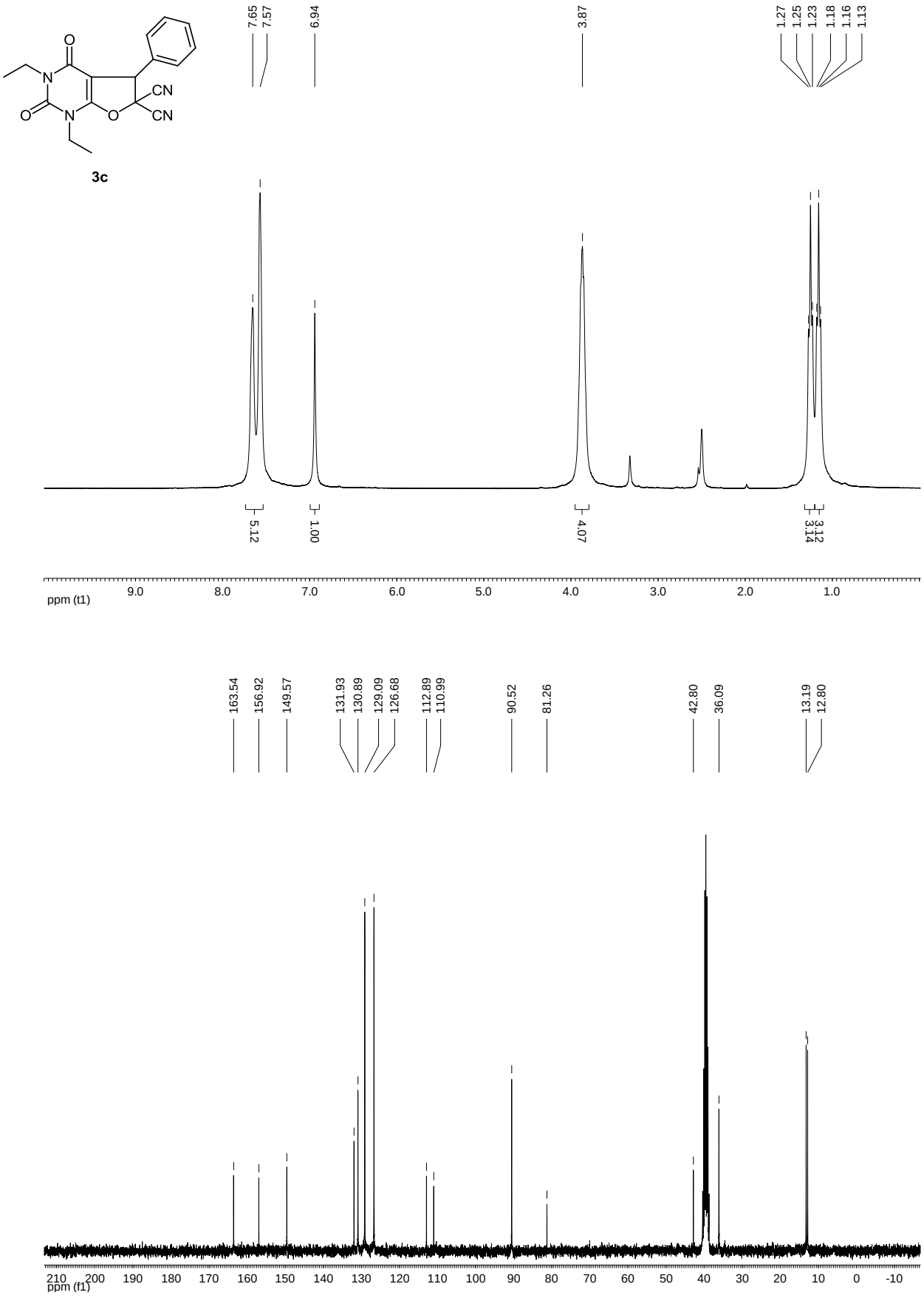




^{1}H and ^{13}C – NMR of compound **3b**:

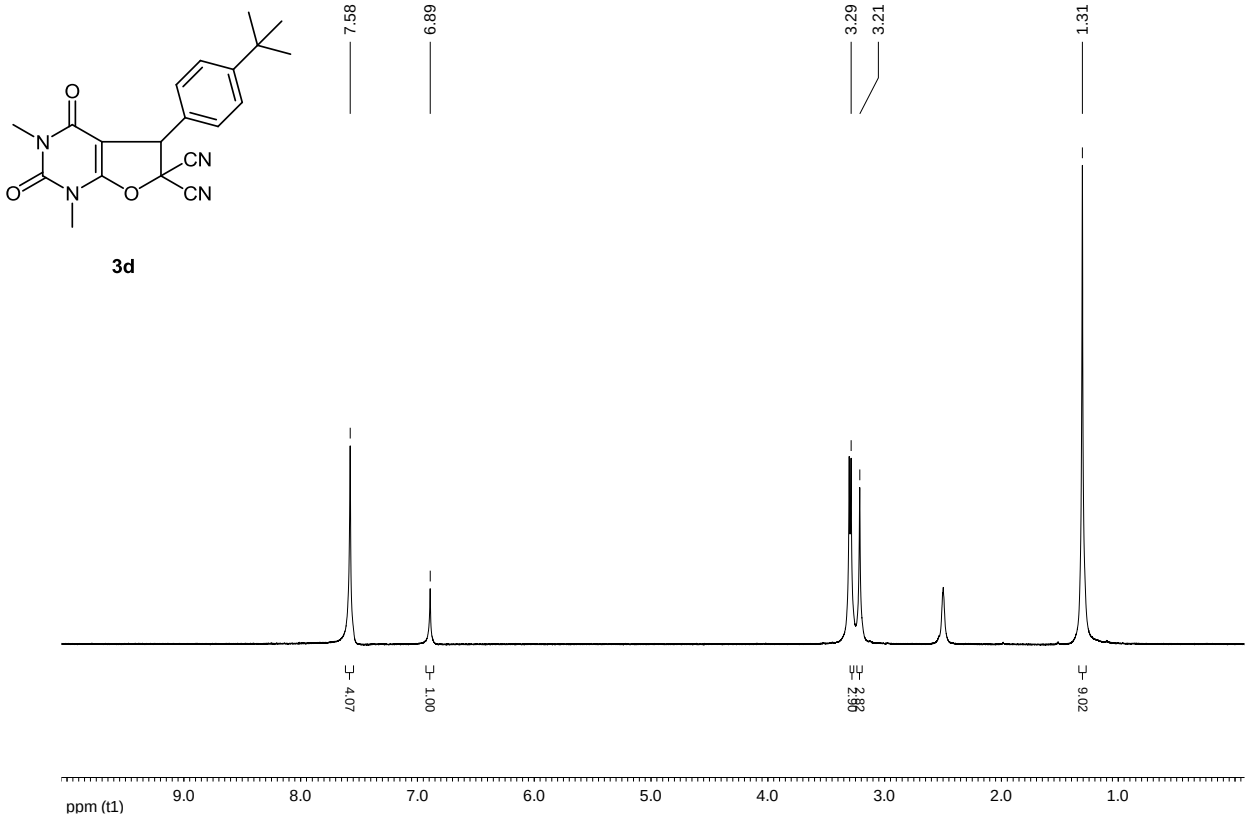


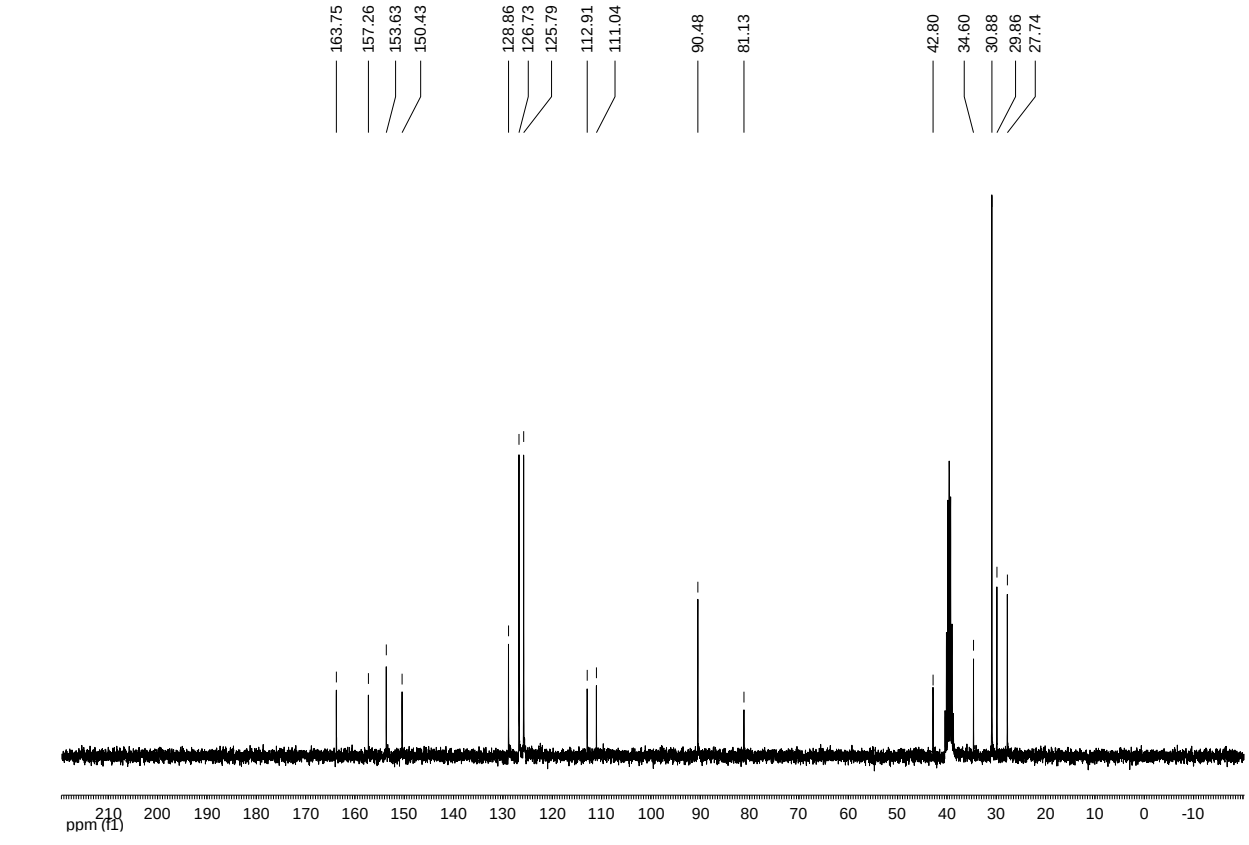
^{1}H and ^{13}C – NMR of compound **3c**:



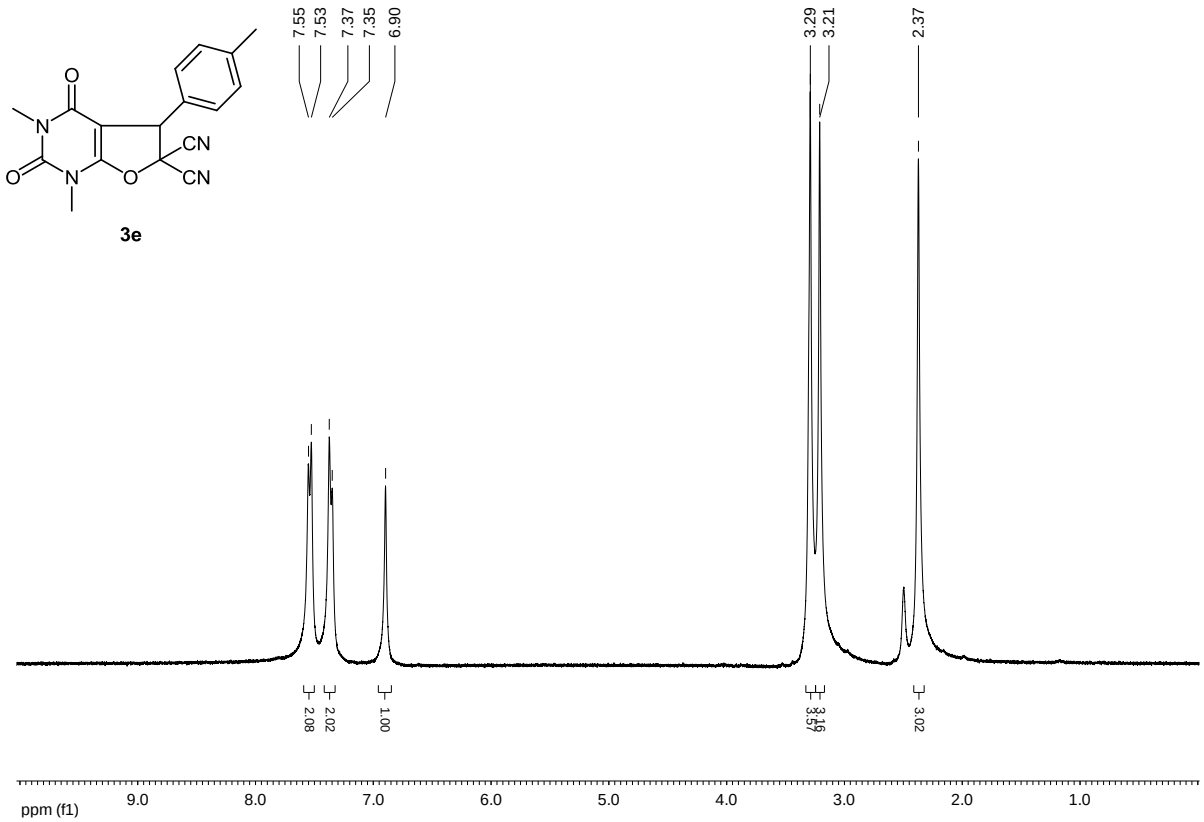
3c

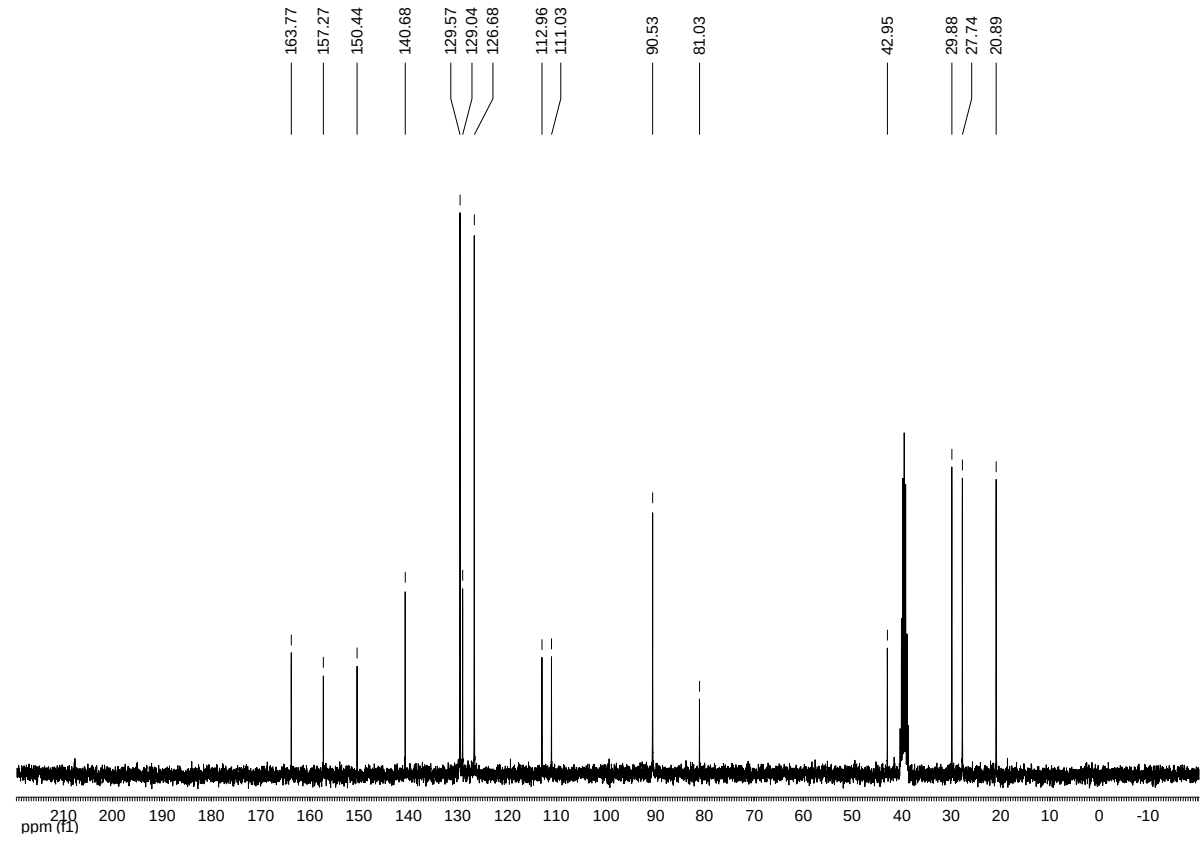
^{1}H and ^{13}C – NMR of compound **3d**:



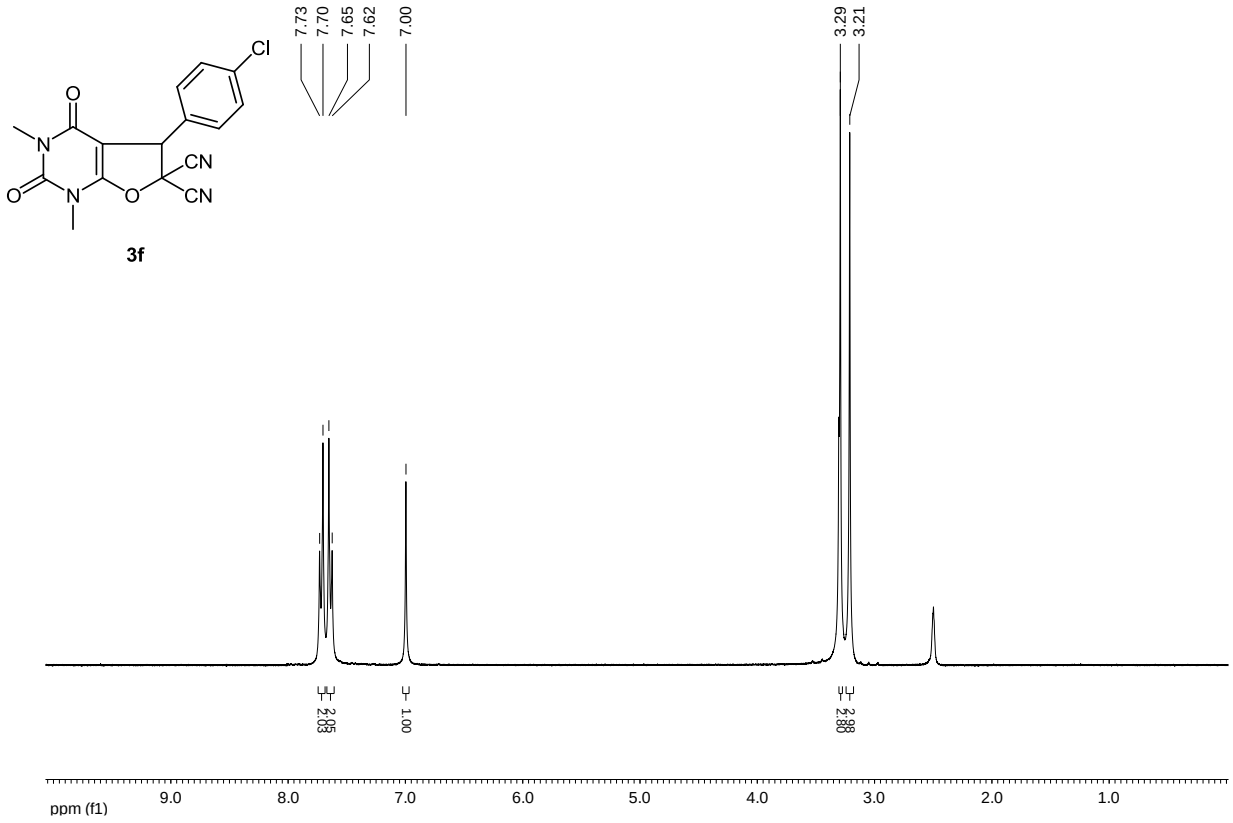


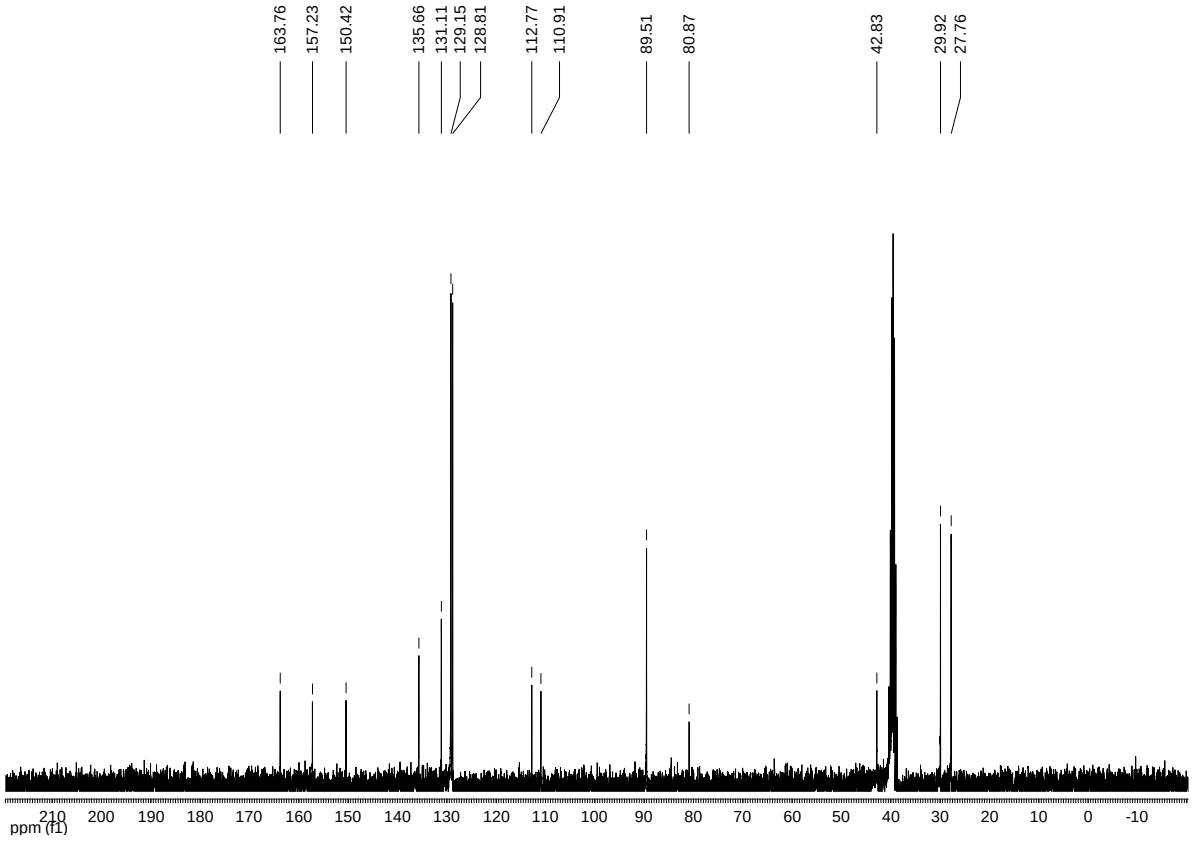
^{1}H and ^{13}C – NMR of compound **3e**:



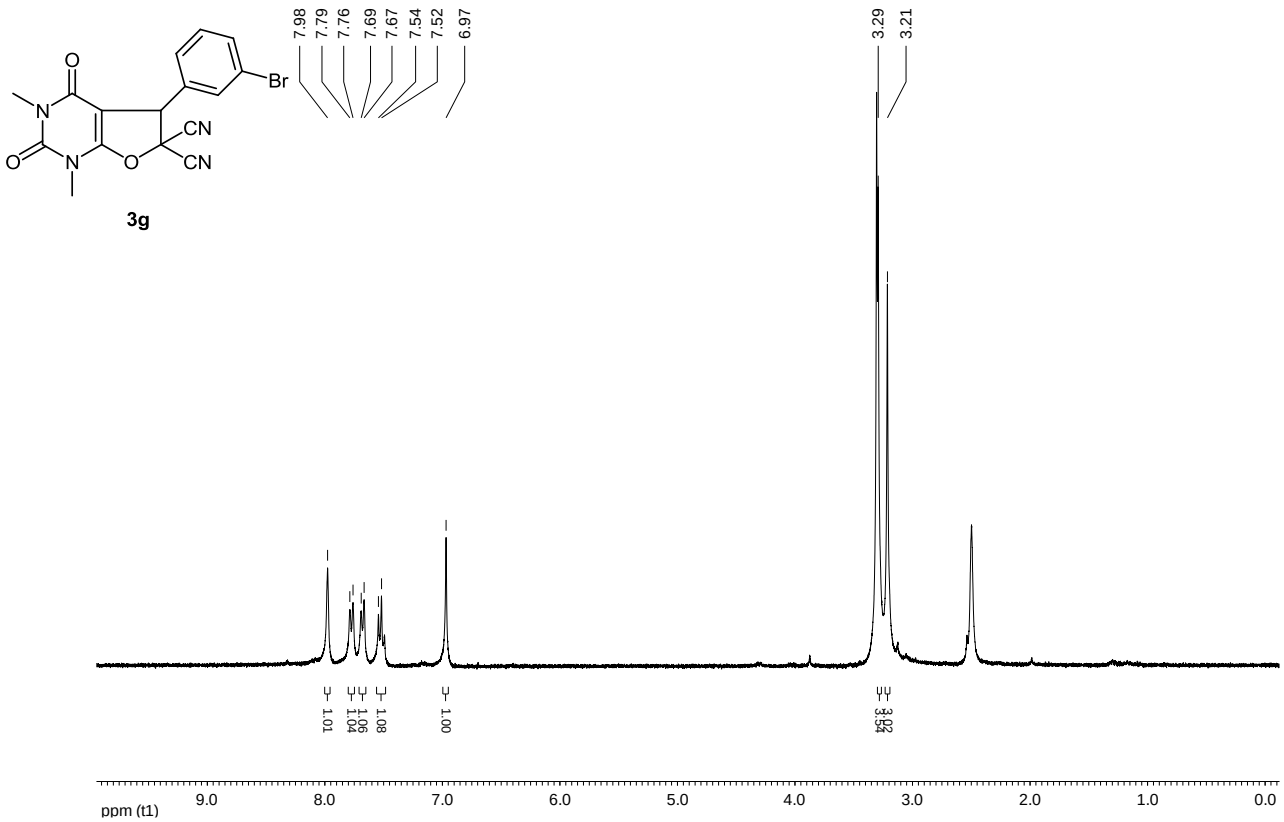


^{1}H and ^{13}C – NMR of compound **3f**:

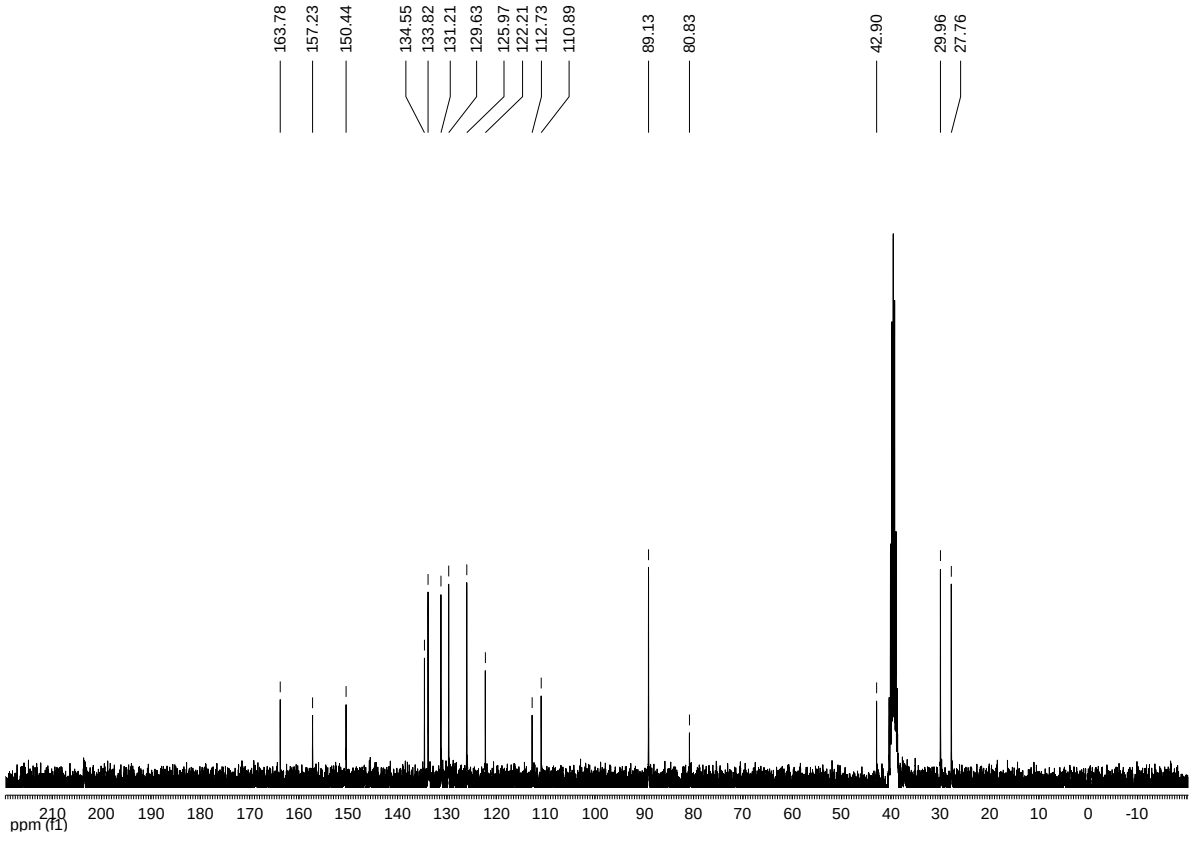




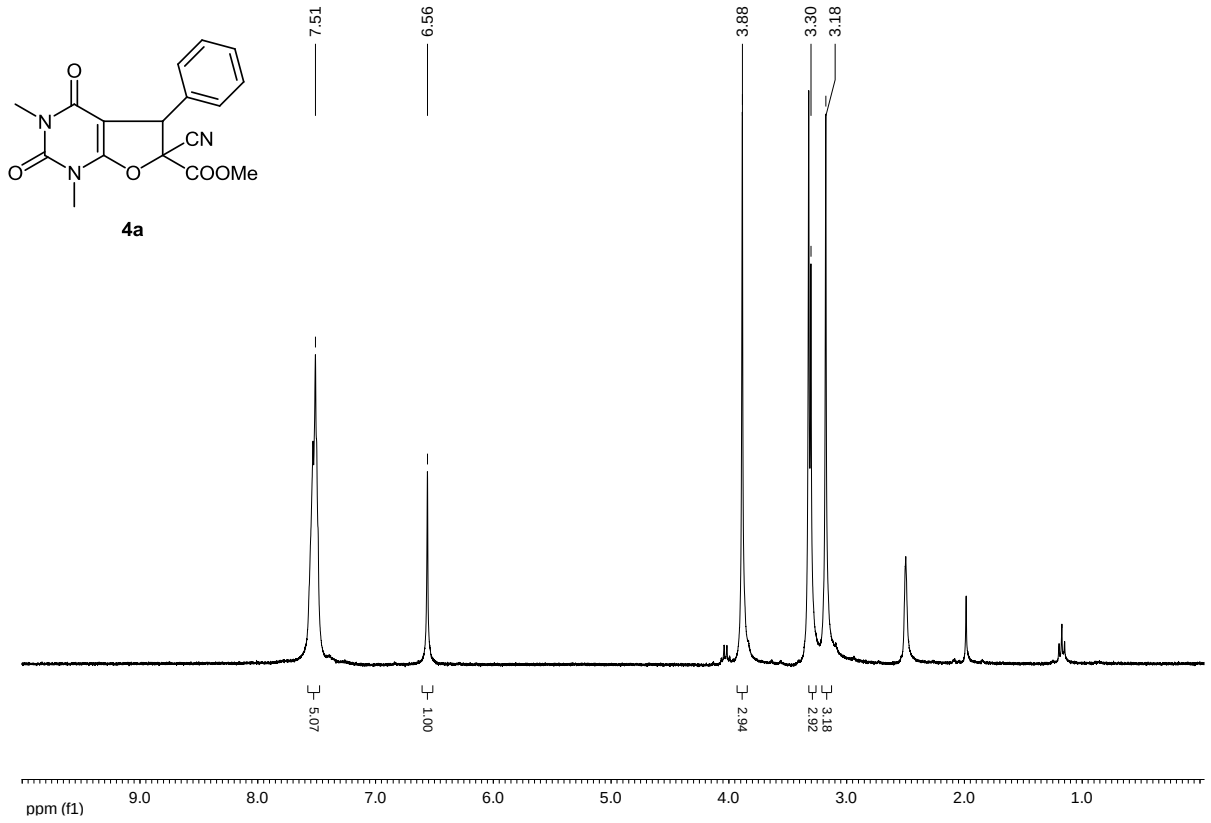
^{1}H and ^{13}C – NMR of compound **3g**:

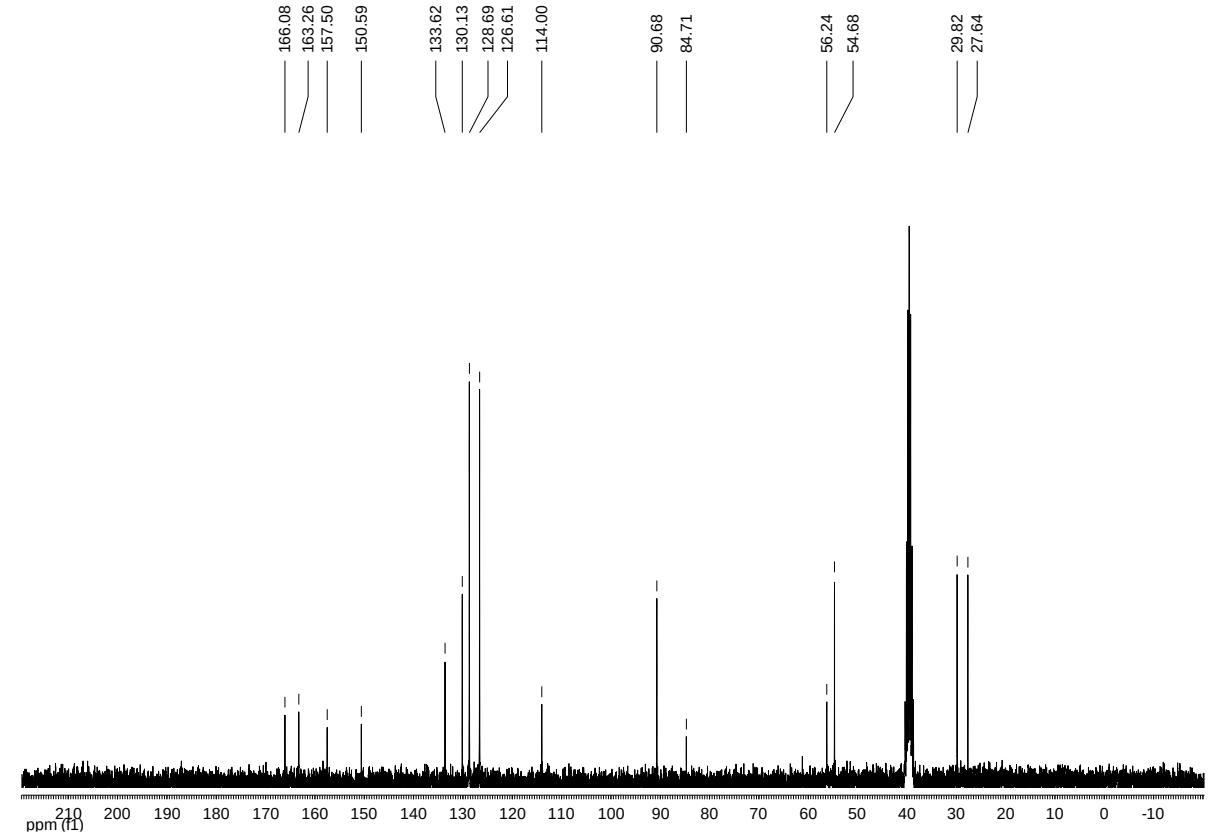


3g

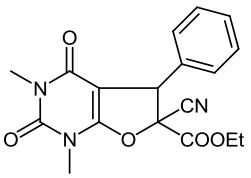


^{1}H and ^{13}C – NMR of compound **4a**:

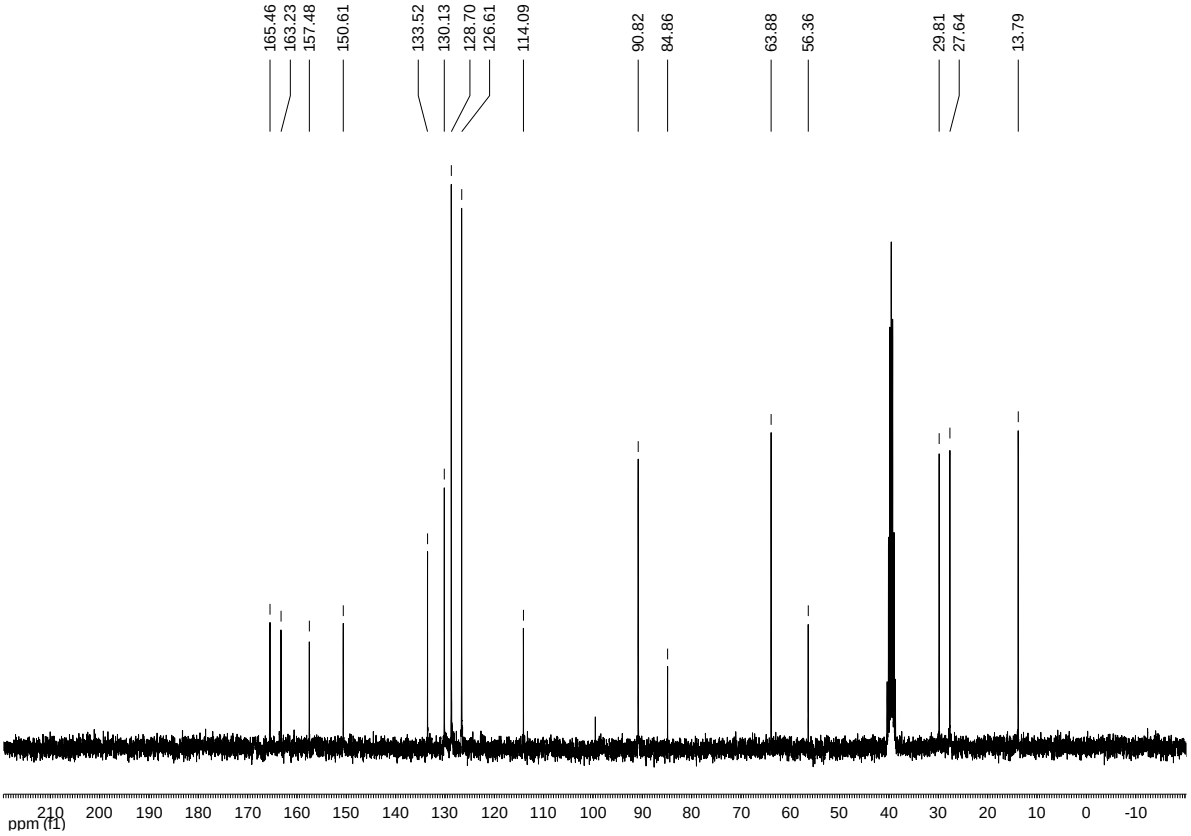




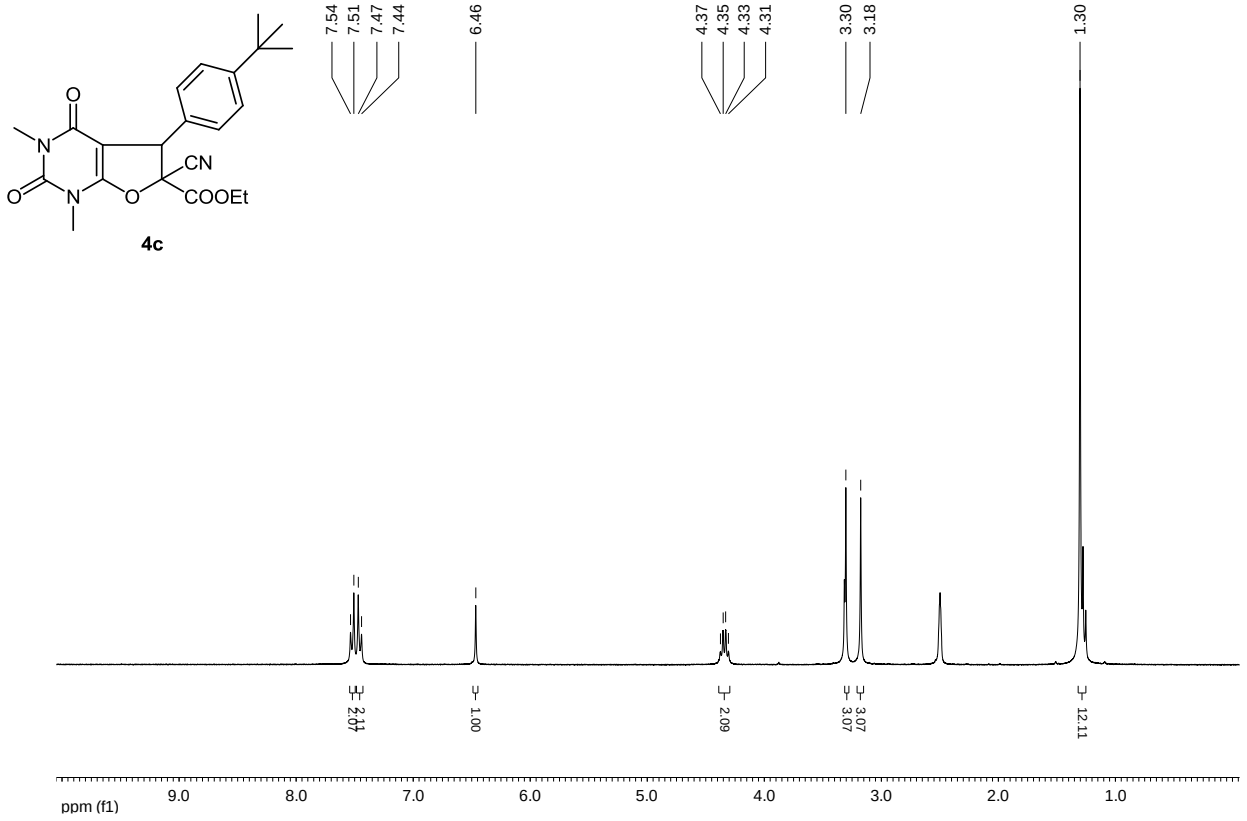
^{1}H and ^{13}C – NMR of compound **4b**:

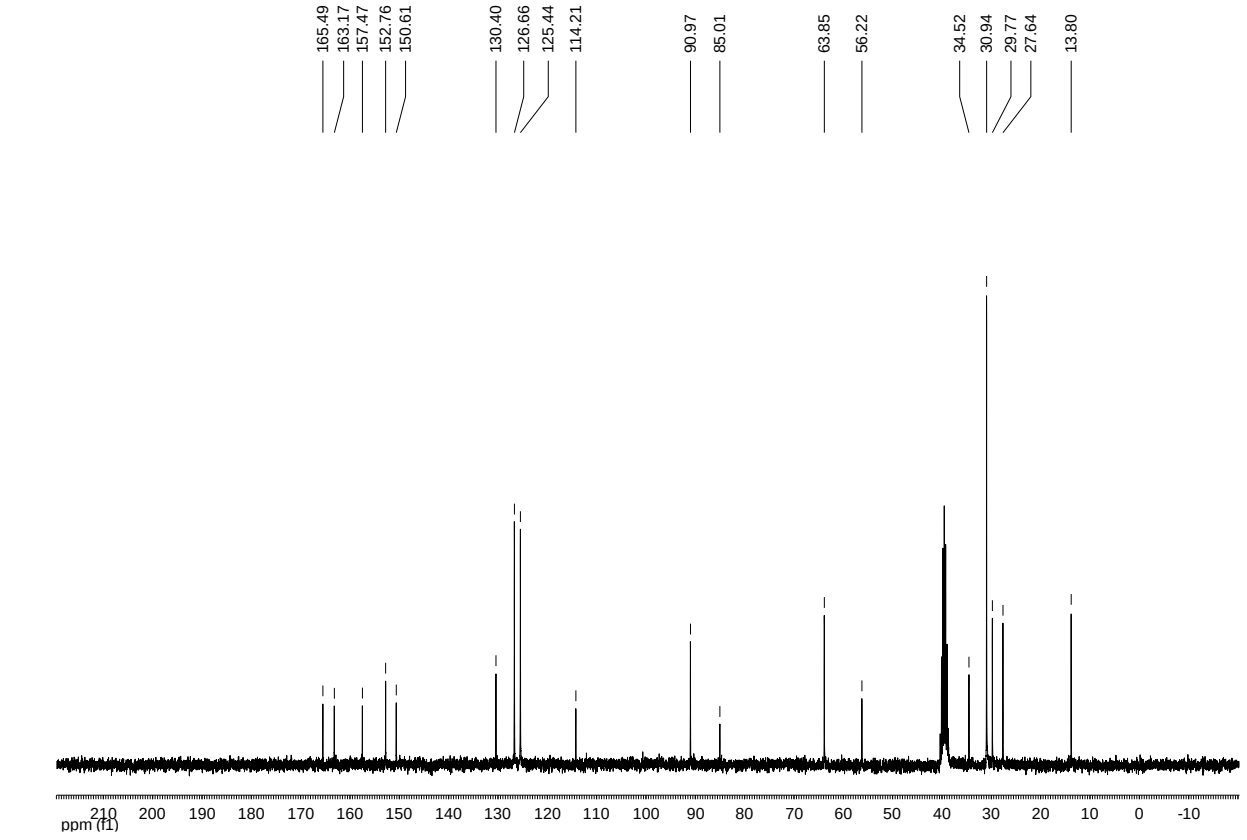


4b

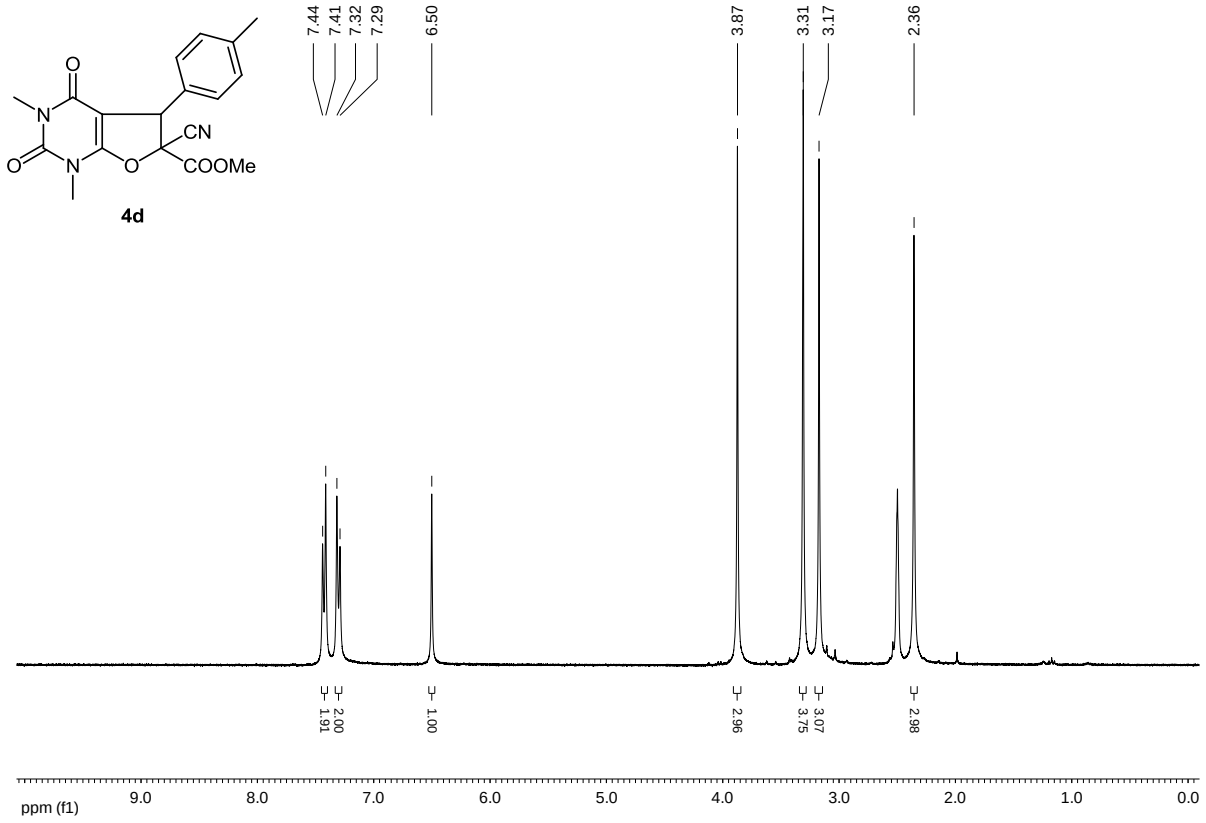


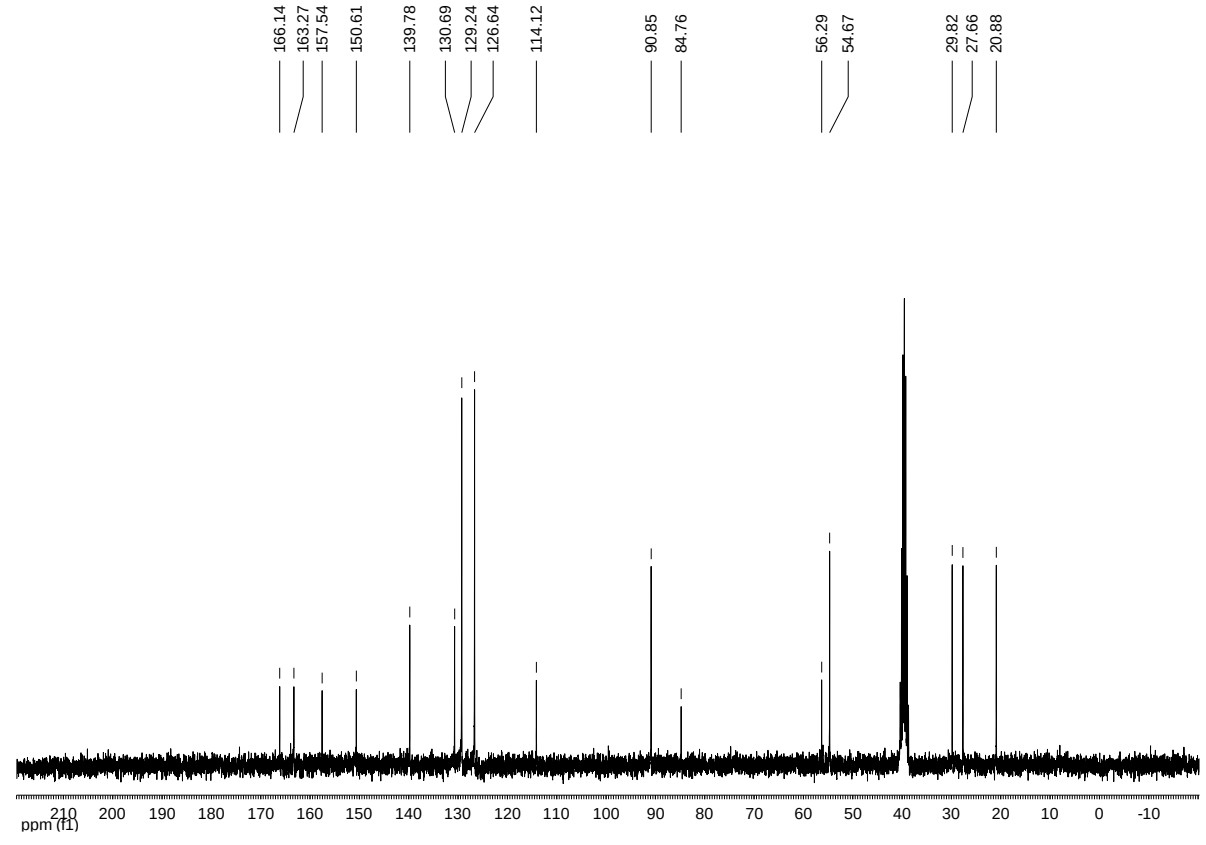
^{1}H and ^{13}C – NMR of compound **4c**:



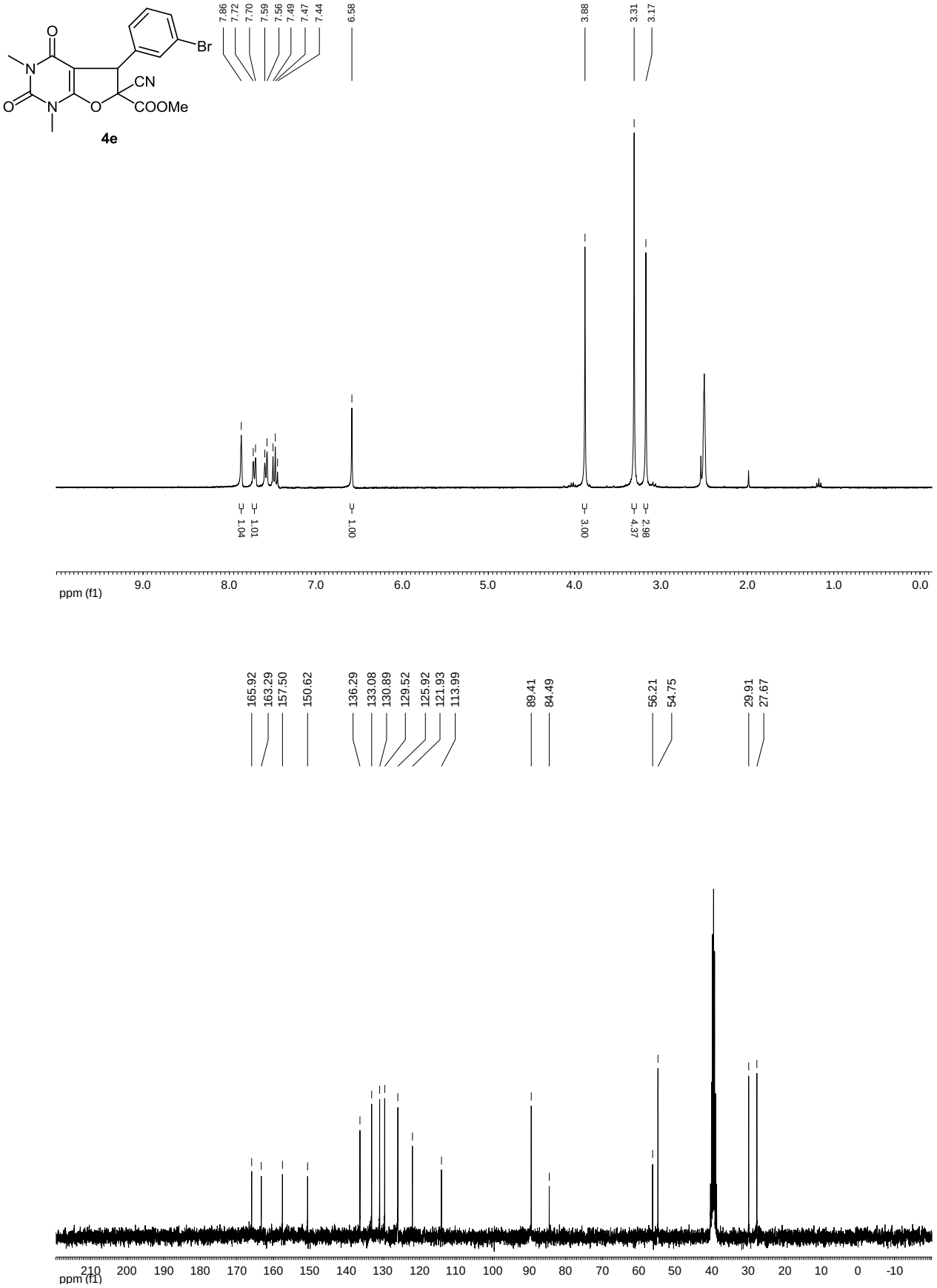


^{1}H and ^{13}C – NMR of compound **4d**:

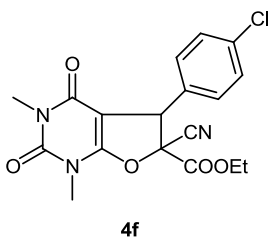




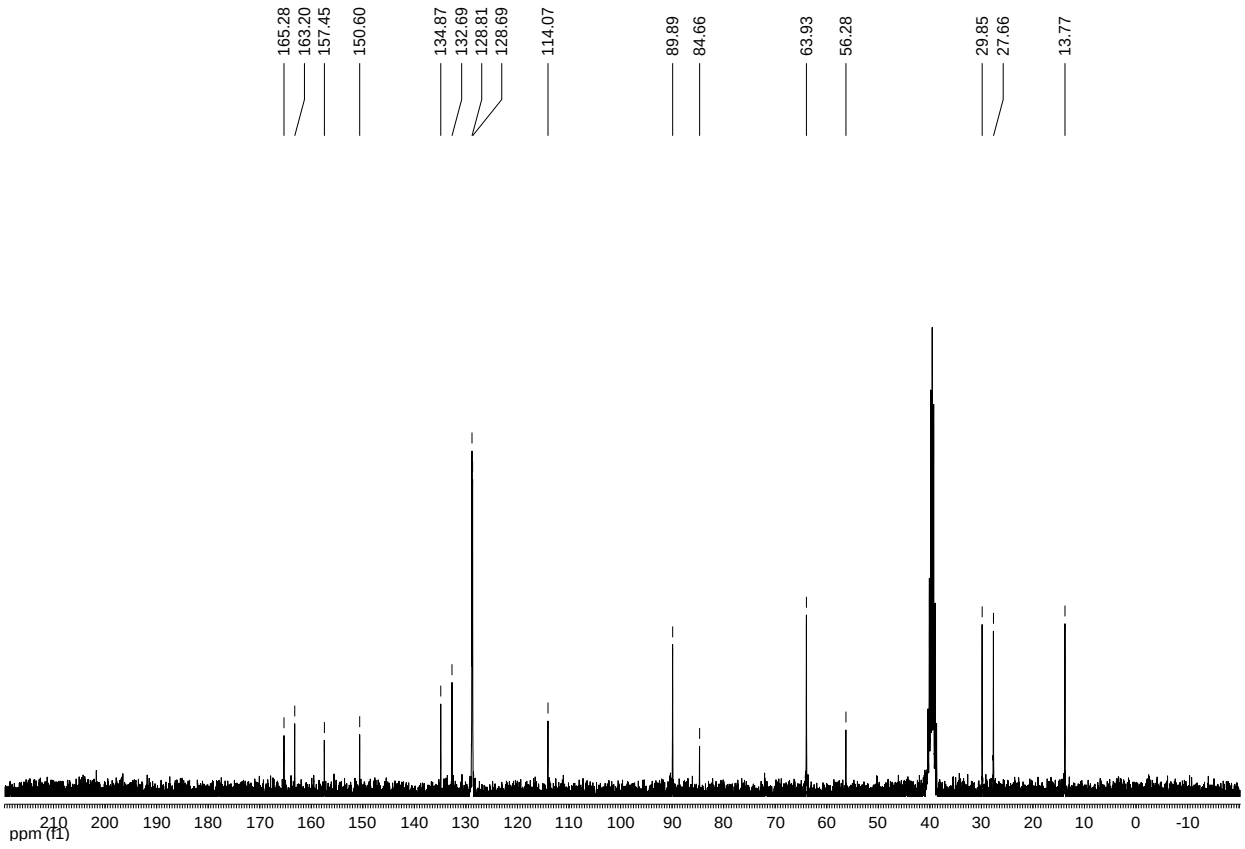
^{1}H and ^{13}C – NMR of compound **4e**:



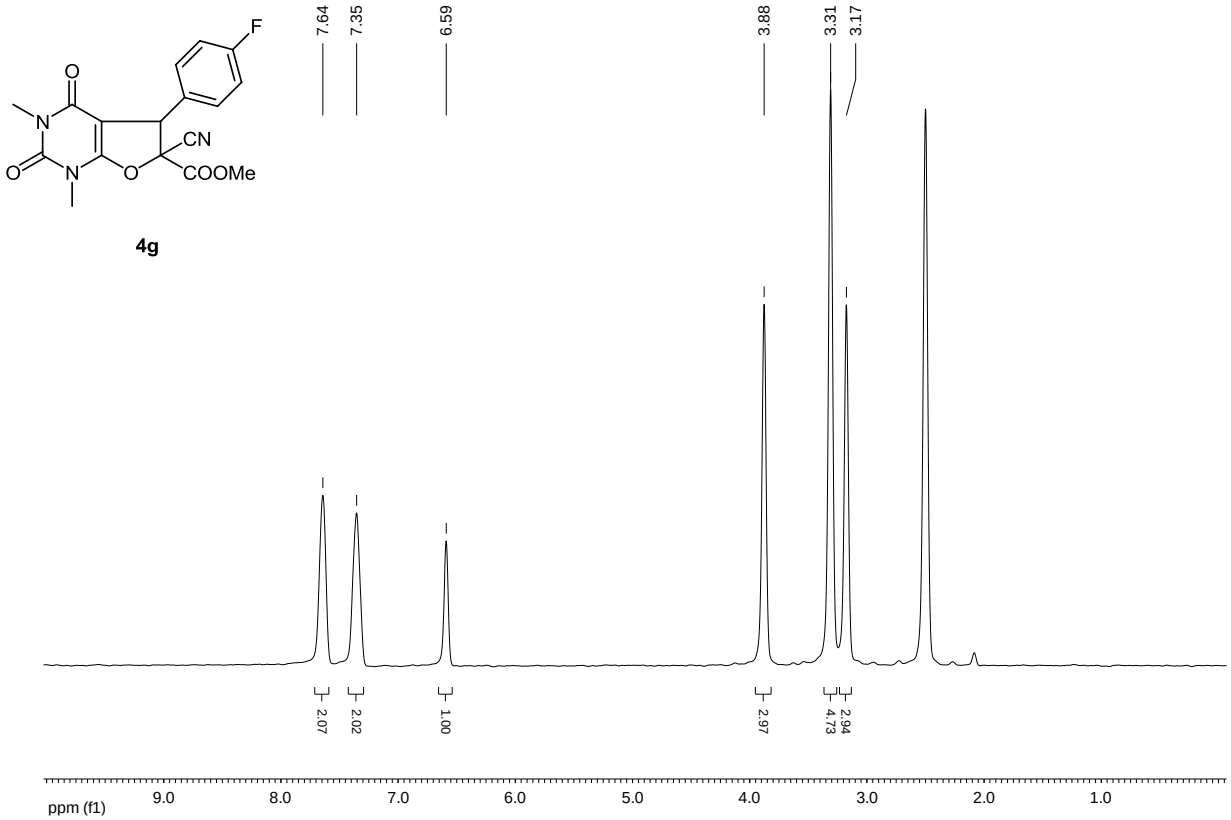
^{1}H and ^{13}C – NMR of compound **4f**:

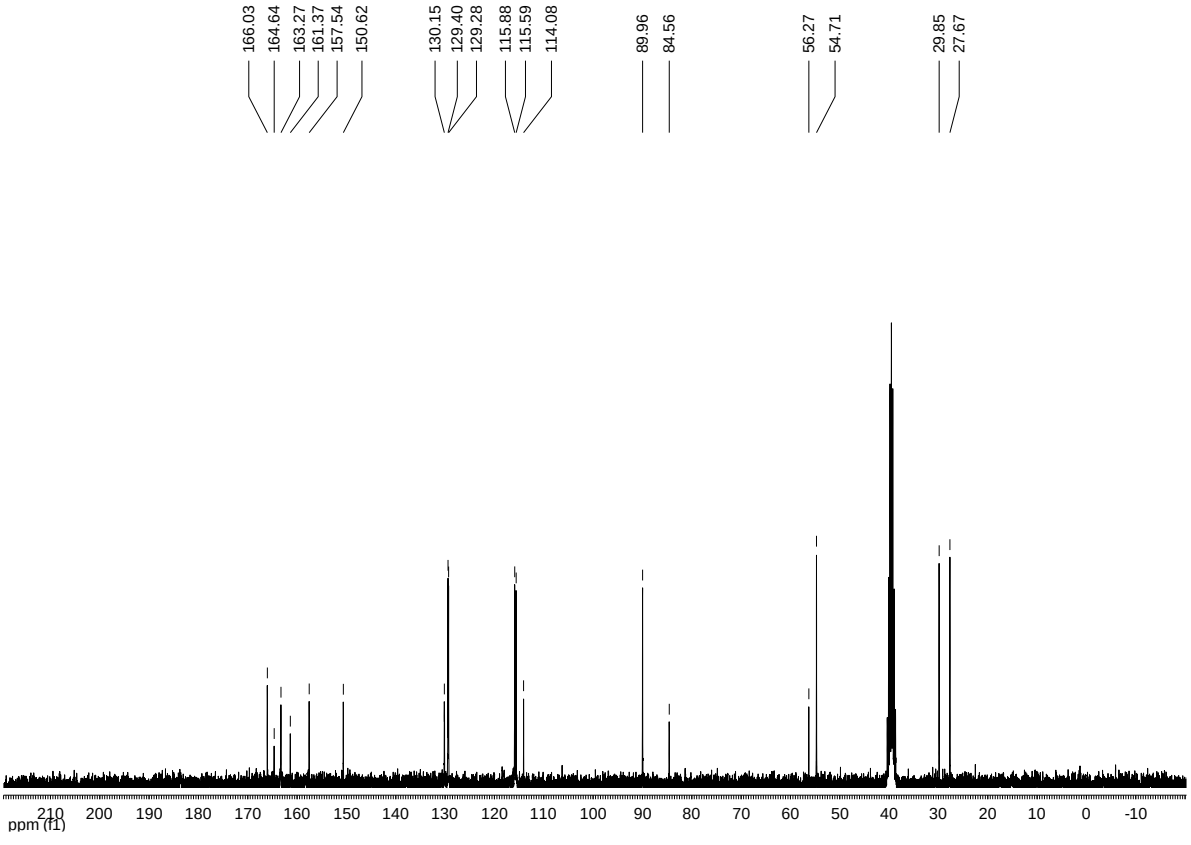


4f



^{1}H and ^{13}C – NMR of compound **4g**:





7. References

1. E.O. Dorofeeva, M.N. Elinson, A.N. Vereshchagin, N.O. Stepanov, I.S. Bushmarinov, P.A. Belyakov, O.O. Sokolova and G.I. Nikishin, *RSC Adv*., 2012, **2**, 4444.
2. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339.
3. Bourhis, L.J., Dolomanov, O.V., Gildea, R.J., Howard, J.A.K., Puschmann, H. *Acta Cryst.*, 2015, **A71**, 59-75.
4. G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112.