Supplementary Information

The spectral data for some selected compounds

2-amino-7,7-dimethyl-5-oxo-4-phenyl-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile ***(4f)****:*

^{1}H NMR (250 MHz, DMSO-*d6*) δ 7.27-7.20 (m, 2H, Ar), 7.15-7.20 (m, 3H, Ar), 6.97 (s, 2H, NH_2), 4.15 (s, 1H, CH), 2.48 (s, 2H, CH_2), 2.21-2.08 (m, 2H, CH_2), 1.00 (s, 3H, CH_3), 0.92 (s, 3H, CH_3).

2-amino-7,7-dimethyl-4-(3-nitrophenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile ***(4h)****:*

^{1}H-NMR (250 MHz, DMSO-*d6*) δ 8.07-8.02 (m, 1H, Ar), 7.95-7.94 (m, 1H, Ar), 7.62 -7.55 (m, 2H, Ar), 7.15 (s, 2H, NH_2), 4.39 (s, 1H, CH), 2.52 (s, 2H, CH_2), 2.27-2.06 (m, 2H, CH_2), 1.01 (s, 3H, CH_3), 0.93 (s, 3H, CH_3). ^{13}C NMR (62.5 MHz, DMSO-*d6*) δ 195.7, 163.1, 158.5, 147.7, 146.9, 134.1, 129.9, 121.7, 121.5, 119.3, 111.7, 57.1, 49,7, 35.3, 31.7, 28.2, 26.6.

2-amino-4-(2,4-dichlorophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile ***(4i)****:*

^{1}H NMR (250 MHz, DMSO-*d6*) δ 7.64 (d, *J* = 8.3 Hz, 2H, Ar), 7.48 (d, *J* = 8.1 Hz, 2H, Ar),7.41 (s, 2H, NH_2), 4.20 (s, 1H, CH), 2.46-2.33 (m, 2H, CH_2), 2.16 (d, *J* = 16.1 Hz, 2H, CH), 2.00 (d, *J* = 16.1 Hz, 2H, CH), 1.02 (s, 3H, CH_3), 0.92 (s, 3H, CH_3). ^{13}C NMR (62.5 MHz, DMSO-*d6*) δ 194.6, 167.6, 153.3, 147.0, 138.8, 134.1, 128.8, 127.9, 126.6, 120.0, 118.6, 57.6, 50.0, 40.9, 34.1, 32.2, 27.4.

2-amino-4-(4-chlorophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile ***(4j)****:*

^{1}H NMR (250 MHz, DMSO-*d6*) δ 7.31 (d, J = 8.2 Hz, 2H, Ar), 7.14 (d, J = 8.5 Hz, 2H, Ar),7.03 (s, 2H, NH_2), 4.16 (s, 1H, CH), 2.47 (s, 2H, CH_2), 2.03-2.26 (m, 2H, CH_2), 0.99 (s, 3H, CH_3), 0.91 (s, 3H, CH_3). ^{13}C NMR (62.5 MHz, DMSO-*d6*) δ 195.6, 162.5, 158.4, 143.6, 131.0, 129.0, 128.2, 119.5, 112.2, 57.6, 55.9, 49.8, 35.0, 31.7, 28.2, 26.7, 18.4.

2-amino-4-(3-nitrophenyl)-5-oxo-4H,5H-pyrano[3,2-c]chromene-3-carbonitrile ***(4m)****:*

^{1}H NMR (250 MHz, DMSO-*d6*) δ 7.73 (d, *J* = 8.2 Hz, 2H, Ar), 7.46 (t, *J* = 8.1 Hz, 2H, Ar),7.31-7.24 (m, 5H, Ar, NH_2), 7.13 (t, *J* = 8.1 Hz, 2H, Ar), 4.71 (s, 1H, CH). ^{13}C NMR (62.5 MHz, DMSO-*d6*) δ 171.6, 167.0, 154.6, 154.6, 153.3, 147.0, 138.8, 134.1, 128.8, 127.9, 126.6, 124.4, 119.9, 119.8, 118.1, 112.1, 107.6, 57.0, 40.9.

6-amino-8-(4-methoxyphenyl)-2,4-dioxo-2,3,4,8-tetrahydro-1H-pyrano[3,2-d]pyrimidine-7-carbonitrile ***(5b)****:*

^{1}H NMR (250 MHz, DMSO-*d6*) δ 7.45 (s, 2H, NH_2), 7.22 (d, *J* = 8.1 Hz, 2H, Ar), 6.84 (d, *J* = 8.2 Hz, 2H, Ar), 4.23 (s, 1H, CH), 3.76 (s, 3H, OCH_3), 3.18 (s, 3H, CH_3), 3.03 (s, 3H, CH_3). ^{13}C NMR (62.5 MHz, DMSO-*d6*) δ 159.0, 152.6, 147.8, 147.5, 146.4, 139.0, 133.0, 128.7, 118.0, 112.7, 61.9, 53.3, 45.8, 40.8, 34.0, 28.9.

7-amino-1,3-dimethyl-5-(3-nitrophenyl)-2,4-dioxo-1,3,4,5-tetrahydro-2H-pyrano [2,3-d]pyrimidine-6-carbonitrile ***(5c)****:*

The colourless crystals, IR (KBr) ν/cm^{-1} 3336, 3196 (NH_2), 2200 (CN), 1689(C=O), 1630, 1529, 1513, 1492 (C=C stretching of aromatic ring). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.17-8.16 (d, 1H, $^4J_{H\text{-}H}$=1Hz), 8.14 (d, 1H, $^4J_{H\text{-}H}$=1Hz), 7.84-7.82 (d, 1H, $^3J_{H\text{-}H}$=8Hz), 7.68-7.64 (t, 1H, $^3J_{H\text{-}H}$=8Hz), 7.53 (2H, s, NH_2), 4.63 (1H, s, CH_2), 3.42(3H, *s*, CH_3), 3.13 (3H, *s*, CH_3).

7-amino-5-(2,4-dichlorophenyl)-1,3-di-methyl-2,4-dioxo-1,3,4,5-tetrahydro-2H-pyrano [2,3-d] pyrimidine-6-carbonitrile ***(5d)****:*

The yellow crystals, IR (KBr) ν/cm^{-1} 3334, 3236 (NH_2), 2221 (CN), 1708, 1660 (C=O), 1551, 1513, 1485 (C=C stretching of aromatic ring). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.09 (2H, s, NH_2), 7.81 (s, 1H), 7.60-7.58 (d, 1H, $^3J_{H\text{-}H}$=8Hz), 7.39-7.37 (d, 1H, $^3J_{H\text{-}H}$=8Hz), 4.40 (1H, s, CH_2), 3.57 (3H, s, CH_3), 3.15 (3H, s, CH_3).

7-amino-1,3-dimethyl-5-(3-nitrophenyl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile ***(5h)****:*

The colourless crystals, IR (KBr) ν/cm^{-1} 3335, 3231 (NH_2), 2225 (CN), 1711(C=O), 1669, 1562, 1468 (C=C stretching of aromatic ring). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.39-8.36 (m, 1H, Ar), 8.23 (t, 1H, $^3J_{H\text{-}H}$=8Hz, Ar), 7.83 (s, 2H, NH_2), 7.82-7.81 (d, 2H, $^3J_{H\text{-}H}$=8Hz, Ar), 3.58(3H, *s*, CH_3), 3.14 (3H, *s*, CH_3)

7-amino-5-(2,4-dichlorophenyl)-1,3-di-methyl-2,4-dioxo-1,2,3,4-tetrahydropyrido -[2,3-d]pyrimidine-6-carbonitrile ***(5i)****:*

The white crystals, IR (KBr) ν/cm^{-1} 3463, 3360 (NH_2), 2215 (CN), 1710, 1685 (C=O), 1563, 1507, 1481 (C=C stretching of aromatic ring). ^{1}H NMR (400 MHz, DMSO- *d6*) δ 8.09 (2H, s, NH_2), 7.81-7.80 (d, 1H, $^4J_{H-H}$=2Hz), 7.60-7.57 (dd, 1H, $^3J_{H-H}$=8Hz, $^4J_{H-H}$=2Hz), 7.39-7.37 (d, 1H, $^3J_{H-H}$=8Hz), 3.56 (3H, *s*, CH_3), 3.15 (3H, *s*, CH_3).

6-amino-8-(4-chlorophenyl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[3,2-d]pyrimidine-7-carbonitrile ***(5j)****:*

^{1}H NMR (250 MHz, DMSO-*d6*) δ 7.23 (d, *J* = 8.2 Hz, 2H, Ar), 6.94 (d, *J* = 8.3 Hz, 2H, Ar), 6.03 (s, 2H, NH_2), 3.73 (s, 3H, CH_3), 3.21 (s, 3H, CH_3). ^{13}C NMR (62.5 MHz, DMSO-*d6*) δ 157.0, 156.1, 151.2, 145.4, 136.3, 135.0, 133.3, 130.6, 128.8, 128.5, 114.7, 90.5, 33.0, 28.8.

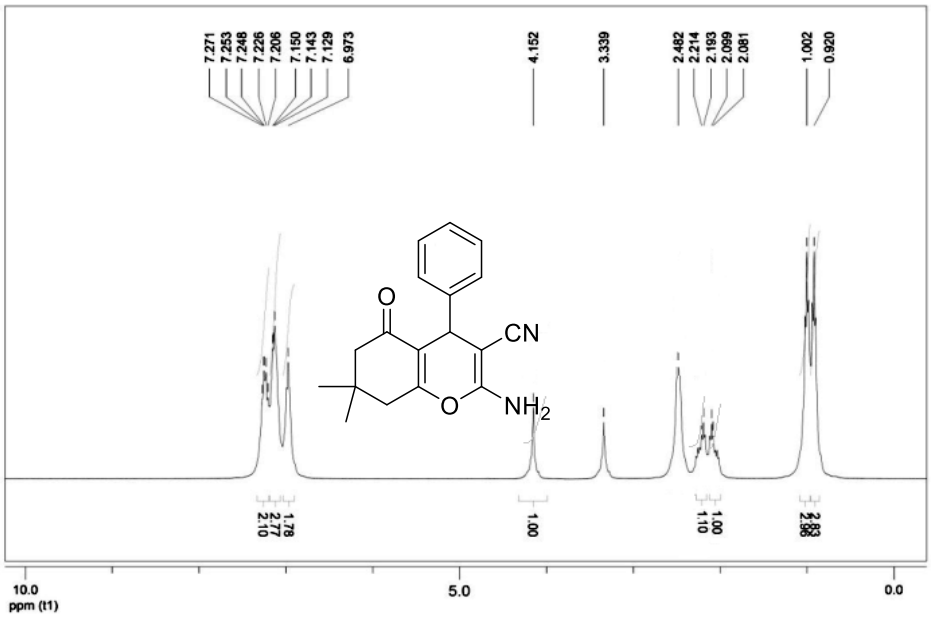


Fig. S1: ^{1}H NMR spectrum (250 MHz, DMSO-d_6) of compound 4f.

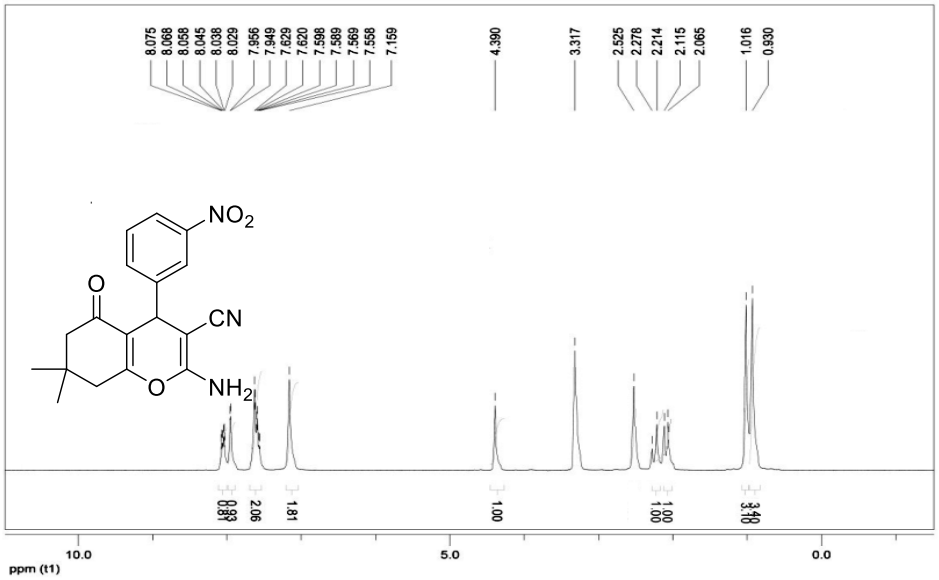


Figure S3. ^{1}H NMR spectrum (250 MHz, DMSO-d_6) of compound 4h

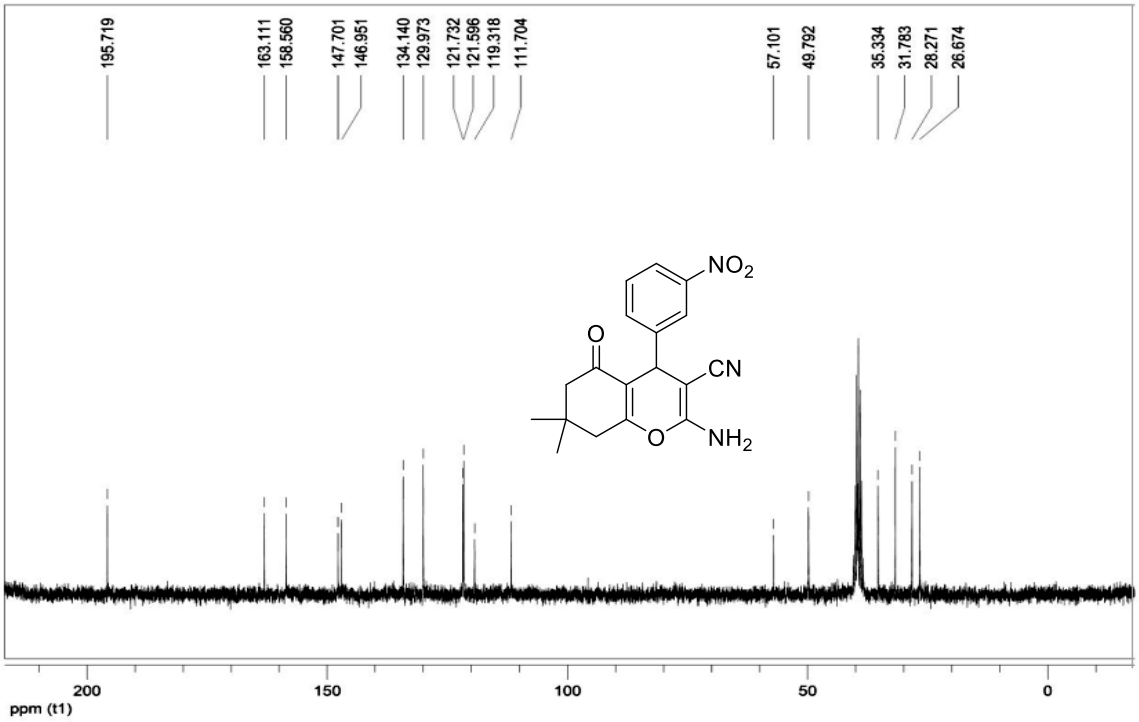


Fig. S4: ^{13}C NMR spectrum (62.5 MHz, DMSO-d_6) of compound 4h

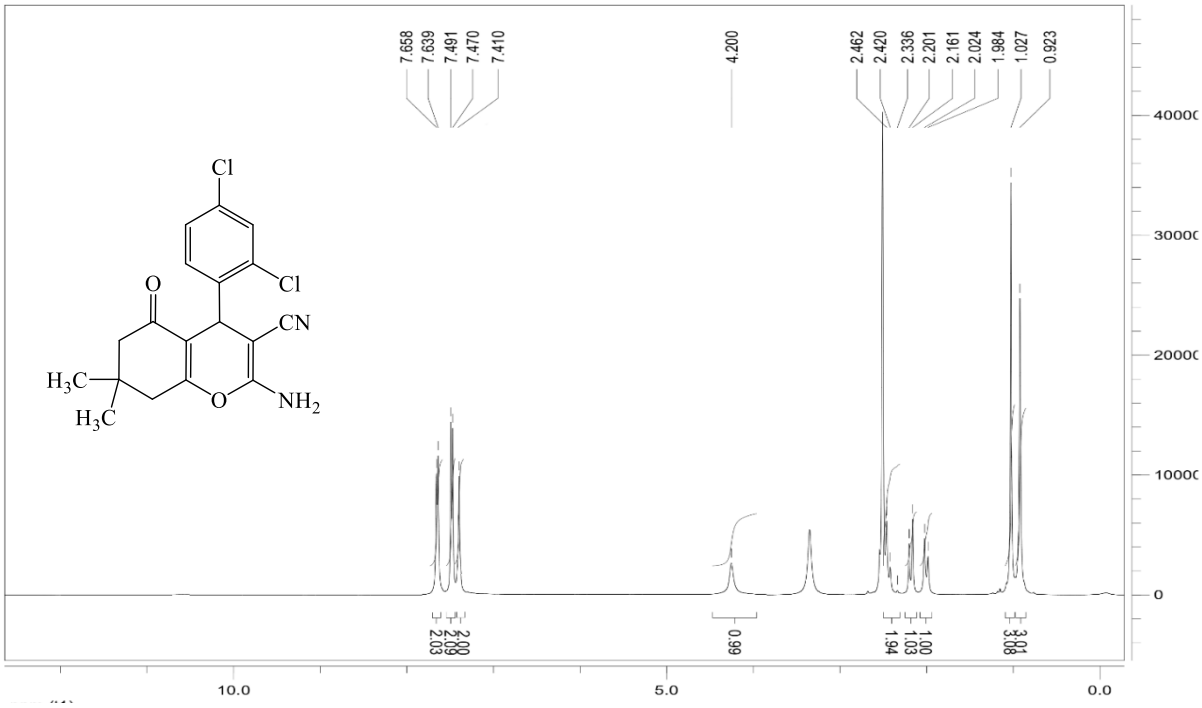


Fig. S5: ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound 4i

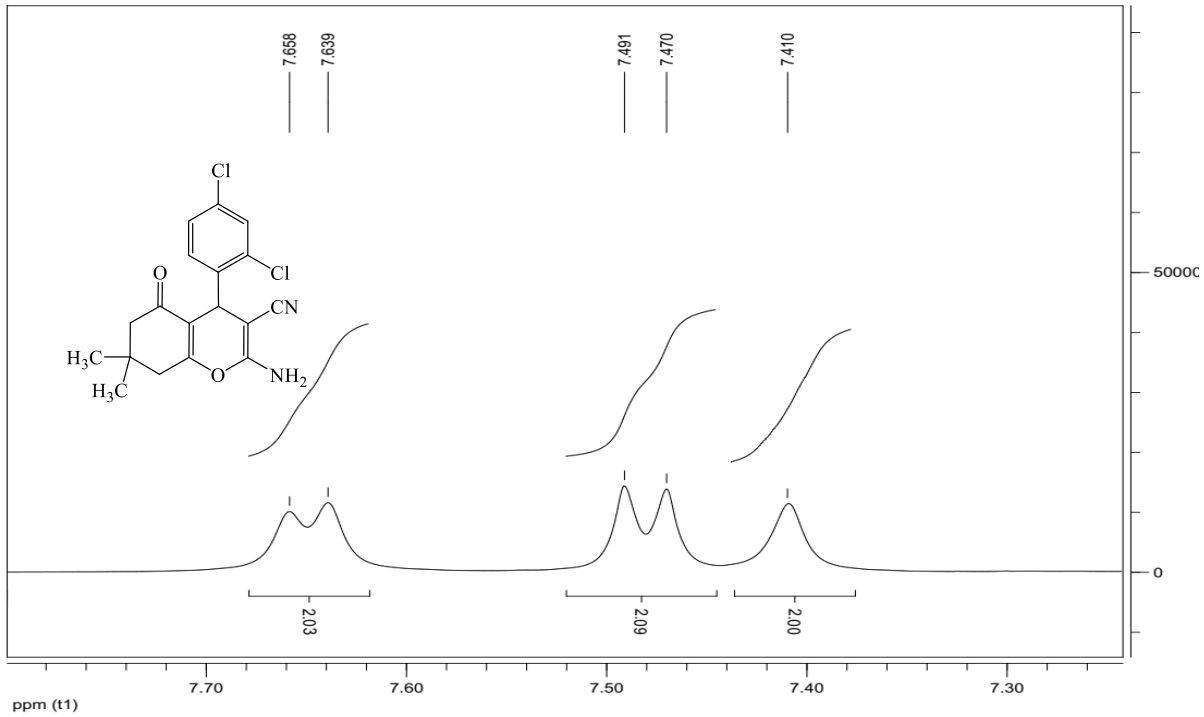


Fig. S6: ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound 4i (Aromatic area).

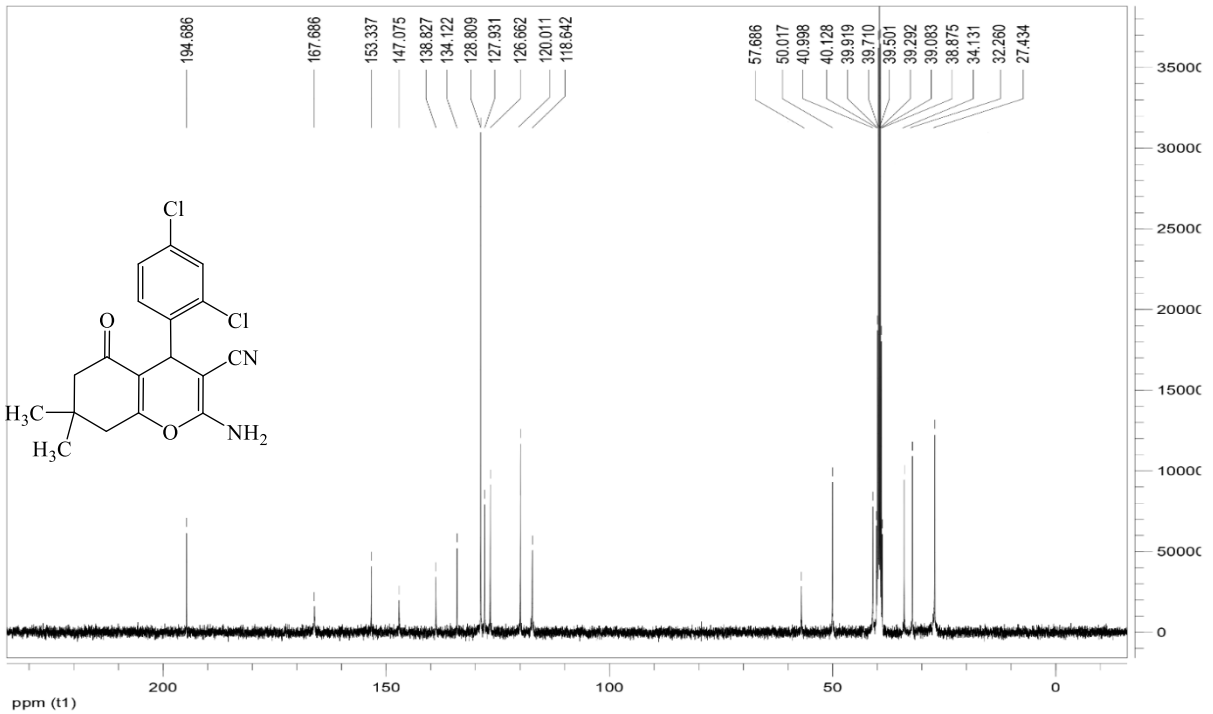


Fig. S7: ^{13}C NMR spectrum (100 MHz, DMSO-d_6) of compound 4i.

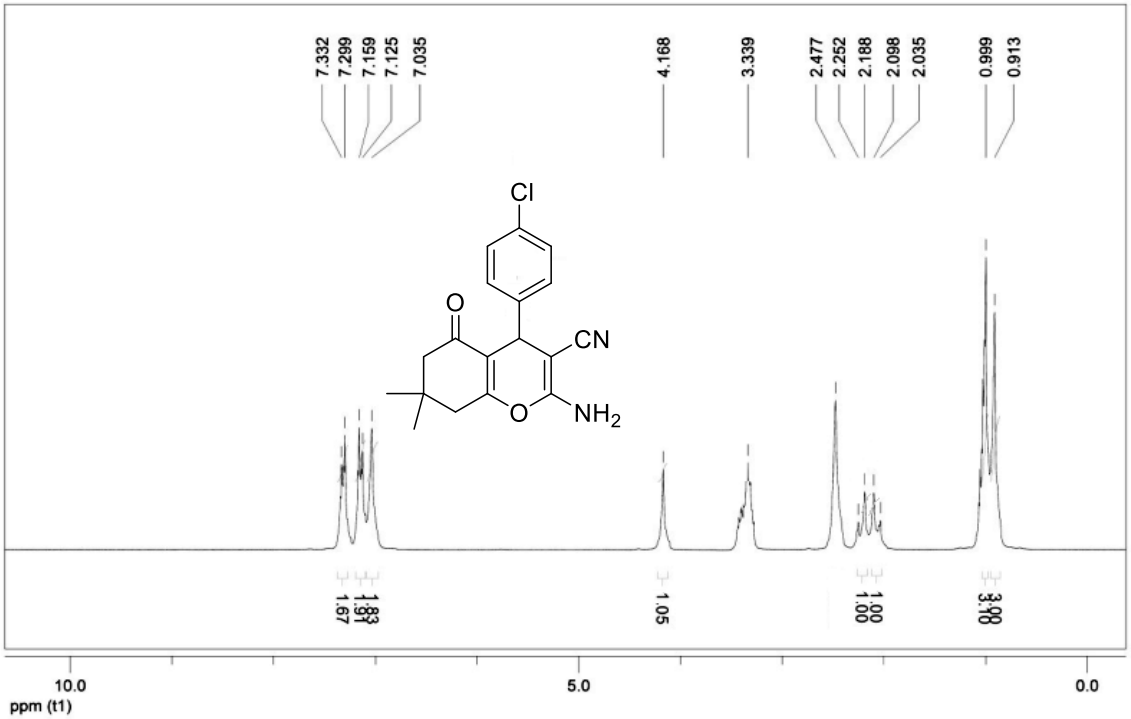


Fig. S8: ^{1}H NMR spectrum (250 MHz, DMSO-d_6) of compound 4j.

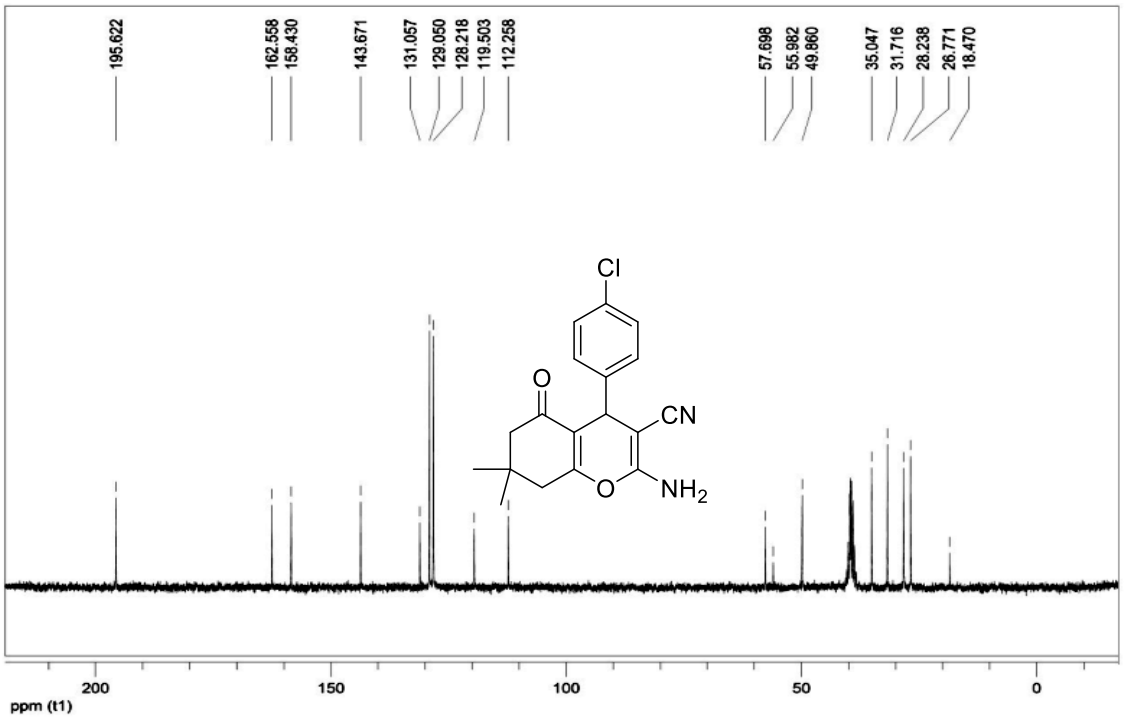


Fig. S9: ^{13}C NMR spectrum (62.5 MHz, DMSO-d_6) of compound 4j.

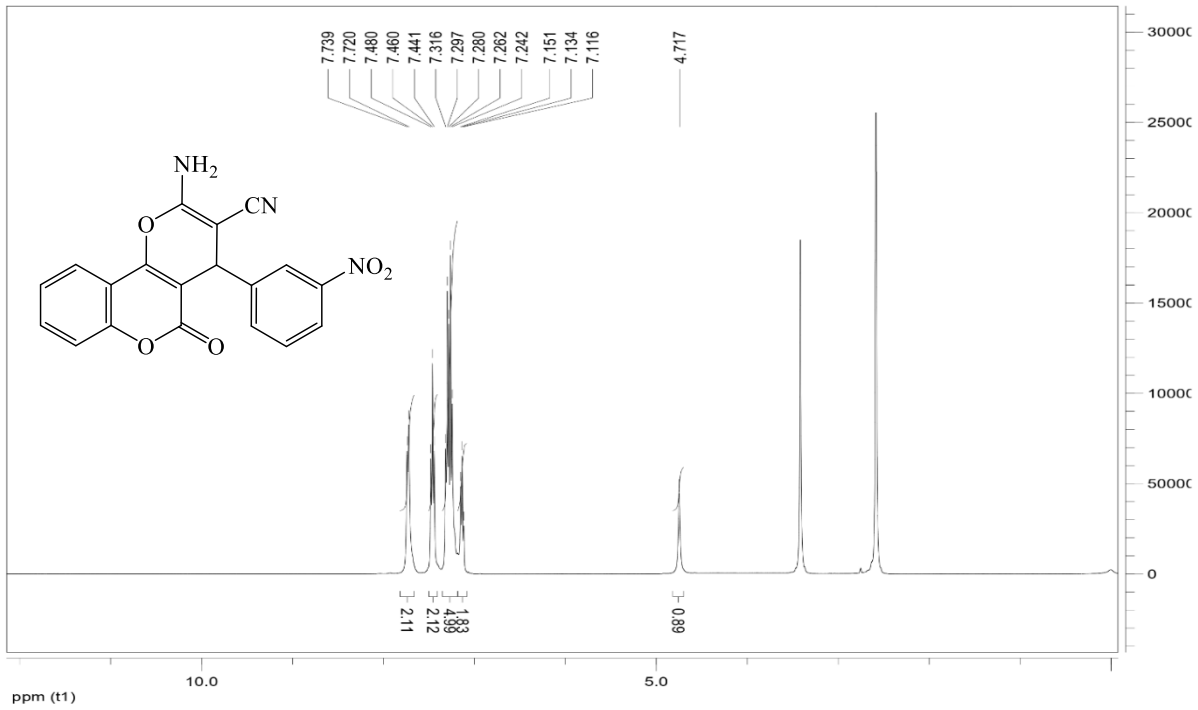


Fig. S10: ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound 4m

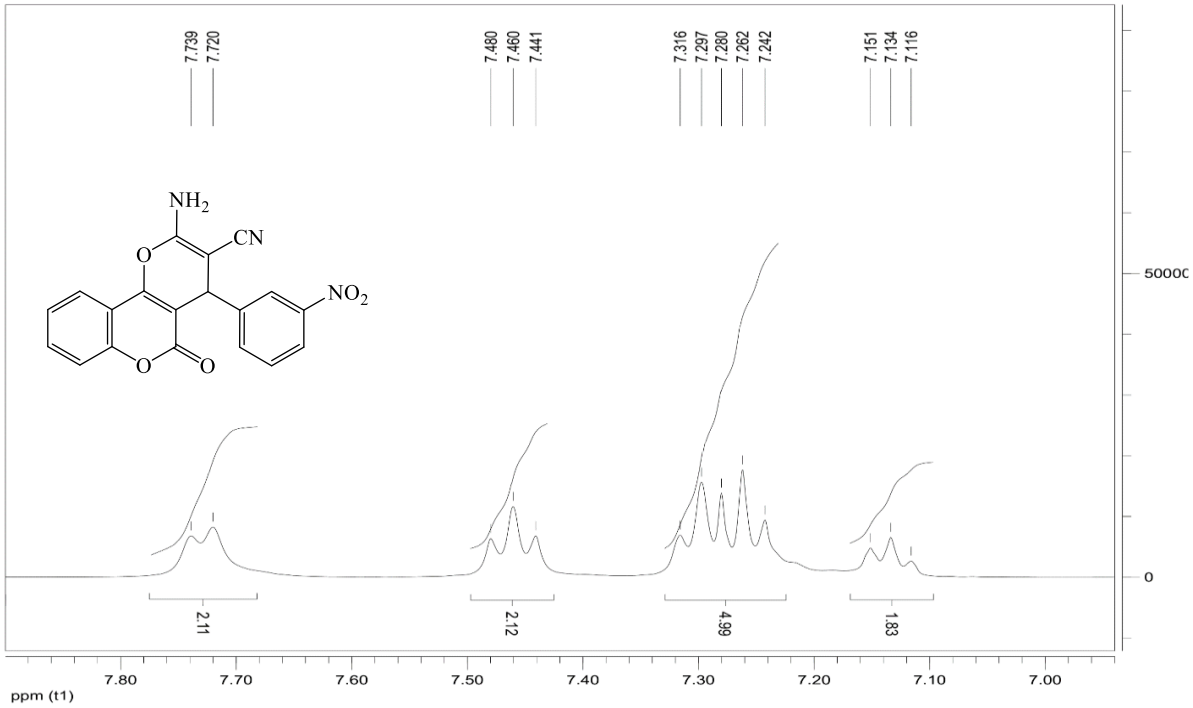


Fig. S11: ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound 4m (Aromatic area)

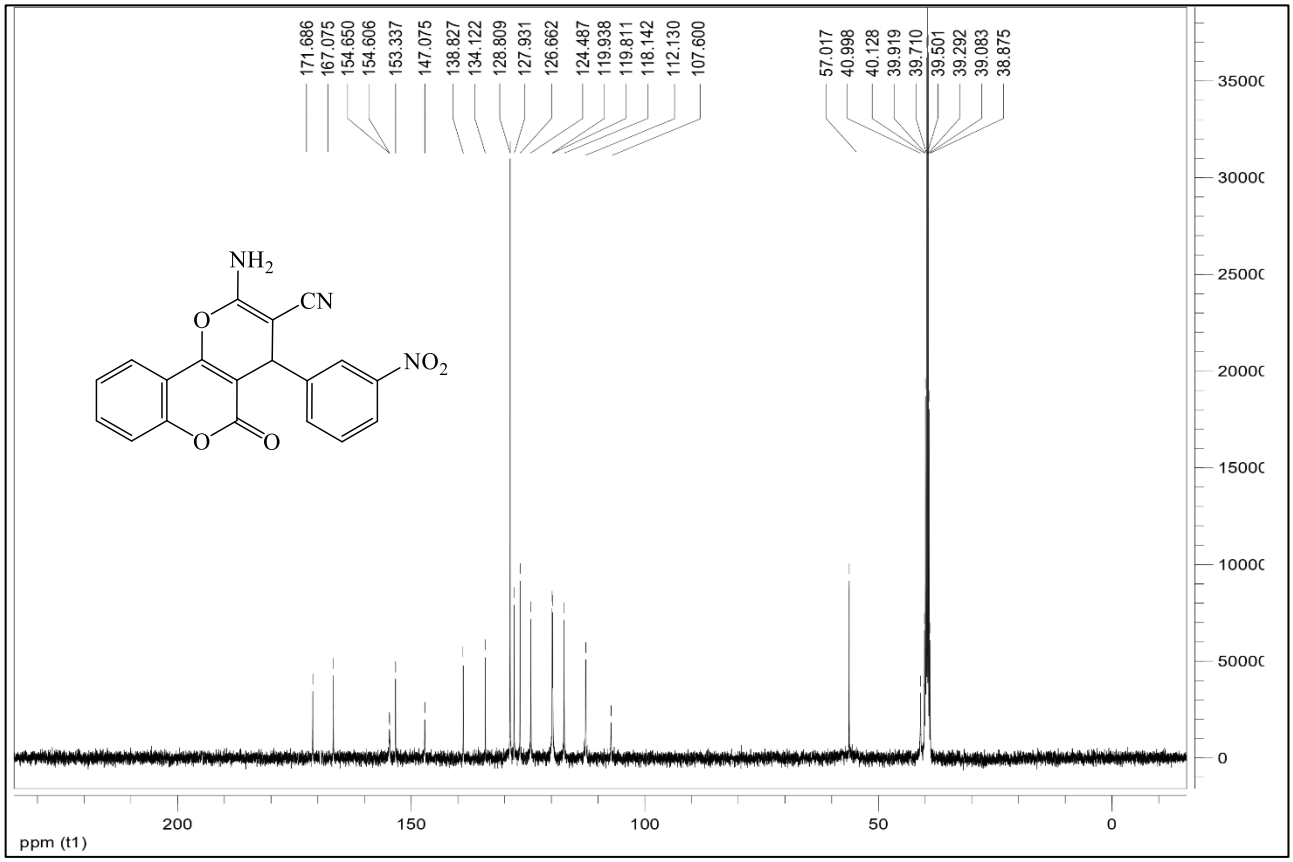


Figure S12. ^{13}C NMR spectrum (100 MHz, DMSO-d_6) of compound **4m**

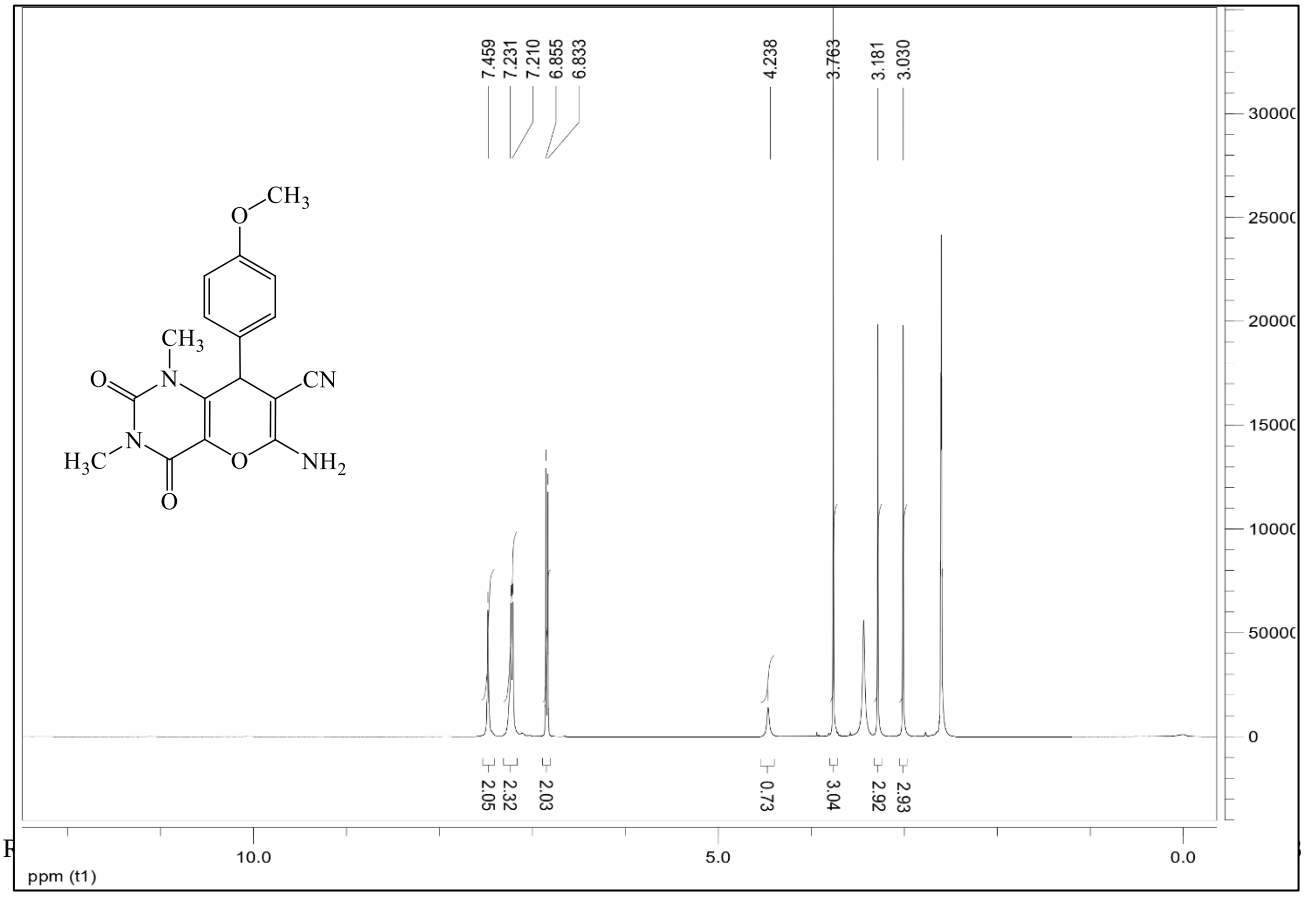


Figure S13. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **5b**

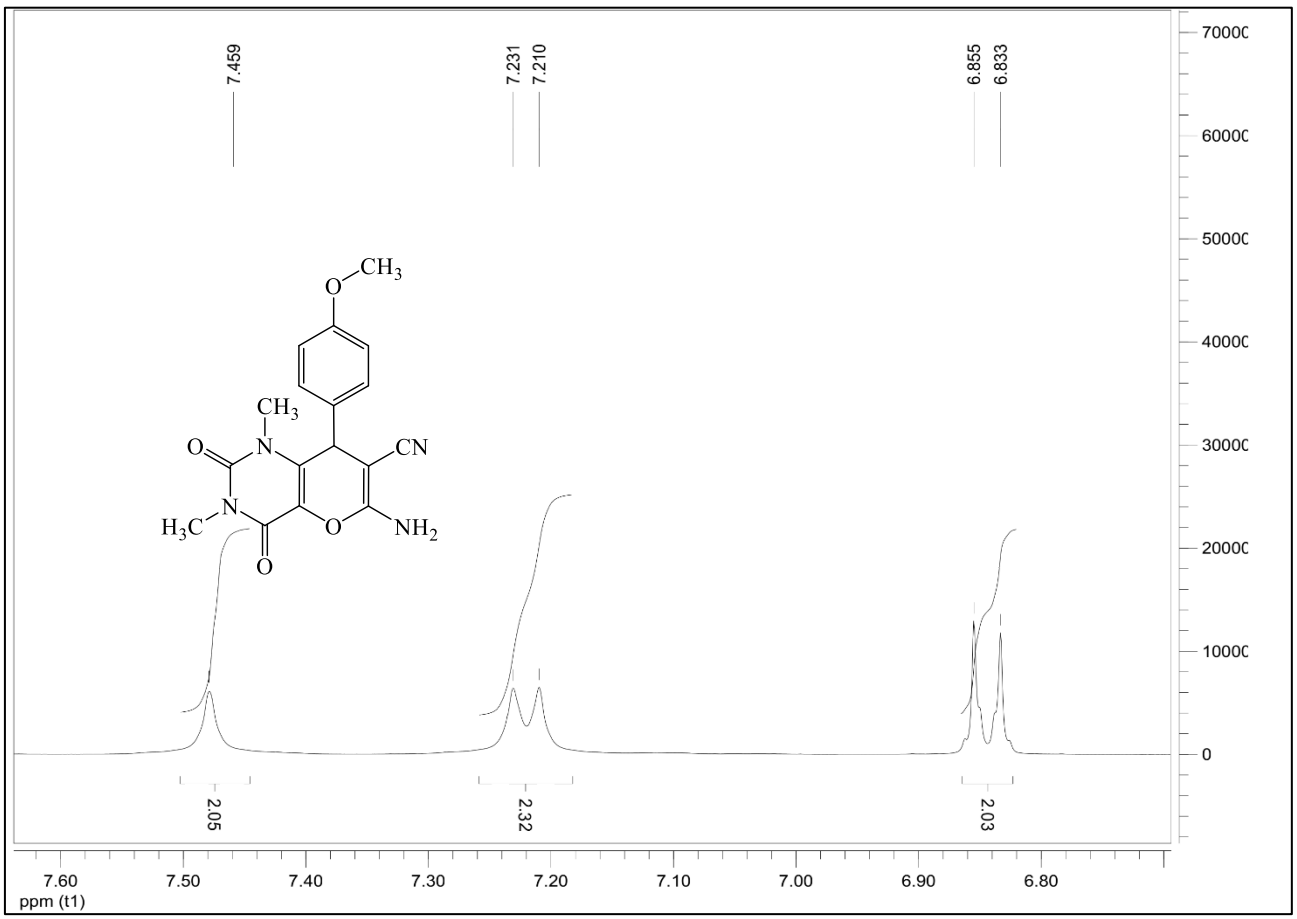


Figure S14. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **5b** (Aromatic area)

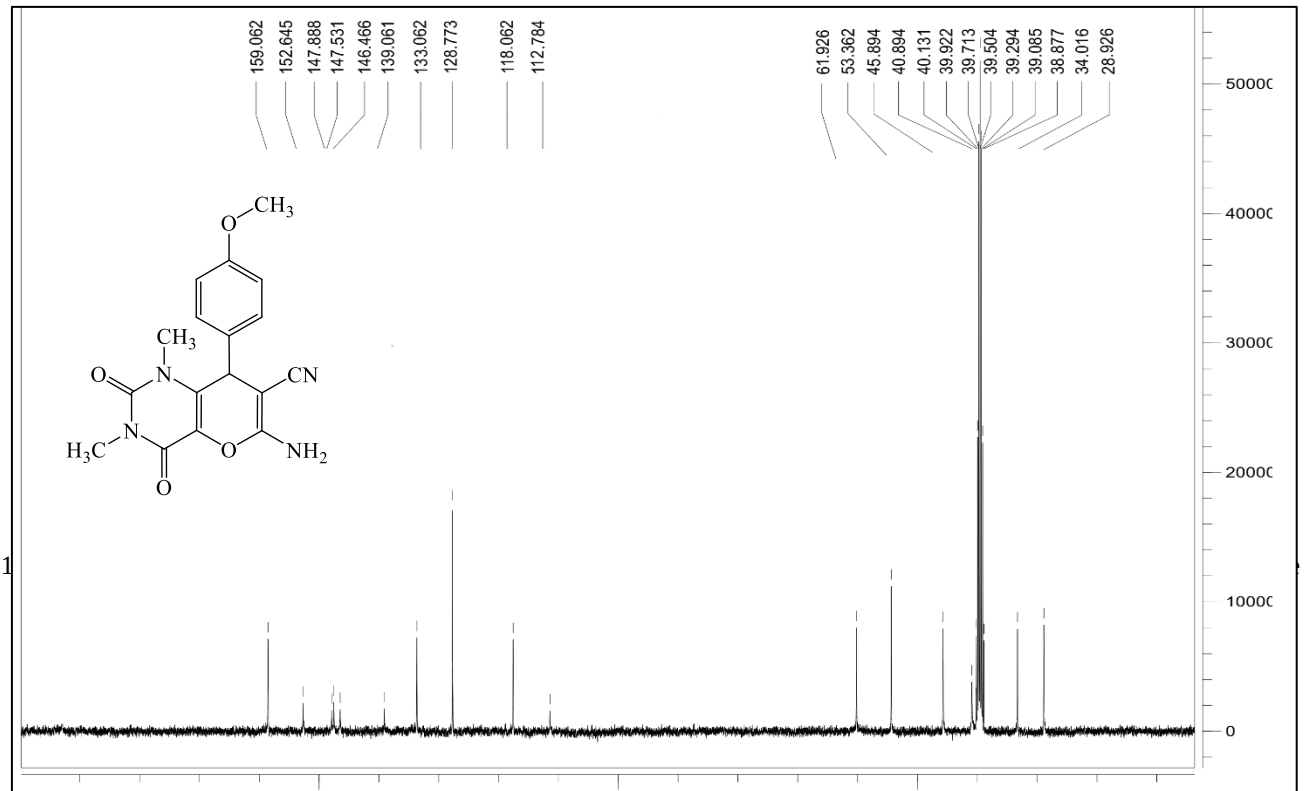


Figure S15. ^{13}C NMR spectrum (100 MHz, DMSO-d_6) of compound **5b**

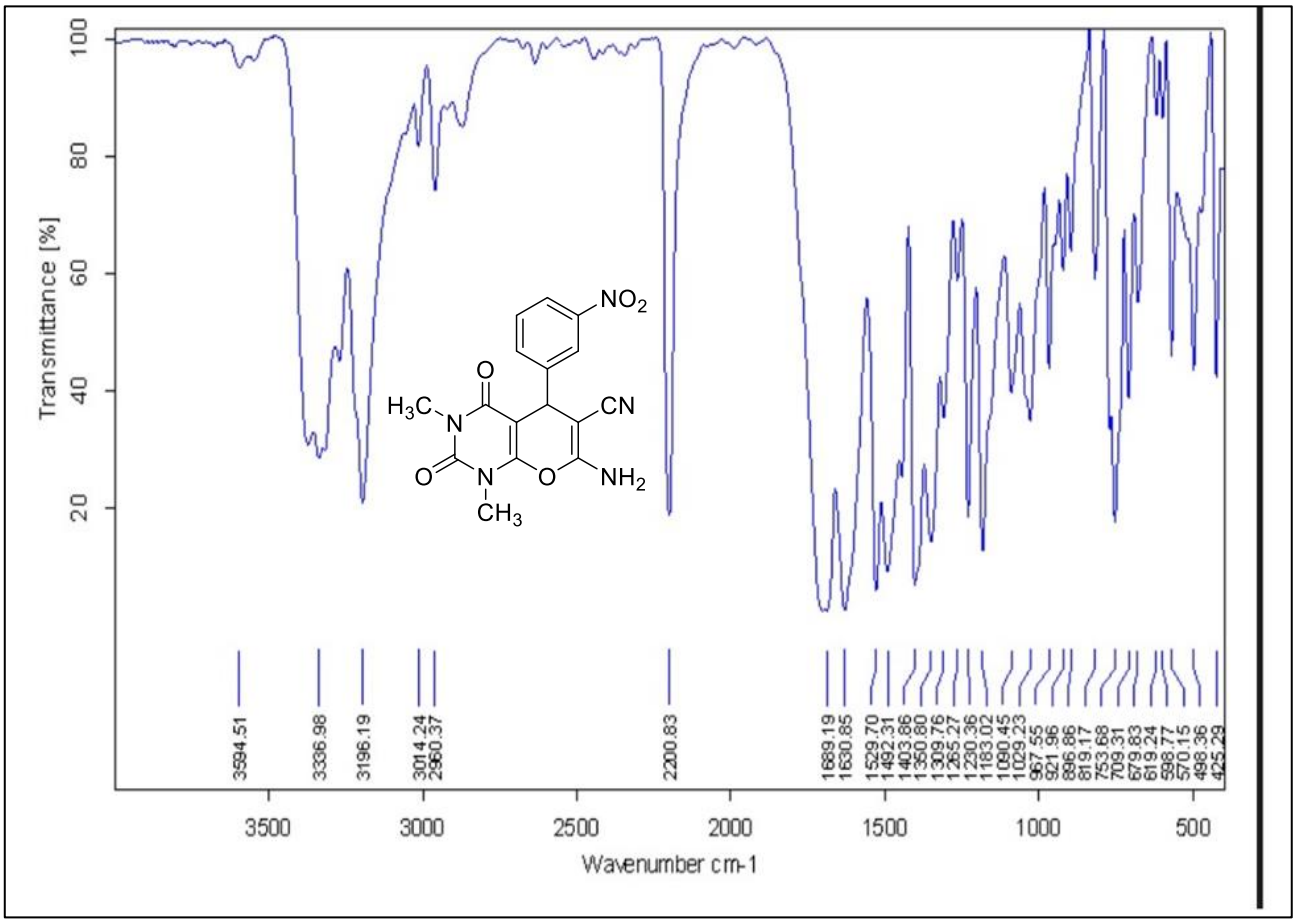
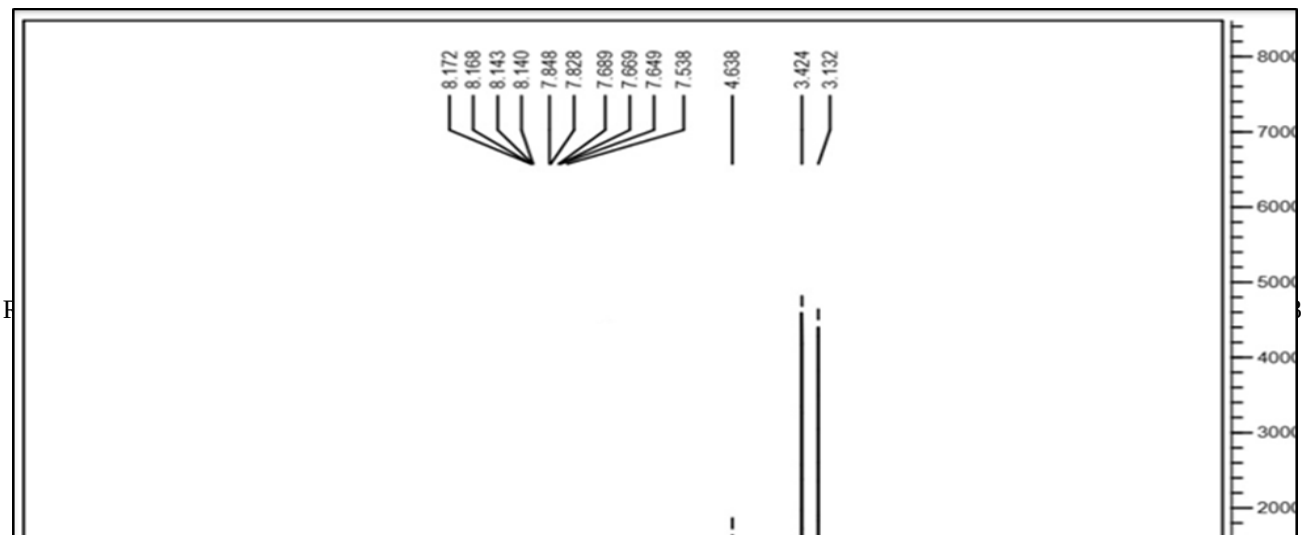


Figure S16. FTIR (KBr) spectrum of compound **5c**



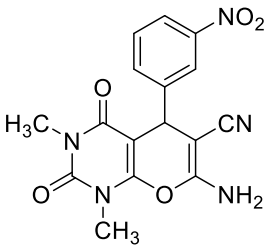


Figure S17. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **5c**

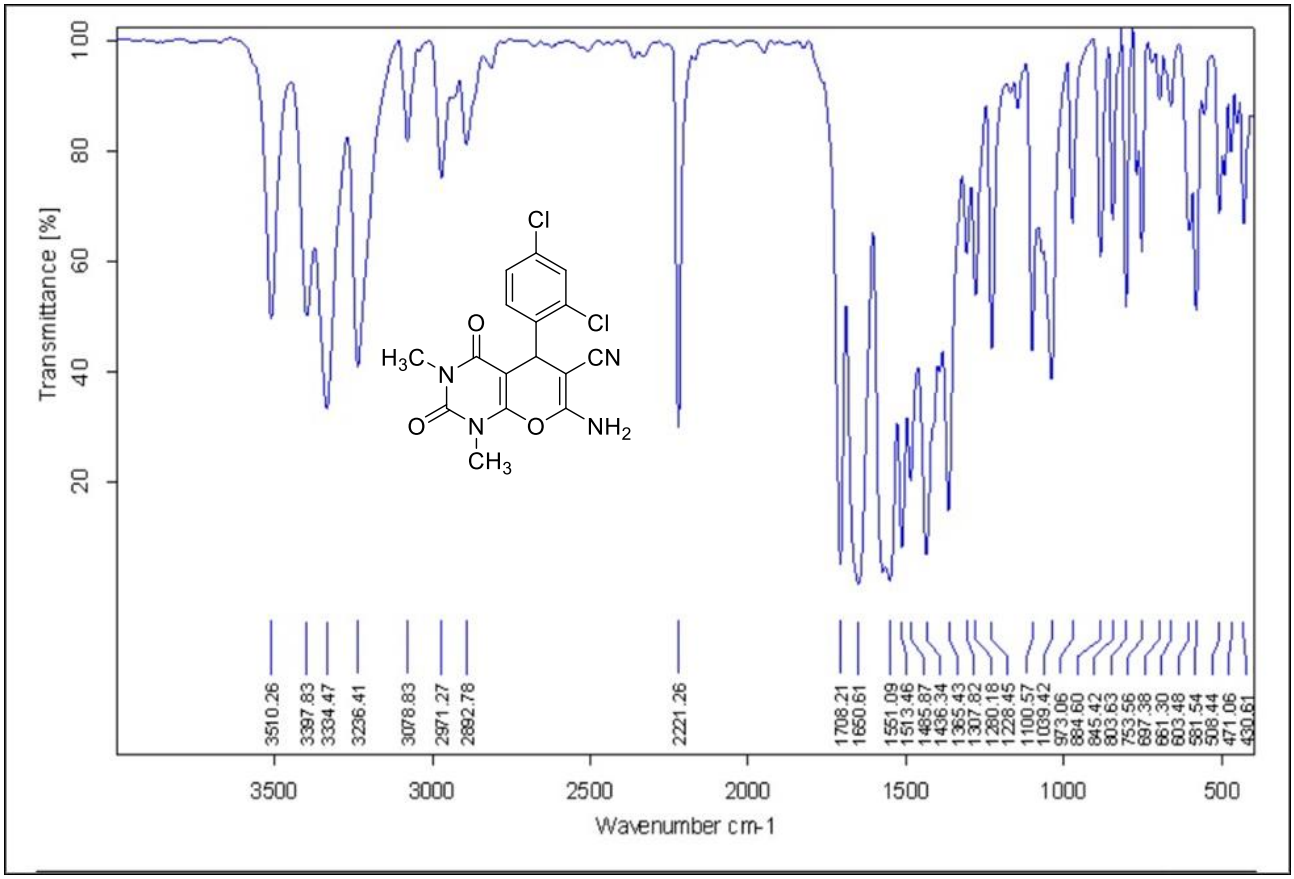
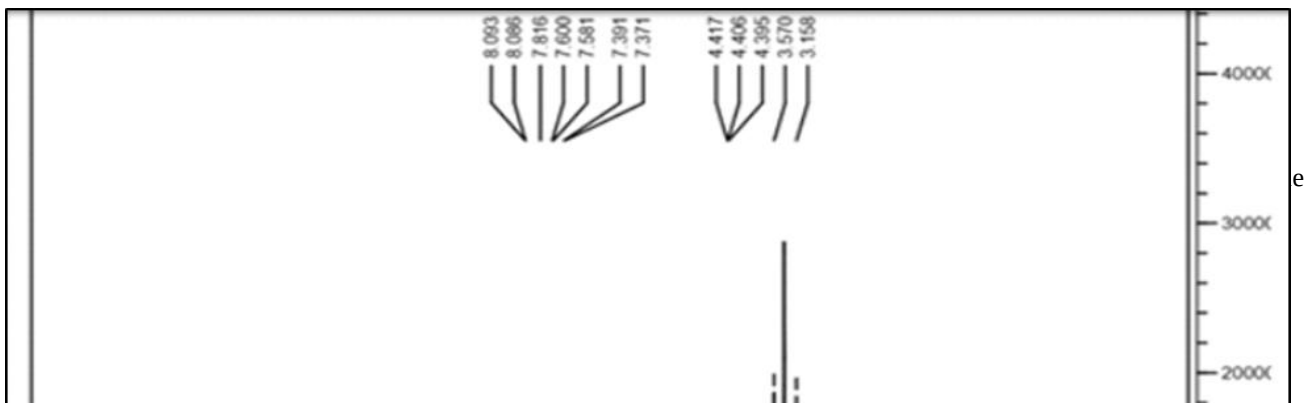


Figure S18. FTIR (KBr) spectrum of compound **5d**



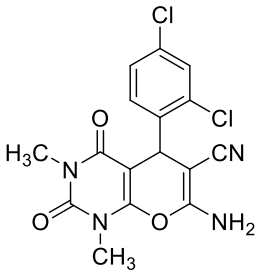


Figure S19. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **5d**

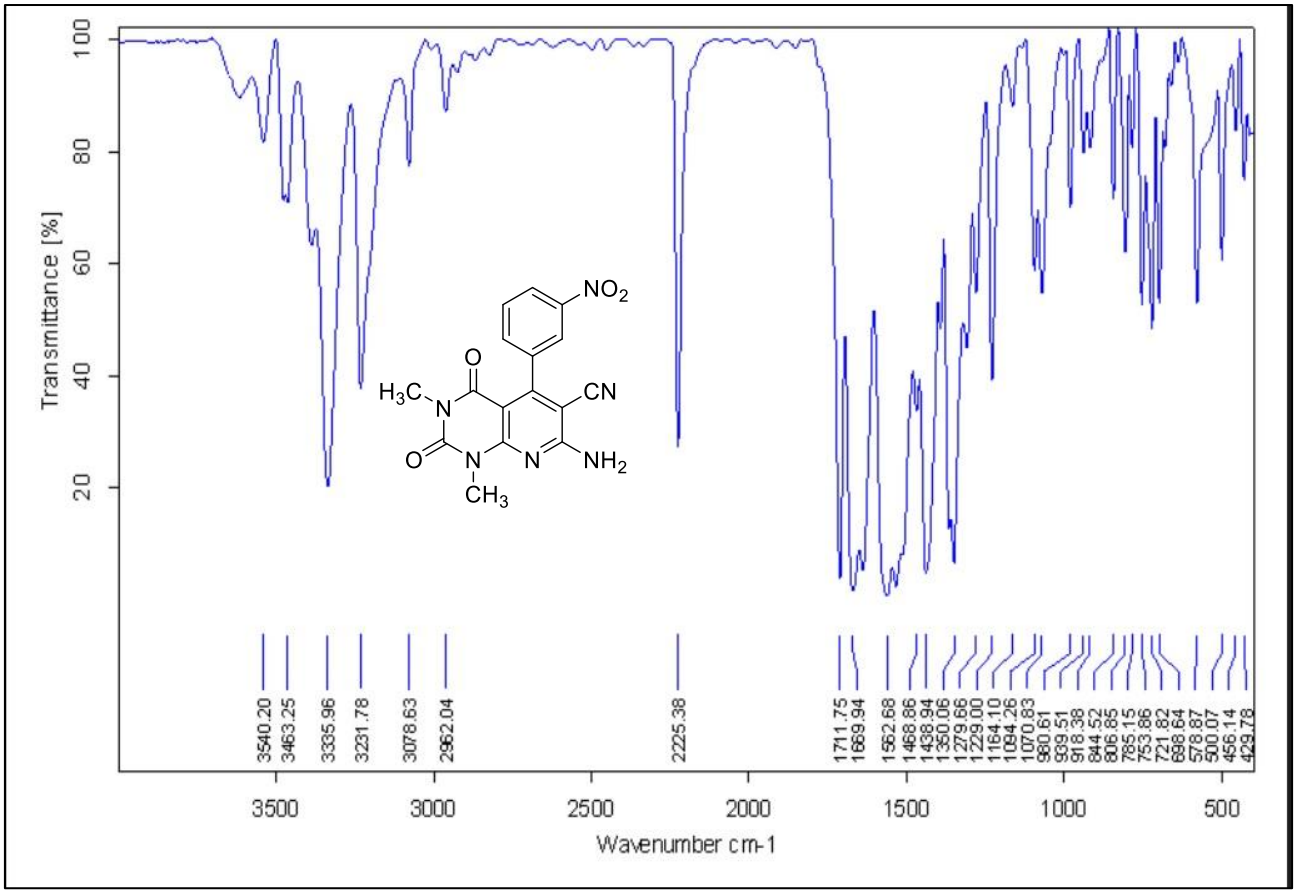


Figure S20. FTIR (KBr) spectrum of compound **5h**

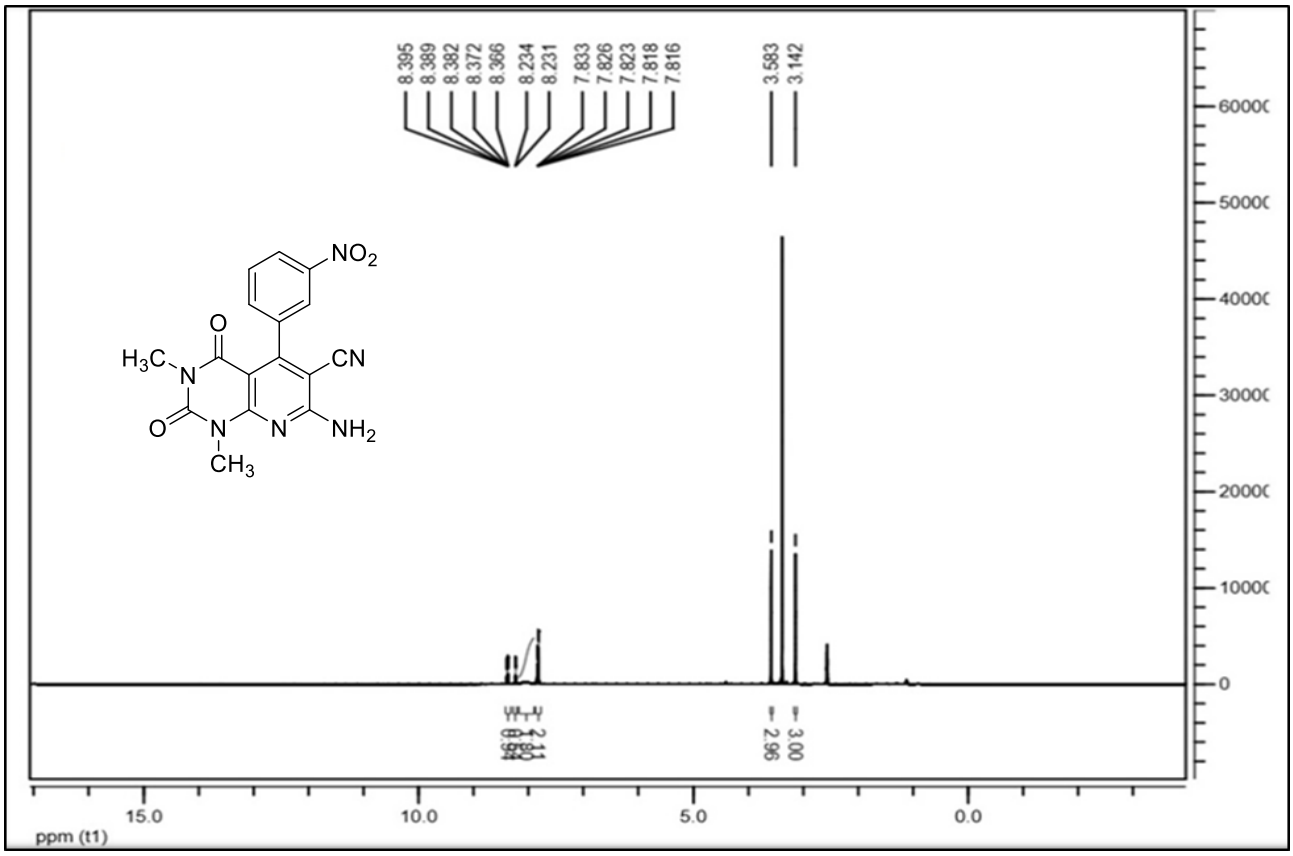


Figure S21. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **5h**

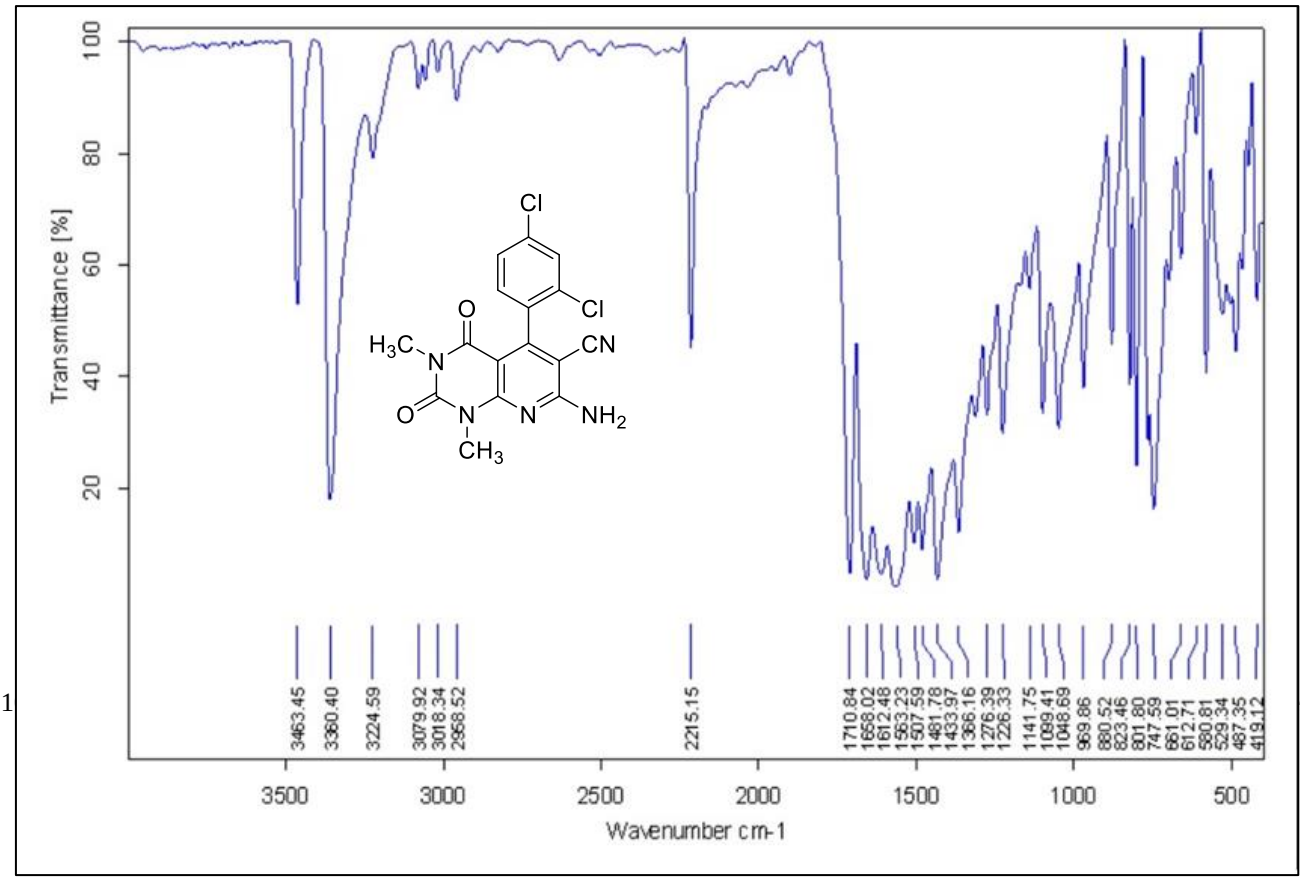


Figure S22. FTIR (KBr) spectrum of compound **5i**

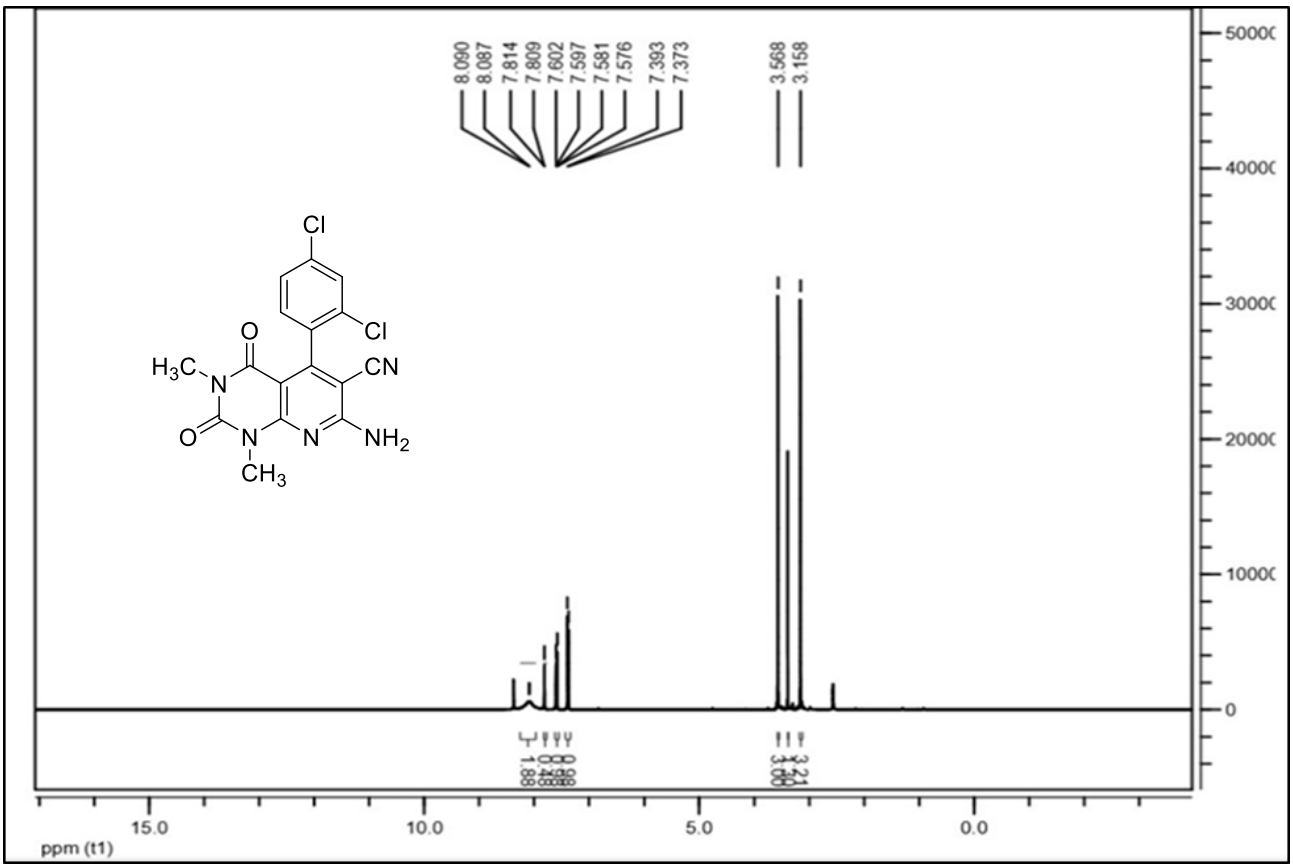


Figure S23. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **5i**

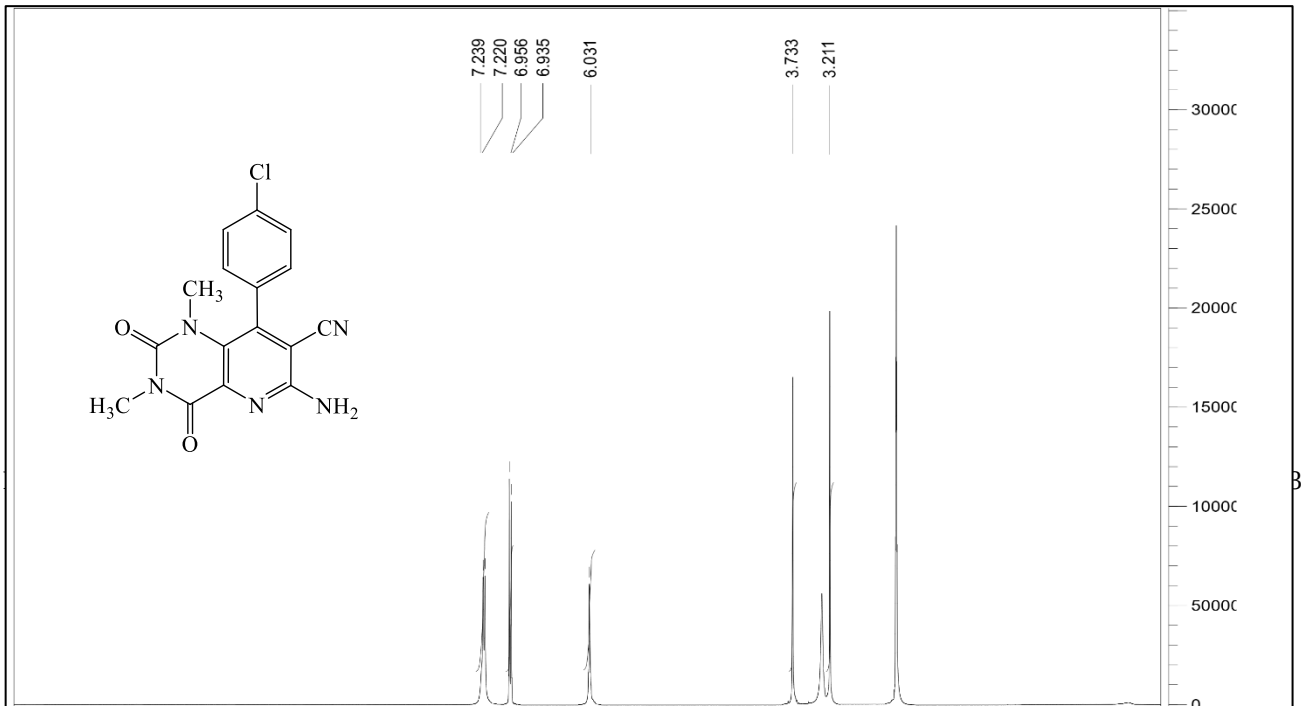


Figure S24. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **5j**

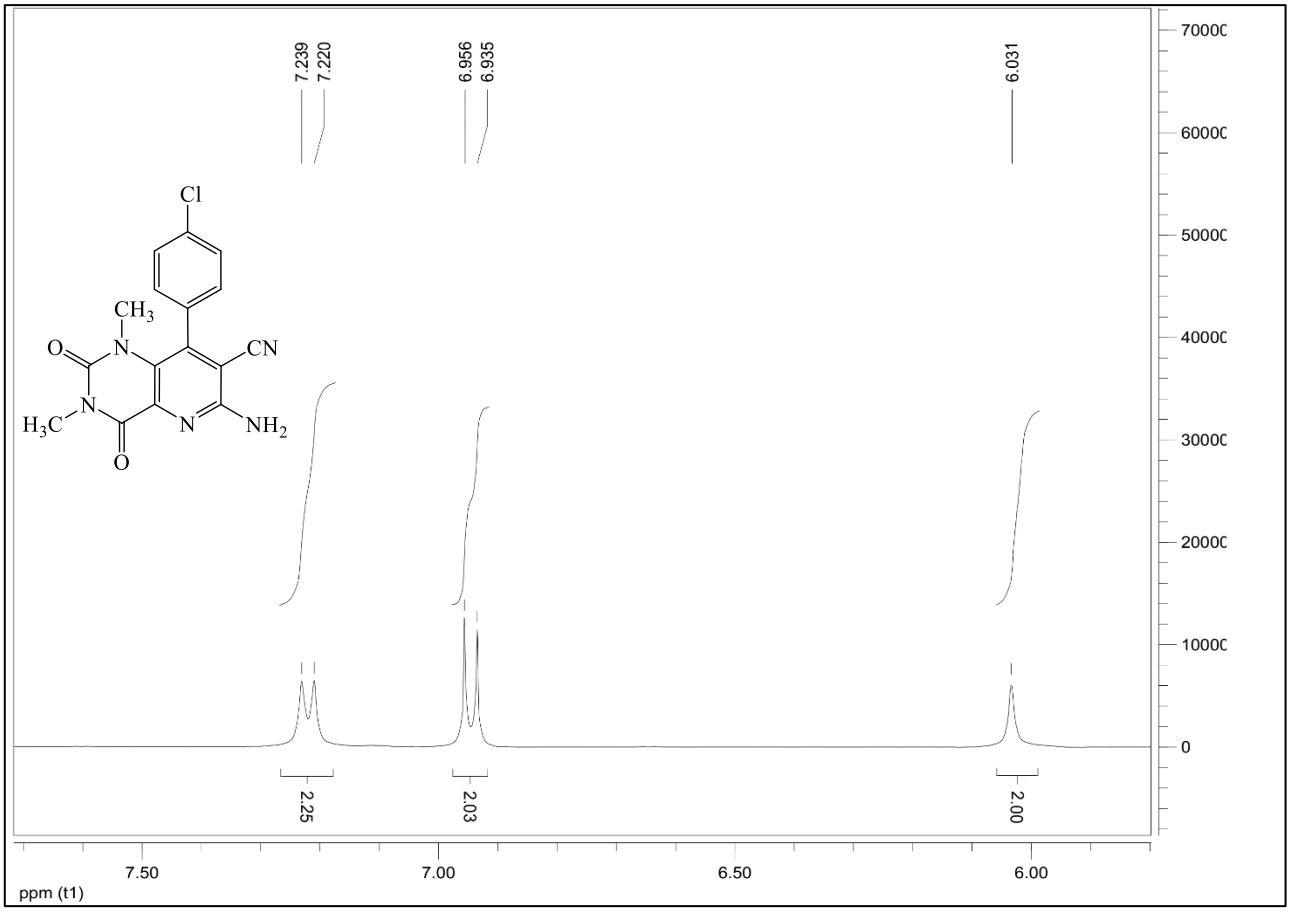
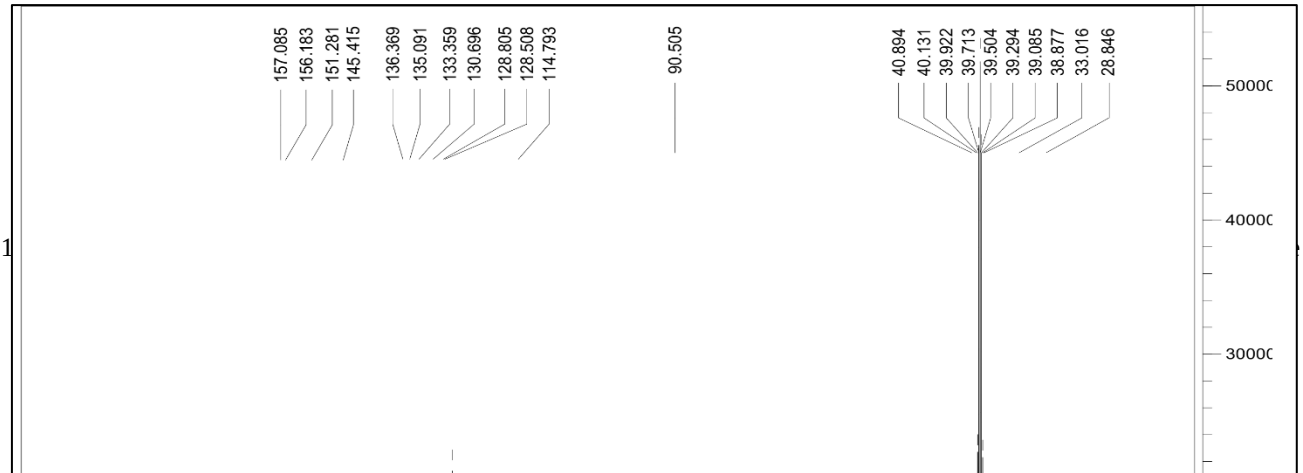


Figure S25. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **5j** (Aromatic area)



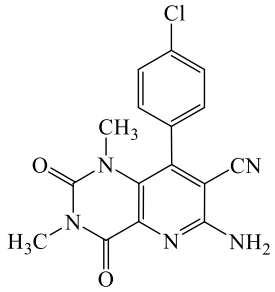


Figure S26. ^{13}C NMR spectrum (100 MHz, DMSO-d_6) of compound **5j**