Supplementary Information

New Fused Imidazo-Pyrimidine and Imidazo-Purine Derived From Maleimide and Nucleobases: One Pot Synthesis, Structure Elucidation, Antioxidant and Antimicrobial Evaluation

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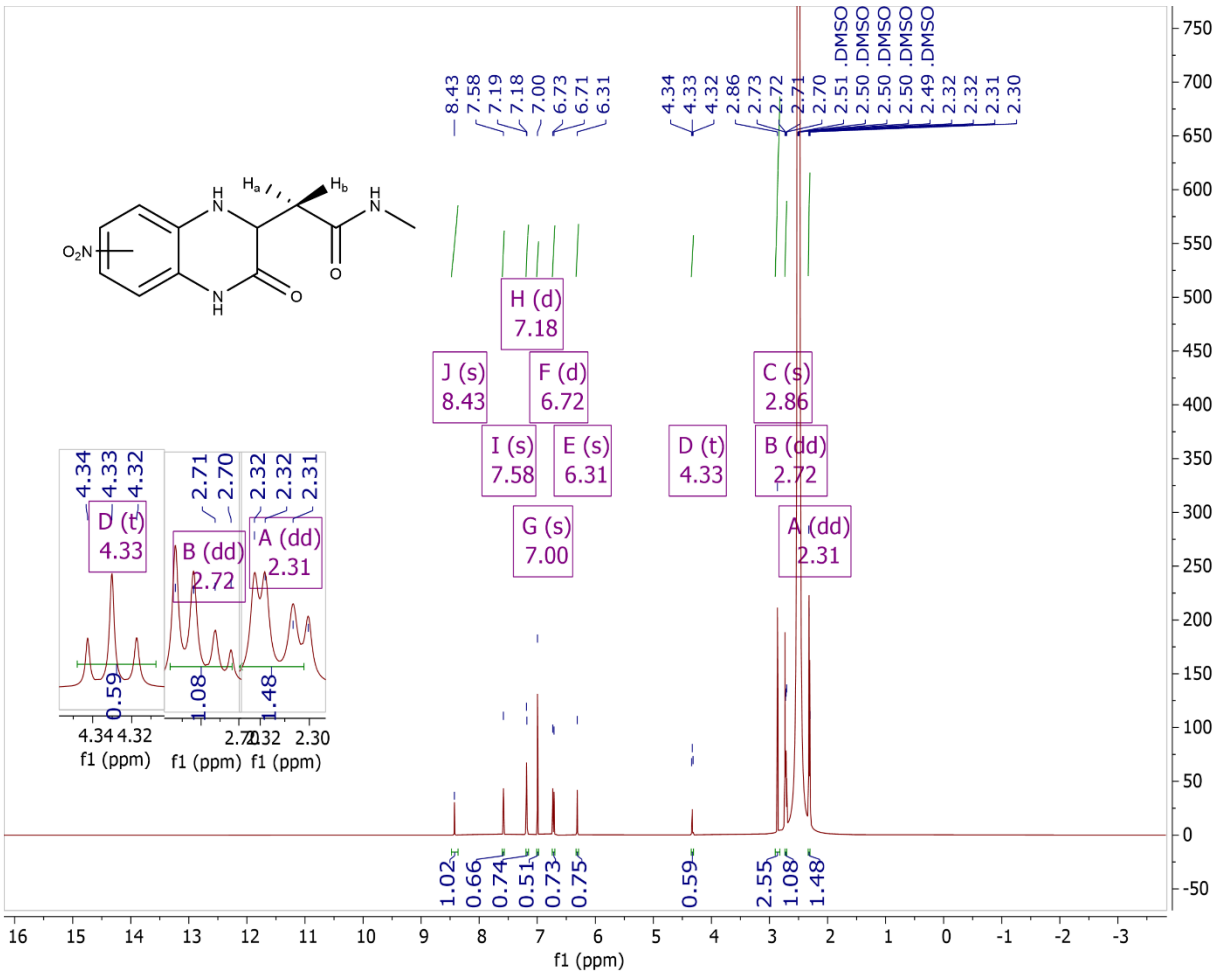
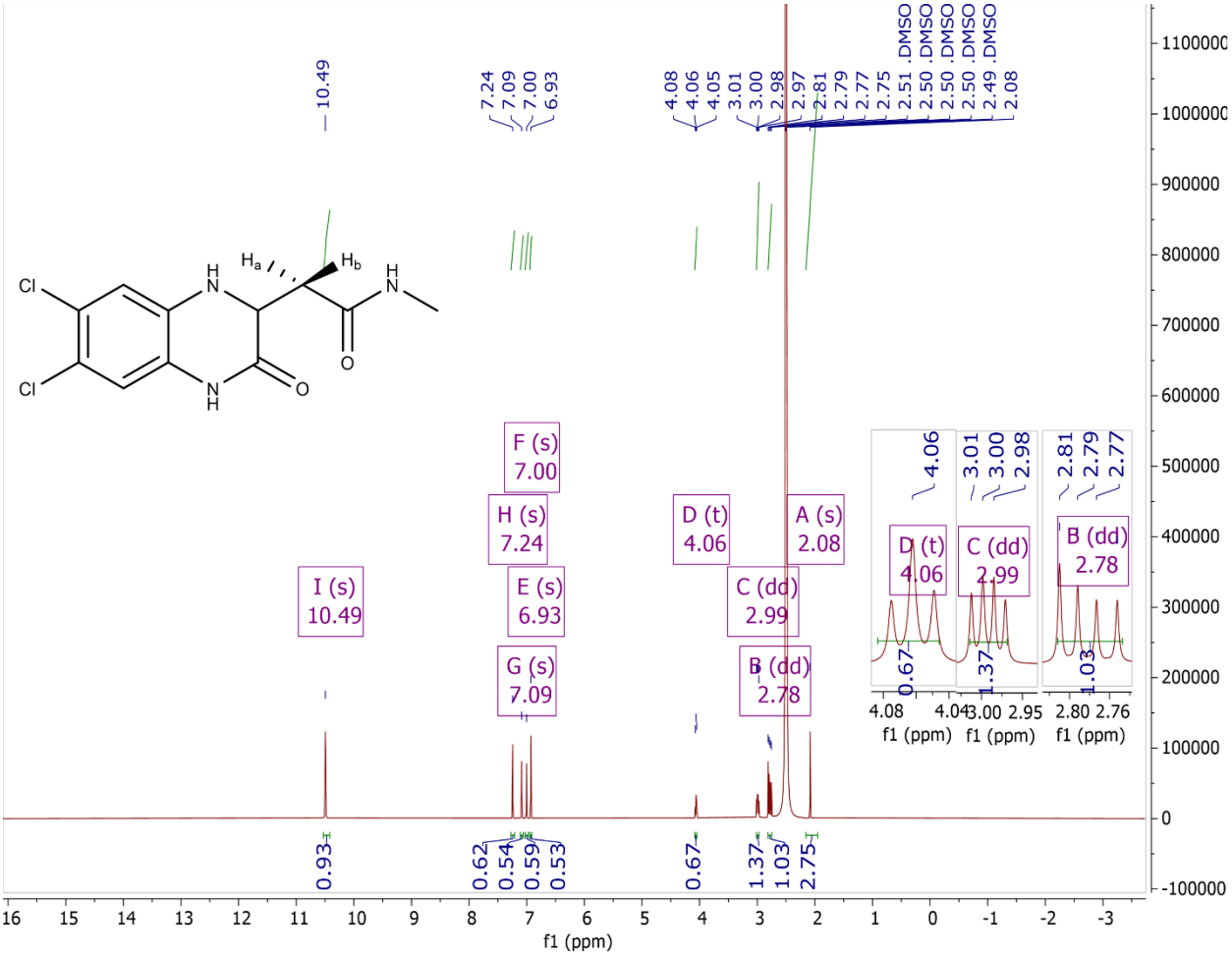
Compound (1e):



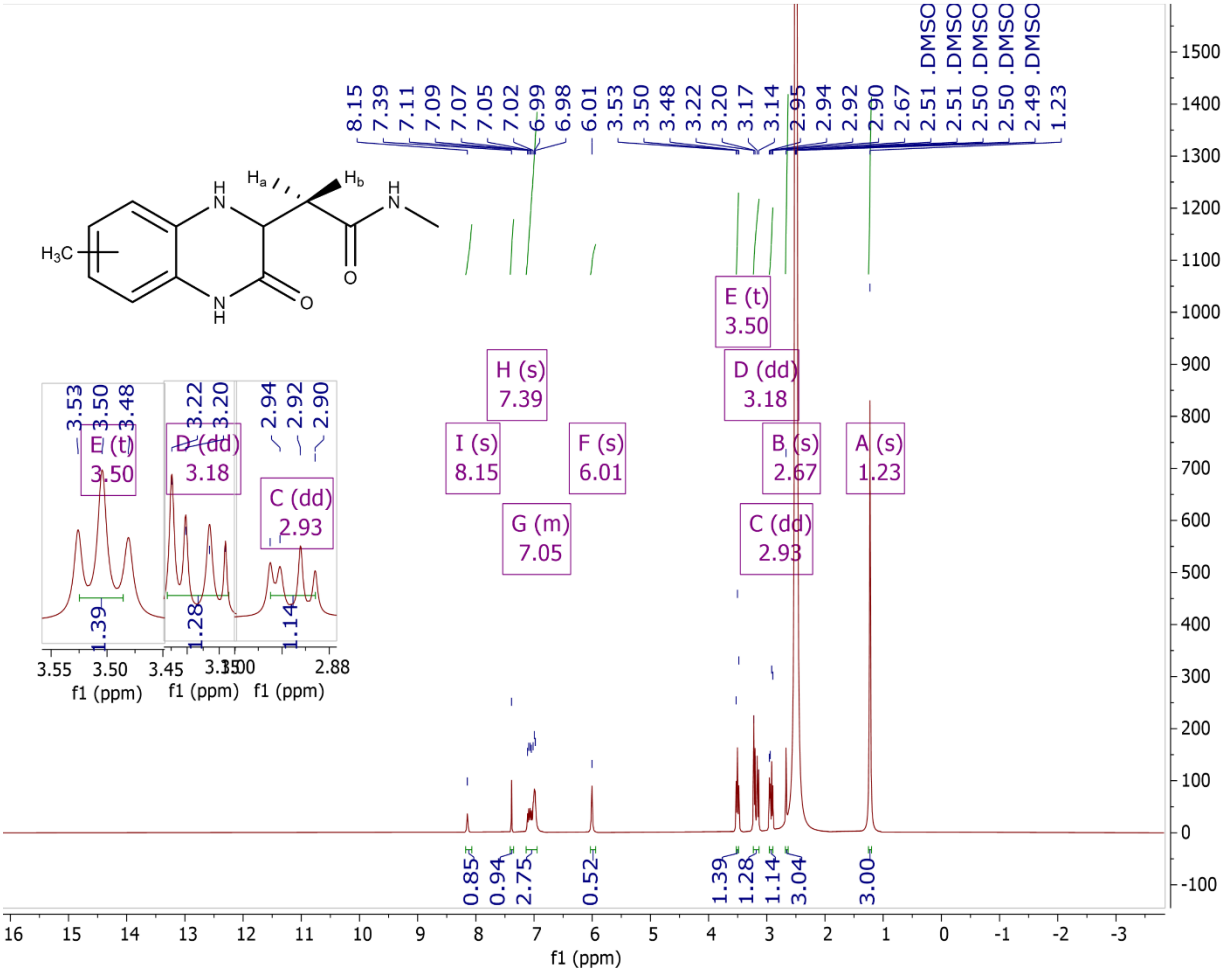
^{1}H NMR (400 MHz, DMSO-*d*$_6$ δ ppm): 8.43 (s, 1H, NHC=O), 7.58 (s, 1H, CH_{arom}), 7.18 (d, *J*= 2.6 Hz, 1H, CH_{arom}), 7.00 (s, 1H, $NHCH_3$), 6.72 (d, *J*= 8.5 Hz, 1H, CH_{arom}), 6.31 (s, 1H, NH), 4.33 (t, *J*= 5.0 Hz, 1H, CH_{ethyl}), 2.86 (s, 3H, CH_3), 2.72 (dd, *J*= 9.4, 4.9 Hz, 1H, H_aCH_b), 2.31 (dd, *J*= 9.4, 4.9 Hz, 1H, H_aCH_b).

Compound (1f): *2-(6,7-dichloro-3-oxo-1,2,3,4-tetrahydroquinoxalin-2-yl)-N-methylacetamide*



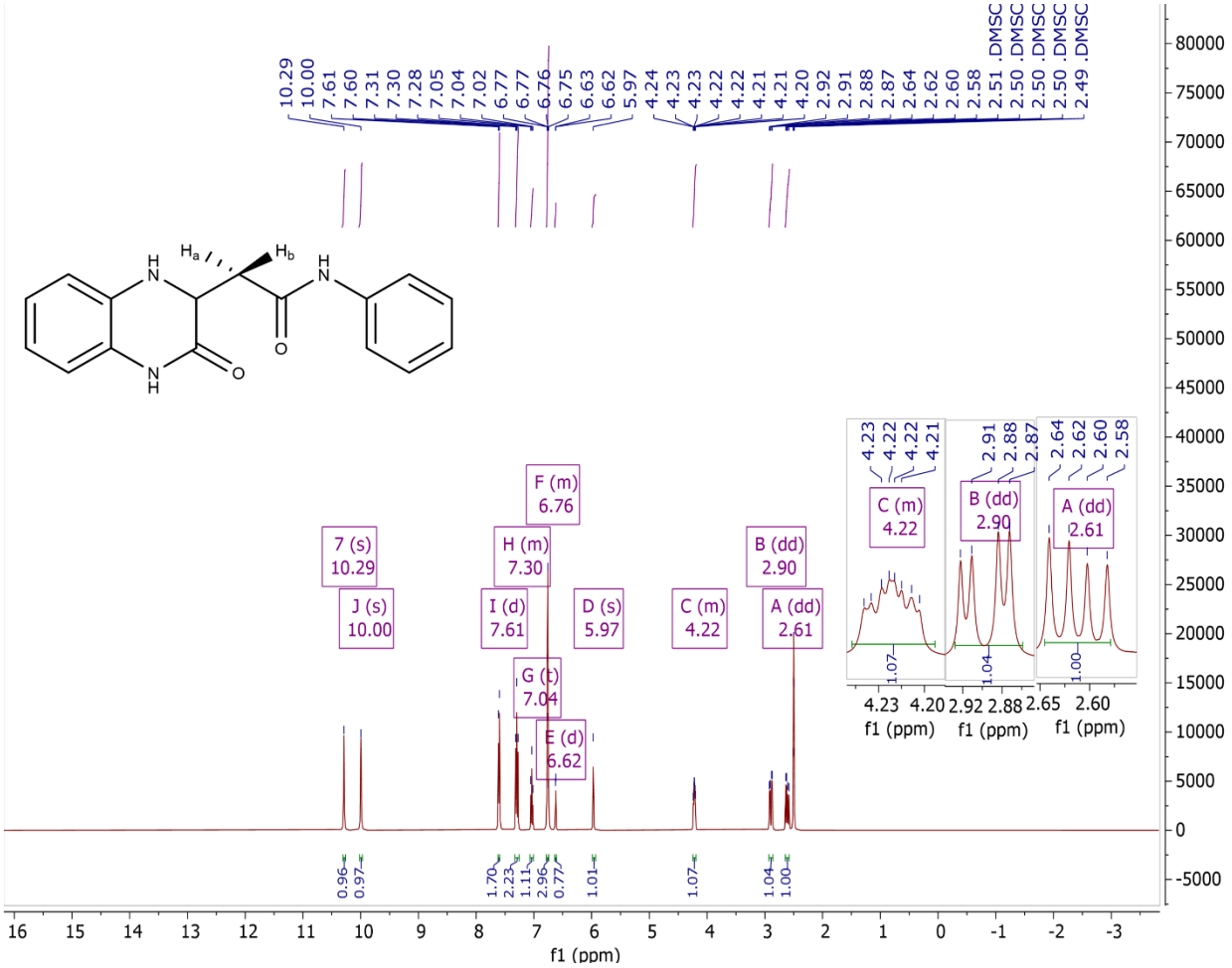
^{1}H NMR (600 MHz, DMSO-*d*$_6$, δ ppm): 10.49 (s, 1H, NHC=O), 7.24 (s, 1H, CH_{arom}), 7.09 (s, 1H, $NHCH_3$), 7.00 (s, 1H, CH_{arom}), 6.93 (s, 1H, NH), 4.06 (t, J = 5.0 Hz, 1H, CH_{ethyl}), 2.99 (dd, J = 9.5, 4.8 Hz, 1H, H_aCH_b), 2.78 (dd, J = 9.5, 4.8 Hz, 1H, H_aCH_b), 2.08 (s, 3H, CH_3).

Compound (1g):

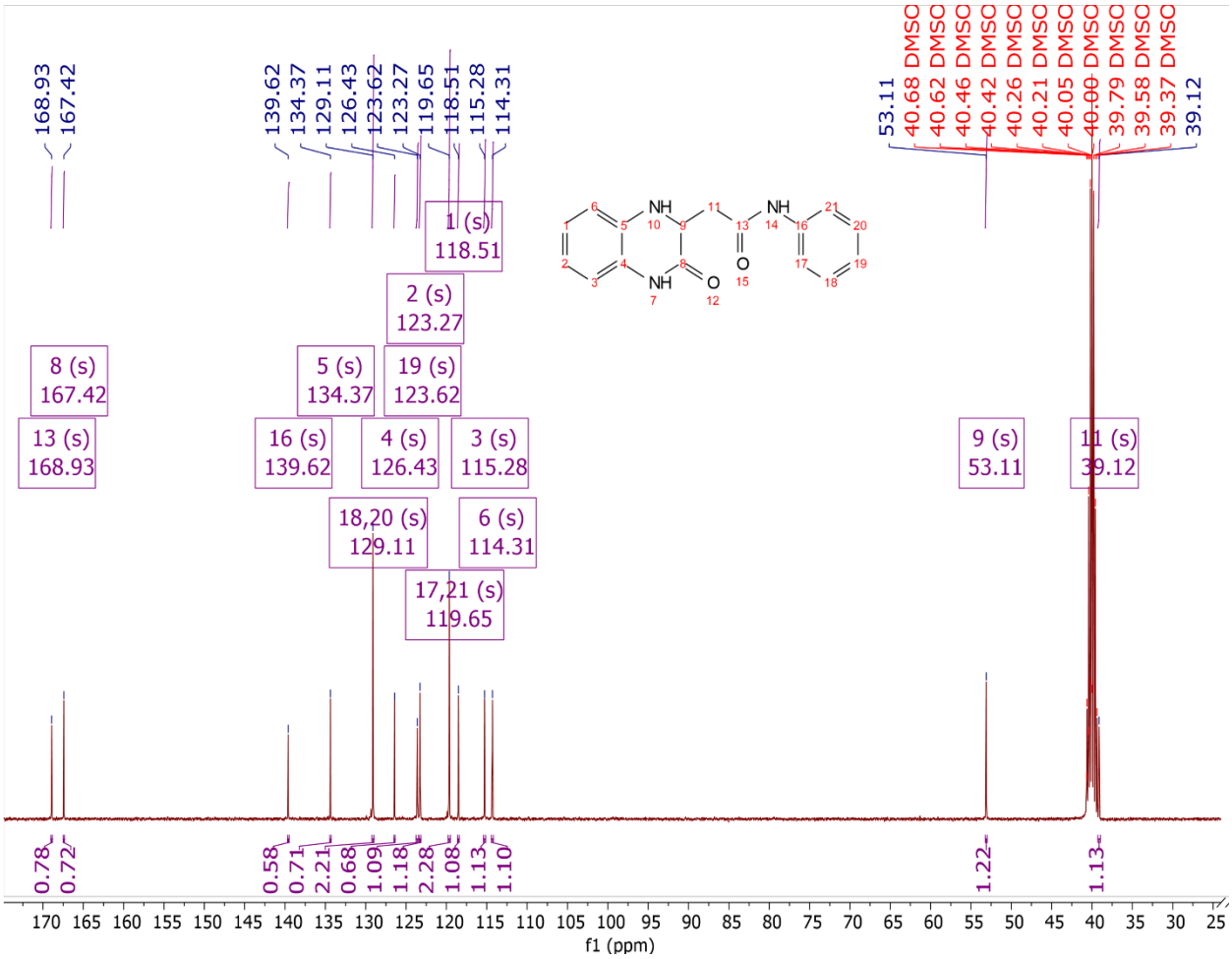


^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.15 (s, 1H, NHC=O), 7.39 (s, 1H, **NH**CH_3), 7.13 – 6.94 (m, 3H, CH_{arom}), 6.01 (s, 1H, NH), 3.50 (t, J = 5.0 Hz, 1H, CH_{ethyl}), 3.18 (dd, J = 9.6, 4.5 Hz, 1H, H_aCH_b), 2.93 (dd, J = 9.6, 4.5 Hz, 1H, H_aCH_b), 2.67 (s, 3H, NH**CH_3**), 1.23 (s, 3H, CH_3).

Compound (1h): *2-(3-oxo-1,2,3,4-tetrahydroquinoxalin-2-yl)-N-phenylacetamide*

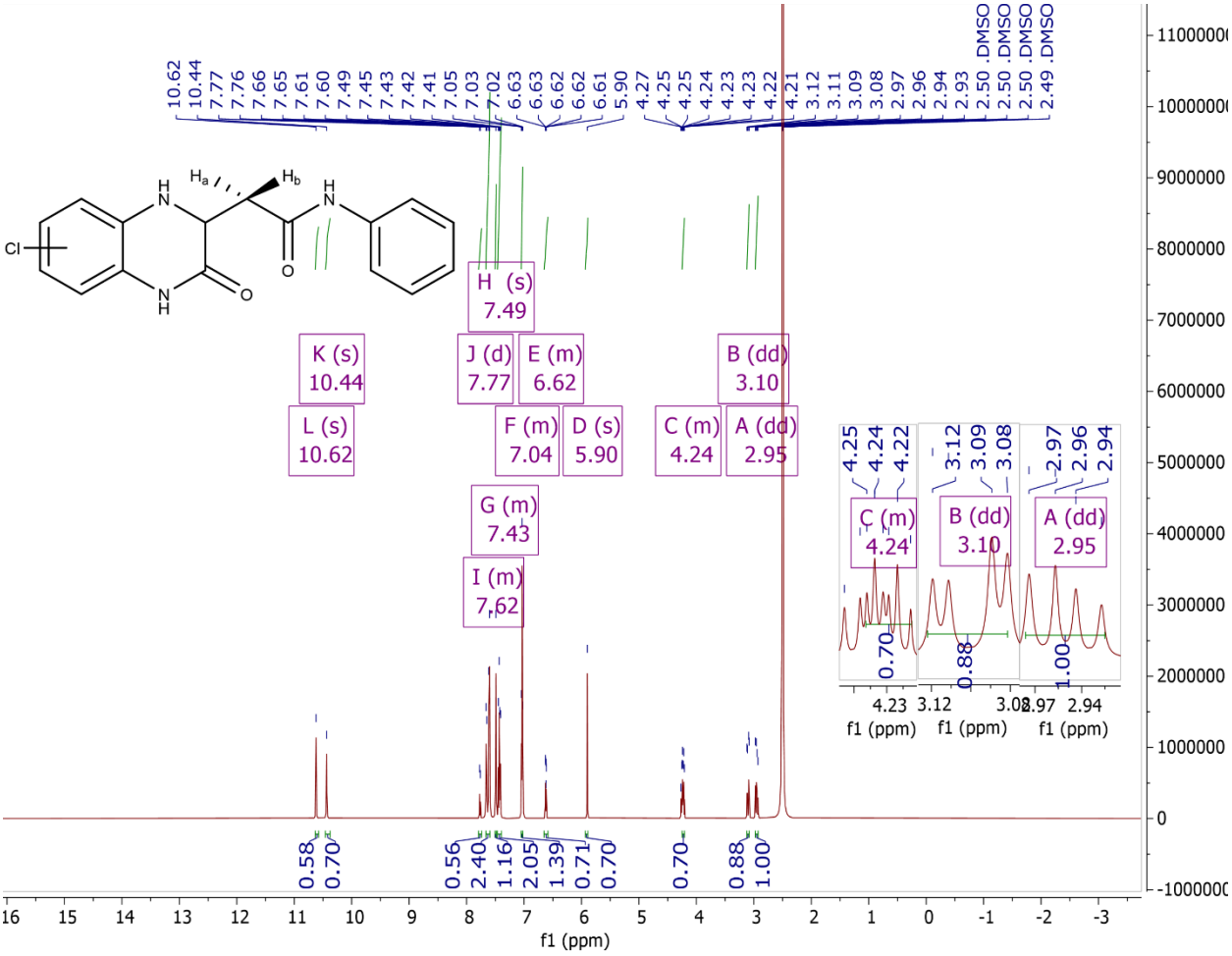


^{1}H NMR (400 MHz, DMSO-d_6, δ ppm):10.29 (s, 1H, NHC=O), 10.00 (s, 1H, NHPh), 7.61 (d, J = 7.3 Hz, 2H, CH_{arom}), 7.32 – 7.27 (m, 2H, CH_{arom}), 7.04 (t, J = 7.4 Hz, 1H, CH_{arom}), 6.78 – 6.74 (m, 3H, CH_{arom}), 6.62 (d, J = 2.6 Hz, 1H, CH_{arom}), 5.97 (s, 1H, NH), 4.25 – 4.19 (m, 1H, CH_{ethyl}), 2.90 (dd, J = 15.4, 4.6 Hz, 1H, H_aCH_b), 2.61 (dd, J = 15.4, 8.0 Hz, 1H, H_aCH_b).



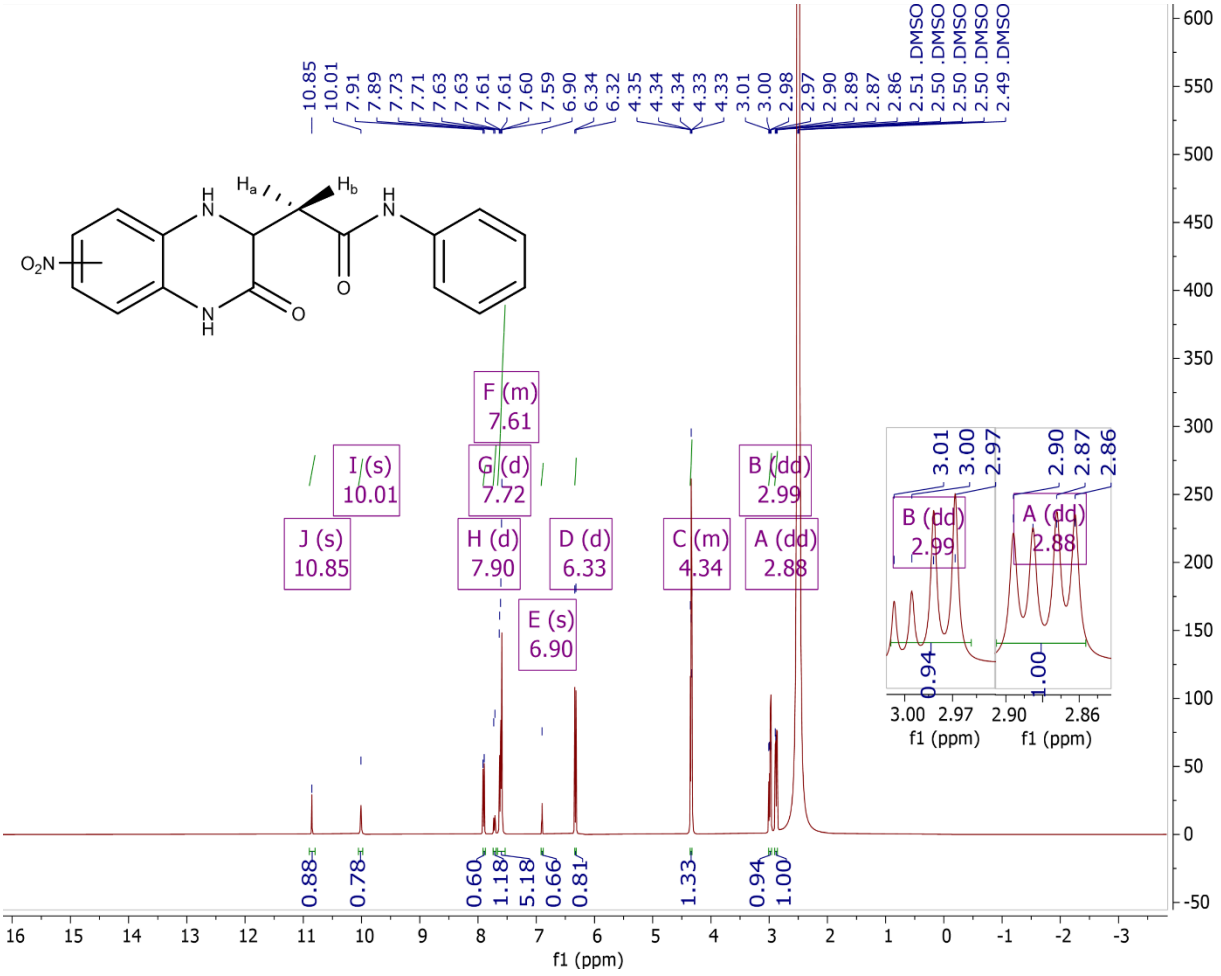
^{13}C NMR (101 MHz, DMSO-*d*$_6$, δ ppm): 168.93 (C=O), 167.42 (C=O), 139.62 (C$_{arom}$), 134.37 (C$_{arom}$), 129.11 (CH$_{arom}$), 126.43 (C$_{arom}$), 123.62 (CH$_{arom}$), 123.27 (CH$_{arom}$), 119.65 (CH$_{arom}$), 118.51 (CH$_{arom}$), 115.28 (CH$_{arom}$), 114.31 (CH$_{arom}$), 53.11 (CH$_{ethyl}$), 39.12 (CH$_2$).

Compound (1i):



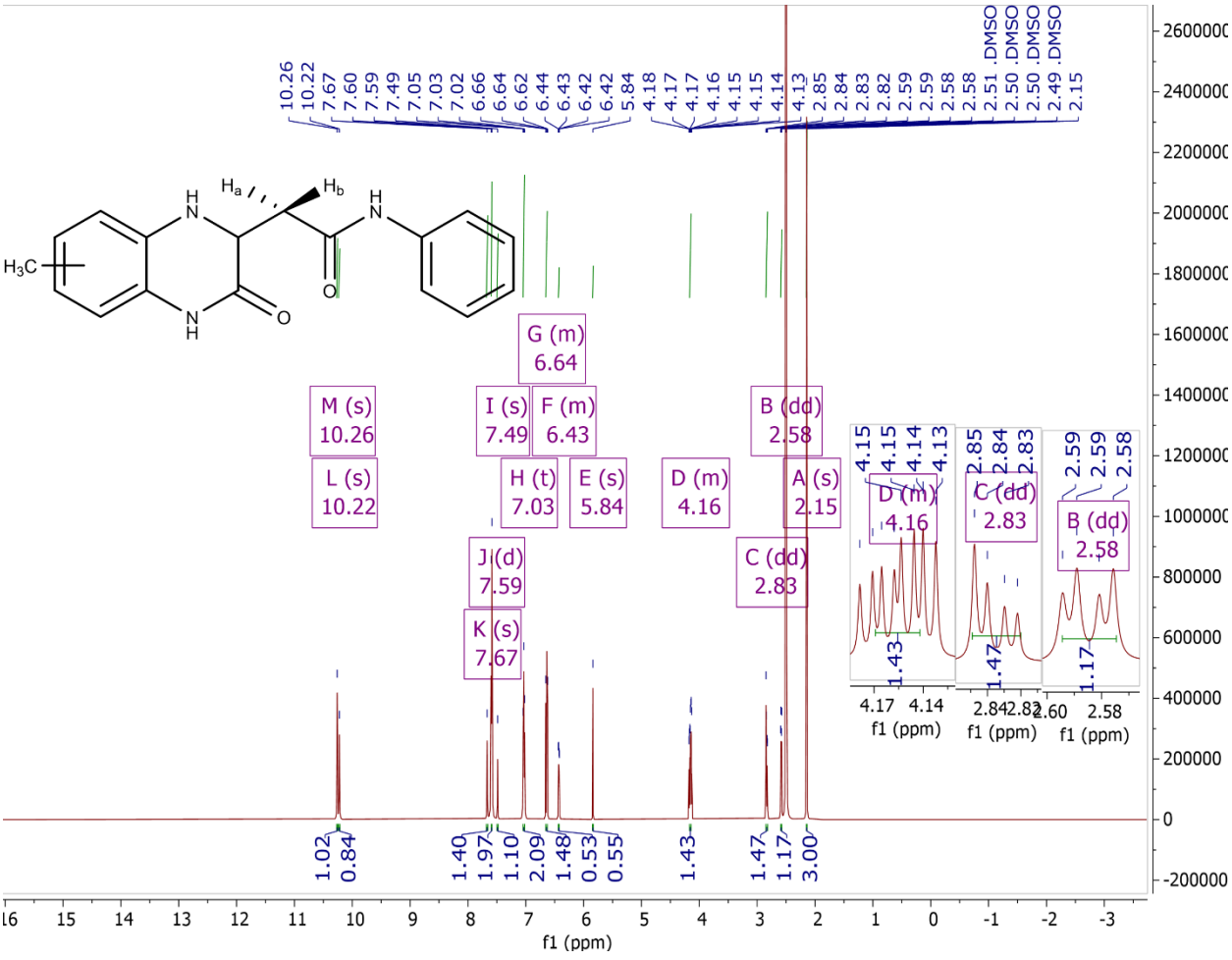
^{1}H NMR (600 MHz, DMSO-*d*$_6$, δ ppm): 10.62 (s, 1H, NHC=O), 10.44 (s, 1H, **NH**Ph), 7.77 (d, *J* = 8.4 Hz, 1H, CH$_{arom}$), 7.67 – 7.60 (m, 2H, CH$_{arom}$), 7.49 (s, 1H, NH), 7.46 – 7.38 (m, 2H, CH$_{arom}$), 7.09 – 6.99 (m, 1H, CH$_{arom}$), 6.66 – 6.58 (m, 1H, CH$_{arom}$), 5.90 (s, 1H, CH$_{arom}$), 4.27 – 4.20 (m, 1H, CH$_{ethyl}$), 3.10 (dd, *J* = 15.7, 4.0 Hz, 1H, **H$_a$**CH$_b$), 2.95 (dd, *J* = 15.7, 8.4 Hz, 1H, H$_a$**CH$_b$**).

Compound (1j):



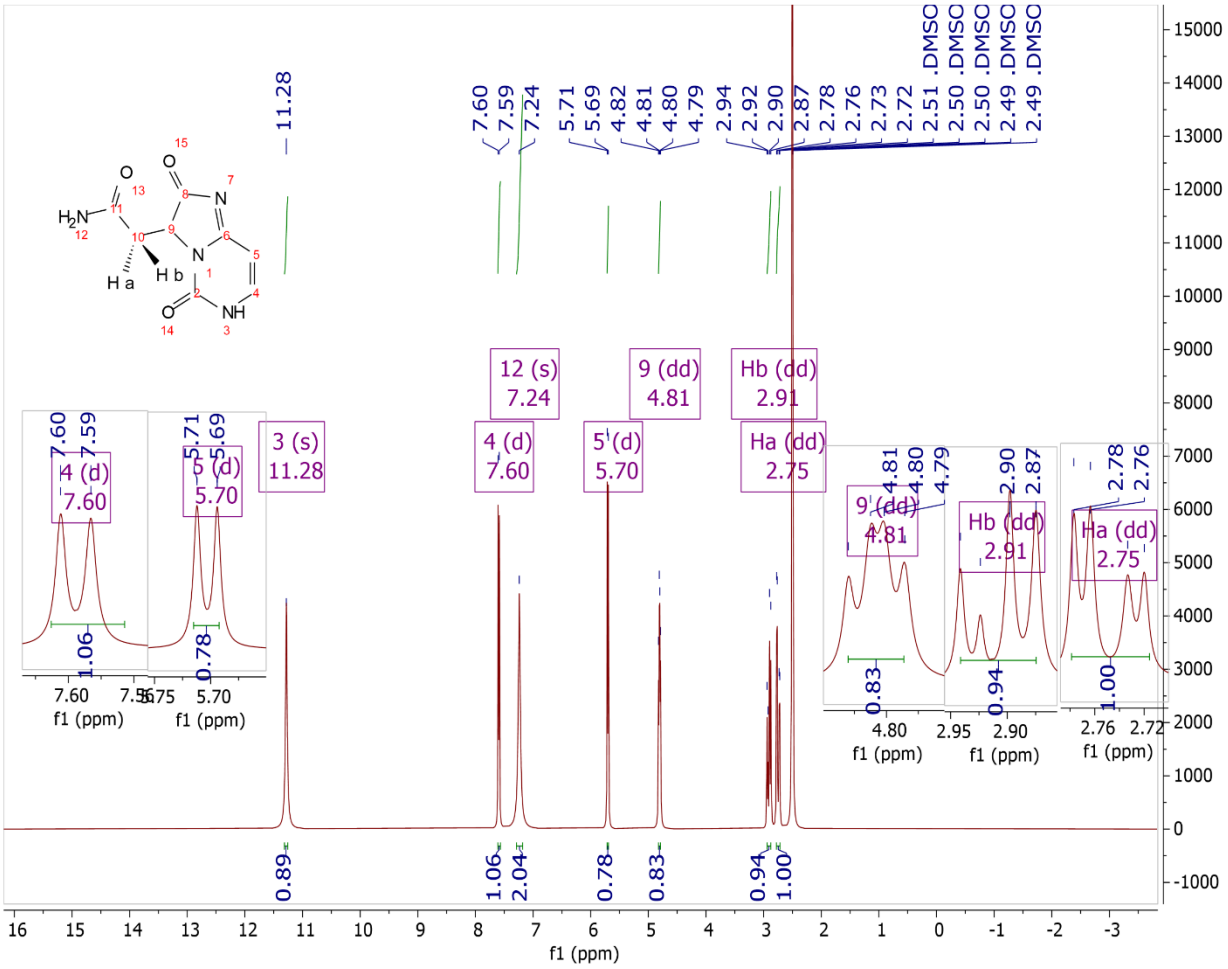
^{1}H NMR (400 MHz, DMSO-*d*$_6$, δ ppm): 10.85 (s, 1H, NHC=O), 10.01 (s, 1H, **NH**Ph), 7.90 (d, *J* = 7.8 Hz, 1H, CH$_{arom}$), 7.72 (d, *J* = 8.7 Hz, 1H, CH$_{arom}$), 7.66 – 7.57 (m, 5H, CH$_{arom}$), 6.90 (s, 1H, NH), 6.33 (d, *J* = 8.4 Hz, 1H, CH$_{arom}$), 4.37 – 4.25 (m, 1H, CH$_{ethyl}$), 2.99 (dd, *J* = 15.3, 4.9 Hz, 1H, **H$_a$C**H$_b$), 2.88 (dd, *J* = 15.3, 8.1 Hz, 1H, H$_a$**CH$_b$**).

Compound (1k):

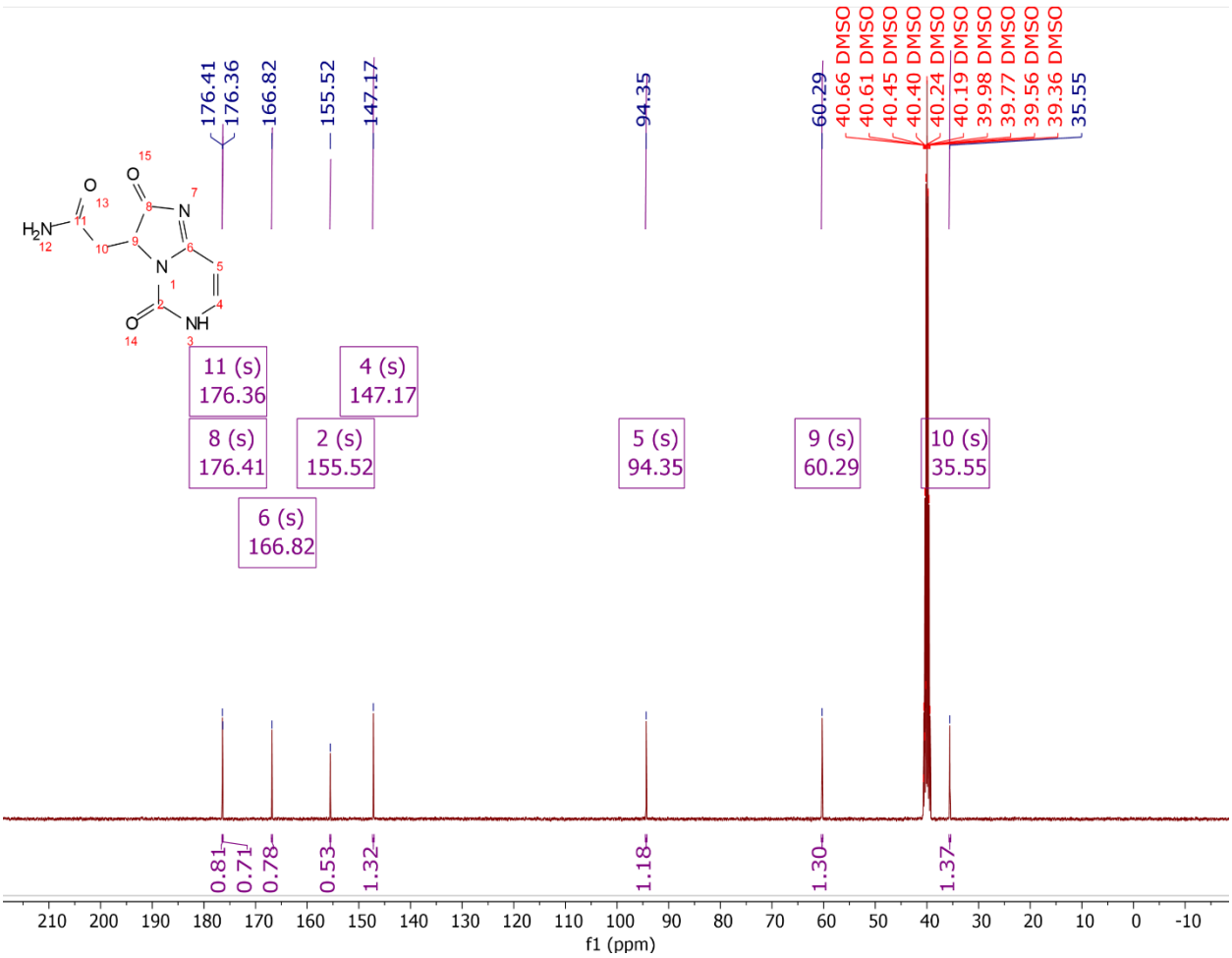


^{1}H NMR (600 MHz, DMSO-*d*$_6$, δ ppm): 10.26 (s, 1H, NHC=O), 10.22 (s, 1H, NHPh), 7.67 (s, 1H, CH_{arom}), 7.59 (d, J = 8.0 Hz, 2H, CH_{arom}), 7.49 (s, 1H, NH), 7.03 (t, J = 7.6 Hz, 2H, CH_{arom}), 6.68 – 6.58 (m, 1H, CH_{arom}), 6.45 – 6.41 (m, 1H, CH_{arom}), 5.84 (s, 1H, CH_{arom}), 4.18 – 4.13 (m, 1H, CH_{ethyl}), 2.83 (dd, J = 15.3, 4.1 Hz, 1H, H_aCH_b), 2.58 (dd, J = 15.3, 8.6 Hz, 1H, H_aCH_b), 2.15 (s, 3H, CH_3).

Compound (2a): *2-(2,5-dioxo-2,3,5,6-tetrahydroimidazo[1,2-c]pyrimidin-3-yl)acetamide*

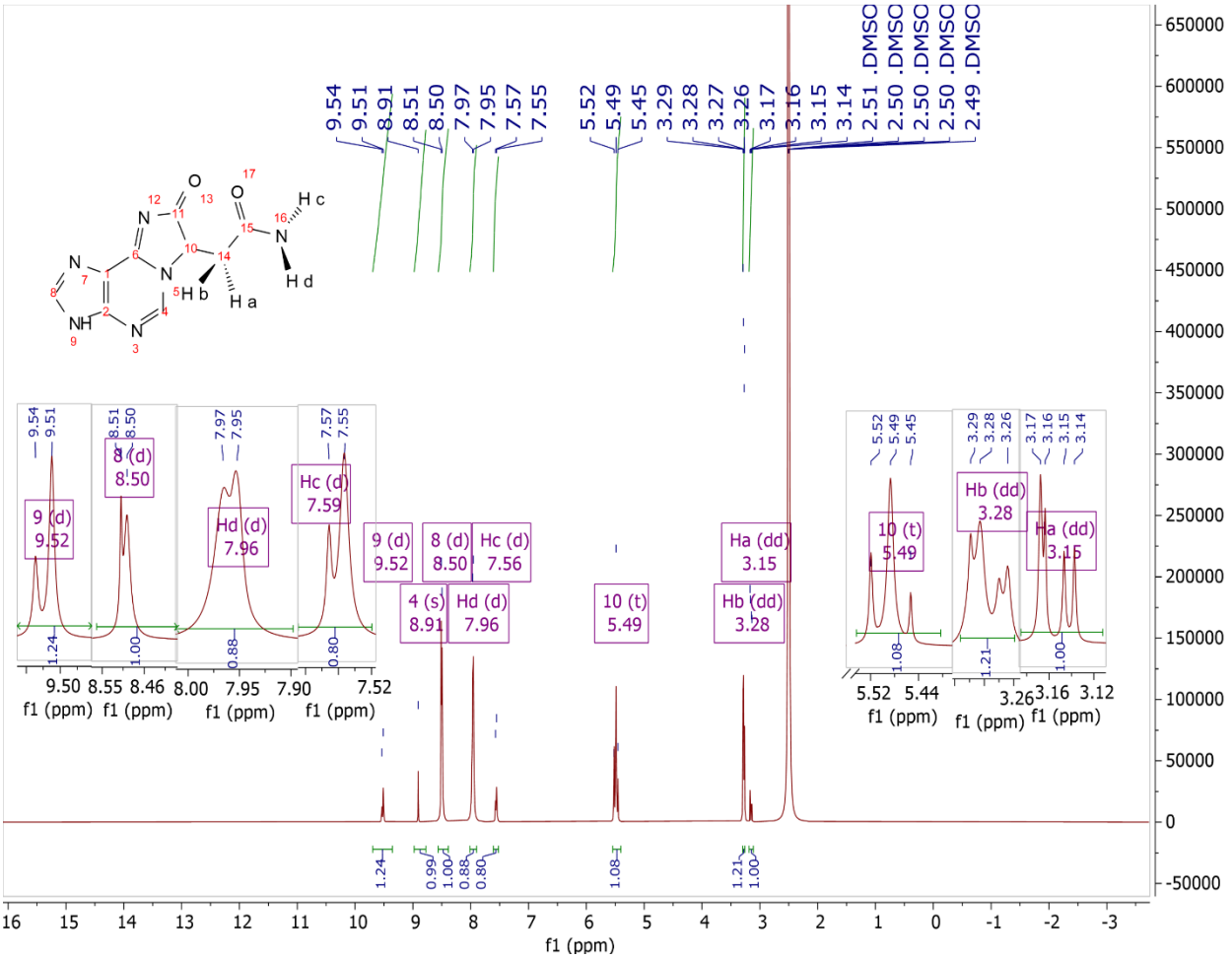


^{1}H NMR (400 MHz, DMSO-*d*$_6$, δ ppm): 11.28 (s, 1H, **NH**), 7.60 (d, *J* = 7.3 Hz, 1H, NH**CH**$_{pyrimidine}$), 7.24 (s, 2H, **NH$_2$**), 5.70 (d, *J* = 7.2 Hz, 1H, **CH**$_{pyrimidine}$), 4.81 (dd, *J* = 8.7, 5.4 Hz, 1H, **CH**$_{imidazole}$), 2.91 (dd, *J* = 17.6, 8.1 Hz, 1H, **H$_a$**CH$_b$), 2.75 (dd, *J* = 17.6, 5.4 Hz, 1H. H$_a$**CH$_b$**).



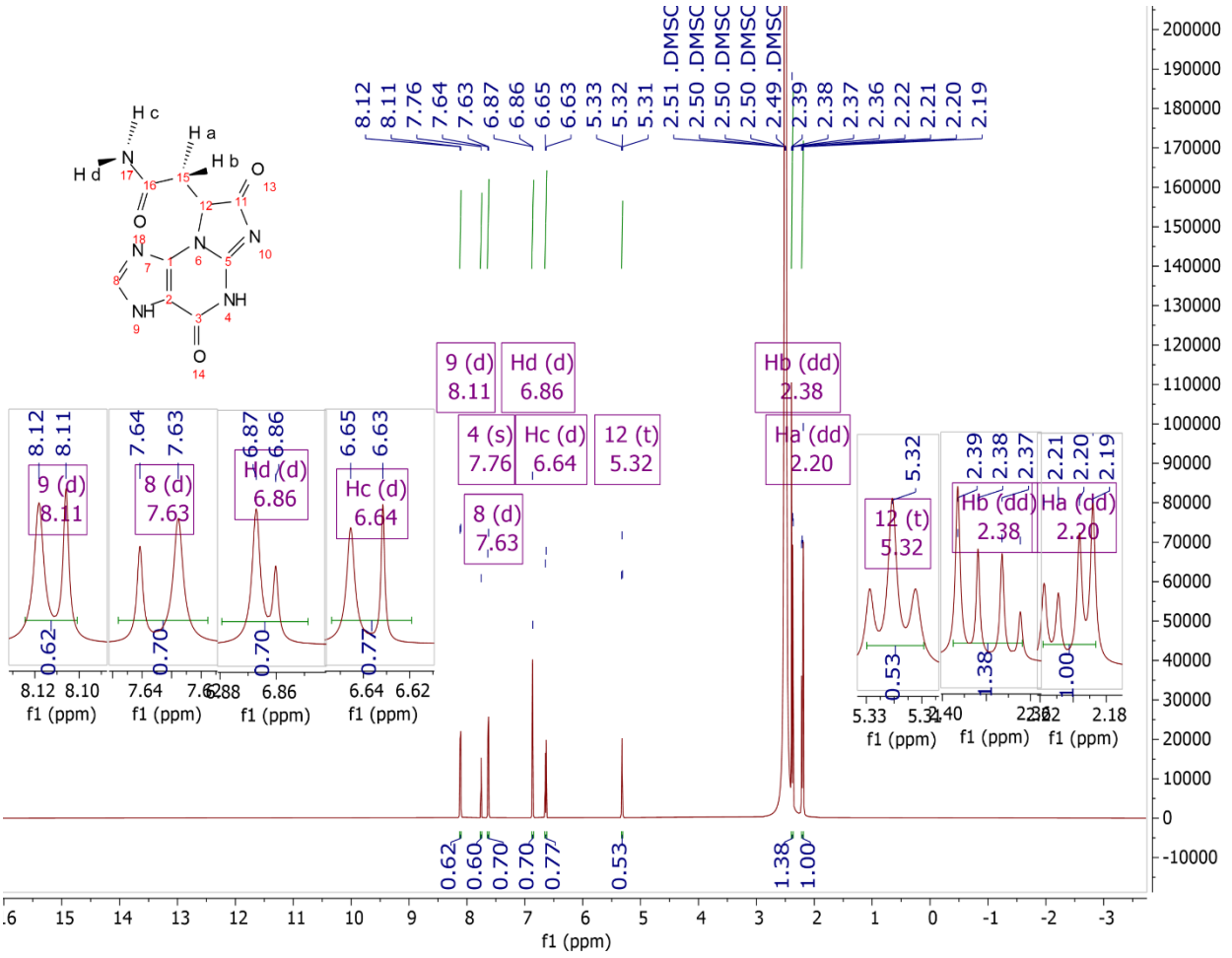
^{13}C NMR (101 MHz, DMSO-d_6, δ ppm): 176.41 (C=O), 176.36 (C=O), 166.82 (C=N), 155.52 (C=O), 147.17 ($CH_{pyrimidine}$), 94.35 ($CH_{pyrimidine}$), 60.29 (CH_{ethyl}), 35.55 (CH_2).

Compound (3a): *2-(7,8-dihydro-8-oxo-3H-imidazo[2,1-i]purin-7-yl)acetamide*



^{1}H NMR (600 MHz, DMSO-*d*$_6$, δ ppm): 9.52 (d, *J* = 14.4 Hz, 1H, **NH**), 8.91 (s, 1H, NH**CH**$_{purine}$), 8.50 (d, *J* = 7.7 Hz, 1H, **CH**$_{purine}$), 7.96 (d, *J* = 5.1 Hz, 1H, **H**$_c$**N**H$_d$), 7.56 (d, *J* = 5.2 Hz, 1H, H$_c$**NH**$_d$), 5.49 (t, *J* = 7.8 Hz, 1H, **CH**$_{imidazole}$), 3.28 (dd, *J* = 14.8, 7.8 Hz, 1H, **H**$_a$**C**H$_b$), 3.15 (dd, *J* = 14.7, 7.8 Hz, 1H, H$_a$**CH**$_b$).

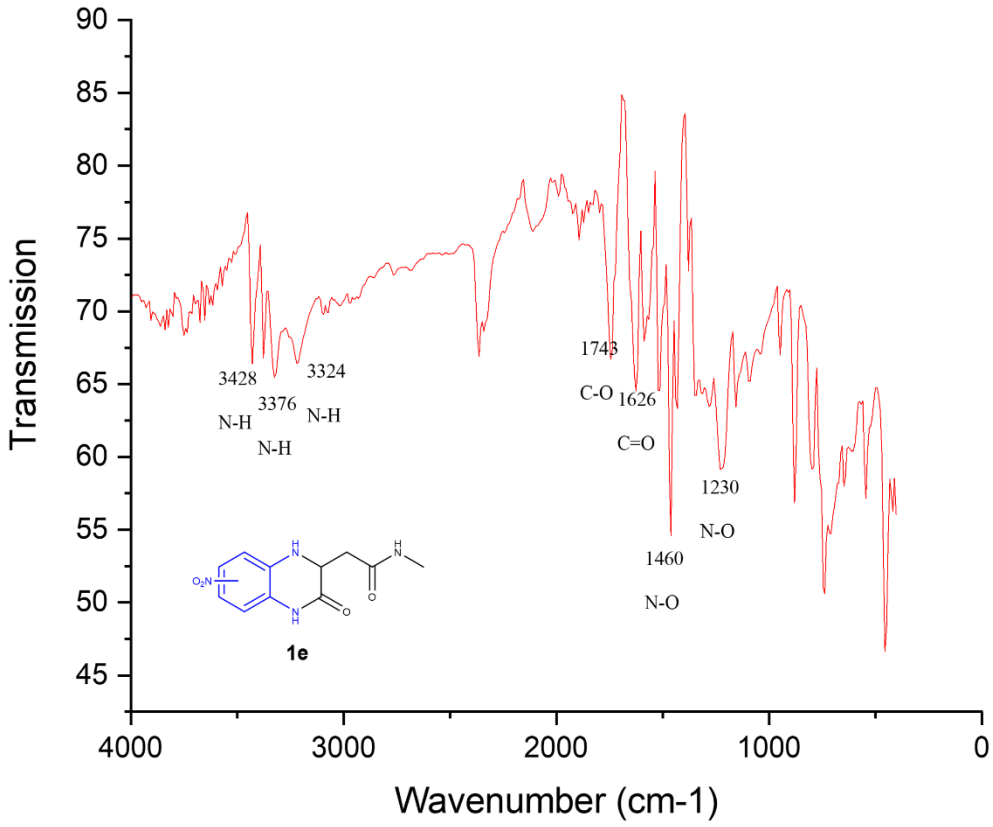
Compound (4a): *2-(4,5,7,8-tetrahydro-4,7-dioxo-3H-imidazo[2,1-b]purin-8-yl)acetamide*



^{1}H NMR (600 MHz, DMSO-d_6, δ ppm): 8.11 (d, J = 7.3 Hz, 1H, **NH**$_{purine}$), 7.76 (s, 1H, **NH**$_{purine}$), 7.63 (d, J = 7.8 Hz, 1H, **CH**$_{purine}$), 6.86 (d, J = 4.2 Hz, 1H, **H**$_c$**N**H$_d$), 6.64 (d, J = 8.4 Hz, 1H, H$_c$**NH**$_d$), 5.32 (t, J = 5.0 Hz, 1H, **CH**$_{imidazole}$), 2.38 (dd, J = 12.8, 5.0 Hz, 1H, **H**$_a$**C**H$_b$), 2.20 (dd, J = 12.7, 5.0 Hz, 1H, H$_a$**CH**$_b$).

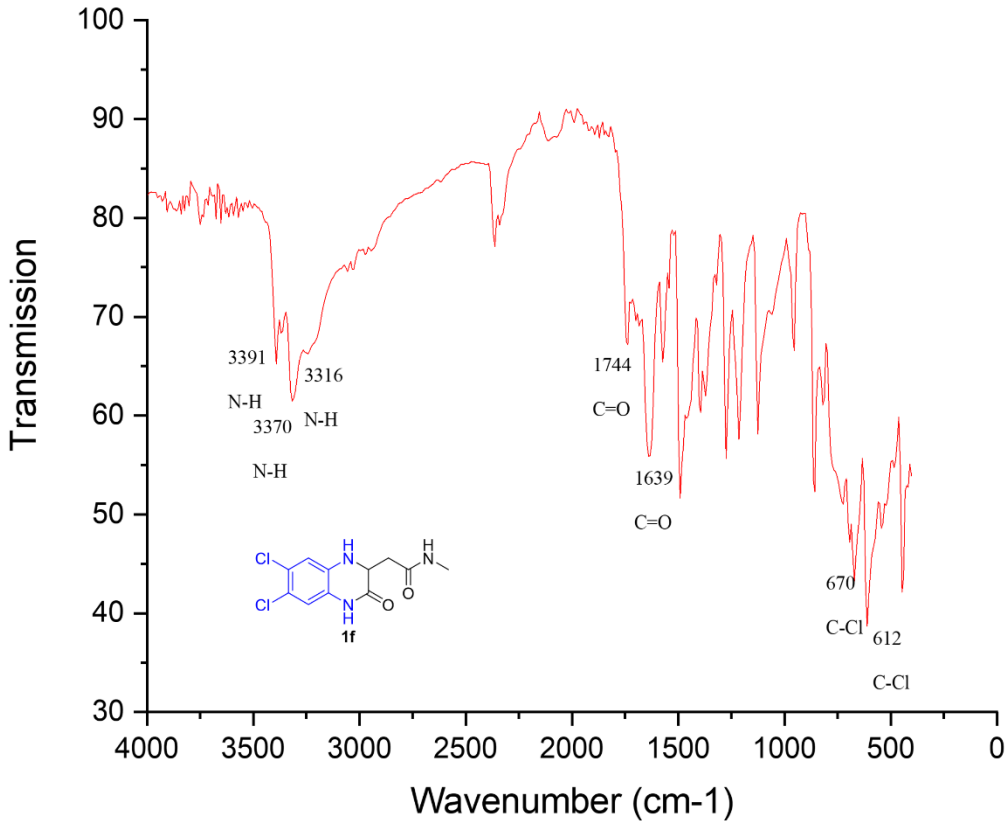
FT-IR spectra

Compound (1e)



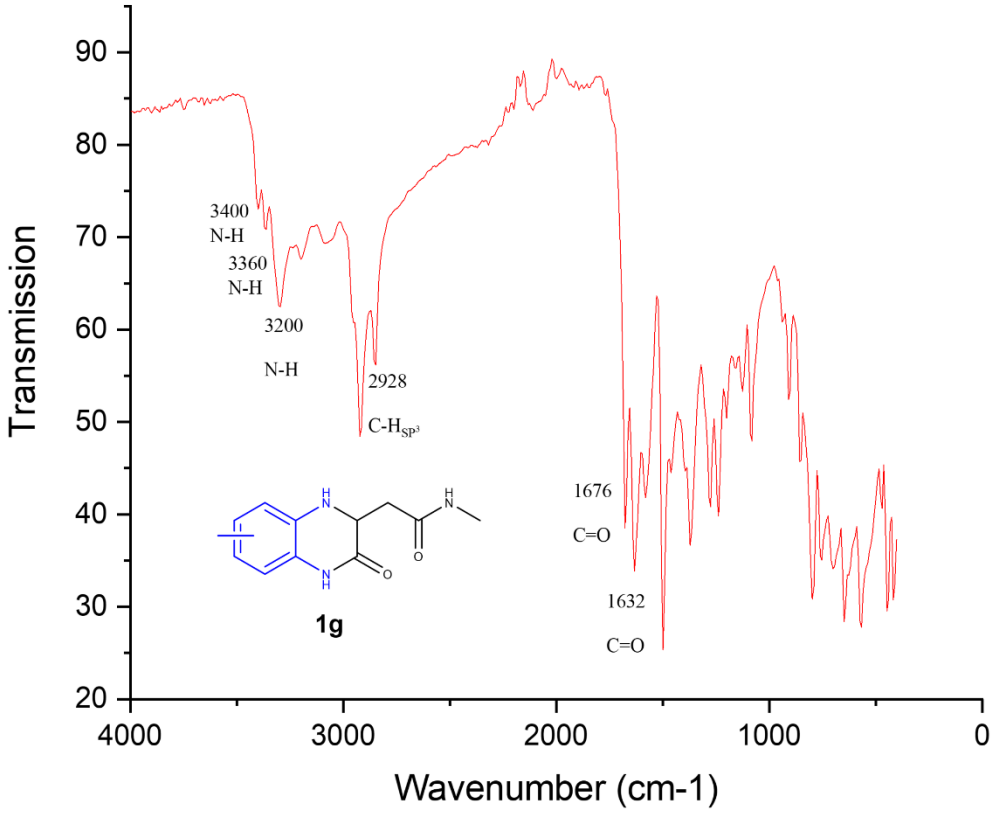
FT-IR (KBr, ῡ cm^{-1}): 3428(NHC=O), 3376($NHCH_3$), 3324(NH), 1743 (C=O), 1626 (C=O), 1460 (N-O) 1230 (N-O).

Compound (1f)



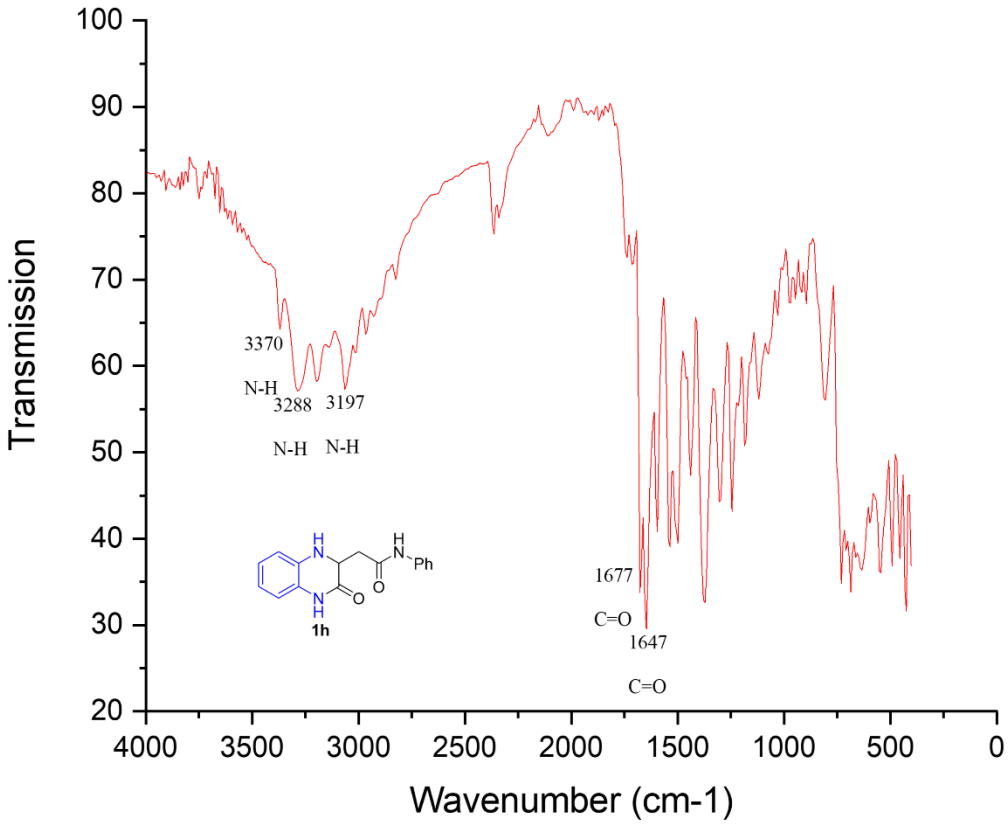
FT-IR (KBr, ῡ cm^{-1}): 3391(NHC=O), 3370($NHCH_3$), 3316(NH), 1744 (C=O), 1639 (C=O), 670 (C-Cl), 612 (C-Cl).

Compound (1g)



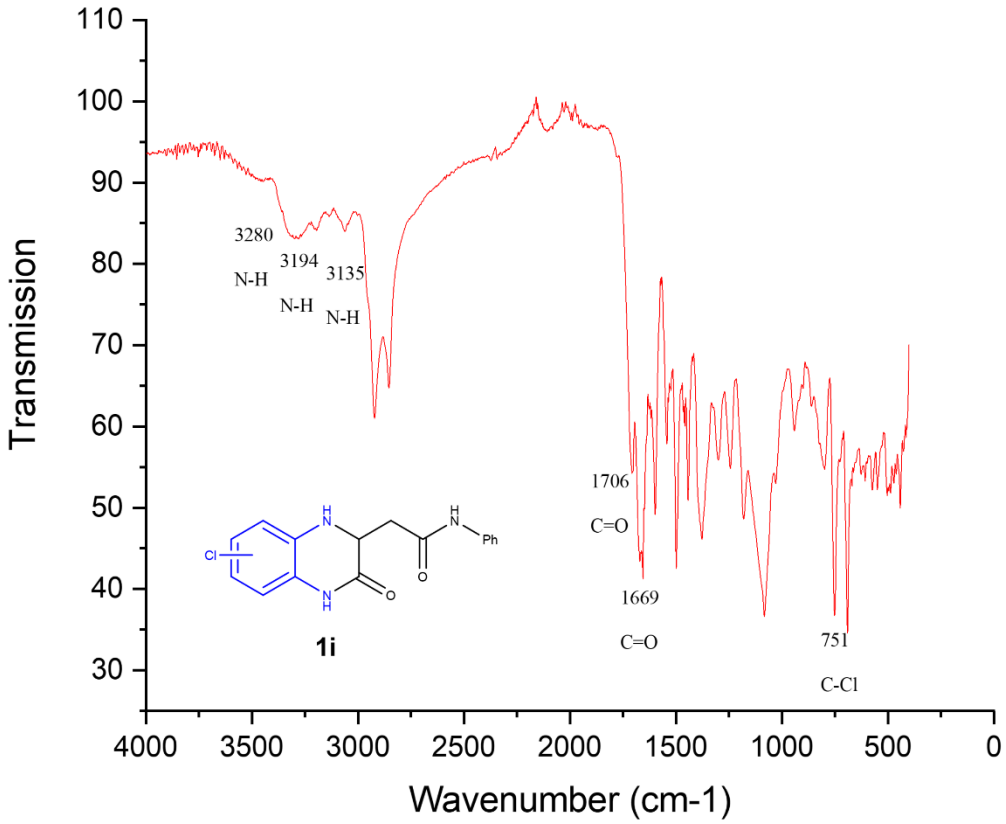
FT-IR (KBr, ῡ cm^{-1}): 3400(NHC=O), 3360(NHCH$_3$), 3200(NH), 2928 (C-H$_{SP}^3$), 1676 (C=O), 1632 (C=O).

Compound (1h)



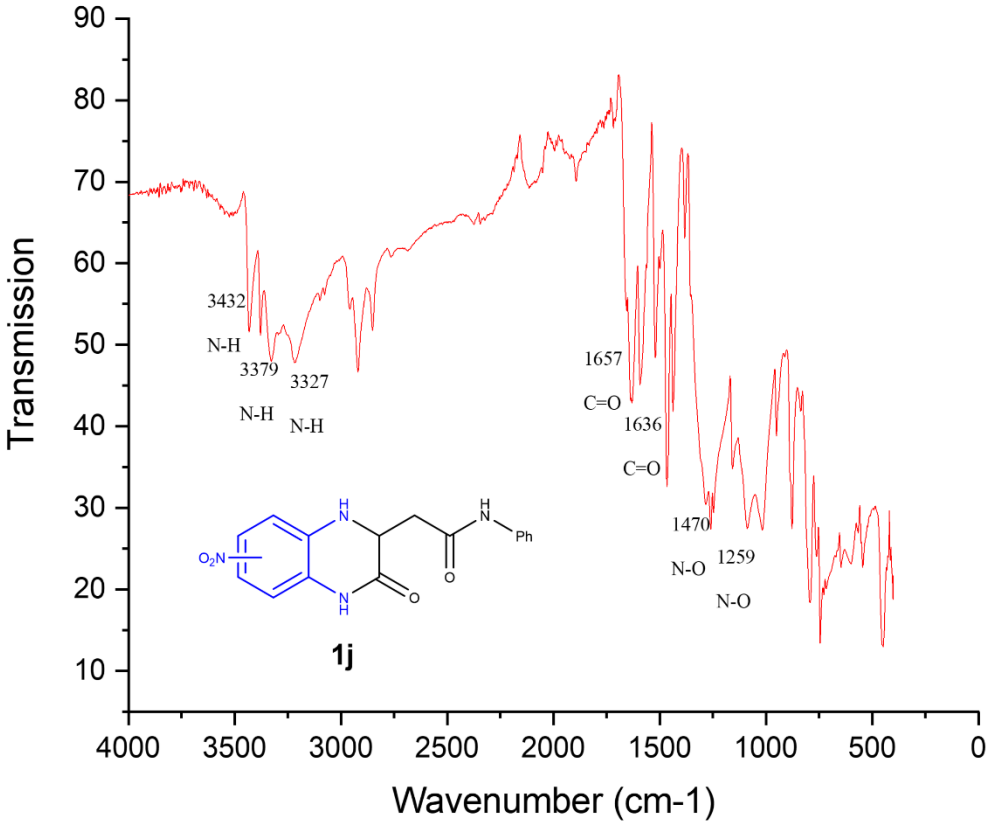
FT-IR (KBr, ῡ cm^{-1}): 3370(NHPh), 3288(NHC=O), 3197 (NH), 1677 (C=O), 1647 (C=O).

Compound (1i)



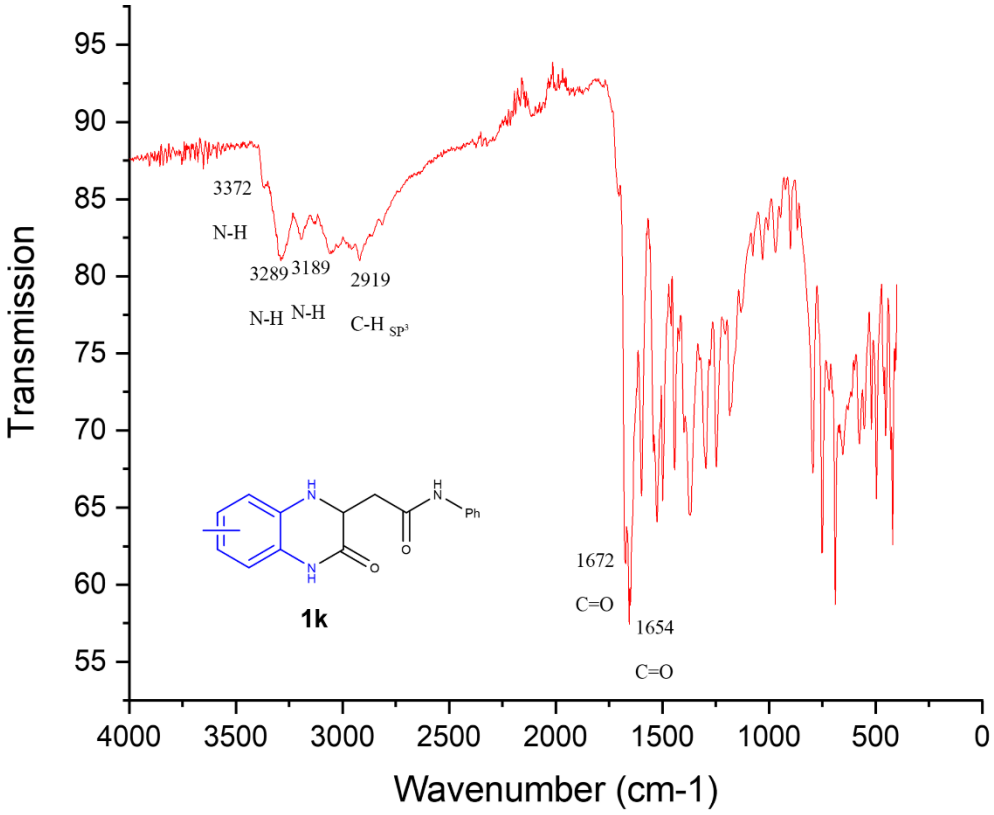
FT-IR (KBr, ῡ cm^{-1}): 3280(NHPh), 3194(NHC=O), 3135(NH), 1706(C=O), 1669(C=O), 751(C-Cl).

Compound (1j)



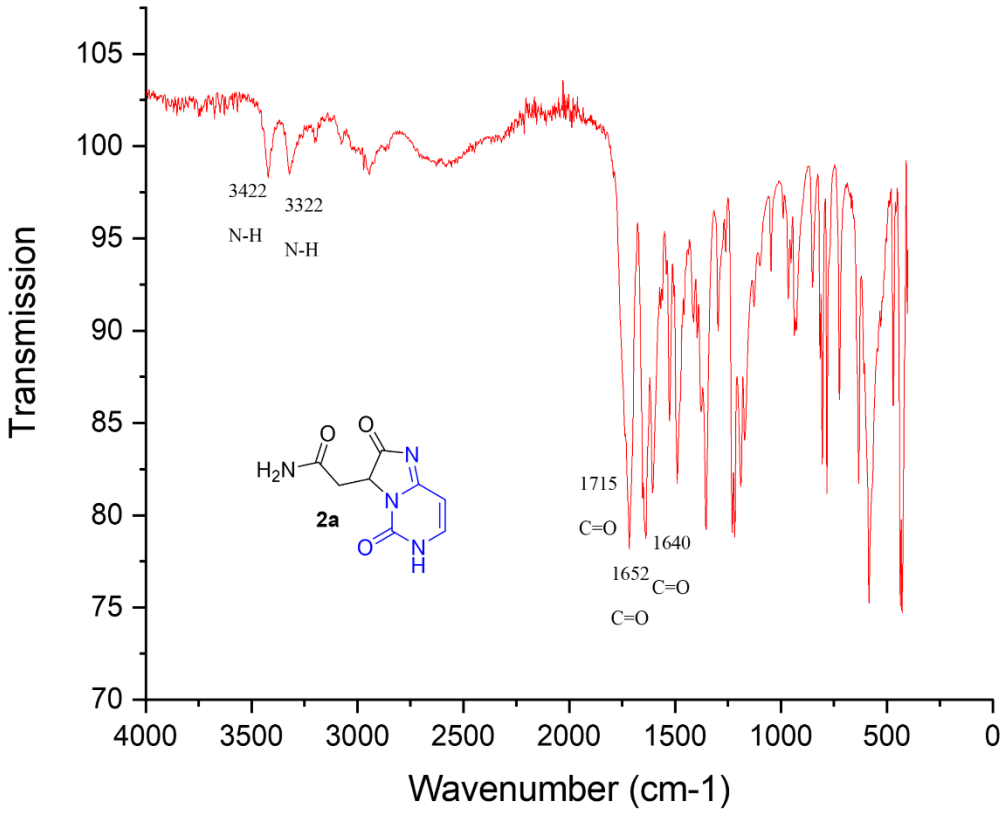
FT-IR (KBr, ῡ cm^{-1}): 3432(NHPh), 3379(NHC=O), 3327(NH), 1657 (C=O), 1636 (C=O), 1470 (N-O), 1259 (N-O).

Compound (1k)



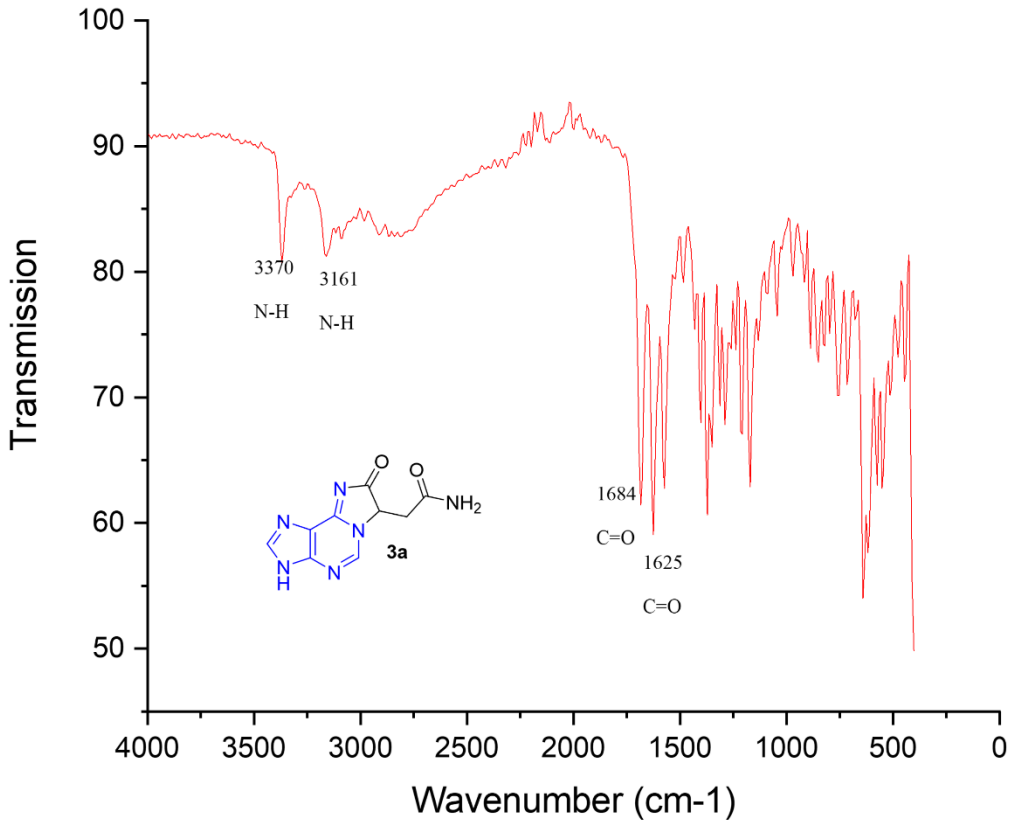
FT-IR (KBr, ῡ cm^{-1}): 3372(NHPh), 3289(NHC=O), 3189(NH), 2919(C-H_{SP^3}), 1672(C=O), 1654(C=O).

Compound (2a)



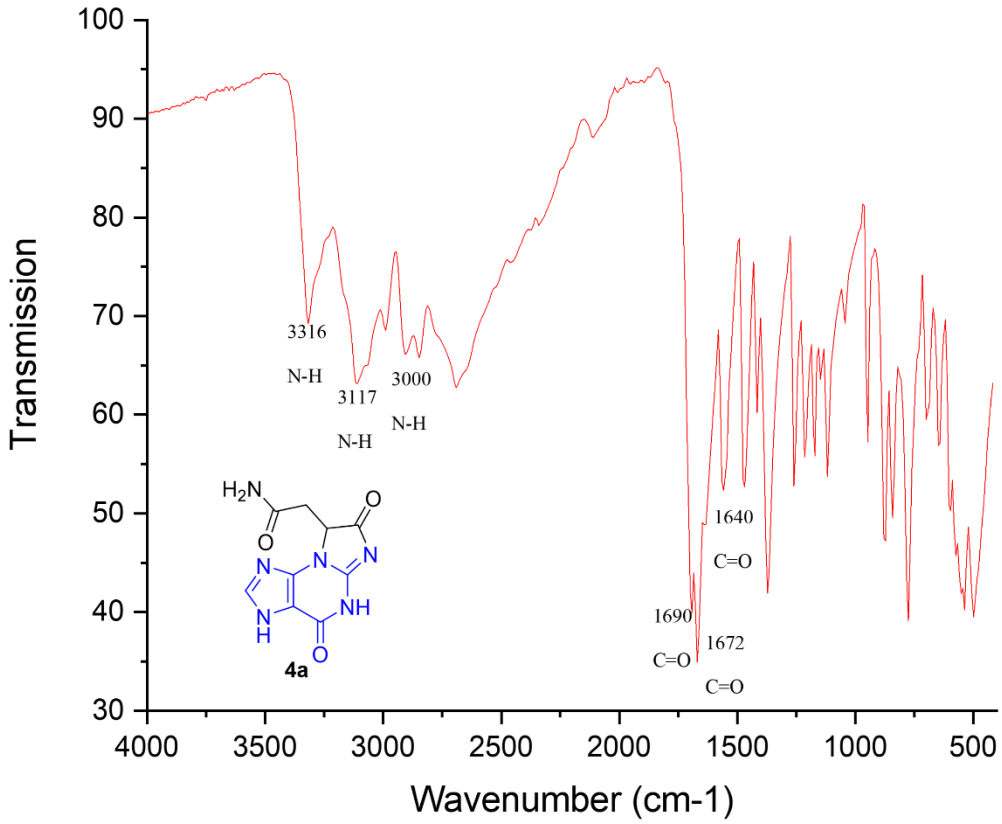
FT-IR (KBr, ῡ cm^{-1}): 3422$(NH_2)_{amide}$, 3322$(NH)_{amide}$, 1715$(C=O)_{amide}$, 1652$(C=O)_{amide}$, 1640$(C=O)_{amide}$.

Compound (3a)



FT-IR (KBr, ῡ cm^{-1}): 3370$(NH_2)_{amide}$, 3161$(NH)_{amine}$, 1685$(C=O)_{amide}$, 1625(C=O).

Compound (4a)



FT-IR (KBr, ῡ cm^{-1}): 3316$(NH)_{amide}$, 3117$(NH_2)_{amide}$, 3000 $(NH)_{amine}$,1690$(C=O)_{amide}$, 1672$(C=O)_{amide}$, 1640$(C=O)_{amide}$.