Supporting Information

A convenient 'NOSE' approach for the synthesis of 6-Amino-1,3-dimethyl-5-indolyl-1*H*-pyrimidine-2,4-dione derivatives catalyzed by nano-Ag

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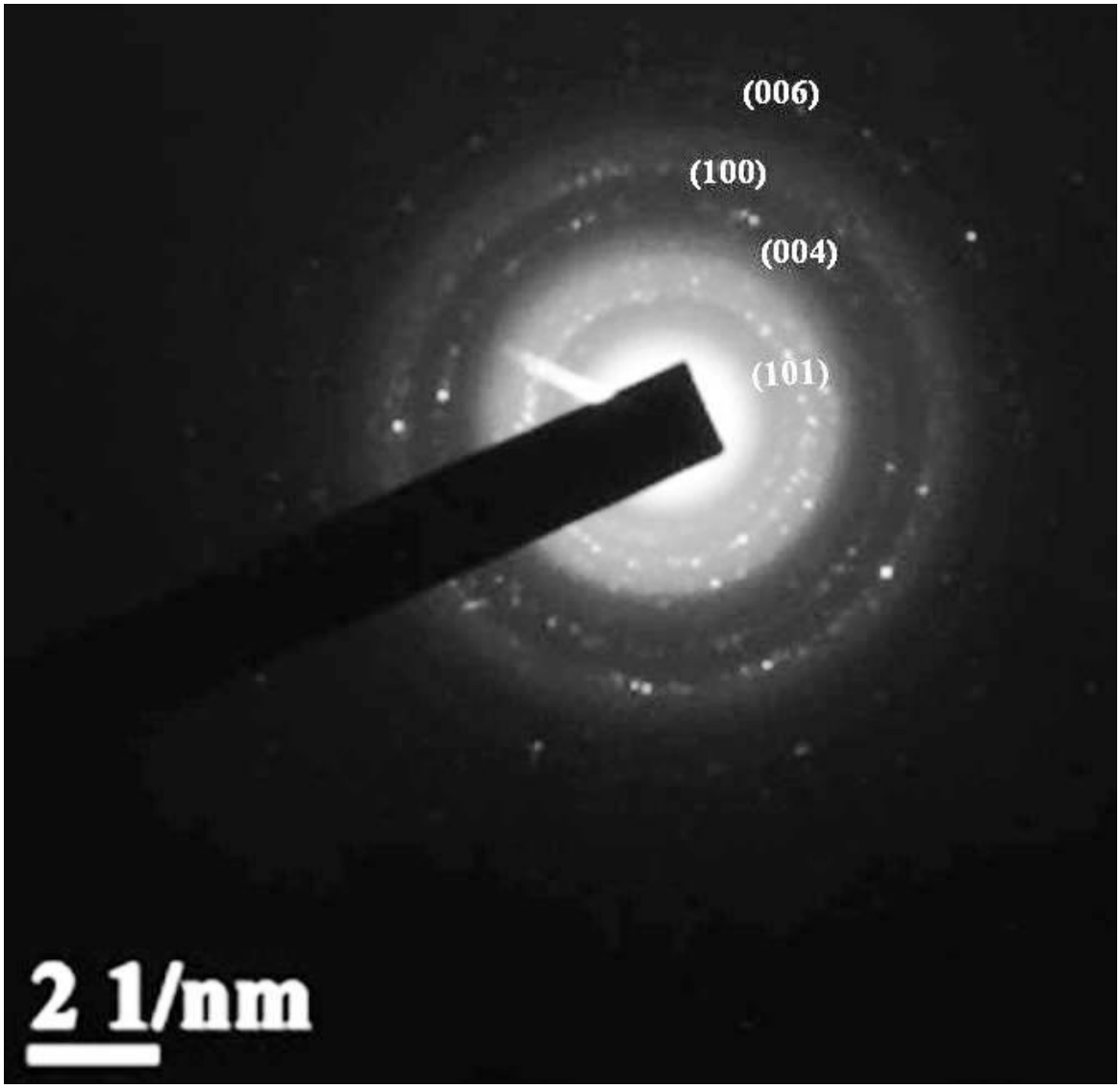
1. General experimental methods

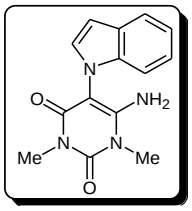
The chemicals and reagents were purchased from Sigma-Aldrich, Merck, M/S S. D. Fine Chemicals Pvt. Ltd. and Loba chemical, and used without further purification. Transmission electron microscopy was performed by (TEM) [CM12, PHILIPS] with energy dispersive spectroscopy (EDS) [OXFORD] and sample preparation facility. The surface morphology and EDX were studied using JEOL scanning electron microscope (model JSM-6390LV SEM). The XRD pattern was recorded with Rigaku X-ray diffractometer. Melting points were determined in a Büchi 504 apparatus. IR spectra were recorded as KBr pallets in a Nicolet (Impact 410) FT-IR spectrophotometer. ^{1}H and ^{13}C NMR spectra were recorded in a 400 MHz NMR spectrophotometer (JEOL, JNM ECS) using tetramethylsilane (TMS) as the internal standard and coupling constants are expressed in Hertz. Elemental analyses were carried out in a Perkin–Elmer CHN analyser (2400 series II). Mass spectra were recorded with a Waters Q-TOF Premier and Aquity UPLC spectrometer. Visualization was accomplished with UV lamp or I_2 stain. Reactions were monitored by thin-layer chromatography using aluminium sheets with silica gel 60 F_{254} (Merck).

2. **Figure S1**: SAED pattern of nano-Ag



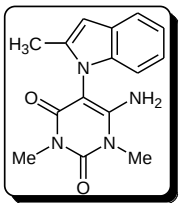
3. Physical and spectroscopic data for all the compounds

6-Amino-5-indol-1-yl-1,3-dimethyl-1*H*-pyrimidine-2,4-dione (Table 2, entry 1)



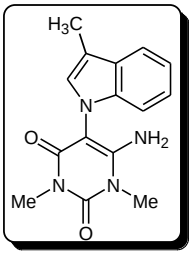
White solid; R_f = 0.44 (30% AcOEt:hexane); mp 98.3-101.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$ TMS): δ 7.63-7.07 (m, 5H, Ar-H), 6.52 (d, *J* = 1.2 Hz, 1H, Ar-H), 6.32 (br, 2H, NH_2), 2.97 (s, 3H, N-CH_3), 2.77 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 164.5, 161.0, 152.1, 141.1, 135.7, 127.7, 124.1, 121.9, 120.6, 119.7, 110.0, 102.4, 81.4, 28.7, 28.1; m/z (GC-MS) 270.11 [M^+]; Anal. Calcd (%) for $C_{14}H_{14}N_4O_2$: C, 62.21; H, 5.22; N, 20.73. Found C, 62.24., H, 5.27, N, 20.71.

6-Amino-1,3-dimethyl-5-(2-methyl-indol-1-yl)-1*H*-pyrimidine-2,4-dione (Table 2, entry 2)



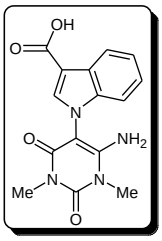
Off white solid; R_f = 0.48 (30% AcOEt:hexane); mp 114.2-118.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$ TMS): δ 7.51 (d, *J* = 8.23 Hz, 1H, Ar-H), 7.16-7.08 (m, 3H, Ar-H), 6.52 (br, 2H, NH_2), 6.13 (s, 1H, Ar-H), 3.18 (s, 3H, N-CH_3), 3.01 (s, 3H, N-CH_3), 2.33 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 162.0, 160.4, 152.2, 142.5, 136.1, 135.3, 129.1, 121.0, 119.7, 116.2, 110.4, 100.4, 81.3, 29.7, 27.5, 13.9; m/z (GC-MS) 284.13 [M^+]; Anal. Calcd (%) for $C_{15}H_{16}N_4O_2$: C, 63.37; H, 5.67; N, 19.71. Found C, 63.40, H, 5.70, N, 19.75.

6-Amino-1,3-dimethyl-5-(3-methyl-indol-1-yl)-1*H*-pyrimidine-2,4-dione (Table 2, entry 3)



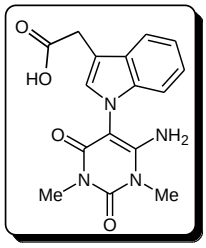
Off white solid; R_f = 0.47 (30% AcOEt:hexane); mp 150.4-153.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$ TMS): δ 7.58-7.13 (m, 4H, Ar-H), 6.96 (s, 1H, Ar-H), 6.54 (br, 2H, NH_2), 2.89 (s, 3H, N-CH_3), 2.70 (s, 3H, N-CH_3), 2.35 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 165.4, 162.1, 152.2, 142.7, 136.1, 135.3, 129.2, 121.2, 119.6, 116.3, 110.3, 100.5, 82.6, 29.8, 27.6, 13.7; m/z (GC-MS) 284.13 [M^+]; Anal. Calcd (%) for $C_{15}H_{16}N_4O_2$: C, 63.37; H, 5.67; N, 19.71. Found C, 63.39, H, 5.69, N, 19.74.

1-(6-Amino-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydro-pyrimidin-5-yl)-1*H*-indole-3-carboxylic acid (Table 2, entry 4)



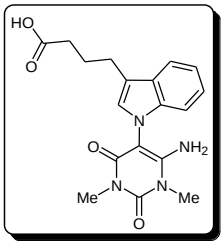
White solid; R_f = 0.41 (30% AcOEt:hexane); mp 222.4-225.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$ TMS): δ 8.12 (br, 1H, OH), 7.41-7.38 (m, 4H, Ar-H), 6.87 (s, 1H, Ar-H), 6.39 (br, 2H, NH_2), 3.41 (s, 3H, N-CH_3), 3.39 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 173.4, 164.6, 161.3, 152.7, 136.4, 123.3, 122.7, 119.3, 118.4, 111.3, 107.7, 82.1, 29.8, 28.6; m/z (GC-MS) 314.10 [M^+]; Anal. Calcd (%) for $C_{14}H_{14}N_4O_2$: C, 57.32; H, 4.49; N, 17.83. Found C, 57.11, H, 4.35, N, 17.54.

[1-(6-Amino-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydro-pyrimidin-5-yl)-1H-indol-3-yl]-acetic acid (Table 2, entry 5)



Pale yellow solid; R_f = 0.39 (30% AcOEt:hexane); mp 210.3-214.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$ TMS): δ 8.07 (br, 1H, OH), 7.34-7.13 (m, 4H, Ar-H), 6.75 (s, 1H, Ar-H), 6.45 (br, 2H, NH_2), 3.80 (s, 2H, CH_2), 3.57 (s, 3H, N-CH_3), 3.33 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 176.3, 164.4, 160.0, 152.3, 136.1, 123.2, 122.4, 119.9, 118.8, 111.2, 107.9, 81.7, 35.8, 29.2, 28.7; m/z (GC-MS) 328.12 [M^+]; Anal. Calcd (%) for $C_{16}H_{16}N_4O_4$: C, 58.53; H, 4.91; N, 17.06. Found C, 58.14, H, 4.55, N, 10.73.

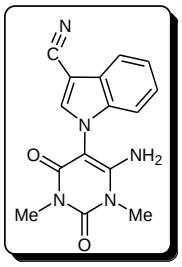
4-[1-(4-Amino-1,3-dimethyl-2,6-dioxo-hexahydro-pyrimidin-5-yl)-1*H*-indol-3-yl]-butyric acid (Table 2, entry 6)



Yellow solid; R_f = 0.37 (30% AcOEt:hexane); mp 186.6-189.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$ TMS): δ 8.09 (br, 1H, OH), 7.60-7.11 (m, 4H, Ar-H), 6.96 (s, 1H, Ar-H), 6.40 (br, 2H, NH_2), 3.18 (s, 3H, N-CH_3), 3.08 (s, 3H, N-CH_3), 2.82 (t, *J* = 7.32 Hz, 2H, CH_2), 2.42 (t, *J* = 7.32 Hz, 2H, CH_2), 2.07-2.03 (m, 2H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 180.0, 165.1, 163.0, 152.9, 136.4, 127.4, 122.0, 121.6, 119.3, 118.9, 115.4, 111.2, 81.8,

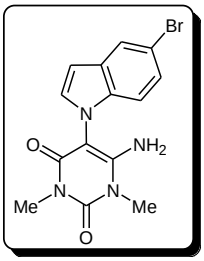
33.6, 29.4, 28.6, 25.1, 24.4; m/z (GC-MS) 328.12 [M^+]; Anal. Calcd (%) for $C_{18}H_{20}N_4O_4$: C, 60.66; H, 5.66; N, 15.72. Found C, 60.32, H, 5.41, N, 15.58.

1-(6-Amino-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydro-pyrimidin-5-yl)-1*H*-indole-3-carbonitrile (Table 2, entry 7)



Brownish yellow viscous oil; R_f = 0.51 (30% AcOEt:hexane); ^{1}H NMR (400 MHz, $CDCl_3$ TMS): δ 7.49 (d, *J* = 7.8 Hz, 1H, Ar-H), 7.24-7.11 (m, H, Ar-H), 6.92 (s, 1H, Ar-H), 6.57 (br, 2H, NH_2), 2.99 (s, 3H, N-CH_3), 2.69 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 164.8, 162.3, 151.0, 136.6, 126.3, 123.5, 123.1, 120.4, 119.1, 118.6, 118.4, 118.0, 112.1, 111.8, 104.4, 84.2, 34.5, 31.1; m/z (GC-MS) 295.11 [M^+]; Anal. Calcd (%) for $C_{15}H_{13}N_5O_2$: C, 61.01; H, 4.44; N, 23.72. Found C, 60.70, H, 4.12, N, 23.41.

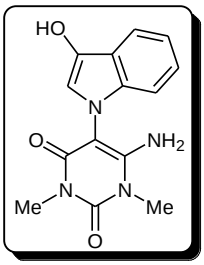
6-Amino-5-(5-bromo-indol-1-yl)-1,3-dimethyl-1*H*-pyrimidine-2,4-dione (Table 2, entry 8)



Yellow solid; R_f = 0.38 (30% AcOEt:hexane); mp 106.0-109.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$ TMS): δ 7.80 (d, *J* = 6.4 Hz, 1H, Ar-H), 7.29-7.22 (m, 3H, Ar-H), 6.08 (br, 2H, NH_2), 2.80 (s, 3H, N-CH_3), 2.70 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ

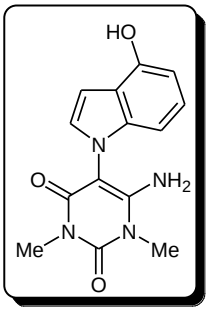
164.1, 162.5, 152.7, 142.1, 134.4, 129.7, 125.4, 124.9, 123.2, 113.1, 112.5, 102.3, 84.2, 29.5, 27.3; m/z (GC-MS) 348.02 [M^+]; Anal. Calcd (%) for $C_{14}H_{13}BrN_4O_2$: C, 48.16; H, 3.75; N, 16.05. Found C, 47.77, H, 3.48, N, 15.71.

6-Amino-5-(3-hydroxy-indol-1-yl)-1,3-dimethyl-1*H*-pyrimidine-2,4-dione (Table 2, entry 9)



Pale yellow solid; R_f = 0.51 (30% AcOEt:hexane); mp 171.2-175.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$ TMS): δ 9.52 (br, 1H, OH), 7.45 (d, *J* = 7.8 Hz, 1H, Ar-H), 7.28-7.14 (m, H, Ar-H), 6.93 (s, 1H, Ar-H), 6.52 (br, 2H, NH_2), 3.11 (s, 3H, N-CH_3), 2.95 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 164.6, 162.4, 152.2, 142.4, 130.5, 128.4, 125.7, 111.6, 104.8, 100.4, 84.2, 33.5, 31.7; m/z (GC-MS) 286.11 [M^+]; Anal. Calcd (%) for $C_{14}H_{14}N_4O_3$: C, 58.73, H, 4.93, N, 19.57. Found C, 58.61, H, 4.88, N, 19.41.

6-Amino-5-(4-hydroxy-indol-1-yl)-1,3-dimethyl-1*H*-pyrimidine-2,4-dione (Table 2, entry 10)

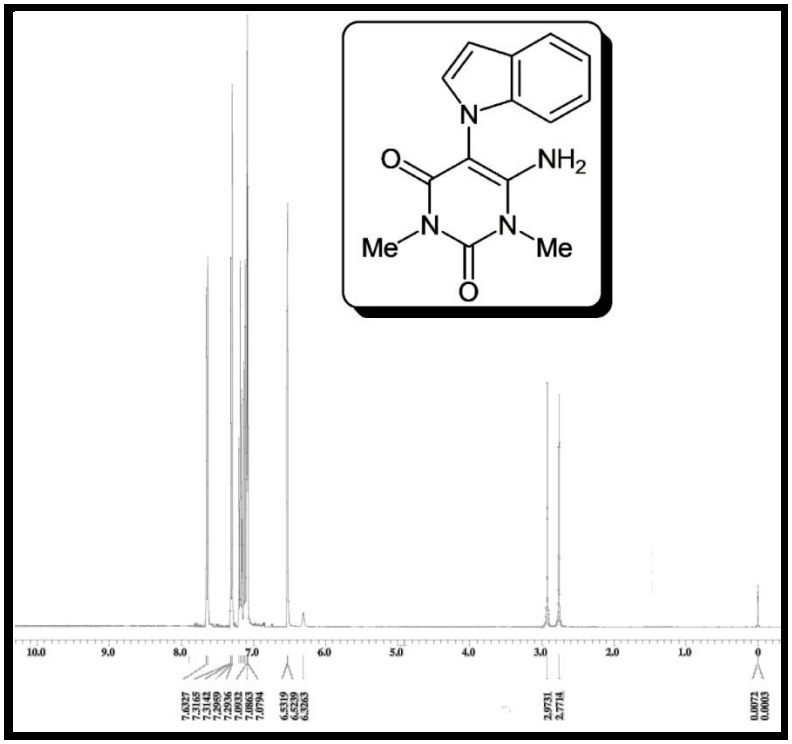


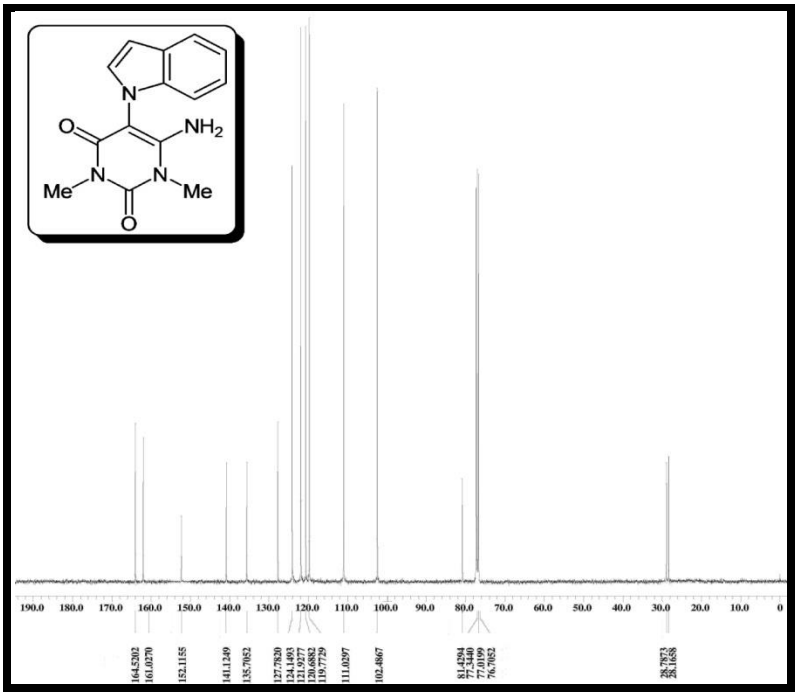
Faint yellow solid; R_f = 0.54 (30% AcOEt:hexane); mp 120.4-123.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$ TMS): δ 9.49 (br, 1H, OH), 8.14-8.04 (m, 1H, Ar-H), 7.18-6.74 (m, 3H, Ar-H), 6.32

(d, J = 6.4 Hz, 1H, Ar-H), 5.84 (br, 2H, NH_2), 3.01 (s, 3H, N-CH_3), 2.79 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 164.0, 162.0, 150.4, 142.2, 130.7, 128.5, 125.0, 111.7, 11.6, 104.5, 100.9, 84.0, 33.7, 31.5; m/z (GC-MS) 286.11 [M^+]; Anal. Calcd (%) for $C_{14}H_{14}N_4O_3$: C, 58.73; H, 4.93; N, 19.57. Found C, 58.42, H, 4.67, N, 19.25.

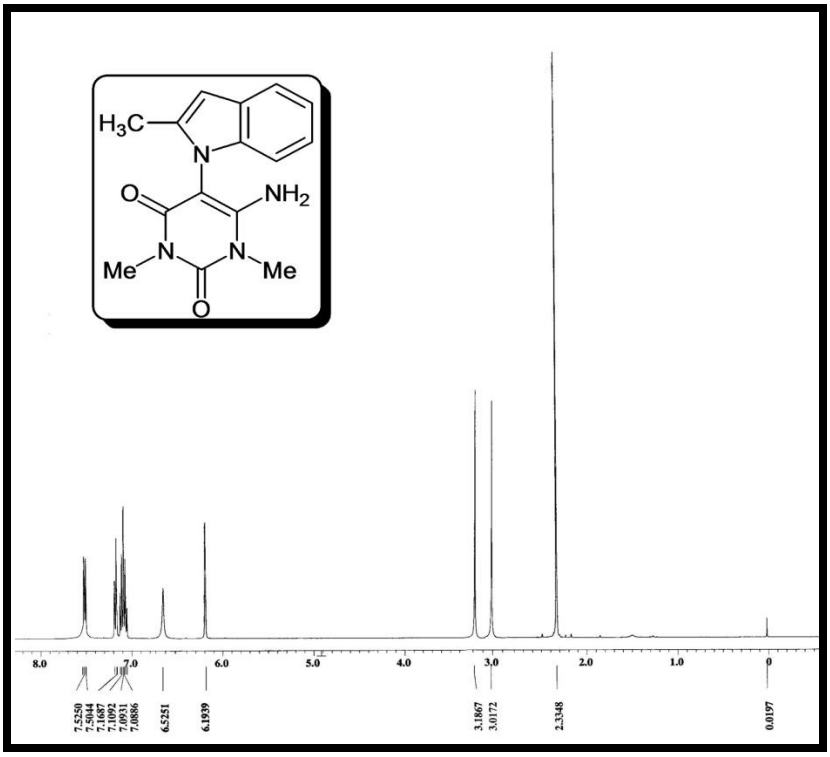
4. ^{1}H and ^{13}C NMR spectra of the selected compounds

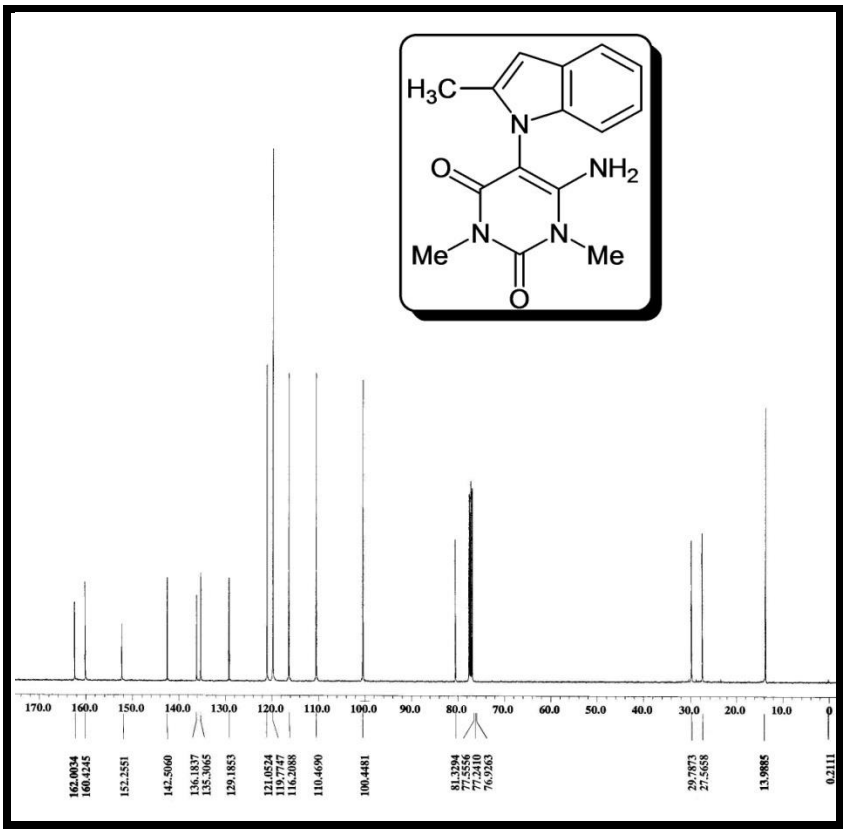
^{1}H and ^{13}C NMR spectra of 6-Amino-5-indol-1-yl-1,3-dimethyl-1*H*-pyrimidine-2,4-dione (Table 2, entry 1)



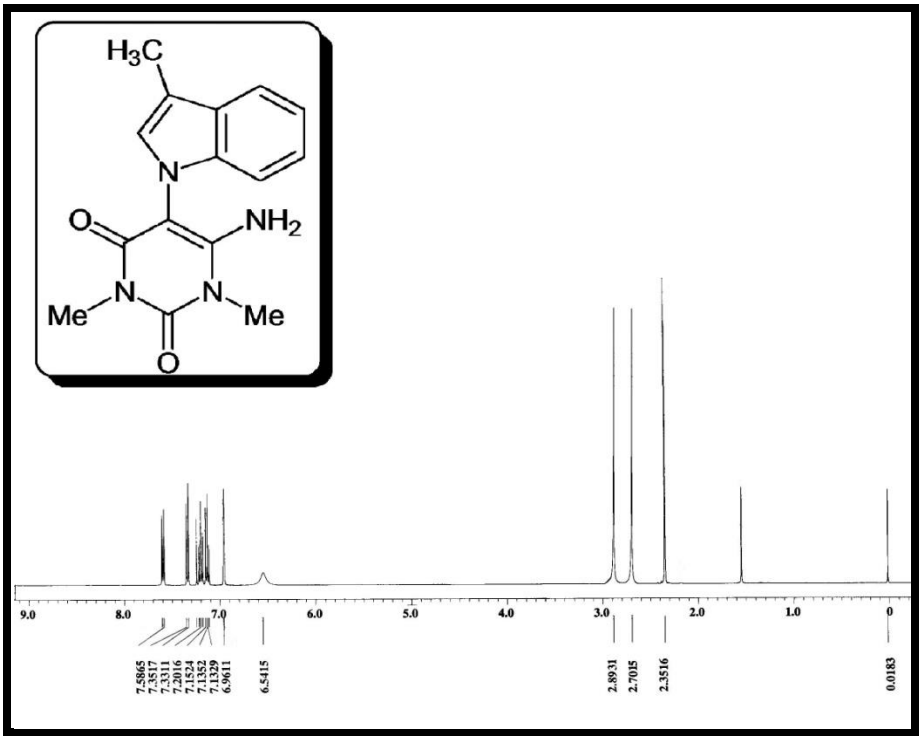


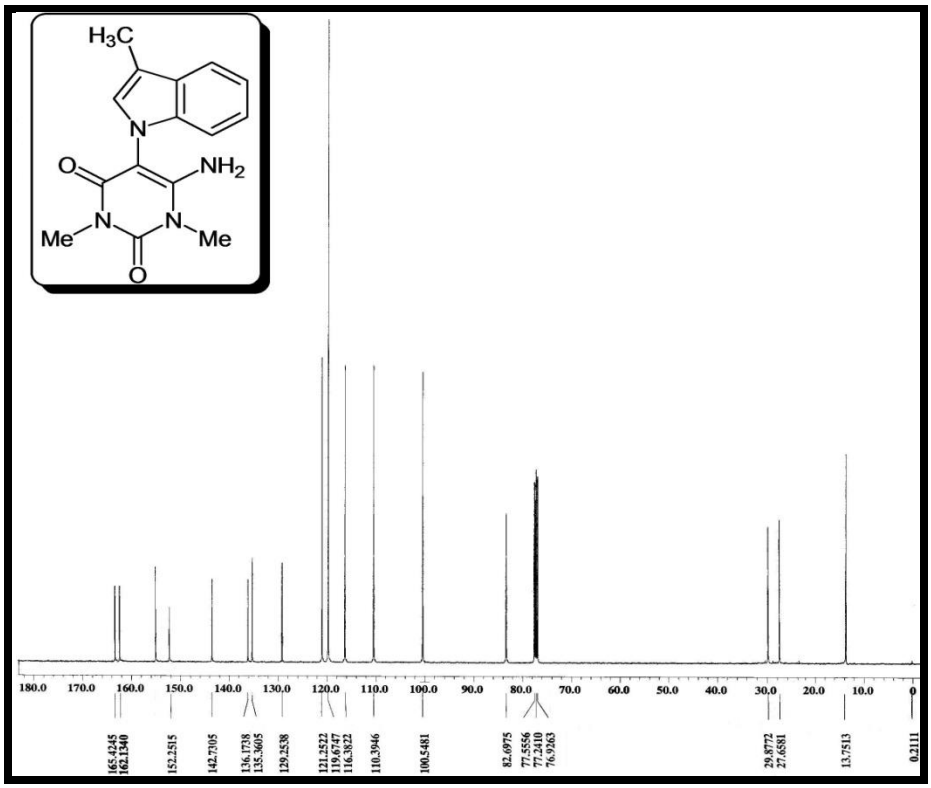
^{1}H and ^{13}C NMR spectra of 6-Amino-1,3-dimethyl-5-(2-methyl-indol-1-yl)-1*H*-pyrimidine-2,4-dione (Table 2, entry 2)



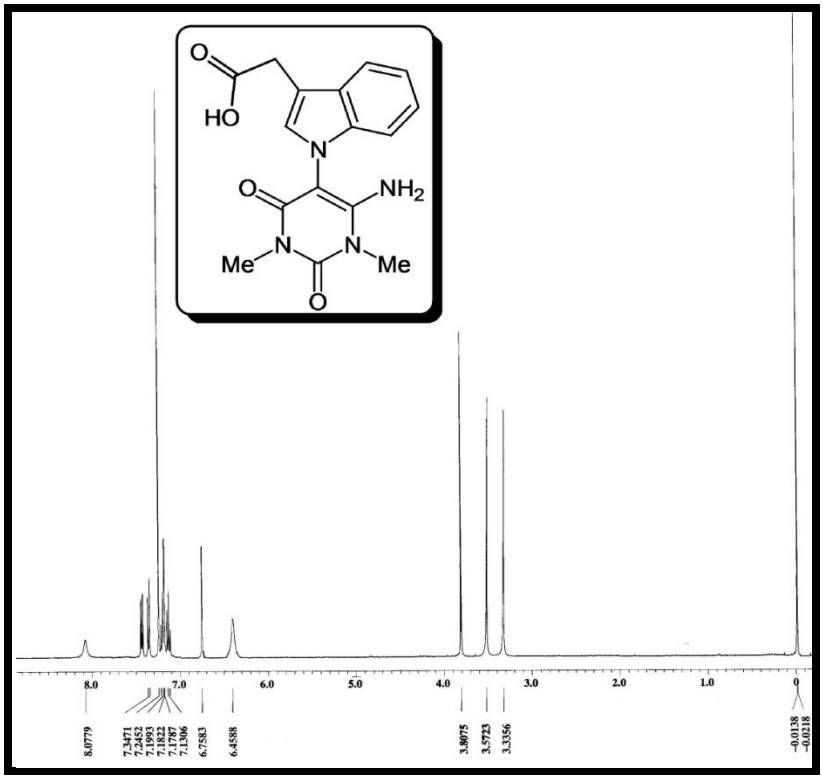


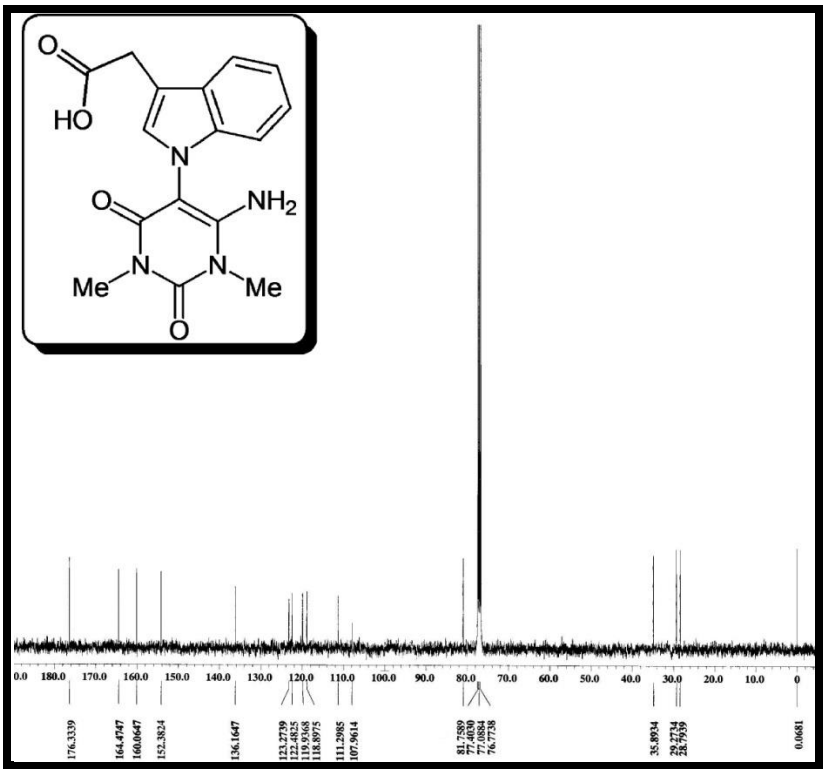
^{1}H and ^{13}C NMR spectra of 6-Amino-1,3-dimethyl-5-(3-methyl-indol-1-yl)-1*H*-pyrimidine-2,4-dione (Table 2, entry 3)



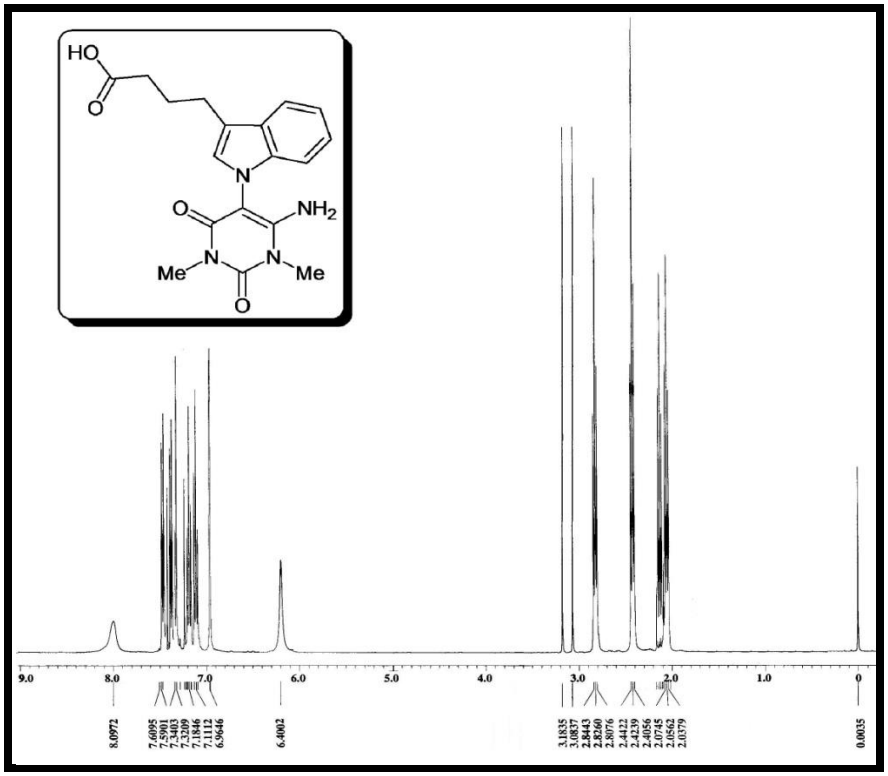


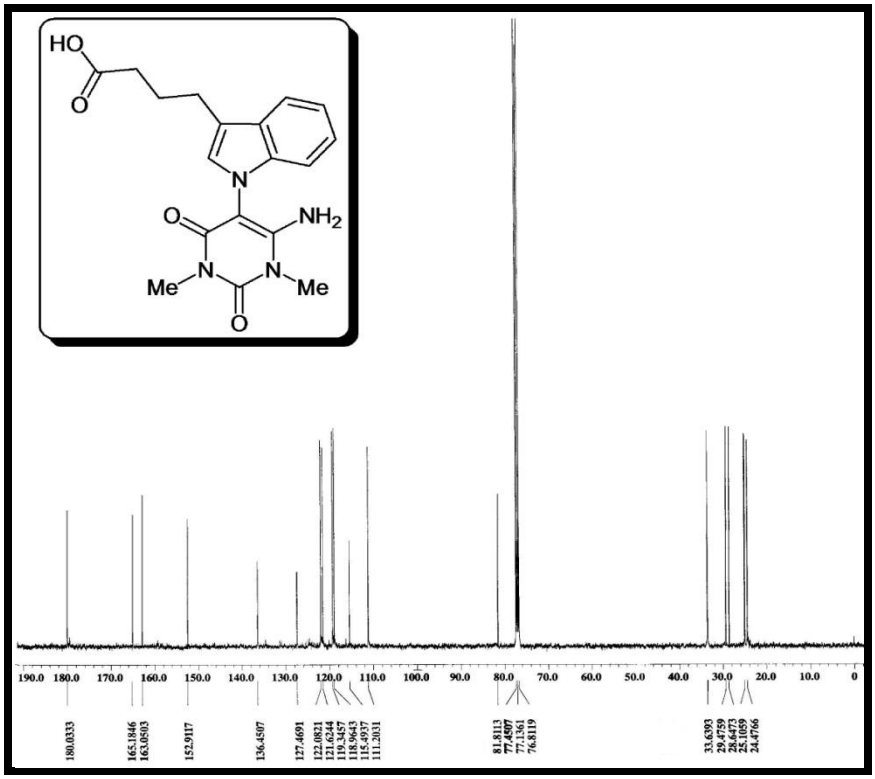
^{1}H and ^{13}C NMR spectra of 6 [1-(6-Amino-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydro-pyrimidin-5-yl)-1H-indol-3-yl]-acetic acid (Table 2, entry 5)



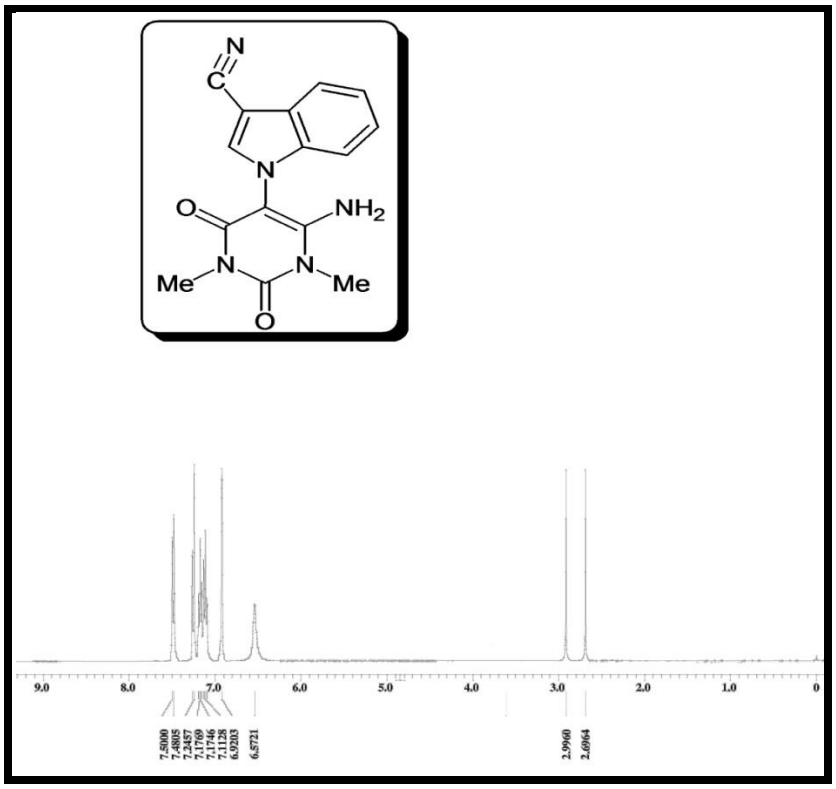


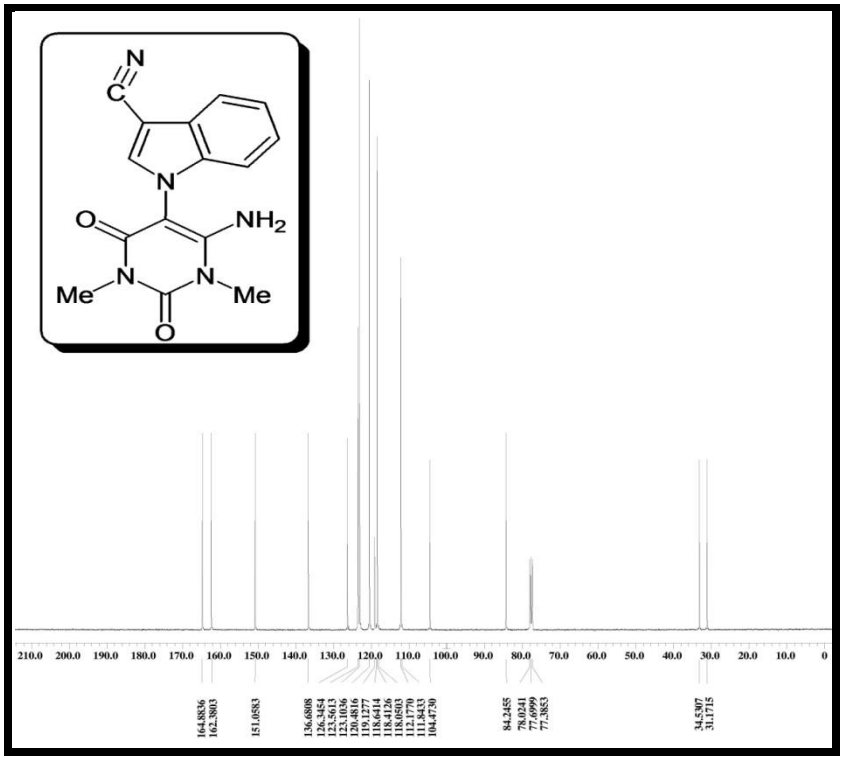
^{1}H and ^{13}C NMR spectra of 4-[1-(4-Amino-1,3-dimethyl-2,6-dioxo-hexahydro-pyrimidin-5-yl)-1*H*-indol-3-yl]-butyric acid (Table 2, entry 6)





^{1}H and ^{13}C NMR spectra of 1-(6-Amino-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydro-pyrimidin-5-yl)-1*H*-indole-3-carbonitrile (Table 2, entry 7)





^{1}H and ^{13}C NMR spectra of 6-Amino-5-(5-bromo-indol-1-yl)-1,3-dimethyl-1*H*-pyrimidine-2,4-dione (Table 2, entry 8)