

## Synthesis, characterization and application of ZnFe<sub>2</sub>O<sub>4</sub> nano- particles as a heterogeneous ditopic catalyst for the synthesis of pyrano[2,3-d]pyrimidines

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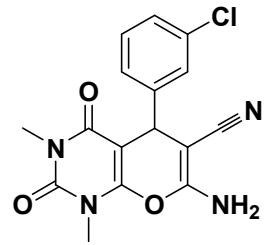
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*Khazaei\_1326@yahoo.com (A. Khazaei),*

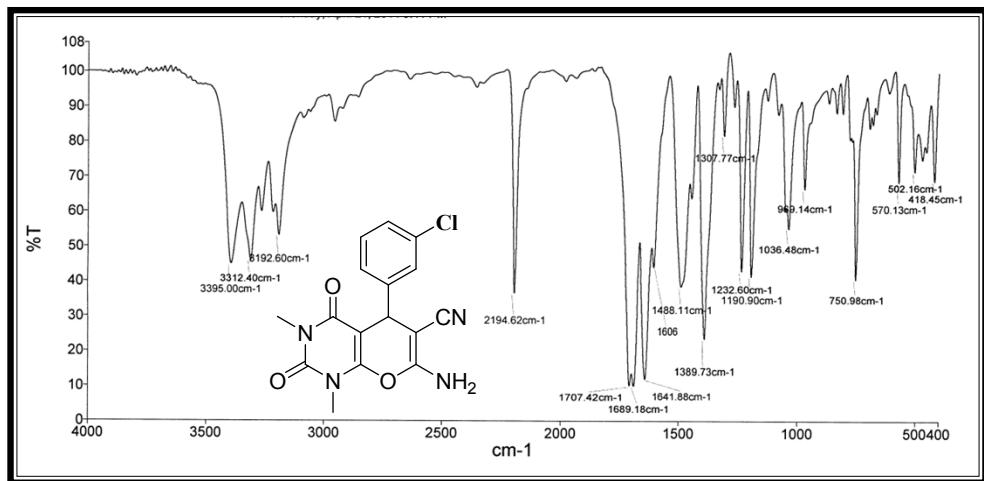
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*Supplementary data:*

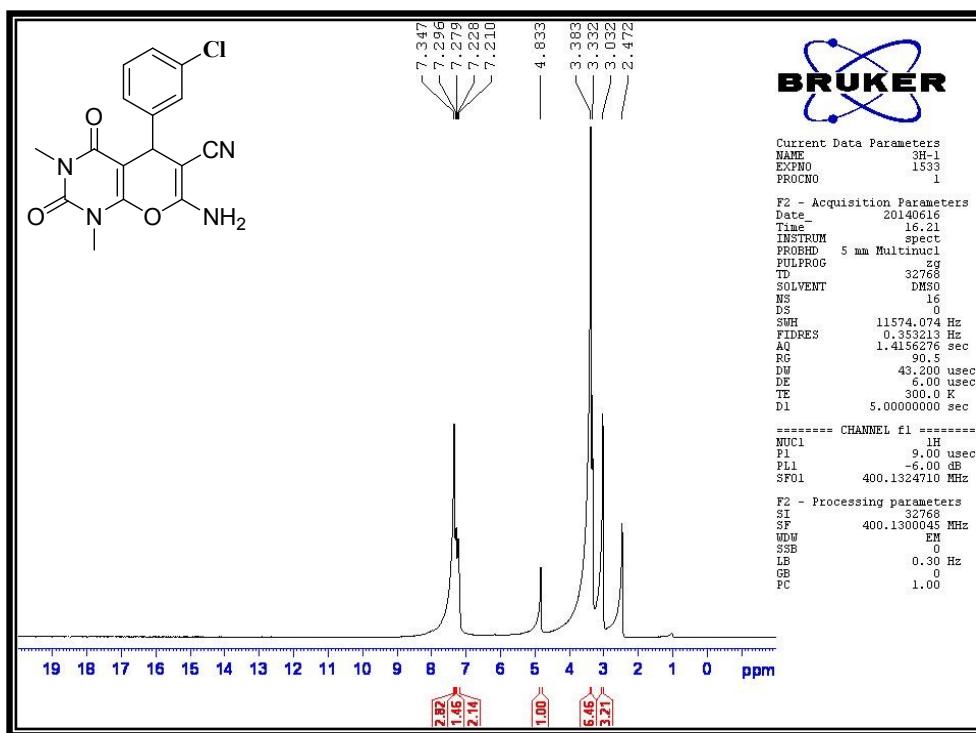
**7-Amino-5-(3-chlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano  
[2,3-d] pyrimidine-6-carbonitrile**



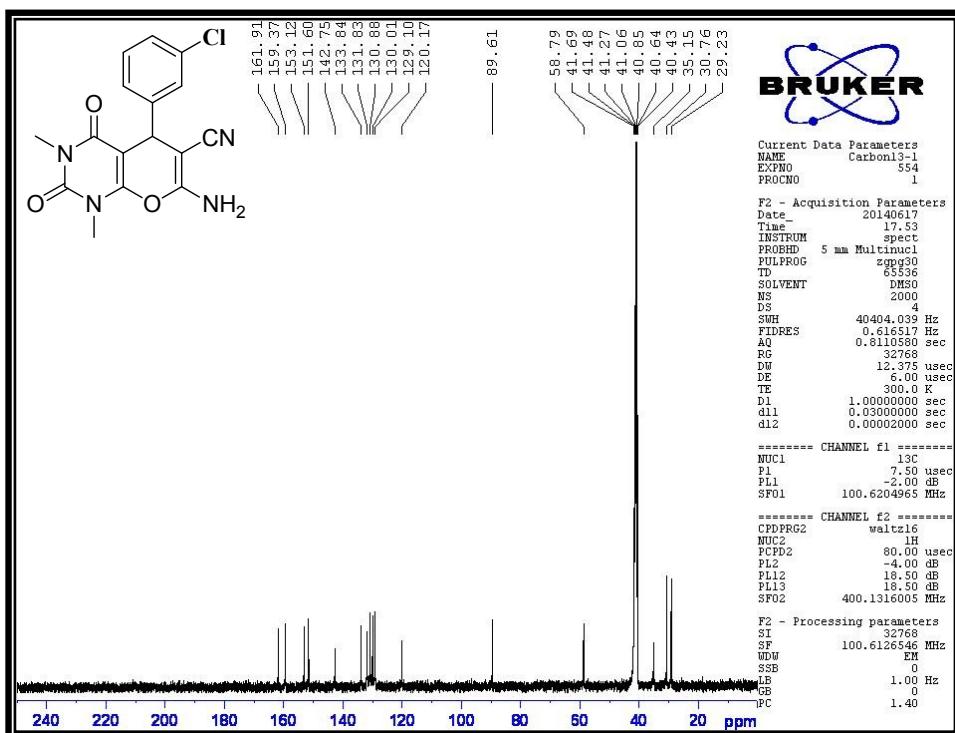
White solid; mp 247-248 °C; IR(KBr,Cm-1)  $\nu_{max}$ = 3395, 3312, 3192, 2194, 1707, 1689, 1641, 1488, 1389, 1232, 1190, 1036, 750, 570;  $^1\text{H}$ NMR(400MHZ,DMSO-d6):  $\delta$ = 3.03 (s,3H,NMe), 3.38 (s,3H,NMe), 4.83 (s,1H,CH), 7.21-7.34 (m,6H,Ar-H and NH<sub>2</sub>);  $^{13}\text{C}$  NMR (100 MHz, DMSO-d6):  $\delta$  = 29.2, 30.7, 35.1, 58.7, 89.6, 120.1, 129.1, 130, 130.8, 131.80, 133.8, 142.7, 151.6, 153.1, 159.3, 161.9 ppm; MS:m/z=345(M<sup>+</sup>)



**Fig. S1.** The IR spectrum of 7-Amino-5-(3-chlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile

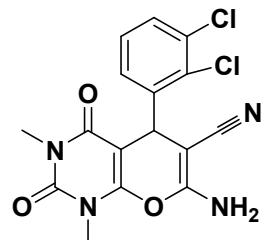


**Fig. S2.** The  $^1\text{H}$  NMR spectrum of 7-Amino-5-(3-chlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d]

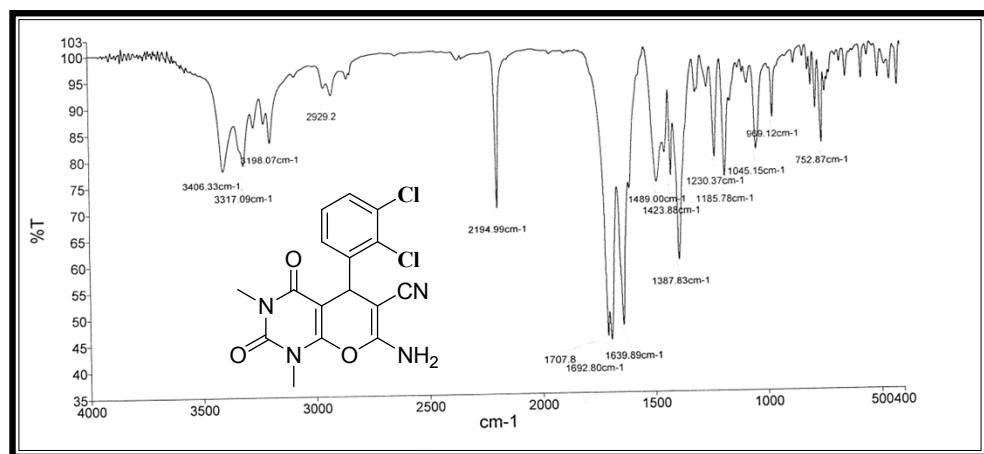


**Fig. S3.** The  $^{13}\text{C}$  NMR spectrum of 7-Amino-5-(3-chlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d]

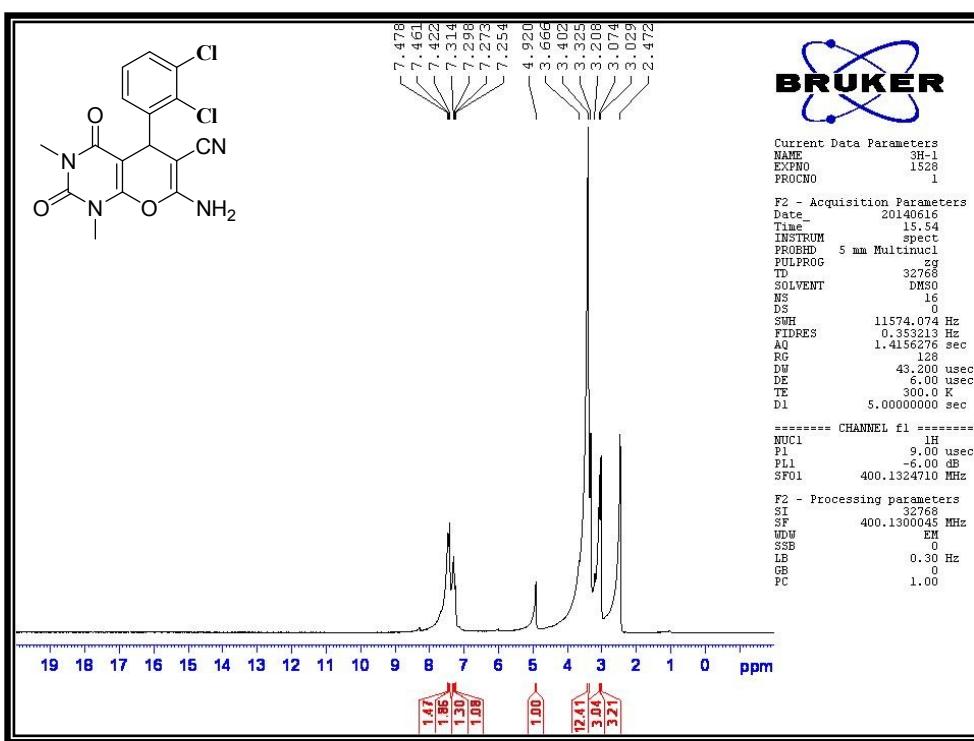
**7-Amino-5-(2,3-dichlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile**



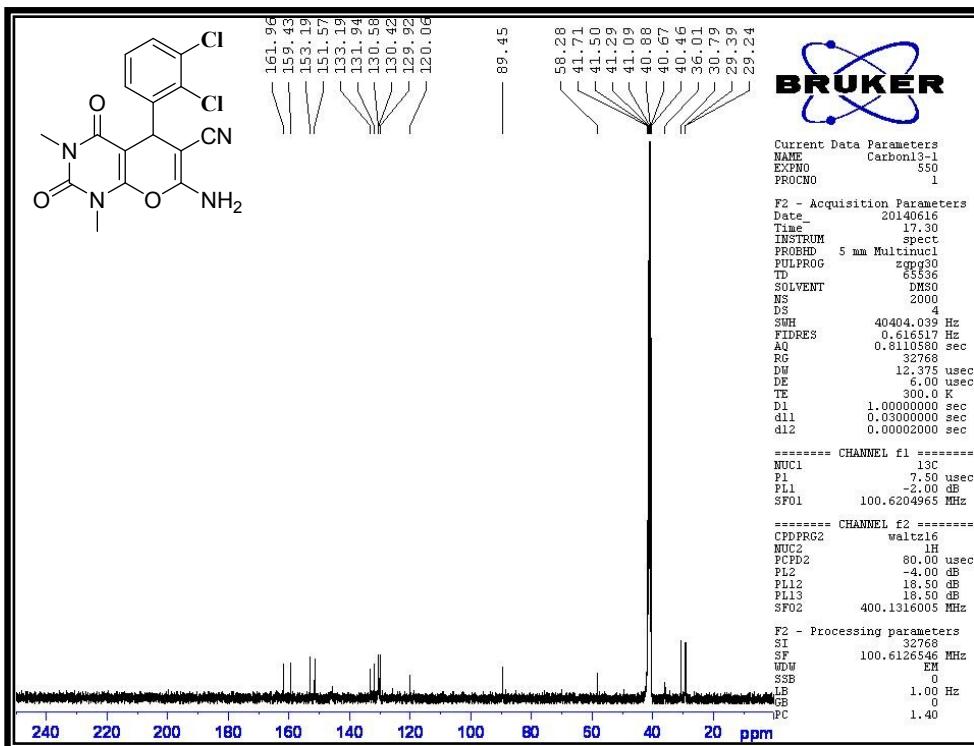
White solid; mp 238 °C ; IR(KBr,Cm<sup>-1</sup>) $\nu_{\text{max}}$ = 3406, 3317, 3198, 2929, 2194, 1707, 1692, 1639, 1489, 1387, 1230, 1185, 1045, 752; <sup>1</sup>H NMR(400MHz,DMSO-d<sub>6</sub>): δ= 3.07(s,3H, NMe), 3.40(s,3H,NMe), 4.92 (s,1H,CH), 7.25-7.47 (m,5H, ,Ar-H and NH2); <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ = 29.2, 30.7, 58.2, 89.4, 120, 129.9, 130.4, 130.5, 131.9, 133.1, 151.5, 153.1, 159.4, 161.9 ppm; MS:m/z=378(M<sup>+</sup>)



**Fig. S4.** The IR spectrum of 7-Amino-5-(2,3-dichlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile

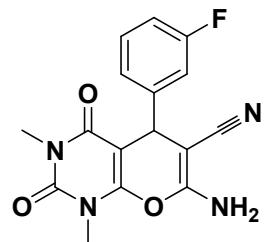


**Fig. S5.** The  $^1\text{H}$  NMR spectrum of 7-Amino-5-(2,3-dichlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyran-6-carbonitrile [2,3-d] pyrimidine-6-carbonitrile

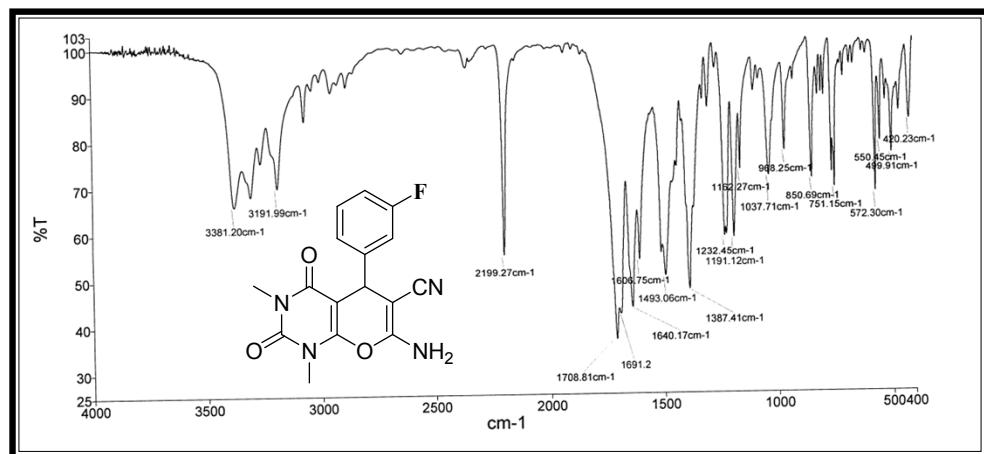


**Fig. S6.** The  $^{13}\text{C}$  NMR spectrum of 7-Amino-5-(2,3-dichlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyran-6-carbonitrile [2,3-d] pyrimidine-6-carbonitrile

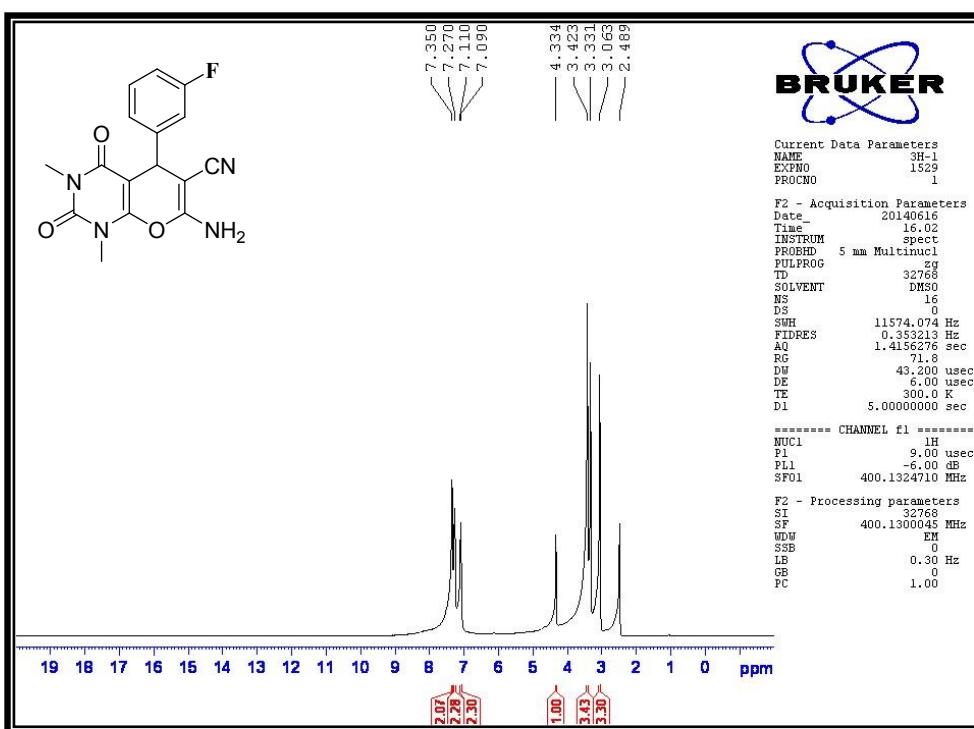
**7-Amino-5-(3-fluorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile**



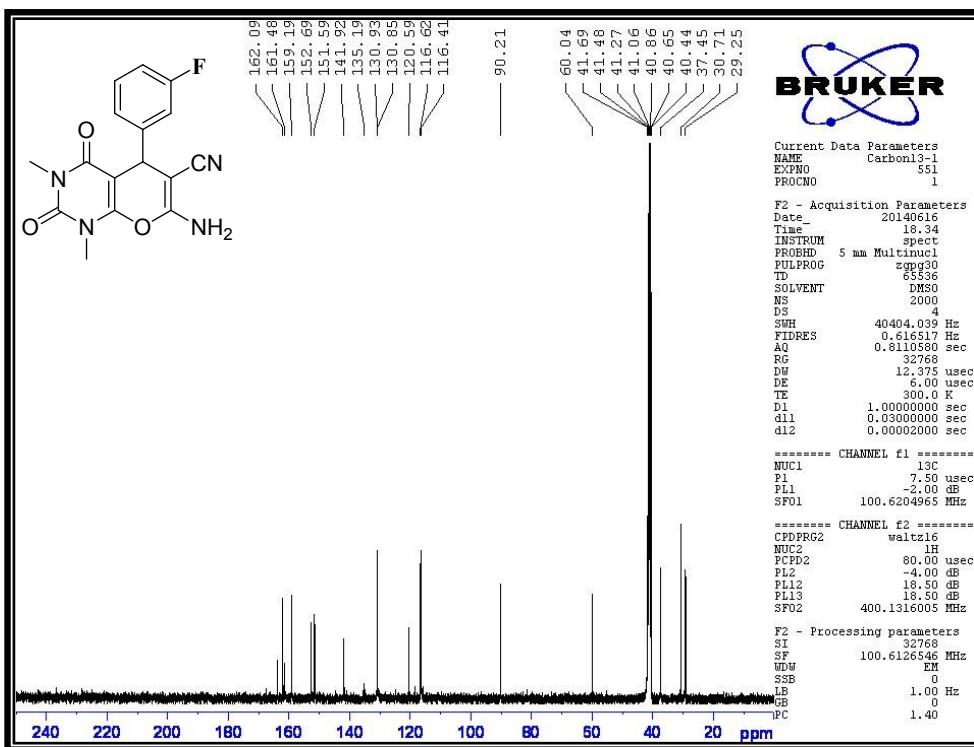
White solid; mp 228-229 °C; IR(KBr,Cm<sup>-1</sup>) $\nu_{\text{max}}$ = 3381,3309 , 3191, 2199, 1708, 1691, 1640, 1493, 1387, 1232, 1191, 1037, 850, 751, 572; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ =3.06(s,3H, NMe), 3.42(s,3H,NMe), 4.33(s,1H,CH), 7.09-7.35 (m,6H, Ar-H and NH<sub>2</sub>); <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ = 29.2, 30.7, 37.4, 60, 90.2, 116.4, 116.6, 120.5, 130.8, 130.9, 135.1, 141.9, 151.5, 152.6, 159.1, 161.4, 162.0 ppm; MS:m/z=328(M<sup>+</sup>)



**Fig. S7.** The IR spectrum of 7-Amino-5-(3-fluorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile

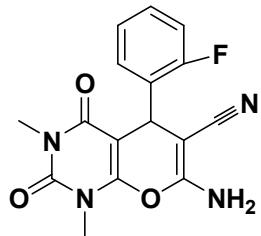


**Fig. S8.** The  $^1\text{H}$  NMR spectrum of 7-Amino-5-(3-fluorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyran-6-carbonitrile [2,3-d] pyrimidine-6-carbonitrile

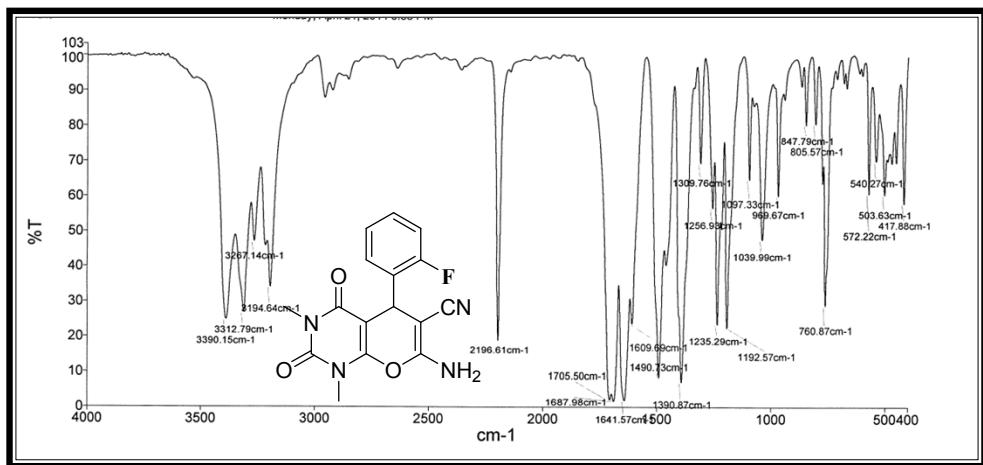


**Fig. S9.** The  $^{13}\text{C}$  NMR spectrum of 7-Amino-5-(3-fluorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyran-6-carbonitrile [2,3-d] pyrimidine-6-carbonitrile

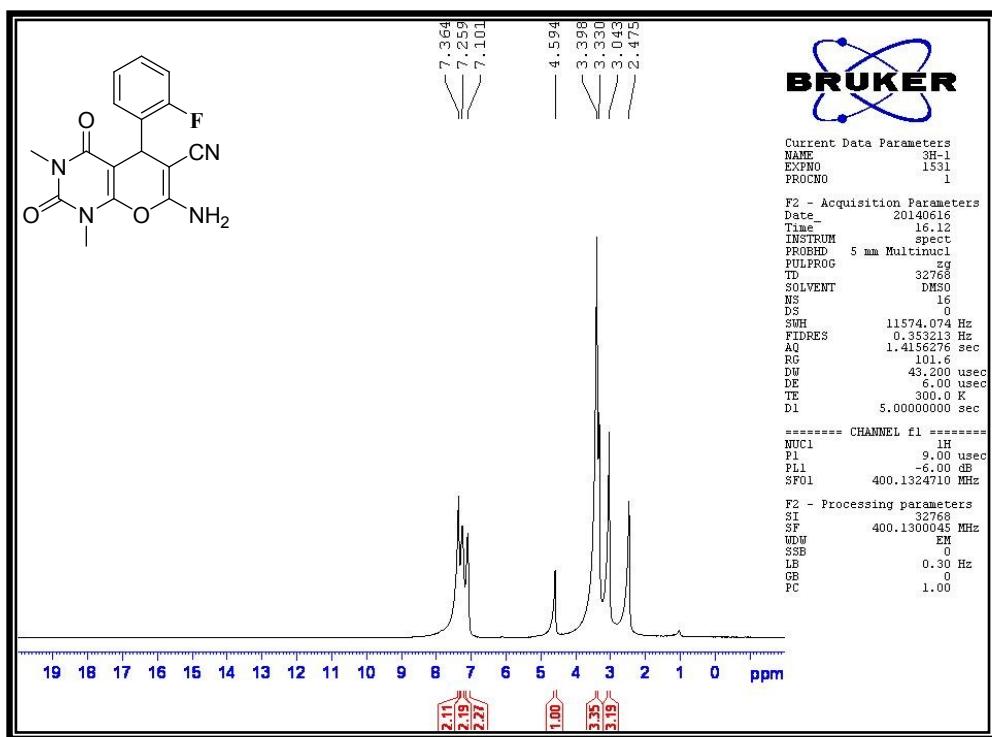
**7-Amino-5-(2-fluorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile**



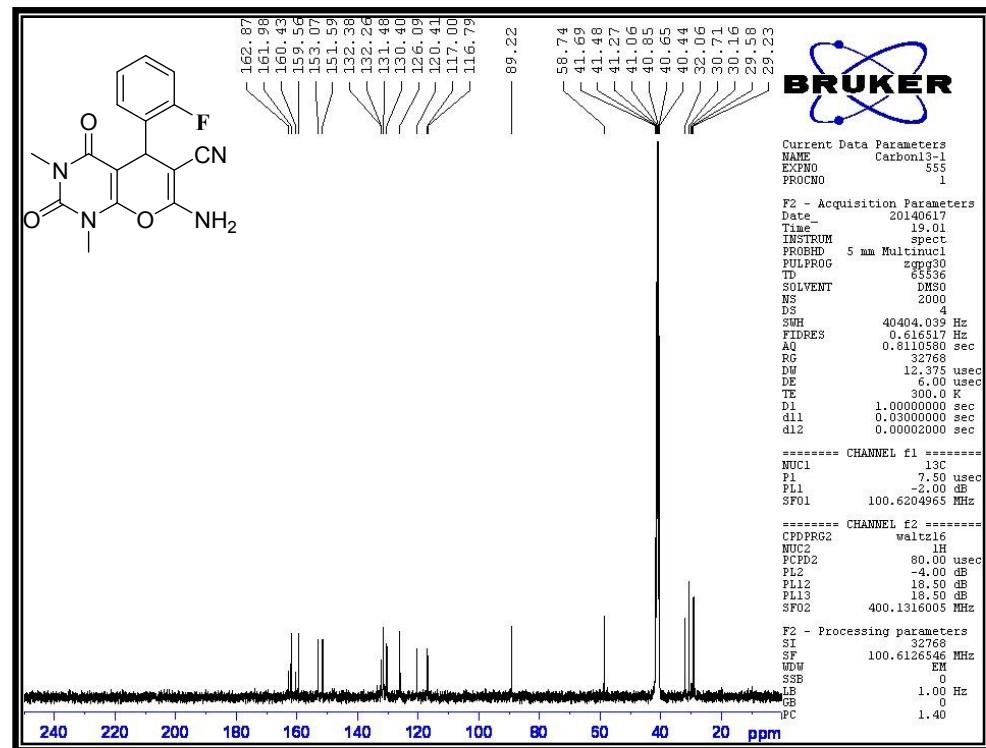
White solid; mp 238-239 °C; IR(KBr,Cm<sup>-1</sup>) $\nu_{\text{max}}$ = 3390, 3312, 3194, 2196, 1705, 1687, 1641, 1490, 1390, 1235, 1192, 1039, 969, 760, 572; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ = 3.04(s,3H,NMe), 3.39(s,3H,NMe), 4.59(s,1H,CH), 7.10-7.36 (m,6H, Ar-H and NH<sub>2</sub>) <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): δ = 29.2, 30.7, 32, 58.7, 89.2, 116.7, 117, 120.4, 126.0, 130.4, 131.4, 132.2, 132.3, 151.5, 153, 159.5, 160.4, 161.9, 162.8 ppm; MS:m/z=328(M<sup>+</sup>)



**Fig. S10.** The IR spectrum of 7-Amino-5-(2-fluorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile

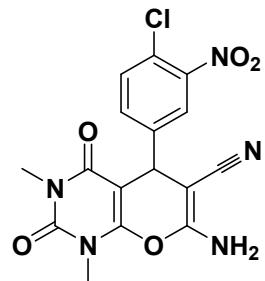


**Fig. S11.** The  $^1\text{H}$  NMR spectrum of 7-Amino-5-(2-fluorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d]

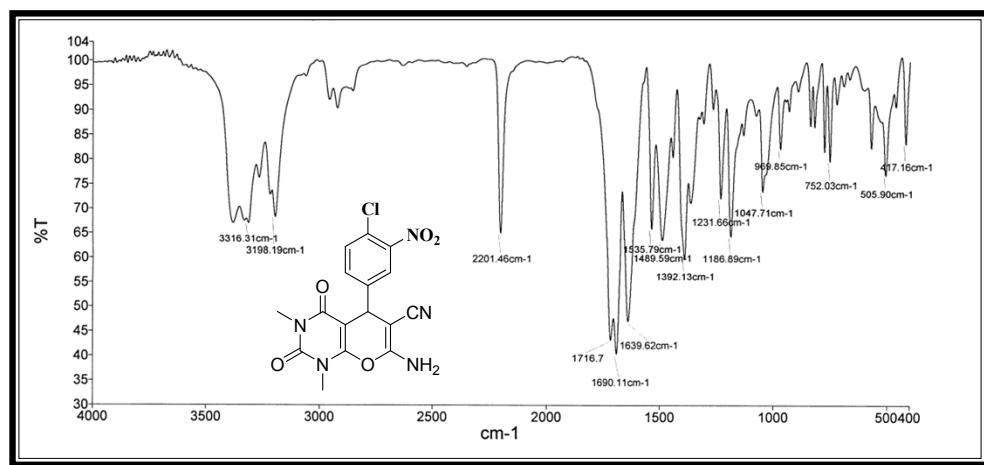


**Fig. S12.** The  $^{13}\text{C}$  NMR spectrum of 7-Amino-5-(2-fluorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d]

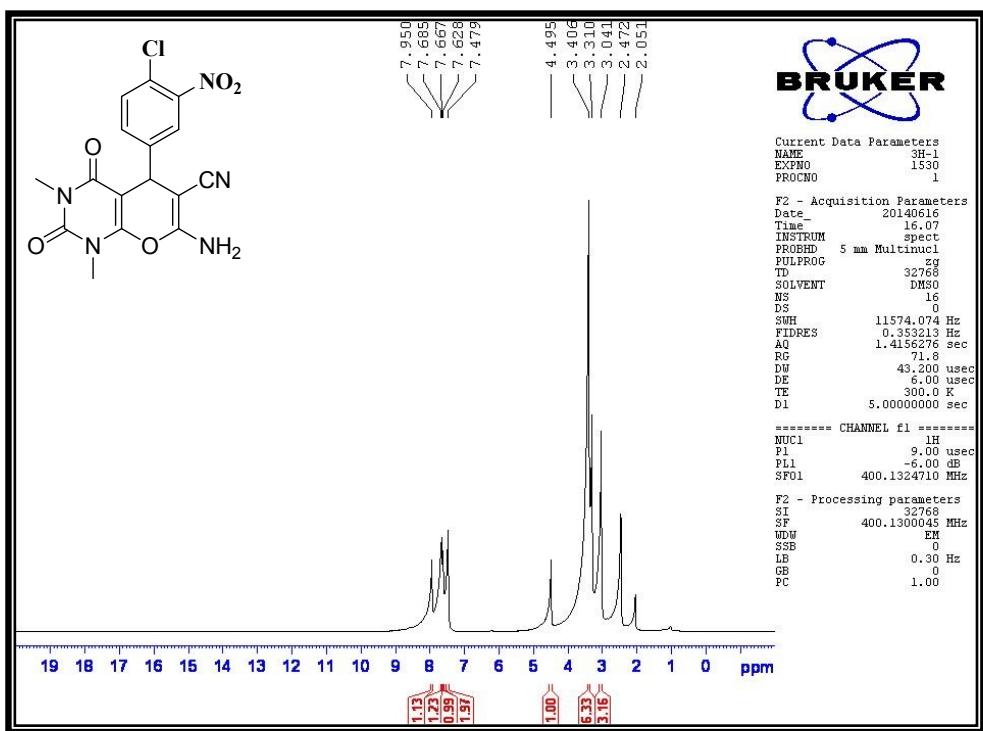
**7-Amino-5-(4-chloro-3-nitrophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile**



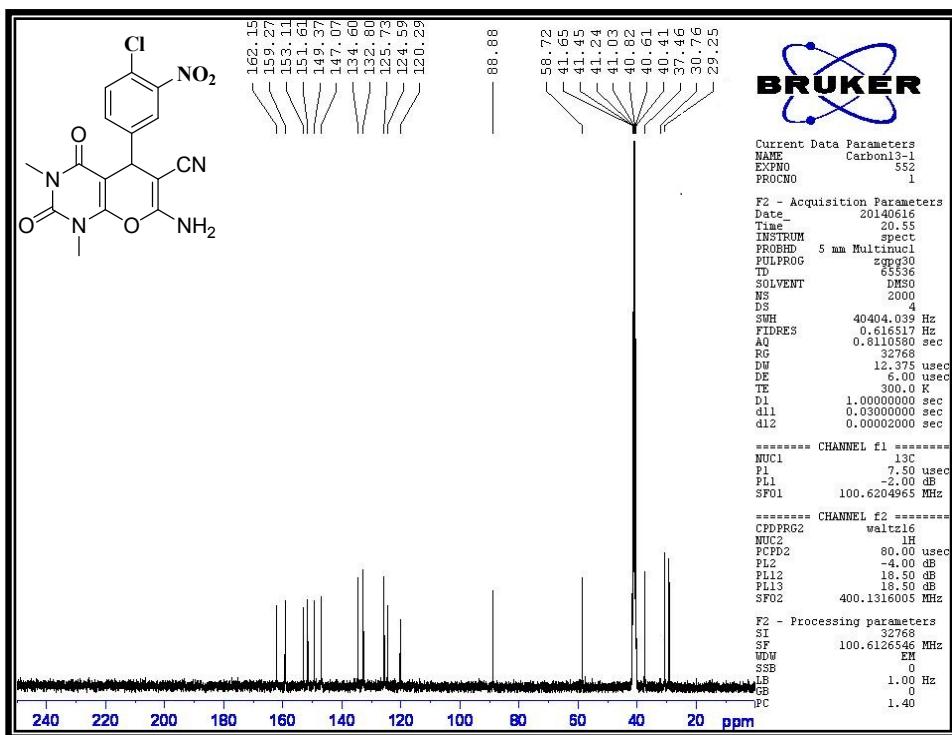
White solid; mp 209-210 °C; IR(KBr,Cm<sup>-1</sup>) $\nu_{\text{max}} = 3395, 3316, 3198, 2201, 1716, 1690, 1639, 1489, 1392, 1231, 1186, 1047, 969, 752, 505$ ; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>):  $\delta = 3.04(\text{s}, 3\text{H}, \text{NMe}), 3.40(\text{s}, 3\text{H}, \text{NMe}), 4.49(\text{s}, 1\text{H}, \text{CH}), 7.47\text{-}7.95(\text{m}, 5\text{H}, \text{NH}_2, \text{Ar-H})$  <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>):  $\delta = 29.2, 30.7, 37.4, 58.7, 88.8, 120.2, 124.5, 125.7, 132.8, 134.6, 147.0, 149.3, 151.6, 153.1, 159.2, 162.1$  ppm; MS:m/z=389(M<sup>+</sup>)



**Fig. S13.** The IR spectrum of 7-Amino-5-(4-chloro-3-nitrophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile

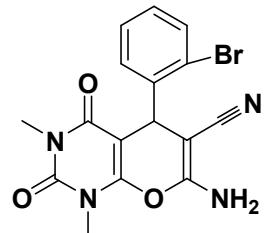


**Fig. S14.** The  $^1\text{H}$  NMR spectrum of 7-Amino-5-(4-chloro-3-nitrophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyran-6-carbonitrile [2,3-d] pyrimidine-6-carbonitrile

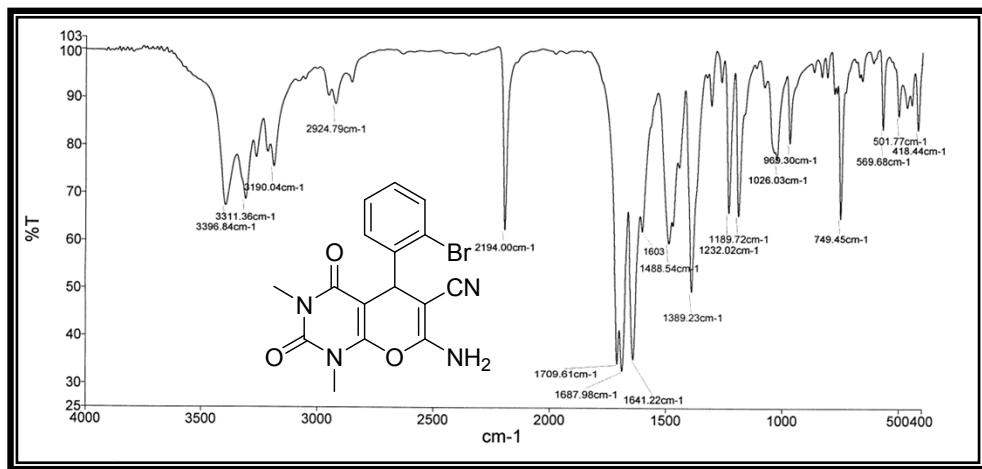


**Fig. S15.** The  $^{13}\text{C}$  NMR spectrum of 7-Amino-5-(4-chloro-3-nitrophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyran-6-carbonitrile [2,3-d] pyrimidine-6-carbonitrile

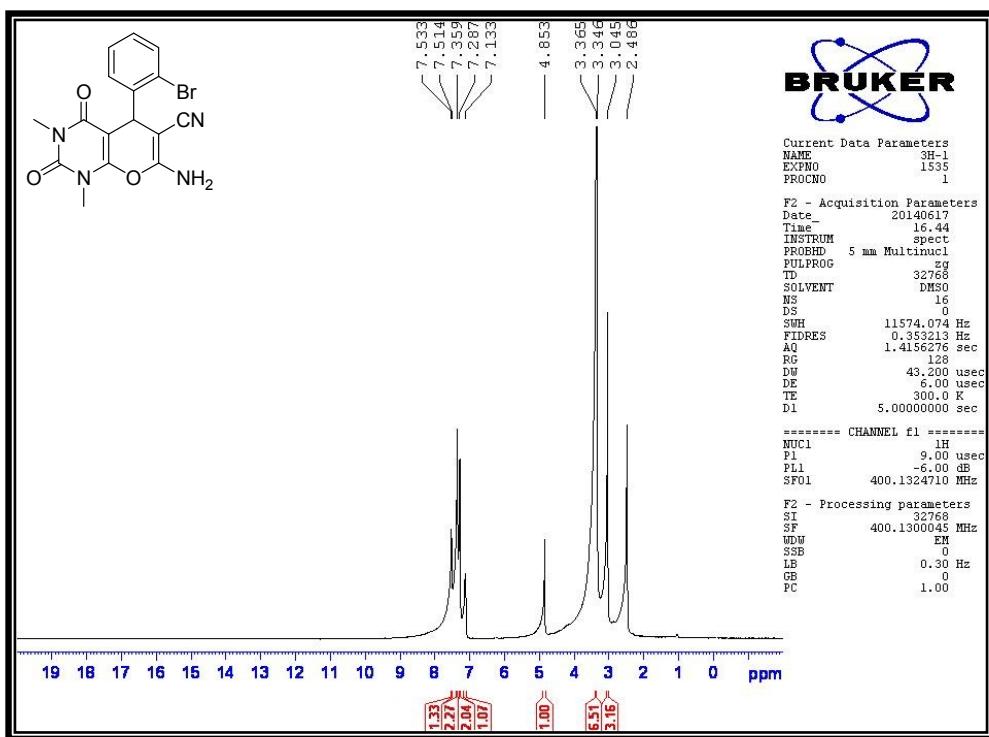
**7-Amino-5-(2-bromophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile**



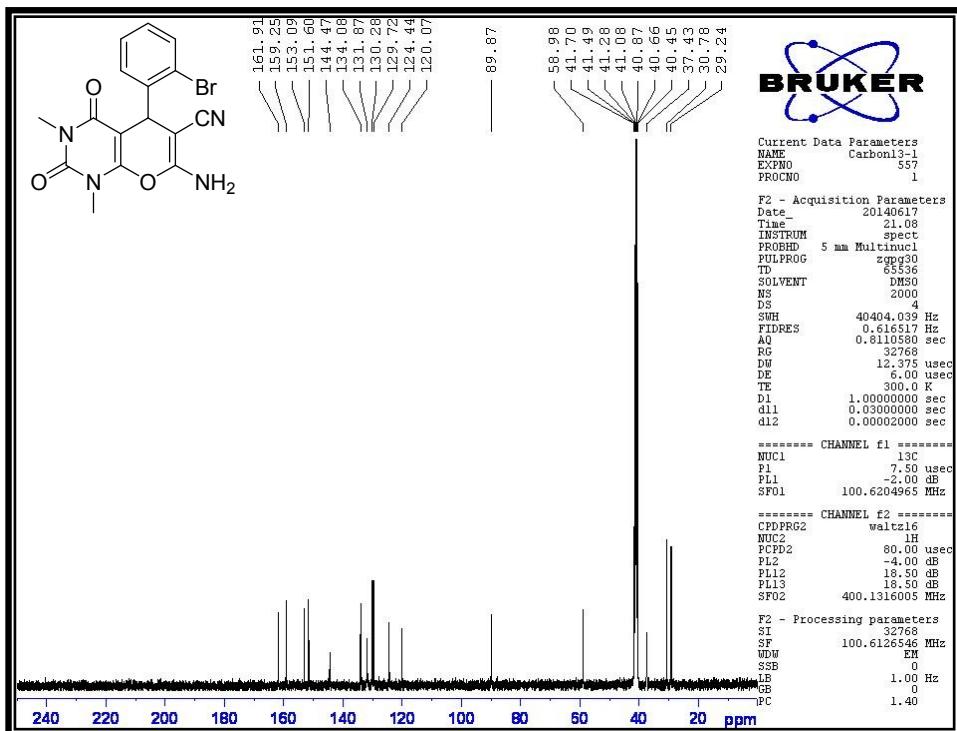
White solid; mp 237-238°C; IR(KBr,Cm<sup>-1</sup>) $\nu_{\text{max}} = 3396, 3311, 3190, 2194, 1709, 1687, 1641, 1488, 1389, 1232, 1189, 1026, 969, 749, 567$ ; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>):  $\delta = 3.04(\text{s}, 3\text{H}, \text{NMe}), 3.34(\text{s}, 3\text{H}, \text{NMe}), 4.85(\text{s}, 1\text{H}, \text{CH}), 7.13\text{-}7.53 (\text{m}, 6\text{H}, \text{NH}_2, \text{Ar-H})$  <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>):  $\delta = 29.2, 30.7, 37.4, 58.9, 89.8, 120, 124.4, 129.7, 130.2, 131.8, 134, 144.4, 151.6, 153, 159.2, 161.9$  ppm; MS:m/z=389(M<sup>+</sup>)



**Fig. S16.** The IR spectrum of 7-Amino-5-(2-bromophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile

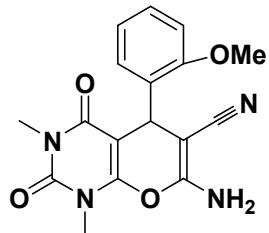


**Fig. S17.** The  $^1\text{H}$  NMR spectrum of 7-Amino-5-(3-bromophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyran-6-carbonitrile [2,3-d]

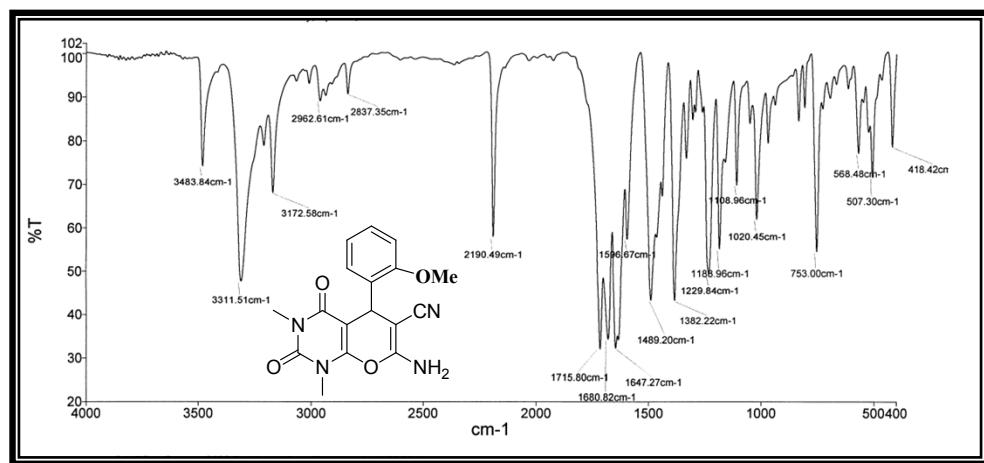


**Fig. S18.** The  $^{13}\text{C}$  NMR spectrum of 7-Amino-5-(3-bromophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyran-6-carbonitrile [2,3-d]

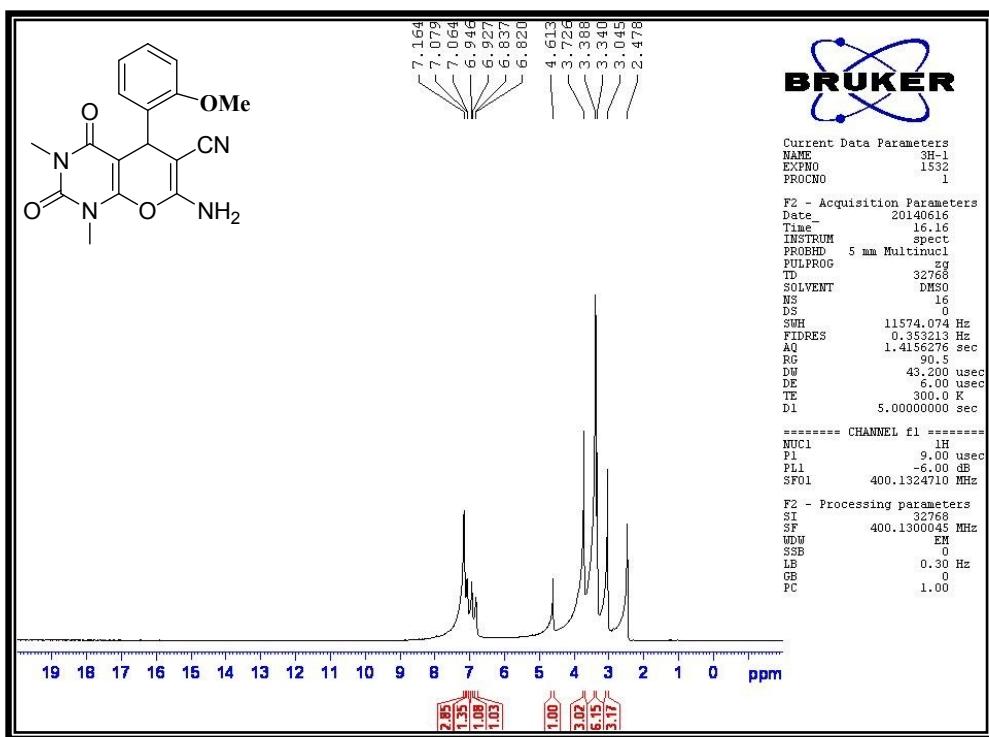
**7-Amino-5-(2-methoxyphenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile**



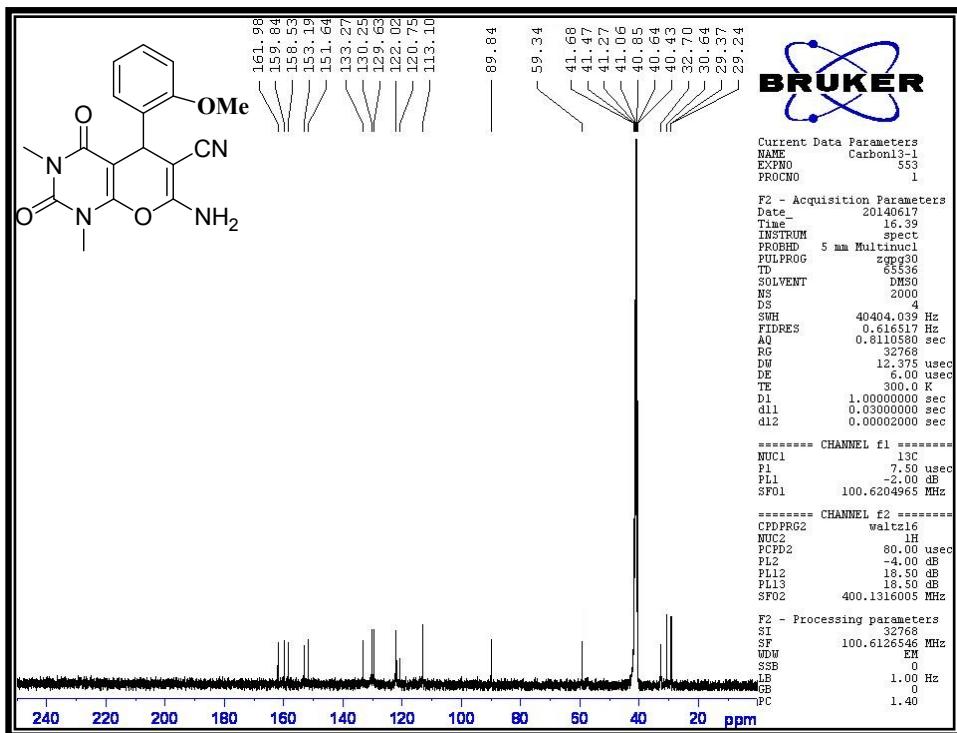
White solid; mp 209-210°C; IR(KBr,Cm<sup>-1</sup>) $\nu_{\text{max}} = 3483, 3311, 3172, 2962, 2190, 1715, 1680, 1642, 1489, 1382, 1229, 1188, 1020, 753, 568$ ; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>):  $\delta = 3.04(\text{s}, 3\text{H}, \text{NMe}), 3.38(\text{s}, 3\text{H}, \text{NMe}), 3.72(\text{s}, 3\text{H}, \text{CH}_3), 4.61(\text{s}, 1\text{H}, \text{CH}), 6.82\text{-}7.16(\text{m}, 6\text{H}, \text{NH}_2, \text{Ar-H})$ ; <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>):  $\delta = 29.2, 30.6, 32.7, 57.2, 59.3, 89.8, 113.1, 120.7, 122, 129.6, 130.2, 133.2, 151.6, 153.1, 158.5, 159.8, 161.9$  ppm; MS:m/z=340(M<sup>+</sup>)



**Fig. S19.** The IR spectrum of 7-Amino-5-(2-methoxyphenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile

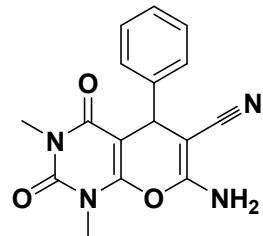


**Fig. S20.** The  $^1\text{H}$  NMR spectrum of 7-Amino-5-(2-methoxyphenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyran-6-carbonitrile [2,3-d] pyrimidine-6-carbonitrile

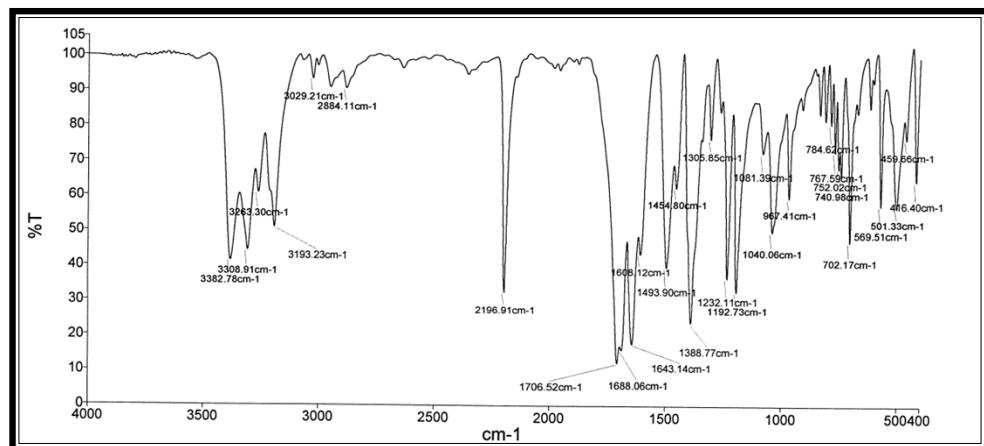


**Fig. S21.** The  $^{13}\text{C}$  NMR spectrum of 7-Amino-5-(2-methoxyphenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyran-6-carbonitrile [2,3-d] pyrimidine-6-carbonitrile

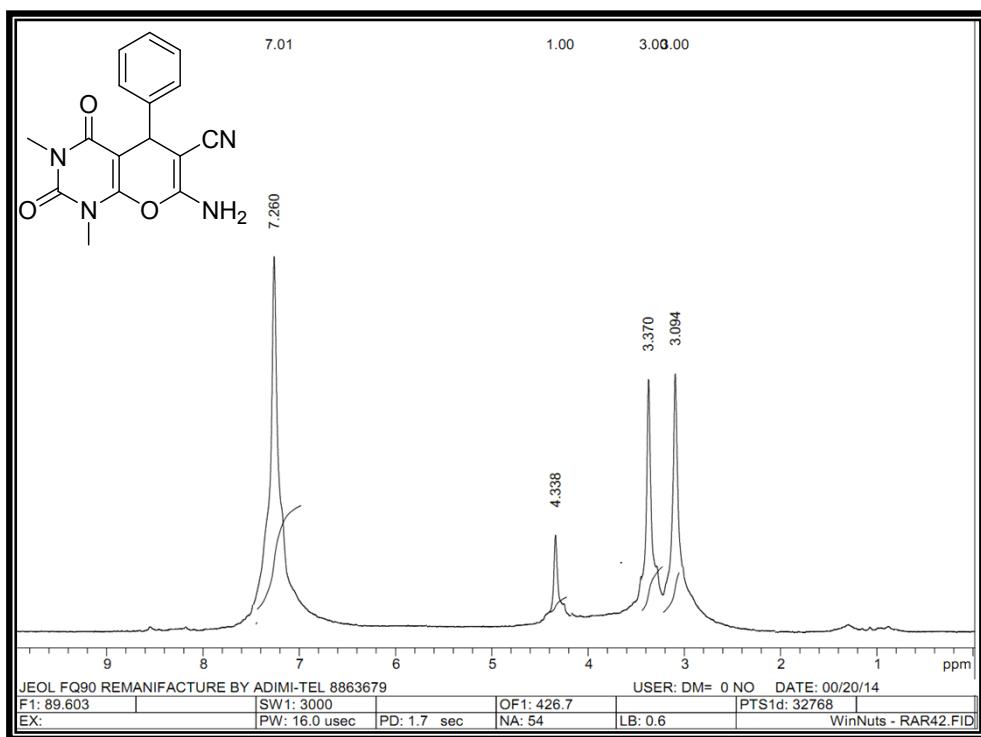
**7-Amino-5-phenyl-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile**



White solid; mp 218-220 °C (mp 210°C ); IR(KBr,Cm<sup>-1</sup>) $\nu_{\text{max}}$ = 3382,3308,3193,2196  
,1706,1688,1643,1493,1388,1232,1192,1040,702,596; <sup>1</sup>HNMR( 90 MHZ,DMSO-d<sub>6</sub>) $\delta$ : 3.09  
(s,3H,NMe), 3.37 (s,3H,NMe), 4.33 (s,1H,CH),6.89-7.50 (m,7H,Ar-H and NH<sub>2</sub>)

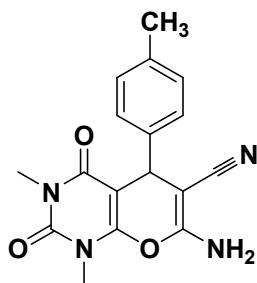


**Fig. S22.** The IR spectrum of 7-Amino-5-phenyl-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile



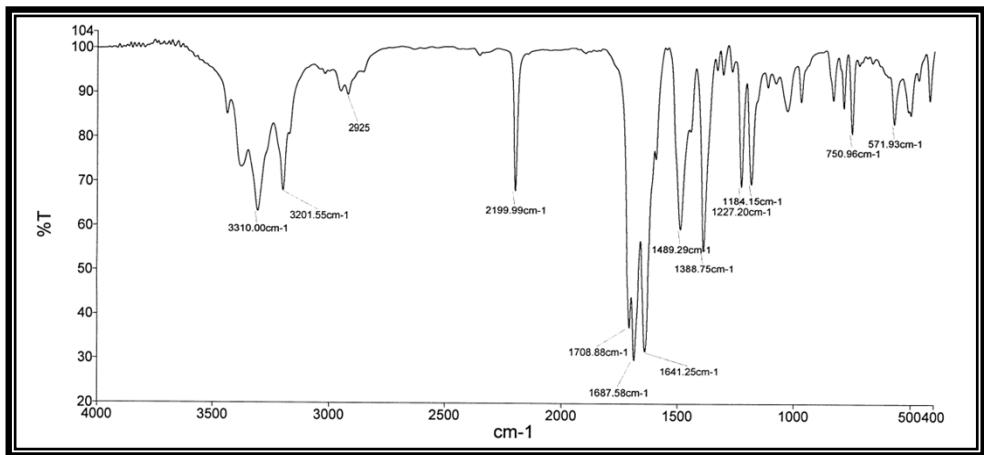
**Fig. S23.** The <sup>1</sup>H NMR spectrum of 7-Amino-5-phenyl-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d]

**7-Amino-5-(4-methylphenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile**

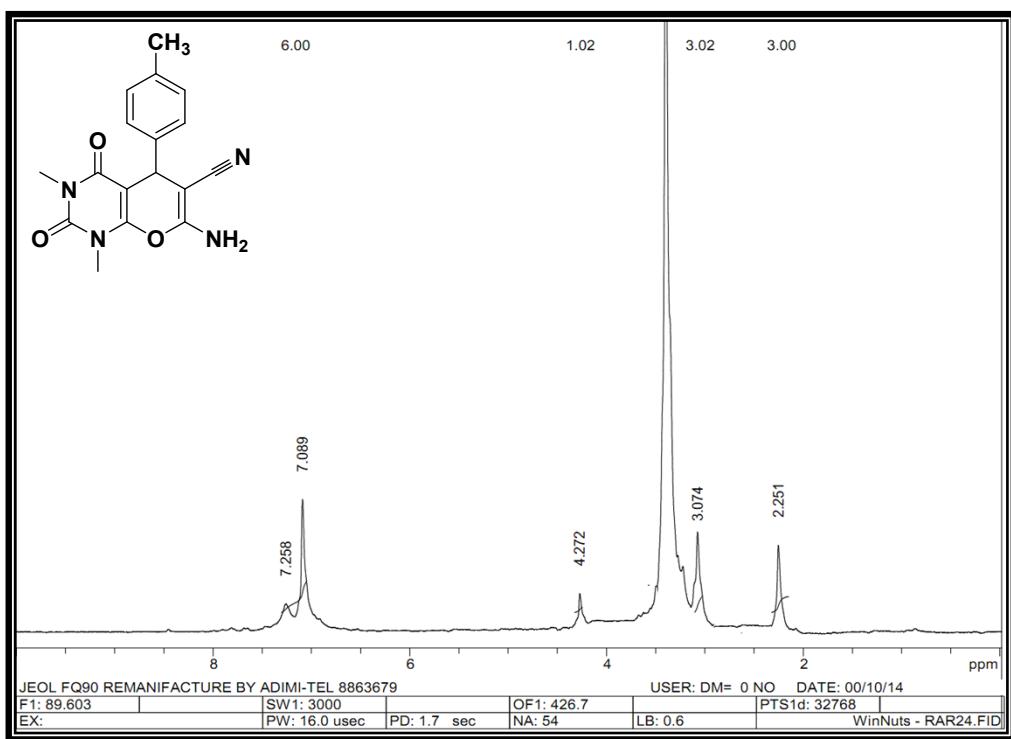


White solid; mp 217-218 °C (mp 221-223°C); IR(KBr,Cm<sup>-1</sup>) $\nu_{\text{max}} = \text{????,} 3310, 3201, 2925, 2199, 1708, 1687, 1641, 1489, 1388, 1227, 1184, 750, 571$ ; <sup>1</sup>HNMR(90 MHZ,DMSO-d<sub>6</sub>) $\delta$ :

2.25 (s,3H, Me), 3.07 (s,3H,NMe), 3.39 (s,3H,NMe), 4.27 (s,1H,CH), 6.93-7.40(m,6H, Ar-H and NH2)

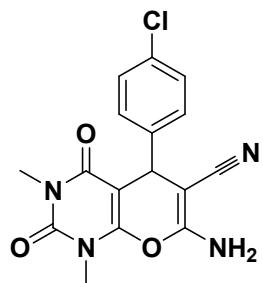


**Fig. S24.** The IR spectrum of 7-Amino-5-(4-methylphenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile



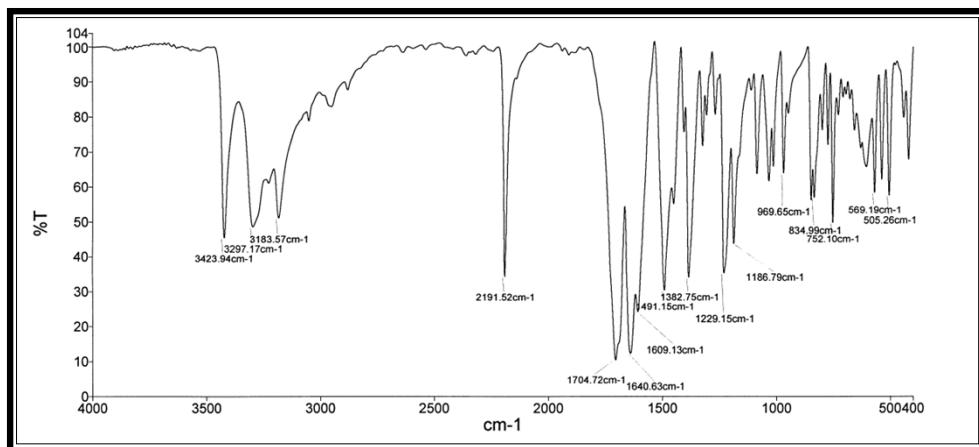
**Fig. S25.** The  $^1\text{H}$  NMR spectrum of 7-Amino-5-(4-methylphenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile

**7-Amino-5-(4-chlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile**

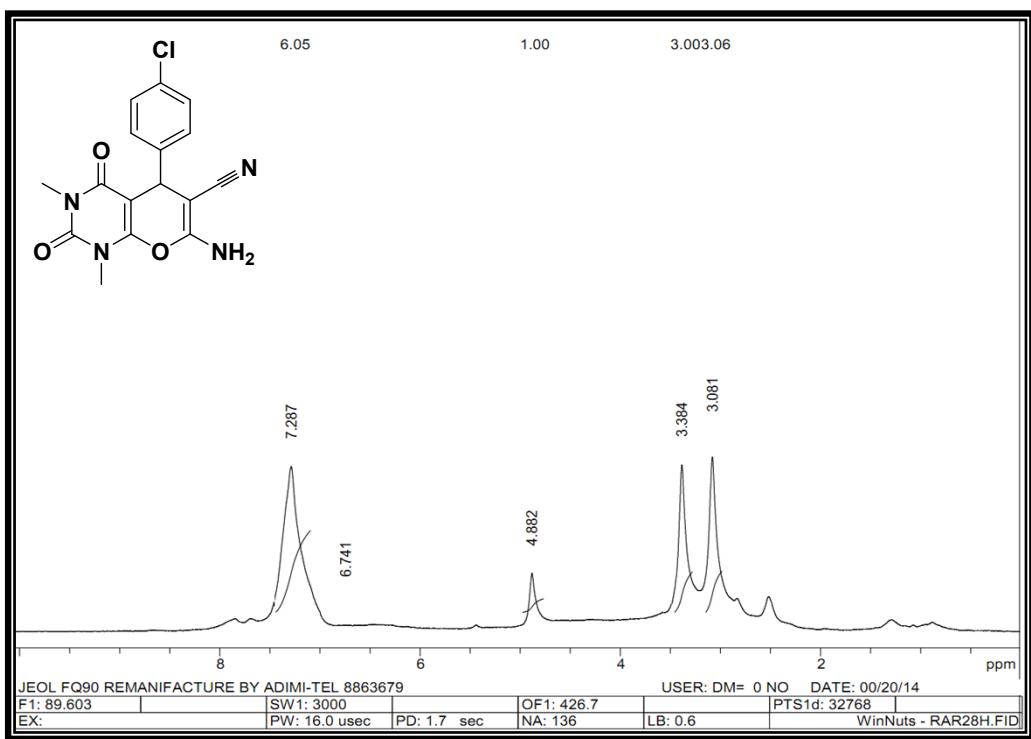


White solid; mp 206 °C (mp 206-208°C ); IR(KBr,Cm<sup>-1</sup>) $\nu_{\text{max}}= 3423, 3297, 3183, 2955, 2191, 1704, 1640, 1491, 1382, 1229, 1186, 969, 834;$

<sup>1</sup>HNMR(90MHZ,DMSO-d<sub>6</sub>) $\delta$ :3.21(s,3H,NMe), 3.47(s,3H,NMe), 4.46(s,1H,CH), 6.73(brs, 2H,NH<sub>2</sub>), 7.25(s,4H, Ar-H)

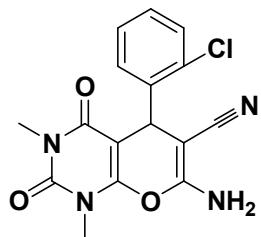


**Fig. S26.** The IR spectrum of 7-Amino-5-(4-chlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile

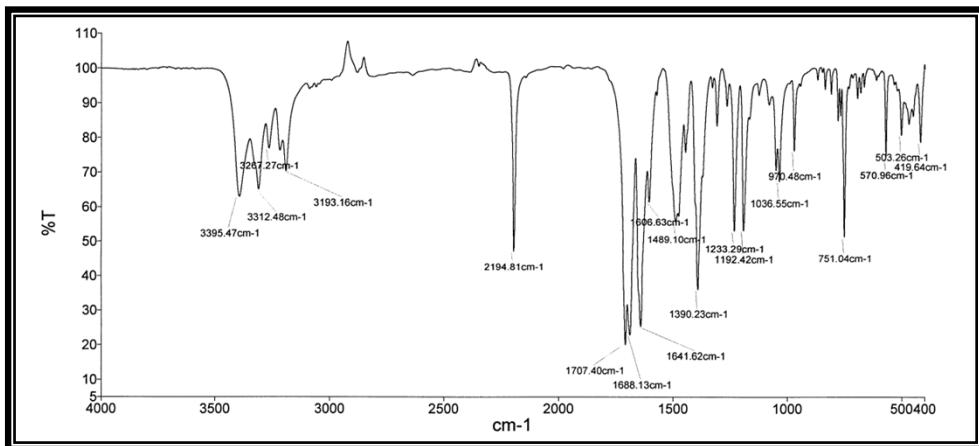


**Fig. S27.** The <sup>1</sup>H NMR spectrum of 7-Amino-5-(4-chlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d]

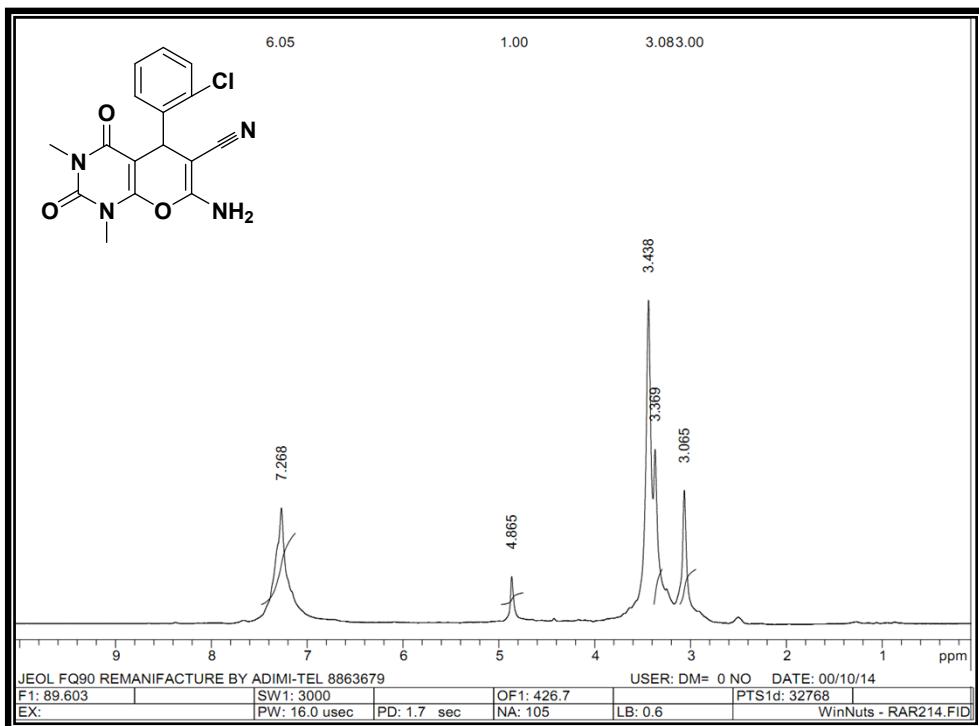
### 7-Amino-5-(2-chlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile



White solid; mp 243-244 °C (mp 238-239°C); IR(KBr, Cm<sup>-1</sup>) ν<sub>max</sub> = 3395, 3312, 3193, 2194, 1707, 1688, 1641, 1489, 1390, 1233, 1192, 1036, 970, 751, 570; <sup>1</sup>HNMR( 400 MHZ, DMSO-d<sub>6</sub>): δ= 3.06 (s,3H,NMe), 3.36 (s,3H,NMe), 4.86 (s,1H,CH), 6.98-7.49(m,5H,Ar-H and NH2)

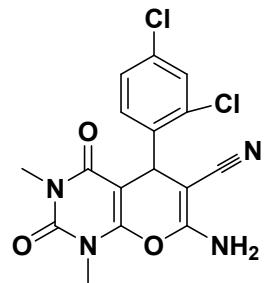


**Fig. S28.** The IR spectrum of 7-Amino-5-(2-chlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile

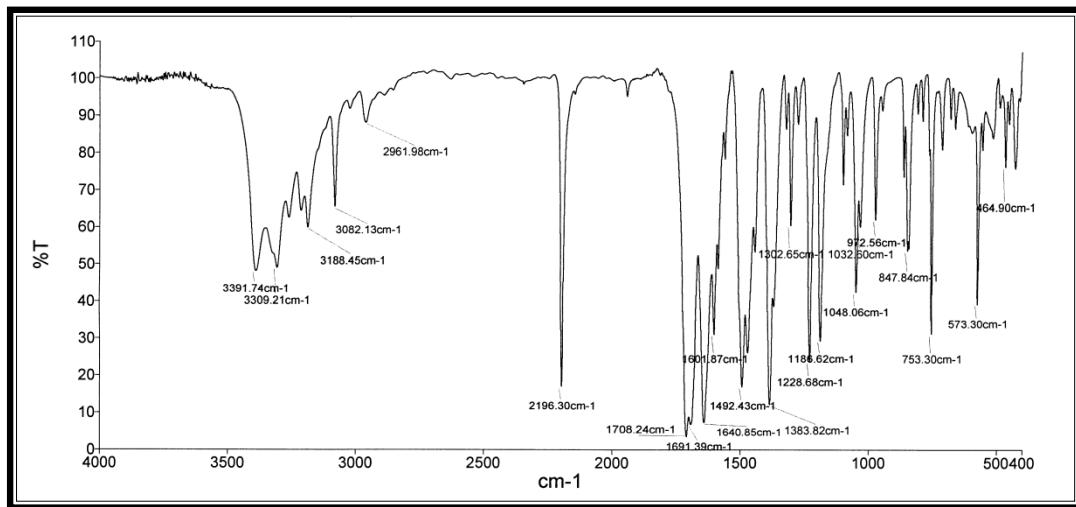


**Fig. S29.** The  $^1\text{H}$  NMR spectrum of 7-Amino-5-(2-chlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile

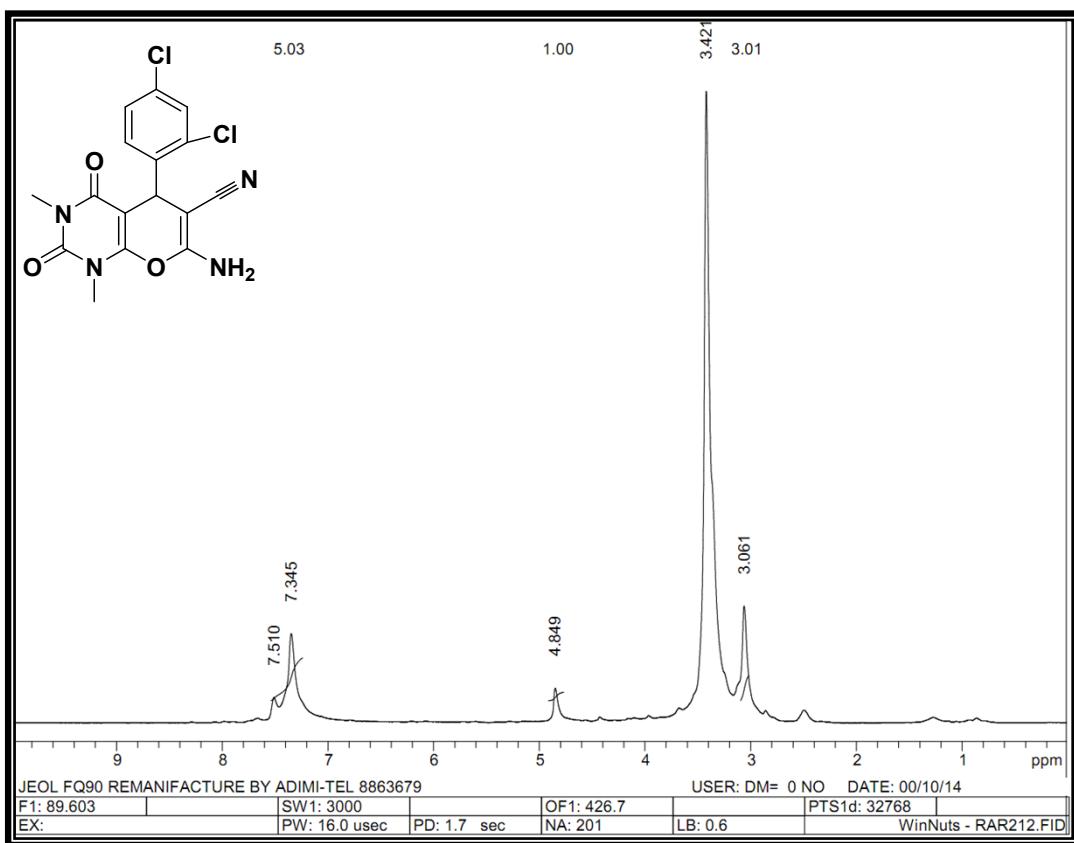
**7-Amino-5-(2,4-dichlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile**



White solid; mp 211-212 °C(mp193-195°C ); IR(KBr,Cm<sup>-1</sup>) $\nu_{max}$ = 3391, 3309, 3188, 3082, 2961, 2196, 1708, 1691, 1640, 1492, 1383, 1228, 1186, 1048, 847, 753, 573;  
<sup>1</sup>HNMR( 90MHZ,DMSO-d<sub>6</sub>):  $\delta$ = 3.06 (s,3H,NMe), 3.37 (s,3H,NMe), 4.84 (s,1H,CH), 6.57-7.50 (m,5H,Ar-H and NH2)

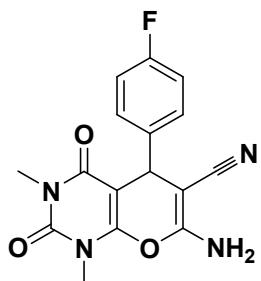


**Fig. S30.** The IR spectrum of 7-Amino-5-(2,4-dichlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile

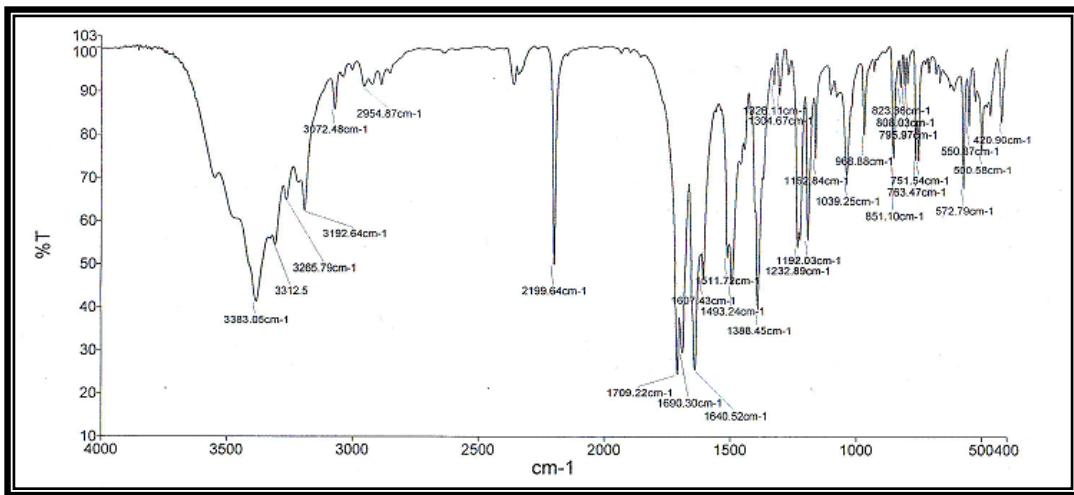


**Fig. S31.** The  $^1\text{H}$  NMR spectrum of 7-Amino-5-(2,4-dichlorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d]

**7-Amino-5-(4-fluorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d]**

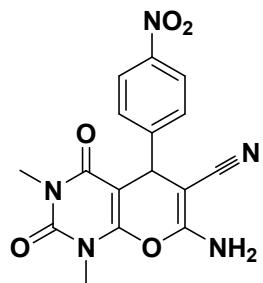


White solid; mp 227-228 °C (mp 230-232°C); IR(KBr,Cm $^{-1}$ ) $\nu_{\text{max}}$ = 3381, 3309, 3192, 2955, 2199, 1709, 1688, 1641, 1493, 1387, 1225, 1191, 1084, 1039

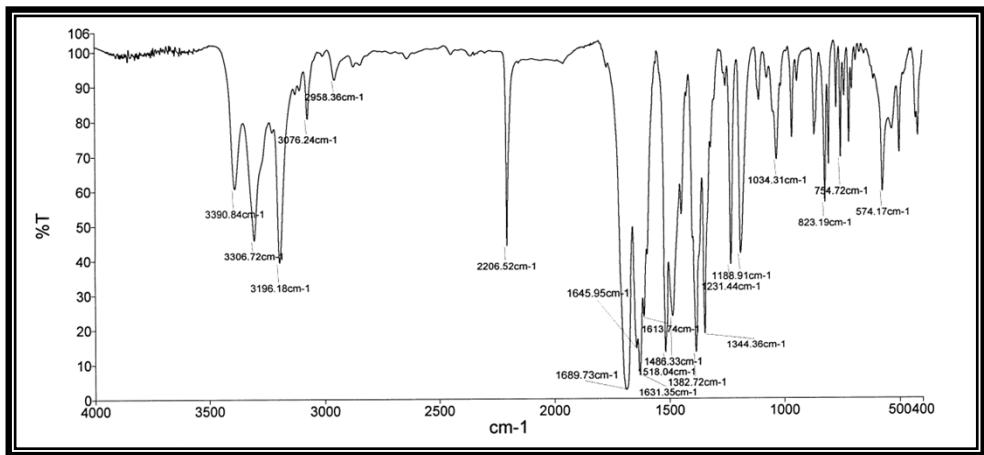


**Fig. S32.** The IR spectrum of 7-Amino-5-(4-fluorophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d]

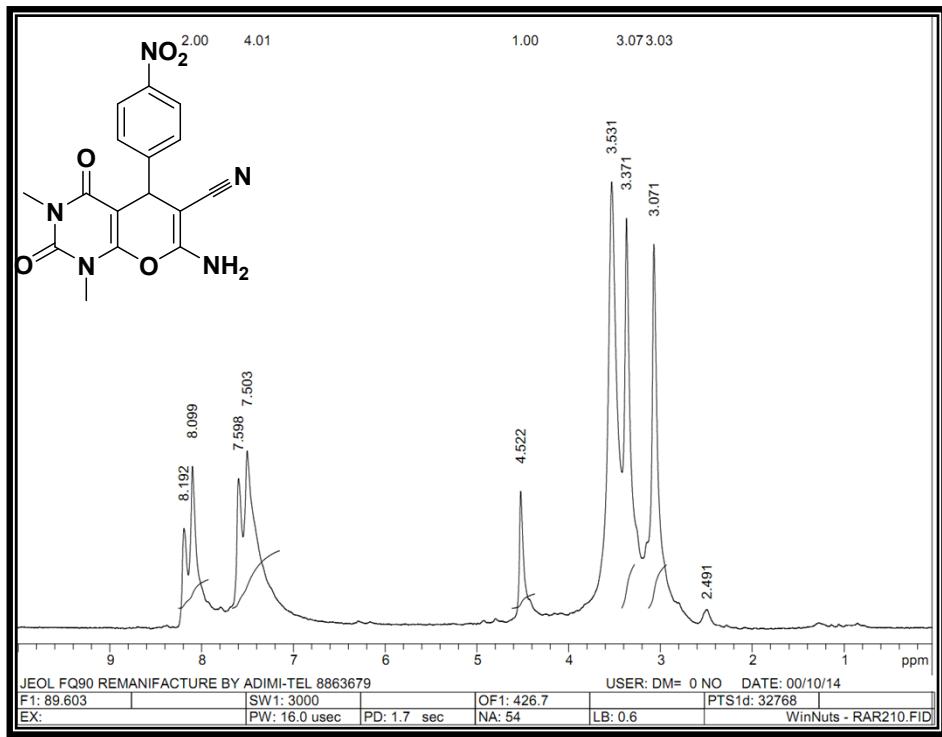
**7-Amino-5-(4-nitrophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile**



White solid; mp 217-219 °C (mp 212°C ); IR(KBr,Cm<sup>-1</sup>) $\nu_{max}$ = 3390, 3306, 3196, 3076, 2958, 2206, 1689, 1645, 1631, 1518, 1486, 1382, 1231, 1188, 1034, 823, 754, 574; <sup>1</sup>HNMR( 90MHZ,DMSO-d<sub>6</sub>): δ= 3.07 (s,3H,NMe), 3.37 (s,3H,NMe), 4.52 (s,1H,CH), 7.18-8.24(m,6H,Ar-H and NH2)

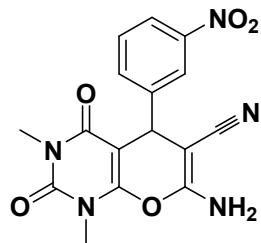


**Fig. S33.** The IR spectrum of 7-Amino-5-(4-nitrophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d] pyrimidine-6-carbonitrile

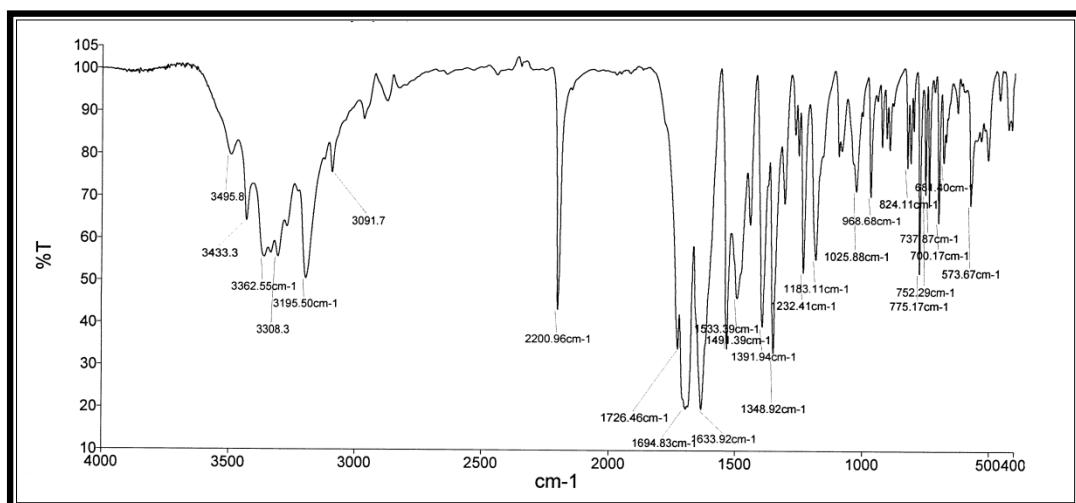


**Fig. S34.** The  $^1\text{H}$  NMR spectrum of 7-Amino-5-(4-nitrophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d] pyrimidine-6-carbonitrile

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

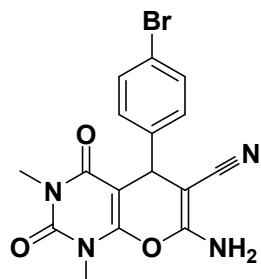


White solid; mp 204 °C; IR(KBr,Cm<sup>-1</sup>) $\nu_{\text{max}} = 3433, 3362, 3308, 3195, 3091, 2200, 1694, 1633, 1491, 1348, 1232, 1183, 1025, 968, 775, 573$

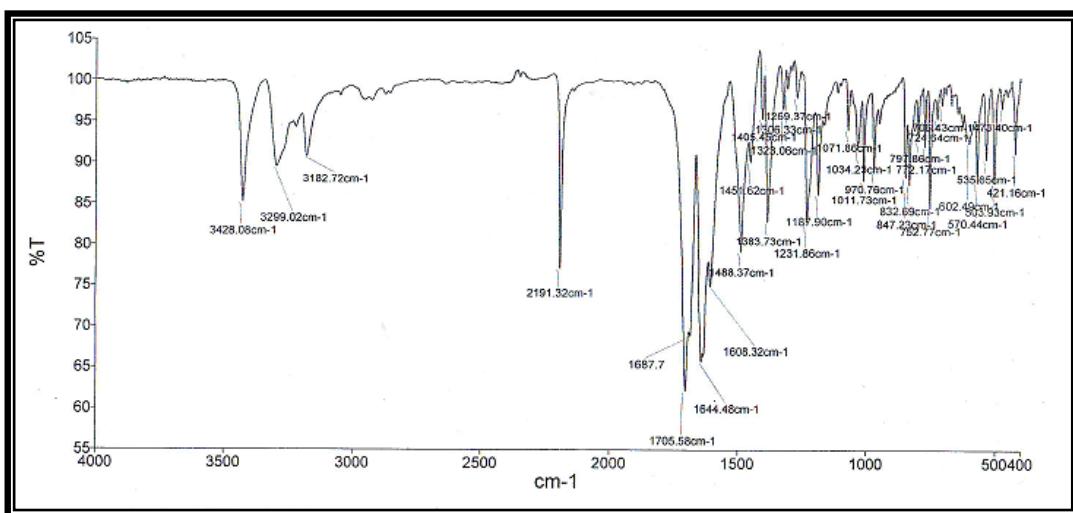


**Fig. S35.** The IR spectrum of 7-Amino-5-(4-bromophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile

**7-Amino-5-(4-bromophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile**

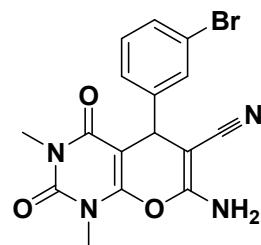


White solid; mp 235 °C (mp 235-237°C); IR(KBr,Cm<sup>-1</sup>) $\nu_{\text{max}} = 3428, 3300, 3184, 2952, 2191, 1705, 1687, 1643, 1607, 1489, 1384, 1231, 1187$

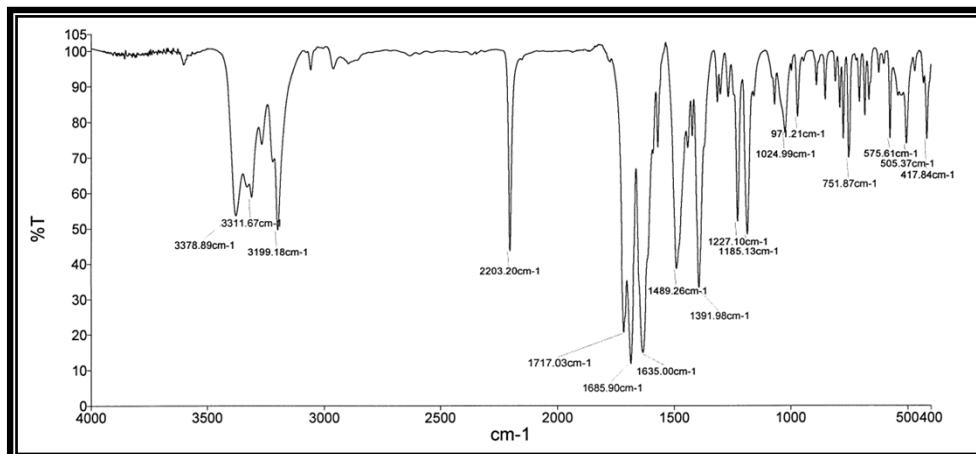


**Fig. S36.** The IR spectrum of 7-Amino-5-(3-nitrophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d]

**7-Amino-5-(3-bromophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d]**

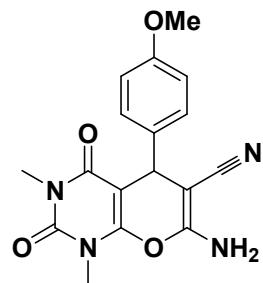


White solid; mp 209°C (mp 217-218°C); IR(KBr,Cm⁻¹)  $\nu_{\text{max}}=3378, 3311, 3199, 2203, 1717, 1685, 1635, 1489, 1391, 1227, 1185, 1024, 971, 751, 575$

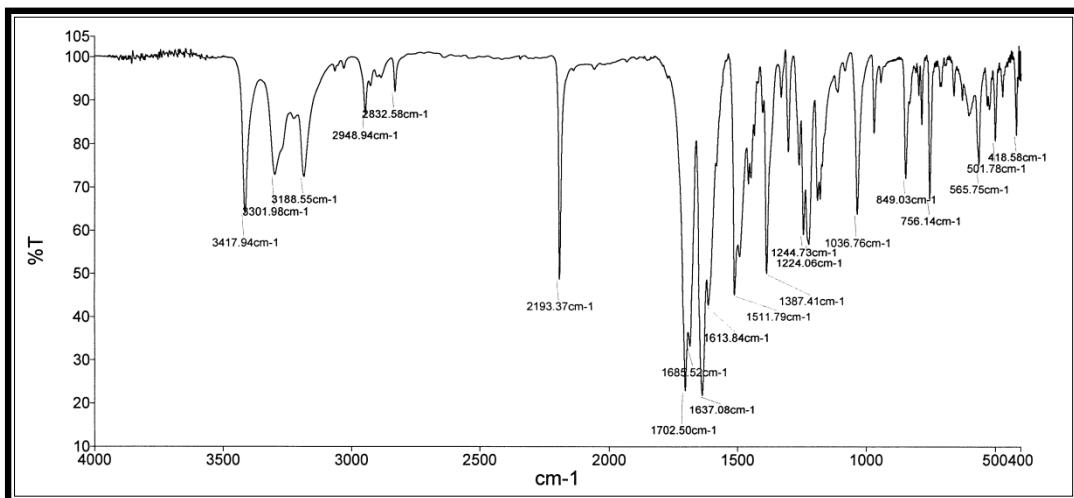


**Fig. S37.** The IR spectrum of 7-Amino-5-(3-bromophenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyranopyrimidine-6-carbonitrile [2,3-d]

**7-Amino-5-(4-methoxyphenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile**



White solid; mp 226-227°C (mp 225-227°C); IR(KBr,Cm<sup>-1</sup>) $\nu_{max}$ =3417, 3301, 3188, 2948, 2832, 2193, 1702, 1685, 1637, 1613, 1511, 1387, 1224, 1036, 849, 756, 565



**Fig. S38.** The IR spectrum of 7-Amino-5-(4-methoxyphenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,5-tetrahydro-1H-pyrano [2,3-d] pyrimidine-6-carbonitrile

