

Supplementary Information

DIPEAc promoted one-pot synthesis of dihydropyrido[2,3-d:6,5-d']dipyrimidinetetraone and pyrimido[4,5 d]pyrimidine derivatives as potent tyrosinase inhibitors and anticancer agents: *in vitro* screening, Molecular docking and ADMET predictions

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Experimental

Chemistry

General: All the chemicals used were of laboratory grade. Melting points of all the synthesized compounds were determined in open capillary tubes and are uncorrected. ¹H NMR and ¹³C NMR spectra were recorded with a Bruker Avance 400 spectrometer operating at 400 and 100 MHz using DMSO-*d*₆ solvent and tetramethylsilane (TMS) as the internal standard and chemical shift in δ ppm. Mass spectra were recorded on a Sciex, Model; API 3000 LCMS/MS Instrument. The progress of reaction was checked by TLC using silica-gel, 60F₂₅₄ aluminum sheets as adsorbent and visualization was accomplished by iodine/ultraviolet light. All compounds were known and IR, ¹H, ¹³C NMR spectra were found to be identical to the ones described in literature.¹⁷

General procedure for the synthesis of dihydropyrido[2,3-*d*:6,5-*d'*]dipyrimidinetetraone (**3a-k**)

A mixture of substituted aldehydes (**1a-k**) (1 mmole), barbituric acid (**2a**) (2 mmole) and ammonium acetate (2 mmole) were added in DIPEAc (5 ml). The resulting mixture was stirred at room temperature. The progress of the reaction was monitored by thin layer chromatography. After 45 min of stirring the reaction mixture was poured on crushed ice. Solid obtained was filtered and washed with water. Dried solid crystallised from ethanol to afford the purified desired product. Synthesized compounds characterized by IR, ¹H, ¹³C NMR spectra and were found to be identical to the ones described in literature.¹⁷

5-(Benzyl)-1,3,5,7,9,10-hexahydropyrimido[5',4'-5,6]pyridine[2,3-*d*]pyrimidine-2,4,6,8-tetraone (**3a**)

White solid, yield 95%; m.p. 279-280 °C; IR (ATR, ν cm⁻¹): 3551 (CONH stretching), 3478 (CONH stretching) 3198 (N-H stretching), 2860 (C-H stretching), 1710, 1680, 1600 (C=O stretching), 1460, 1221, 1010, 830, 780. ¹H NMR (400 MHz, DMSO-*d*₆, ppm): 11.53 (s, 2H, NH), 11.22 (s, 2H, NH), 10.02 (br.s, NH), 7.11-7.15 (d, 2H, Ar-H), 7.26-7.31 (m, 3H, Ar-H), 5.95 (s, 1H, pyrimidine). ¹³CNMR (100 MHz, DMSO-*d*₆, ppm): 169.87 (2C), 163.74 (2C), 154.23 (2C), 146.79, 138.71, 129.13 (2C), 128.43 (2C), 125.54, 87.89, 41.36. Mass (LCMS): m/z 326 [M+H]⁺. Anal. calcd. For C₁₅H₁₁N₅O₄: N: 21.53; C: 55.39; H: 3.41; Found: N: 21.49; C: 55.40; H: 3.47%.

5-(4-Methoxyphenyl)-1,3,5,7,9,10-hexahydropyrimido[5',4'-5,6]pyridine [2,3-d] pyrimidine-2,4,6,8-tetraone (**3b**)

White solid, yield 91%; mp >300 °C; IR (ATR, ν cm^{-1}): 3559 (CONH stretching), 3477 (CONH stretching) 3195 (N-H stretching), 2859 (C-H stretching), 1718, 1683, 1609 (C=O stretching), 1465, 1228, 1022, 826, 785. ^1H NMR (400 MHz, DMSO-*d*₆, ppm): 10.08 (s, br. 2H, NH), 7.12-7.29 (m, 4H, Ar-H), 5.99 (s, 2H, NH) 4.86 (s, 1H, pyrimidine), 3.75 (s, 3H, OCH₃). ^{13}C NMR (100 MHz, DMSO-*d*₆, ppm): 169.92 (2C), 163.38 (2C), 157.28, 154.56 (2C), 146.49, 138.31, 130.73 (2C), 118.51 (2C), 87.45, 59.16, 41.32. Mass (LCMS): m/z 356 [M+H]⁺. Anal. calcd. For C₁₆H₁₃N₅O₅: N: 19.71, C: 54.09, H: 3.69; Found: N: 19.67; C: 54.14; H: 3.67%.

5-(4-Methylphenyl)-1,3,5,7,9,10-hexahydropyrimido[5',4'-5,6]pyridine [2,3-d] pyrimidine-2,4,6,8-tetraone (**3c**)

White solid, yield 89 %; mp 290-292 °C; IR (ATR, ν cm^{-1}): 3560 (CONH stretching), 3469 (CONH stretching) 3187 (N-H stretching), 2843 (C-H stretching), 1705, 1675, 1623 (C=O stretching), 1463, 1230, 1063, 824, 781. ^1H NMR (400 MHz, DMSO-*d*₆, ppm): 10.12 (s, br. 2H, NH), 7.09-7.25 (m, 4H, Ar-H), 5.98 (s, 2H, NH) 4.89 (s, 1H, pyrimidine), 2.46 (s, 3H, OCH₃). ^{13}C NMR (100 MHz, DMSO-*d*₆, ppm): 169.57 (2C), 162.98 (2C), 157.24, 154.57 (2C), 139.51, 138.75, 130.23 (2C), 124.13 (2C), 87.78, 41.32, 37.38. Mass (LCMS): m/z 340 [M+H]⁺. Anal. calcd. For C₁₆H₁₃N₅O₄: N: 20.64, C: 56.64; H: 3.86; Found: N: 20.67; C: 55.87; H: 3.85%.

5-(4-Chlorophenyl)-1,3,5,7,9,10-hexahydropyrimido[5',4'-5,6]pyridine[2,3-d]pyrimidine-2,4,6,8-tetraone (**3d**)

White solid, yield 92 %; mp >300 °C; IR (ATR, ν cm^{-1}): 3572 (CONH stretching), 3468 (CONH stretching) 3178 (N-H stretching), 2851 (C-H stretching), 1709, 1672, 1630 (C=O stretching), 1465, 1238, 1071, 822, 780. ^1H NMR (400 MHz, DMSO-*d*₆, ppm): 11.39 (s, 2H, NH), 11.32 (s, 2H, NH), 10.37 (s, 1H, NH) 7.12-7.33 (m, 4H, Ar-H), 5.04 (s, 1H, pyrimidine). ^{13}C NMR (100 MHz, DMSO-*d*₆, ppm): 169.23 (2C), 162.76 (2C), 157.29, 154.55 (2C), 138.49, 137.68, 131.65 (2C), 123.27 (2C), 88.35, 37.21.

5-(3-Chlorophenyl)-1,3,5,7,9,10-hexahydropyrimido[5',4'-5,6]pyridine[2,3-d]pyrimidine-2,4,6,8-tetraone (**3e**)

White solid, yield 91 %; mp >300 °C; IR (ATR, ν cm^{-1}): 3571 (CONH stretching), 3469 (CONH stretching) 3180 (N-H stretching), 2853 (C-H stretching), 1711, 1673, 1629 (C=O stretching), 1467, 1240, 825, 787. ^1H NMR (400 MHz, DMSO-*d*₆, ppm): 11.30 (s, 2H, NH), 11.28 (s, 2H, NH), 10.35 (s, 1H, NH) 7.09-7.19 (m, 4H, Ar-H), 5.06 (s, 1H, pyrimidine). ^{13}C NMR (100 MHz, DMSO-*d*₆, ppm): 169.29 (2C), 161.89 (2C), 156.54, 154.52 (2C), 138.47, 137.89, 133.45 (2C), 122.78 (2C), 88.37, 37.22.

5-(4-Hydroxyphenyl)-1,3,5,7,9,10-hexahydropyrimido[5',4'-5,6]pyridine[2,3-d]pyrimidine-2,4,6,8-tetraone (**3f**)

Yellow solid, yield 95 %; mp >300 °C; IR (ATR, ν cm^{-1}): 3270 (CONH stretching), 3190 (N-H stretching), 2812 (C-H stretching), 1727, 1667 (C=O stretching), 1535, 1444, 1284, 885, 786. ^1H NMR (400 MHz, CDCl₃, ppm): 11.49 (s, 2H, NH), 11.25 (s, 2H, NH), 10.18 (s, 1H, NH) 7.21-7.40 (m, 2H, Ar-H), 7.18-7.20 (m, 2H, Ar-H) 5.18 (s, 1H, pyrimidine). ^{13}C NMR (100 MHz, DMSO-*d*₆, ppm): 159.96, 158.39, 153.82, 152.53, 143.74, 128.94, 128.04, 127.54, 125.08, 122.89, 119.67, 116.96, 113.35, 82.38, 37.37. Mass (LCMS): m/z 342 [M+H]⁺. Anal. calcd. For C₁₅H₁₁N₅O₅: N: 20.52; C: 52.79; H: 3.25; Found: N: 20.58; C: 52.80; H: 3.22%.

5-(2-Hydroxyphenyl)-1,3,5,7,9,10-hexahydropyrimido[5',4'-5,6]pyridine[2,3-d]pyrimidine-2,4,6,8-tetraone (**3g**)

Yellow solid, yield 87 %; mp 261-263 °C; IR (ATR, ν cm^{-1}): 3289 (CONH stretching), 3267 (N-H stretching), 2854 (C-H stretching), 1753, 1632 (C=O stretching), 1587, 1459, 1234, 853, 779. ^1H NMR (400 MHz, DMSO-*d*₆, ppm): 11.36 (s, 2H, NH), 11.21 (s, 2H, NH), 10.23 (s, 1H, NH) 7.23-7.45 (m, 2H, Ar-H), 7.09-7.19 (m, 2H, Ar-H) 5.12 (s, 1H, pyrimidine). ^{13}C NMR (100 MHz, DMSO-*d*₆, ppm): 168.96, 159.34, 153.37, 152.32, 144.67, 134.23, 128.75, 127.32, 125.89, 122.43, 121.67, 116.32, 115.76, 88.12, 37.40.

5-(2-Nitro phenyl)-1,3,5,7,9,10-hexahydropyrimido[5',4'-5,6]pyridine[2,3-d]pyrimidine-2,4,6,8-tetraone (**3h**)

White solid, yield 88 %; mp 256-258 °C; IR (ATR, ν cm^{-1}): 3343 (CONH stretching), 3421 (CONH stretching) 3183 (N-H stretching), 2870 (C-H stretching), 1743, 1662, 1629 (C=O stretching), 1470, 1237, 870, 795. ^1H NMR (400 MHz, DMSO-*d*₆, ppm): 11.39 (s, 2H, NH),

11.27 (s, 2H, NH), 10.48 (s, 1H, NH) 7.11-7.25 (m, 4H, Ar-H), 5.08 (s, 1H, pyrimidine). ¹³CNMR (100 MHz, DMSO-*d*₆, ppm): 168.96, 162.39, 158.82, 152.76, 143.32, 129.31, 128.64, 127.90, 125.32, 122.12, 121.67, 116.96, 115.42, 84.21, 37.46.

5-(4-(Dimethylamino) phenyl) -9,10-dihydropyrido [2,3-d:6,5-d'] dipyrimidine 2,4,6,8(1H,3H,5H,7H)-tetraone (**3i**)

Orange solid, yield 90 %; mp 286-288 °C; IR (ATR, ν cm⁻¹): 3414 (CONH stretching), 3160 (N-H stretching), 2817 (C-H stretching), 1657 (C=O stretching), 1458, 1243, 854, 791. ¹H NMR (400 MHz, CDCl₃, ppm): 11.51 (s, 2H, NH), 11.29 (s, 2H, NH), 10.51 (s, 1H, NH) 7.61-7.82 (m, 2H, Ar-H), 7.12-7.42 (m, 2H, Ar-H), 5.06 (s, 1H, pyrimidine), 2.45 (s, 6H, CH₃). ¹³CNMR (100 MHz, DMSO-*d*₆, ppm): 162.74 (2C), 158.85 (2C), 142.23, 136.06 (2C), 129.30, 127.49, 120.19 (2C), 111.28 (2C), 85.87, 50.40, 35.59. Mass (LCMS): *m/z* 369 [M+H]⁺. Anal. calcd. For C₁₇H₁₆N₆O₄: N: 22.82; C: 55.43; H: 4.38; Found: N: 22.88; C: 55.46; H: 4.40%.

5-(3,4-Dimethoxyphenyl)-9,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,5H,7H)-tetraone (**3j**)

Pale yellow solid, yield 89 %; mp 294-296 °C; IR (ATR, ν cm⁻¹): 3325 (CONH stretching), 3145 (N-H stretching), 2865 (C-H stretching), 1720, 1689 (C=O stretching), 1426, 1267, 880, 787. ¹H NMR (400 MHz, DMSO-*d*₆, ppm): 11.39 (s, 2H, NH), 11.24 (s, 2H, NH), 10.34 (s, 1H, NH) 7.09-7.78 (m, 3H, Ar-H), 5.13 (s, 1H, pyrimidine), 3.57 (s, 6H, OCH₃), 2.33 (s, 3H, CH₃). ¹³CNMR (100 MHz, DMSO-*d*₆, ppm): 167.45 (2C), 159.48 (2C), 142.76, 136.64 (2C), 129.27, 127.68, 121.89, 120.65, 118.49 (2C), 85.59, 55.87, 37.13.

5-Butyl-9,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,5H,7H)-tetraone (**3k**)

Yellow solid, yield 87 %; mp 232-234 °C; IR (ATR, ν cm⁻¹): 3176 (CONH stretching), 2870 (C-H stretching), 1767, 1659 (C=O stretching), 1489, 1245, 838, 723. ¹H NMR (400 MHz, DMSO-*d*₆, ppm): 11.32 (s, 2H, NH), 11.29 (s, 2H, NH), 10.17 (s, 1H, NH), 3.67 (t, 1H, *J* = 7.1 Hz, pyrimidine), 1.58-1.48 (m, 2H, CH₂), 1.27-1.23 (m, 2H, CH₂), 1.18-1.12 (m, 2H, CH₂), 0.89 (t, 3H, *J* = 7.2 Hz, CH₃). ¹³C NMR (100 MHz, DMSO-*d*₆ ppm): 168.76 (2C), 162.82 (2C), 154.50 (2C), 87.35, 36.45, 31.17, 25.35, 18.04, 14.25.

General Procedure for the synthesis of pyrimido(-4,5-d) pyrimidine (**4a-g**)

A mixture of substituted aldehydes (**1a-k**) (1 mmole), barbituric acid (**2a**) (2 mmole) and urea (2 mmole) were added in DIPEAc (5 ml). The resulting mixture was stirred at room temperature. The progress of the reaction was monitored by thin layer chromatography. After 45 min of stirring the reaction mixture was poured on crushed ice. Solid obtained was filtered and washed with water. Dried solid crystallized from ethanol to afford the purified desired product. Synthesized compounds characterized by IR, ¹H, ¹³C NMR spectra and were found to be identical to the ones described in literature.¹⁷

5,6-Dihydro-5-(benzyl)pyrimido[4,5-d]pyrimidine-2,4,7(1H,3H,8H)-trione (**4a**).

Off white solid, yield 92 %; mp 245-247 °C; IR (ATR, ν cm⁻¹): 3525 (CONH stretching), 2372 (C-H stretching), 1672, 1623 (C=O stretching), 1453, 1227, 1063, 827, 793. ¹H NMR (400 MHz, DMSO-*d*₆, ppm): 11.28 (s, 1H, NH), 11.25 (s, 1H, NH), 8.39 (s, 1H, NH), 7.23-7.35 (m, 5H, A-H), 5.47 (s, 1H). ¹³CNMR (100 MHz, DMSO-*d*₆, ppm): 163.69, 157.24, 154.57, 143.35, 138.75, 128.23 (2C), 127.41 (2C), 124.13, 90.71, 47.28. Mass (LCMS): m/z 259 [M+H]⁺. Anal. calcd. For C₁₂H₁₀N₄O₃: N: 21.70, C: 55.81; H: 3.90; Found: N: 21.69; C: 55.85; H: 3.90%.

5,6-Dihydro-5-(4-methoxyphenyl)pyrimido[4,5-d]pyrimidine-2,4,7(1H,3H,8H)-trione (**4b**)

Yellow solid, yield 83 %; mp 285-286 °C; IR (ATR, ν cm⁻¹): 3478 (CONH stretching), 2372 (C-H stretching), 1672, 1623 (C=O stretching), 1452, 1235, 1067, 854, 790. ¹H NMR (400 MHz, DMSO-*d*₆, ppm): 11.27 (s, 1H, NH), 11.25 (s, 1H, NH), 8.36 (s, 1H, NH), 7.12-7.27 (m, 4H, A-H), 5.43 (s, 1H), 3.54 (s, 3H OCH₃). ¹³CNMR (100 MHz, DMSO-*d*₆, ppm): 163.39, 157.53, 154.86, 143.23, 138.90, 128.74 (2C), 126.31 (2C), 124.24, 90.49, 59.59, 47.28. Mass (LCMS): m/z 290 [M+H]⁺. Anal. calcd. For C₁₃H₁₂N₄O₄: N: 19.44, C: 54.17, H: 4.20; Found: N: 19.44; C: 54.15; H: 4.27%.

5,6-Dihydro-5-(4-hydroxyphenyl)pyrimido[4,5-d]pyrimidine-2,4,7(1H,3H,8H)-trione (**4c**)

White solid, yield 90 %; mp 211-213 °C; IR (ATR, ν cm⁻¹): 3354 (CONH stretching), 2382 (C-H stretching), 1754, 1687 (C=O stretching), 1467, 1260, 1035, 867, 796. ¹H NMR (400 MHz, DMSO-*d*₆, ppm): 11.25 (s, 1H, NH), 11.19 (s, 1H, NH), 8.37 (s, 1H, NH), 7.09-7.26 (m, 4H, A-H), 5.39 (s, 1H). ¹³CNMR (100 MHz, DMSO-*d*₆, ppm): 167.45, 157.61, 154.69, 141.78, 137.99,

128.54 (2C), 127.78 (2C), 125.81, 89.47, 47.25. Mass (LCMS): m/z 275 $[M+H]^+$. Anal. calcd. For $C_{12}H_{10}N_4O_4$: N: 20.43, C: 52.56; H: 3.68; Found: N: 20.4 C: 52.59; H: 3.70 %.

5,6-Dihydro-5-(3-hydroxy-4-methoxyphenyl)pyrimido[4,5-d]pyrimidine-2,4,7(1H,3H,8H)-trione **(4d)**

Yellow solid, yield 89 %; mp 275-277 °C; IR (ATR, ν cm^{-1}): 3287 (CONH stretching), 2380 (C-H stretching), 1772, 1654 (C=O stretching), 1467, 1284, 1085, 836, 787. 1H NMR (400 MHz, DMSO-*d*₆, ppm): 11.26 (s, 1H, NH), 11.22 (s, 1H, NH), 8.35 (s, 1H, NH), 7.10-7.26 (m, 3H, A-H), 5.41 (s, 1H), 3.57 (s, 3H OCH₃). ^{13}C NMR (100 MHz, DMSO-*d*₆, ppm): 167.45, 158.49, 155.31, 149.62, 137.68, 127.32 (2C), 126.36, 125.67, 124.56, 89.89, 59.67, 47.25. Mass (LCMS): m/z 305 $[M+H]^+$. Anal. calcd. For $C_{13}H_{12}N_4O_5$: N: 18.41, C: 51.32; H: 3.98; Found: N: 18.45, C: 51.31; H: 3.95; %.

5,6-Dihydro-5-(4-bromophenyl)pyrimido[4,5-d]pyrimidine-2,4,7(1H,3H,8H)-trione **(4e)**

Off White solid, yield 91 %; mp 212-214 °C; IR (ATR, ν cm^{-1}): 3467 (CONH stretching), 2386 (C-H stretching), 1665, 1634 (C=O stretching), 1451, 1247, 1079, 832, 793. 1H NMR (400 MHz, DMSO-*d*₆, ppm): 11.26 (s, 1H, NH), 11.24 (s, 1H, NH), 8.37 (s, 1H, NH), 7.14-7.30 (m, 4H, A-H), 5.47 (s, 1H). ^{13}C NMR (100 MHz, DMSO-*d*₆, ppm): 165.43, 157.47, 154.23, 143.75, 138.79, 127.54 (2C), 126.98 (2C), 124.43, 90.27, 47.30. Mass (LCMS): m/z 336 $[M+H]^+$. Anal. calcd. For $C_{12}H_9BrN_4O_3$: N: 16.62; C: 42.75; H: 2.69; Found: N: 16.60; C: 42.77; H: 2.71%.

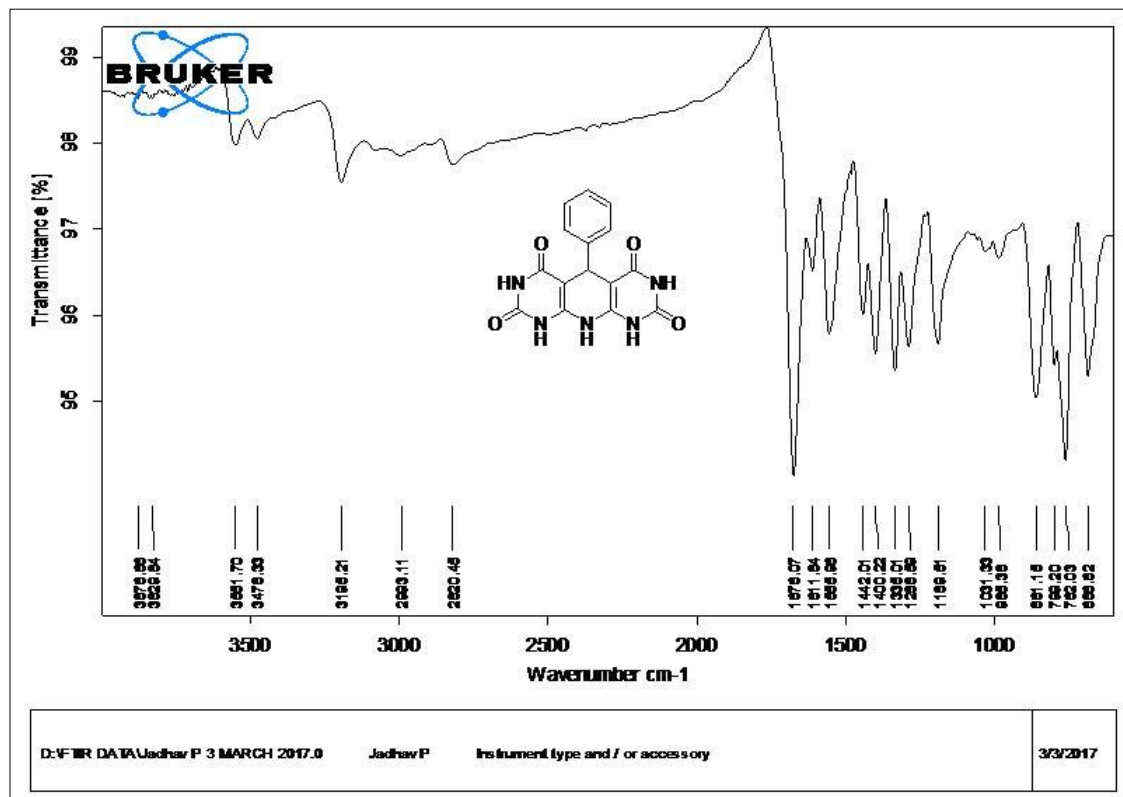
5-(4-(Dimethylamino)phenyl)-5,6-dihydropyrimido[4,5-d]pyrimidine-2,4,7(1H,3H,8H)-trione **(4f)**

Yellow solid, yield 84 %; mp 256-258 °C; IR (ATR, ν cm^{-1}): 3356 (CONH stretching), 2367 (C-H stretching), 1734, 1668 (C=O stretching), 1446, 1237, 1067, 854, 790. 1H NMR (400 MHz, DMSO-*d*₆, ppm): 11.27 (s, 1H, NH), 11.25 (s, 1H, NH), 8.36 (s, 1H, NH), 7.12-7.27 (m, 4H, A-H), 5.46 (s, 1H), 2.89 (s, 6H CH₃). ^{13}C NMR (100 MHz, DMSO-*d*₆, ppm): 165.67, 157.54, 154.23, 143.98, 140.57, 127.43 (2C), 126.59 (2C), 124.35, 90.17, 59.58, 47.22. Mass (LCMS): m/z 302 $[M+H]^+$. Anal. calcd. For $C_{14}H_{15}N_5O_3$: N: 23.24; C: 55.81; H: 5.02; Found: N: 23.26; C: 55.80; H: 5.07%.

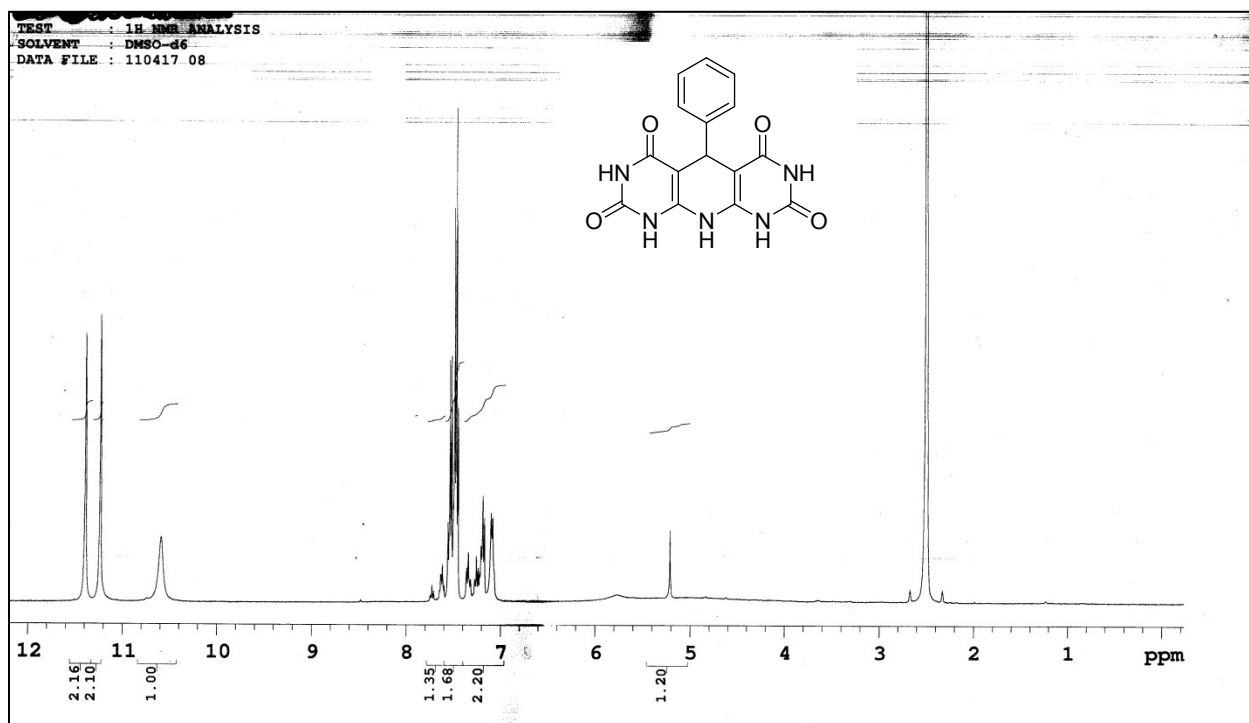
5-(Furan-2-yl)-5,6-dihydropyrimido[4,5-d]pyrimidine-2,4,7(1H,3H,8H)-trione (**4g**)

Yellow solid, yield 86 %; mp 274-276 °C; IR (ATR, ν cm^{-1}): 3265 (CONH stretching), 2381 (C-H stretching), 1680, 1646 (C=O stretching), 1454, 1276, 1089, 834, 787. ^1H NMR (400 MHz, DMSO-*d*₆, ppm): 11.28 (s, 1H, NH), 11.26 (s, 1H, NH), 8.31 (s, 1H, NH), 7.08-7.18 (m, 3H, A-H), 5.39 (s, 1H). ^{13}C NMR (100 MHz, DMSO-*d*₆, ppm): 167.46, 158.89, 154.87, 145.65, 127.78 (2C), 126.61, 124.65, 88.79, 47.25. Mass (LCMS): m/z 249 $[\text{M}+\text{H}]^+$. Anal. calcd. For $\text{C}_{10}\text{H}_8\text{N}_4\text{O}_4$: N: 22.57; C: 48.39; H: 3.25; Found: N: 22.60; C: 48.35; H: 3.30%.

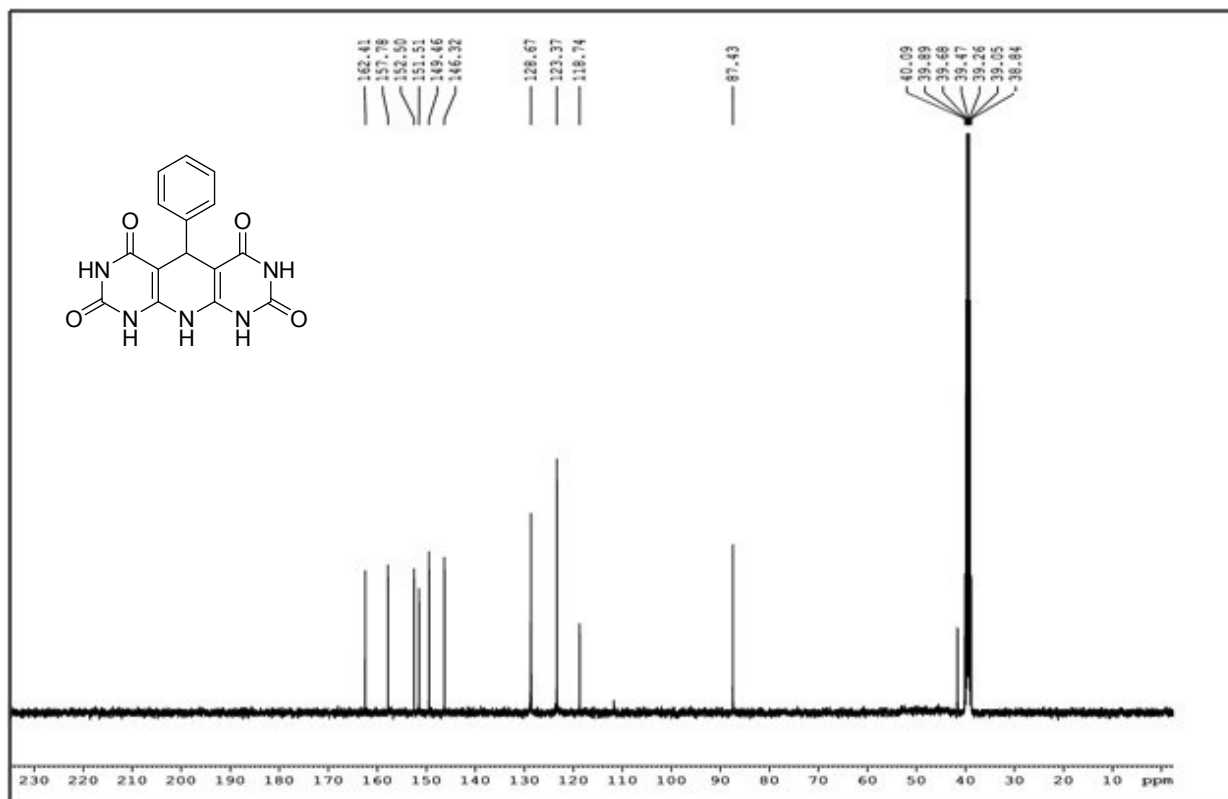
IR spectrum of Compound (3a)



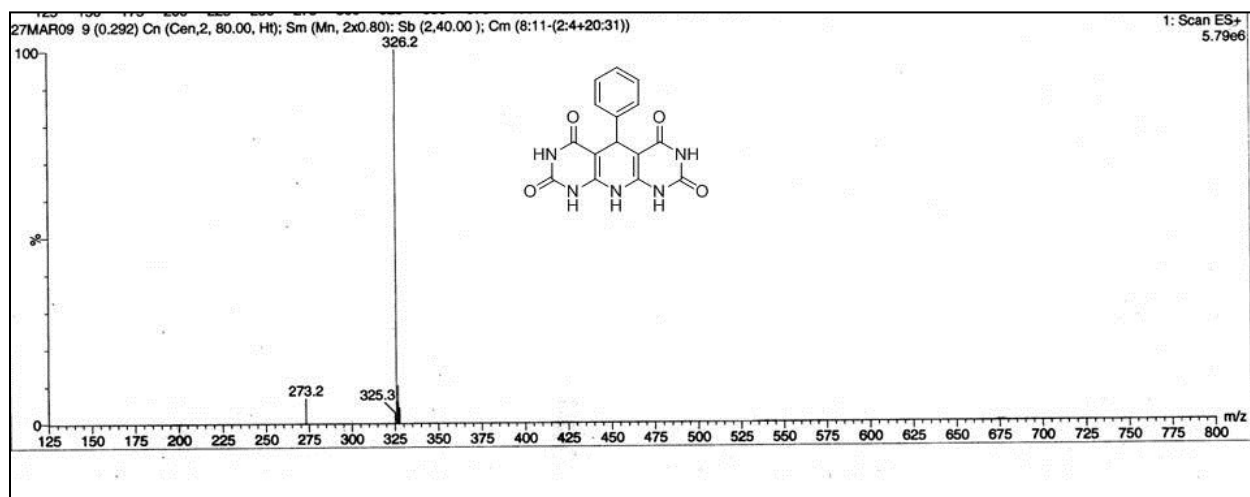
¹H NMR of Compound (3a)



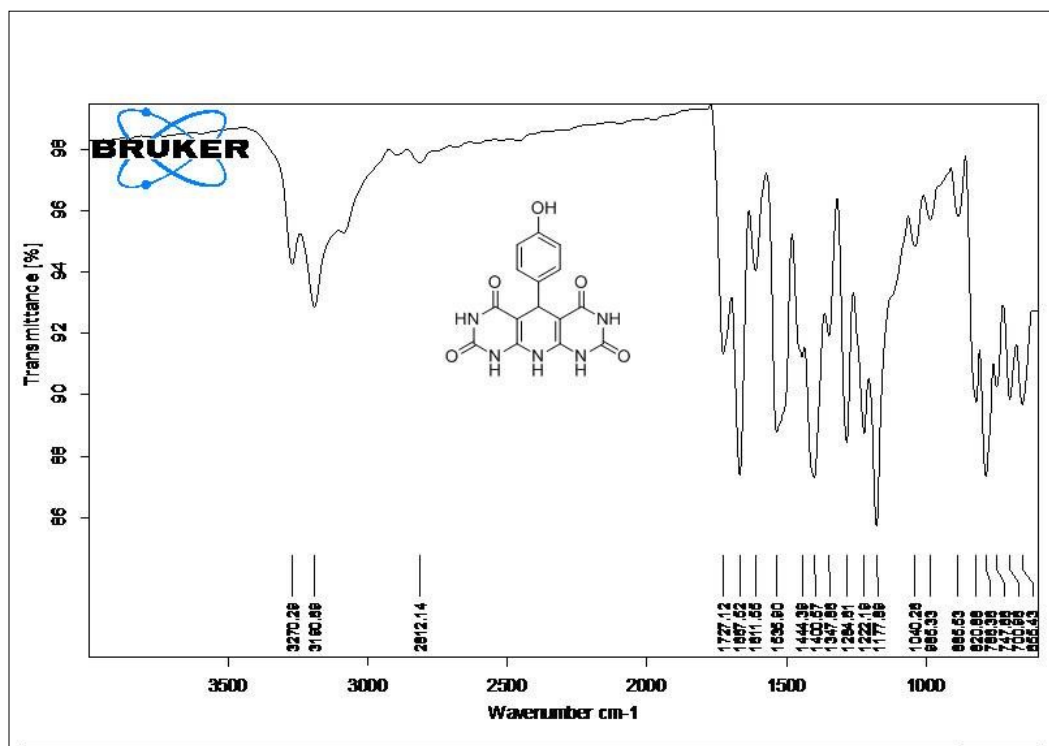
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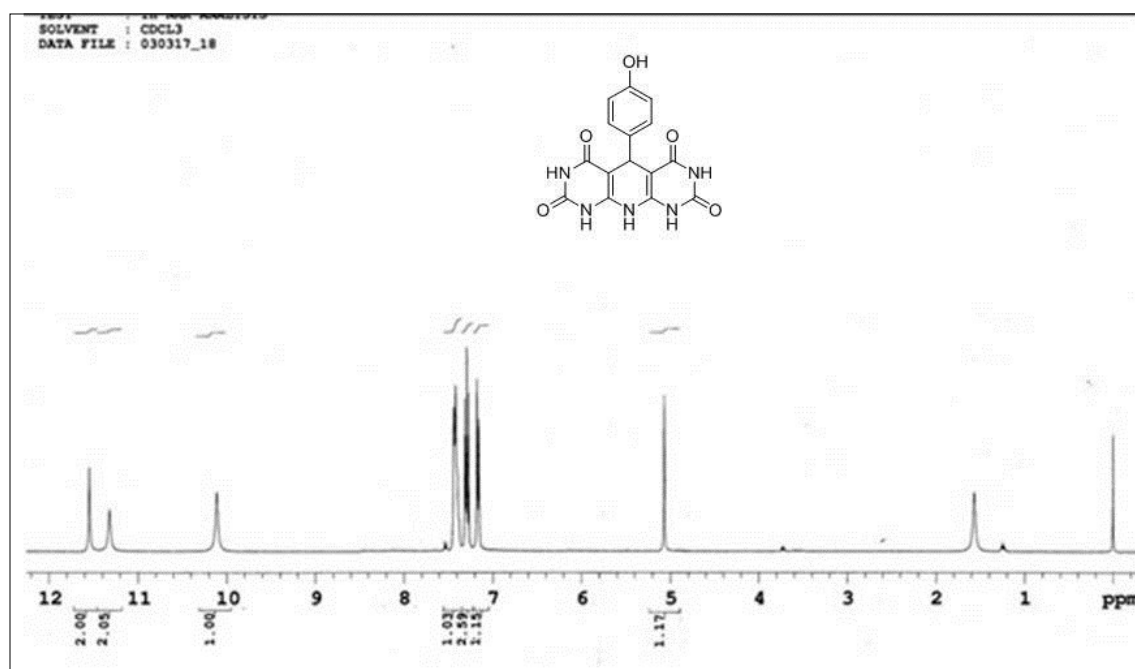
Mass of Compound (3a)



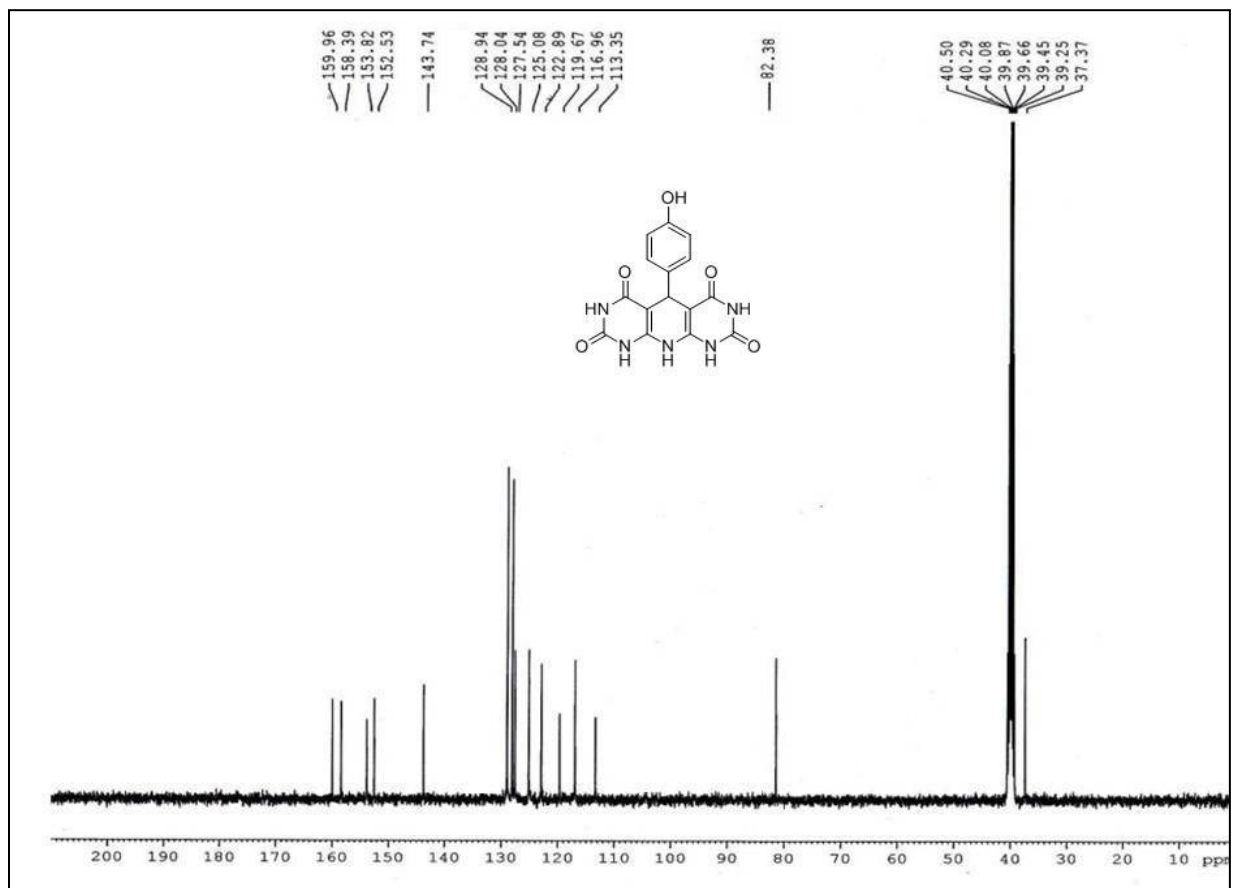
IR spectrum of Compound (3f)



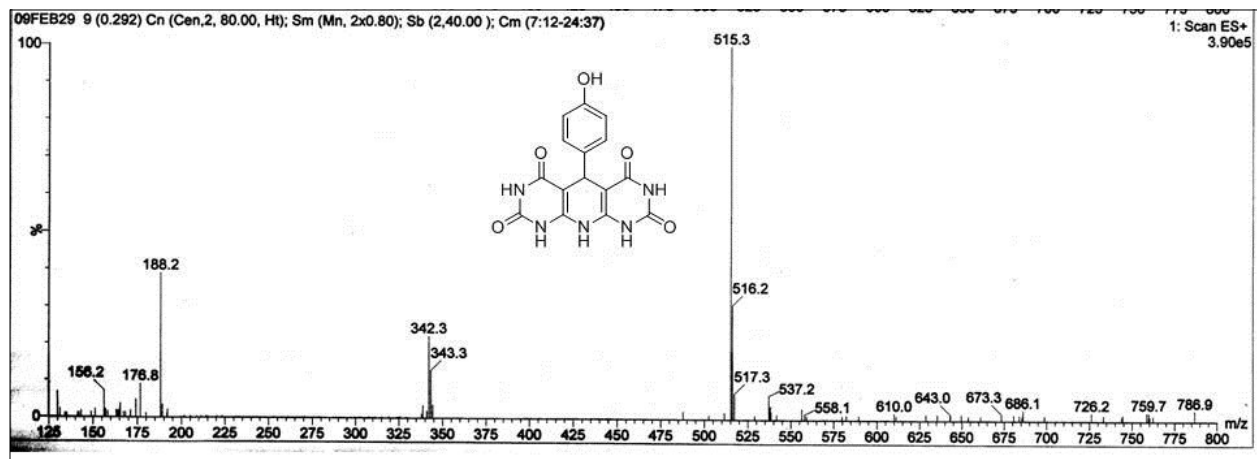
¹H NMR of Compound (3f)



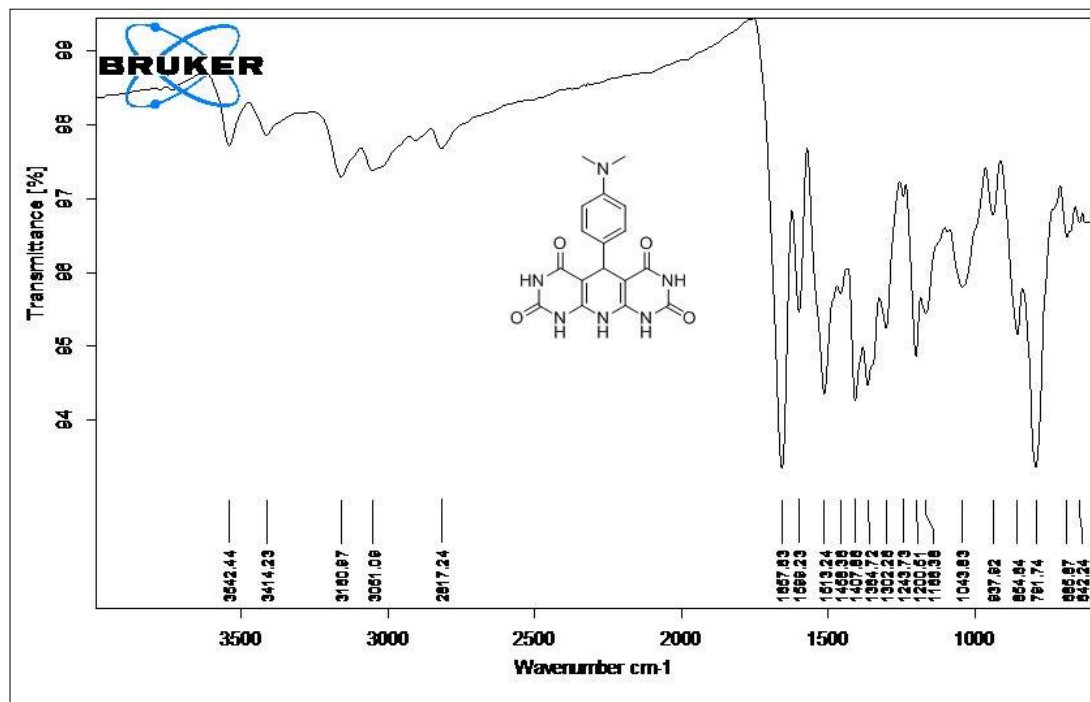
¹³C NMR of Compound (3f)



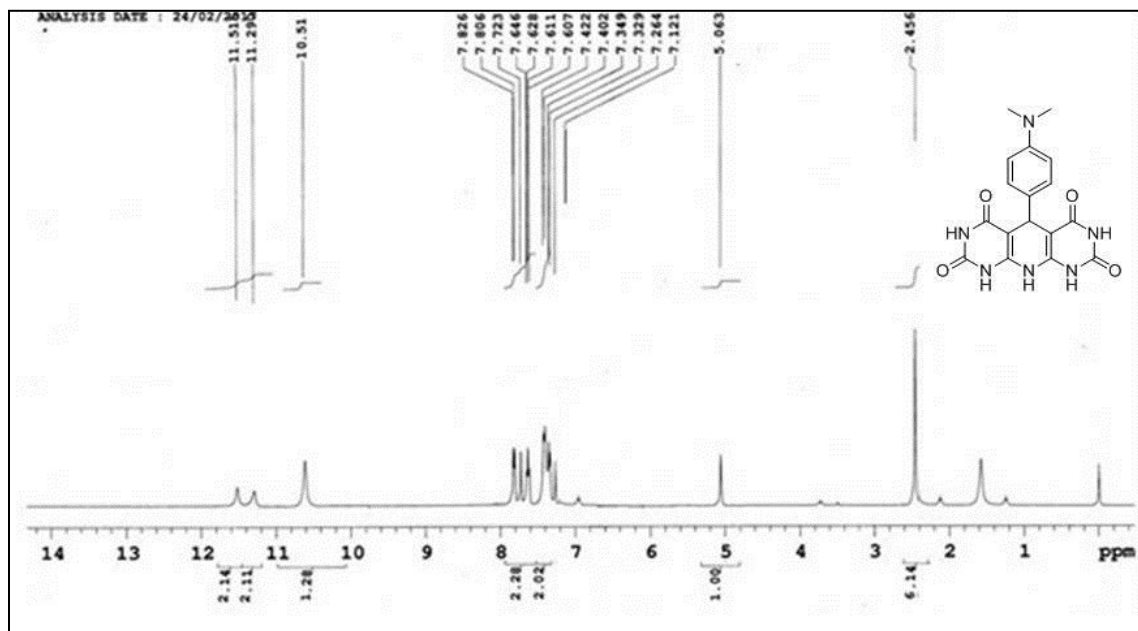
Mass of Compound (3f)



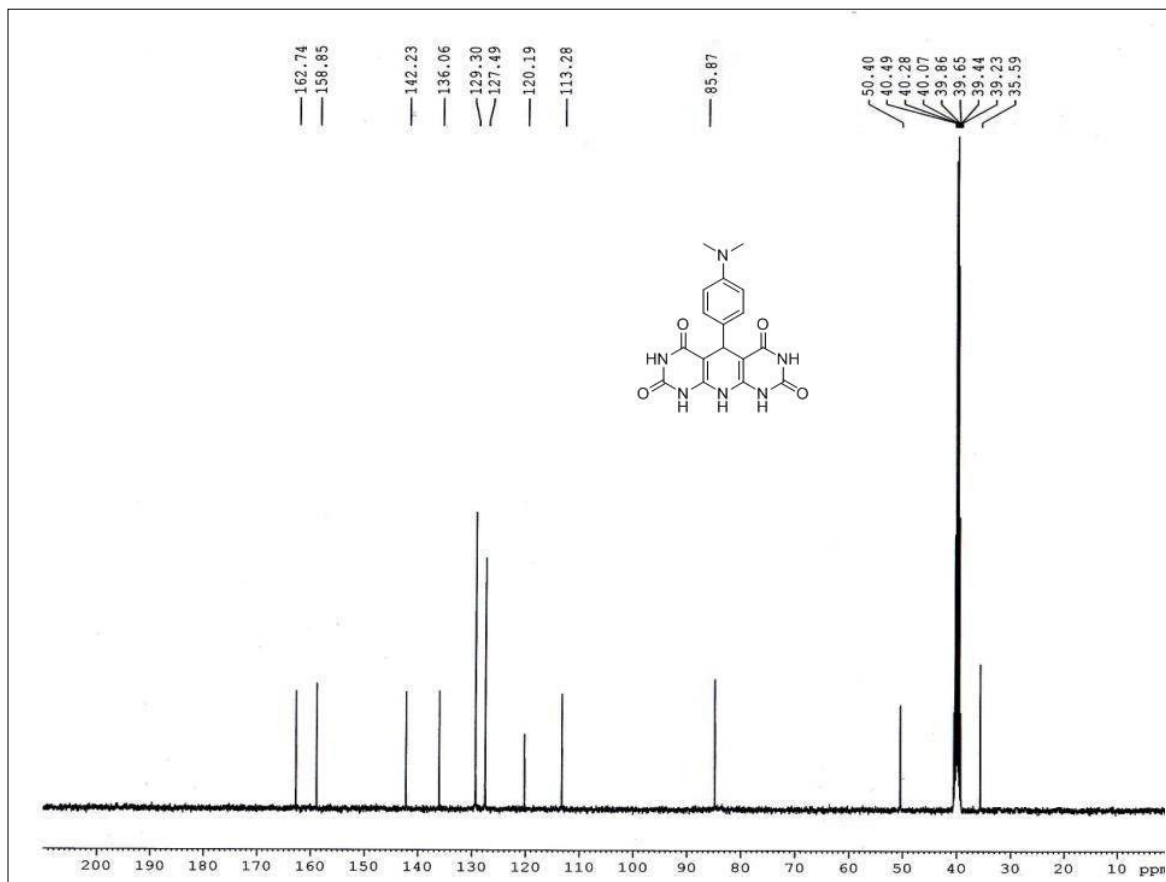
IR spectrum of Compound (3i)



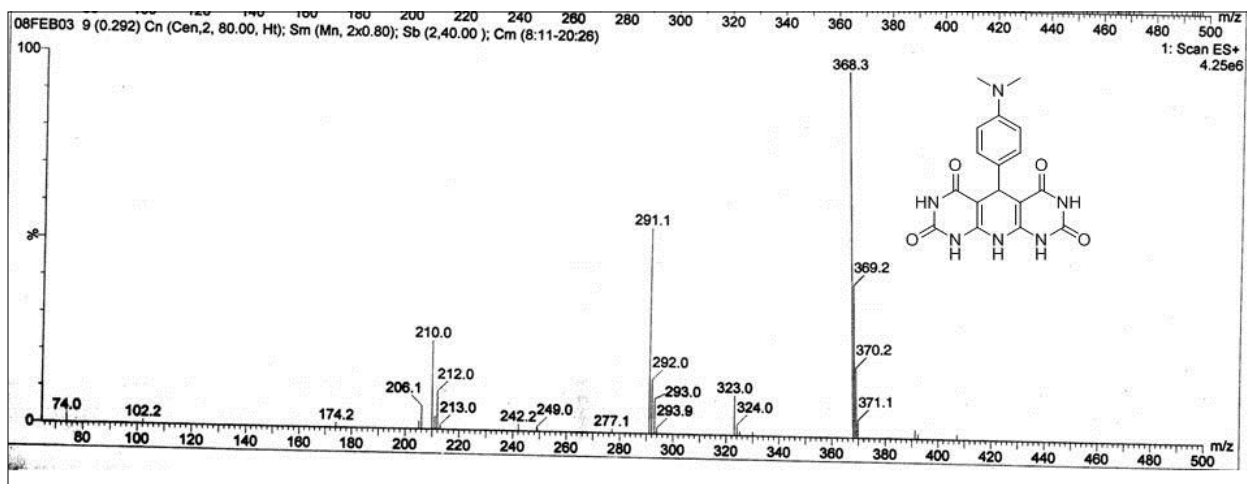
¹H NMR of Compound (3i)



¹³C NMR of Compound (3i)



Mass of Compound (3f)



References

- [1] (a) S.V. Shinde, W.N. Jadhav, N.N. Karade, *Oriental J Chem*, 26(1) (2010) 307-317; (b) A.H. Katgaonkar, S.A. Sadaphal, K.F. Shelke, B.B. Shingate, M.S. Shingare, *Ukrainica Bioorganica Acta*, 1 (2009) 3-7; (c) S. Rostamizadeh, L. Tahershamsi, N.J. Zekri, *Iran Chem Soc*, 12 (2015) 1381-1389; (d) R.A. Mekheimer, A.A. Hameed, K. Sadek, *Green Chem*, 10 (2008) 592-593; (e) G. Cooke, V.M. Rotello, *Chem. Soc. Rev.* 31, (2002) 275-286; (f) N. Azizi, A.M. Alireza, K. Amiri, H. Ghafurires, *Chem Intermed*, 38 (2012) 2271-2275.