

## Supporting Information

### **Hollow mesoporous magnetic silica-based nanocomposite supported with copper ferrite functionalized with phosphomolybdic acid as nanocatalyst for synthesis of 1,4-dihydropyridines**

Mahla Dadaei, Hossein Naeimi\*

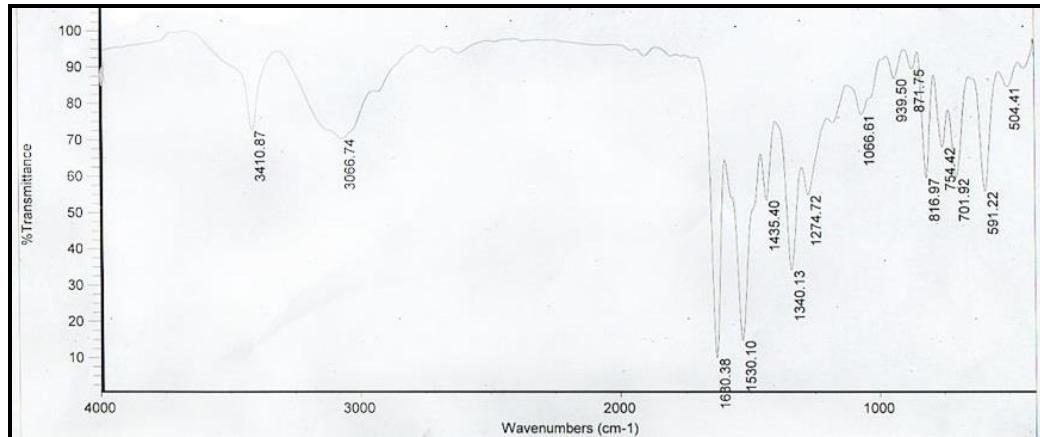
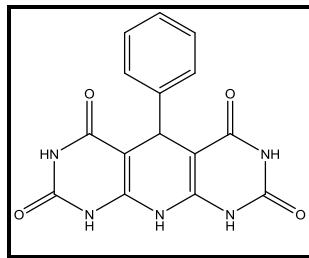
### **Experimental section**

#### **General information**

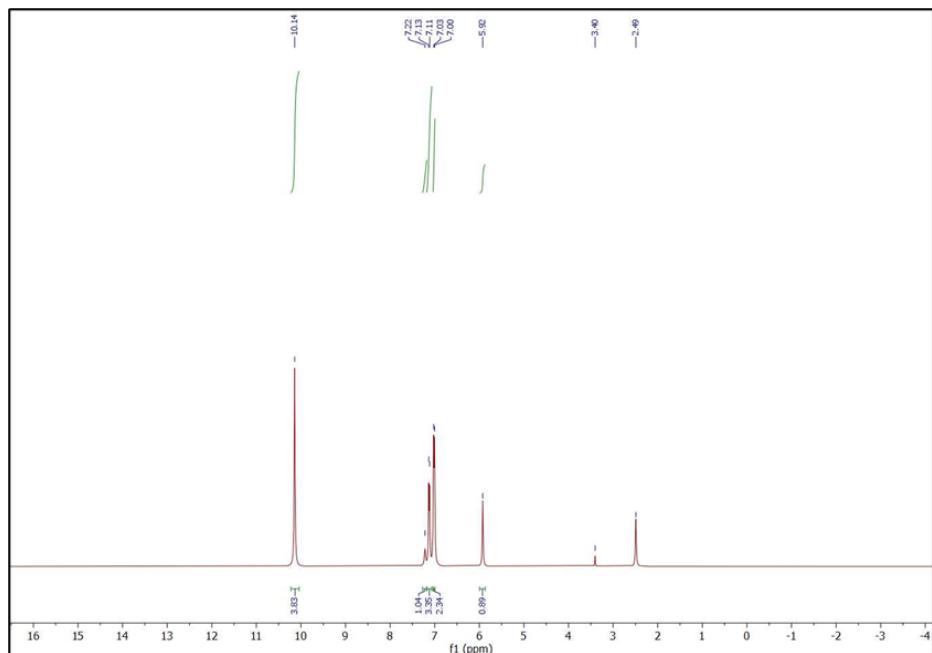
The chemicals used in this study were purchased from Fluka and Merck Chemical Companies and used without further purification. The nanostructures were characterized using a Holland Philips X’Pert X-ray powder diffractometer (XRD) with Cu K $\alpha$  radiation ( $\lambda = 0.154056$  nm), operated at a scanning rate of  $2^\circ$  min $^{-1}$  over a  $2\theta$  range of  $10^\circ$  to  $100^\circ$ . Fourier-transform infrared (FT-IR) spectra were recorded using KBr pellets on a Perkin-Elmer 781 spectrophotometer and a Nicolet Impact 400 FT-IR spectrometer.  $^1$ H NMR spectra were recorded in DMSO-d $_6$  on a Bruker DRX-400 spectrometer using tetramethylsilane (TMS) as an internal standard. The morphology of the nanocomposites was examined using scanning electron microscopy (SEM, SIGMA VP). Elemental analysis of the catalyst was carried out by energy-dispersive X-ray spectroscopy (EDX) using an Oxford Instruments system. Magnetic properties of the nanoparticles were measured using a vibrating sample magnetometer (VSM, PPMS-9T) at 300 K at Kashan University, Iran. Thermo Gravimetric Analysis (TGA) was performed using a thermal analyser TGA 1100 Sanaf electronic industries. The Brunauer–Emmett–Teller (BET) analysis was performed using a Belsorp Mini X. Melting points were determined using a Yanagimoto micro melting point apparatus and are reported uncorrected. The purity of the substrates and the progress of the reactions were monitored by thin-layer chromatography (TLC) on silica gel plates (Polygram SILG/UV 254, Merck).

**Synthesis of 1,4-dihydropyridin derivatives using hollow mesoporous silica-coated copper ferrite nanocatalyst functionalized with phosphomolybdic acid**

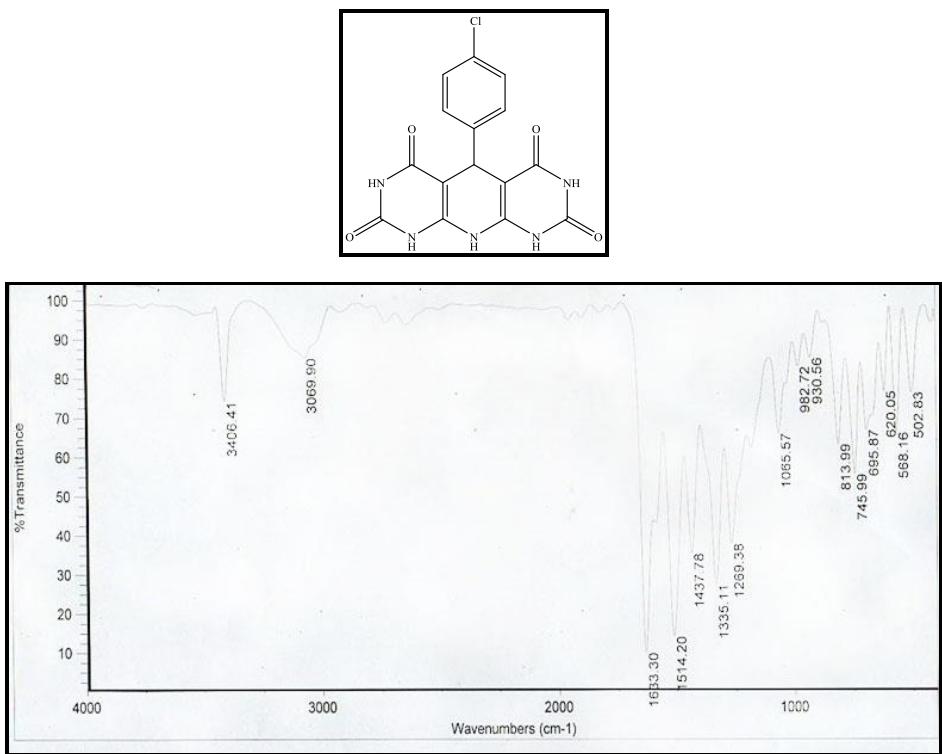
In a 25 mL round-bottom flask, barbituric acid (1 mmol), an appropriate aldehyde derivative (0.5 mmol), ammonium acetate (0.6 mmol), and the synthesized nanocatalyst (30 mg) were added. Ethanol (5 mL) was then introduced into the reaction vessel, and the mixture was stirred at 75 °C using a magnetic stirrer. The progress of the reaction was monitored by thin-layer chromatography (TLC). Upon completion, the nanocatalyst was separated from the reaction mixture using an external magnet. The resulting crude product was washed with hot ethanol to obtain a purified compound. The recovered catalyst was washed sequentially with double-distilled water and ethanol, followed by drying in an oven at 80 °C. The dried catalyst was stored for reuse in subsequent reactions.



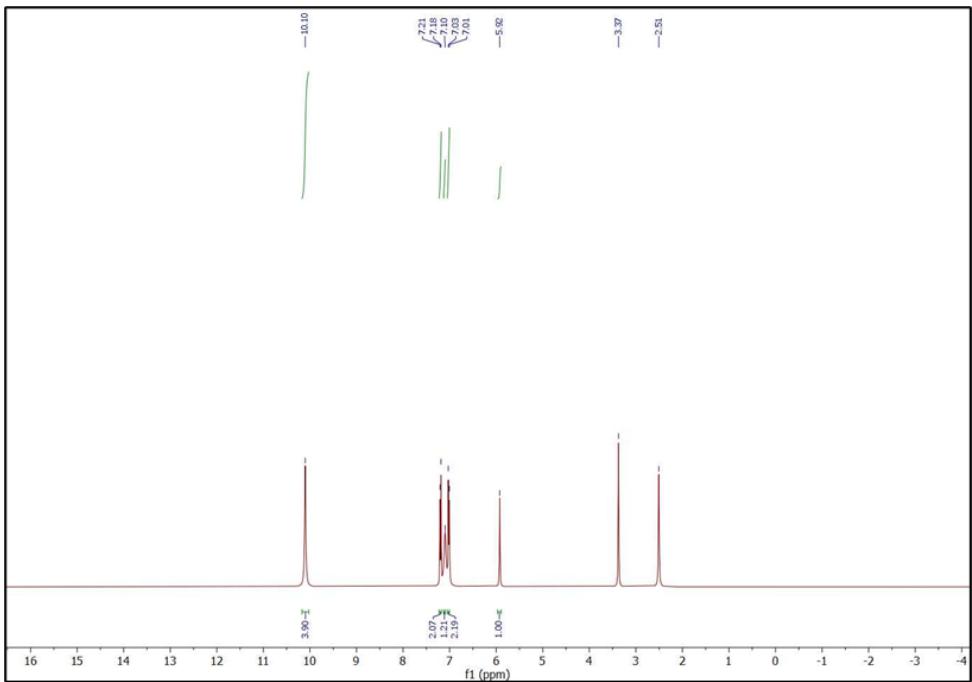
FT-IR of 5-phenyl-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4a**)



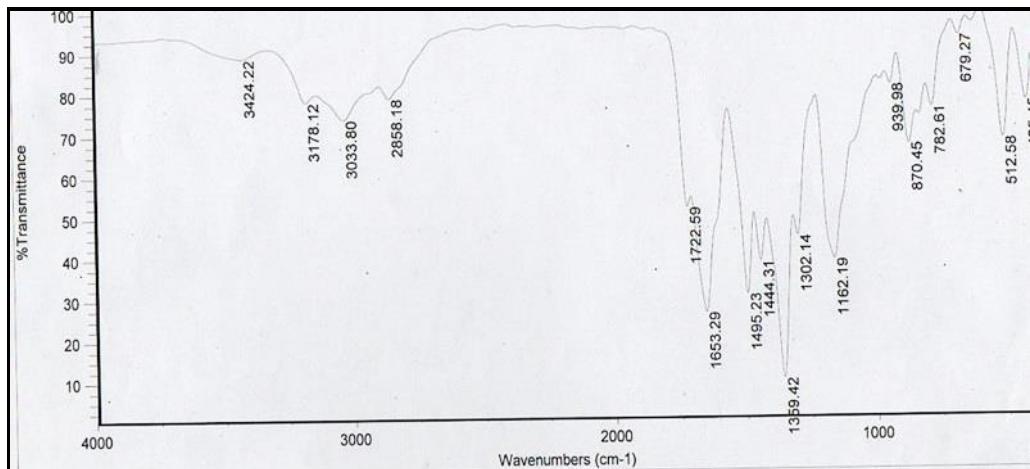
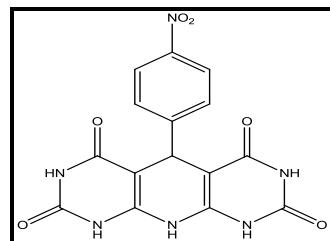
<sup>1</sup>H NMR of 5-phenyl-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4a**)



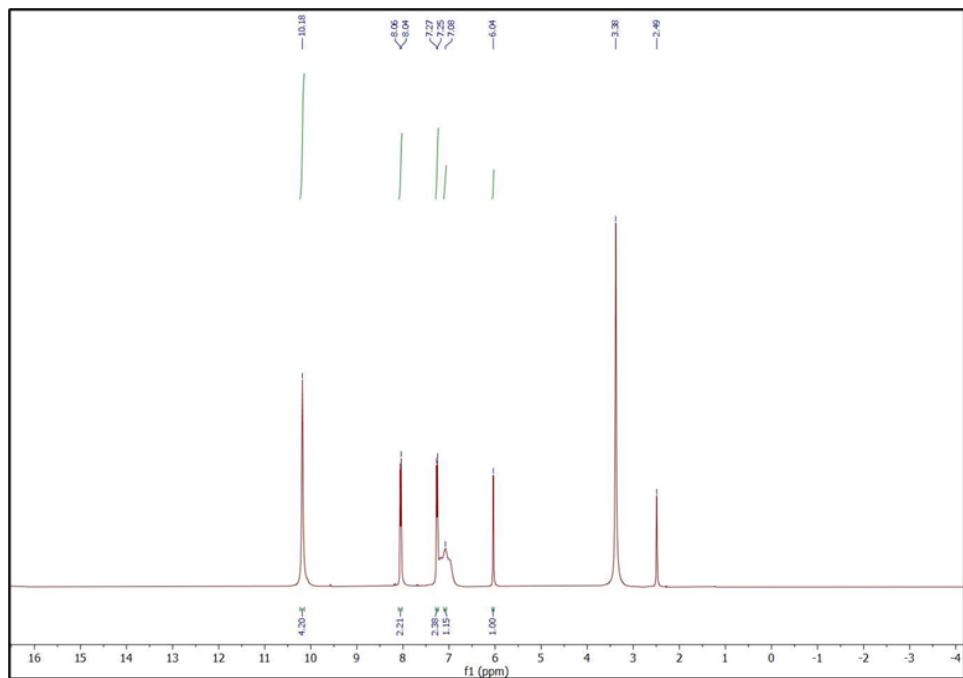
FT-IR of 5-(4-chlorophenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4b**)



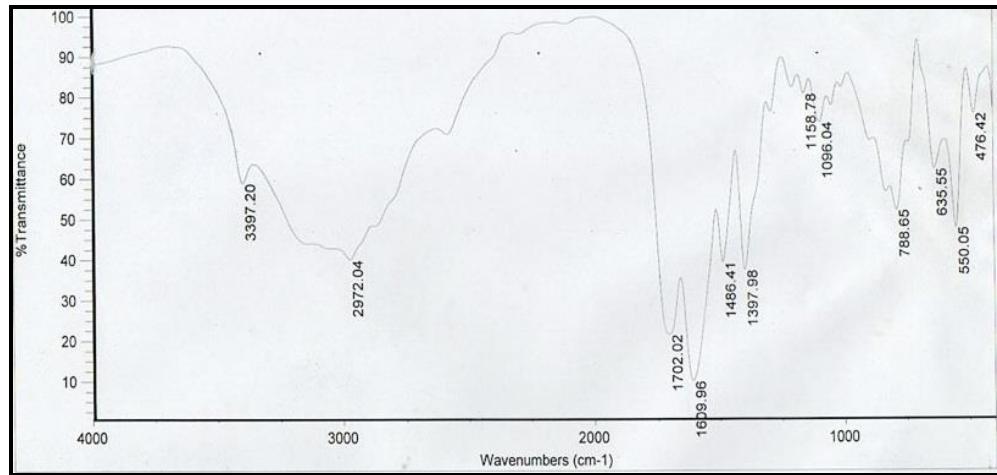
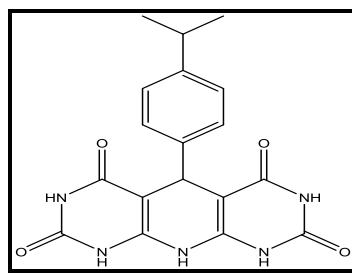
<sup>1</sup>H NMR of 5-(4-chlorophenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4b**)



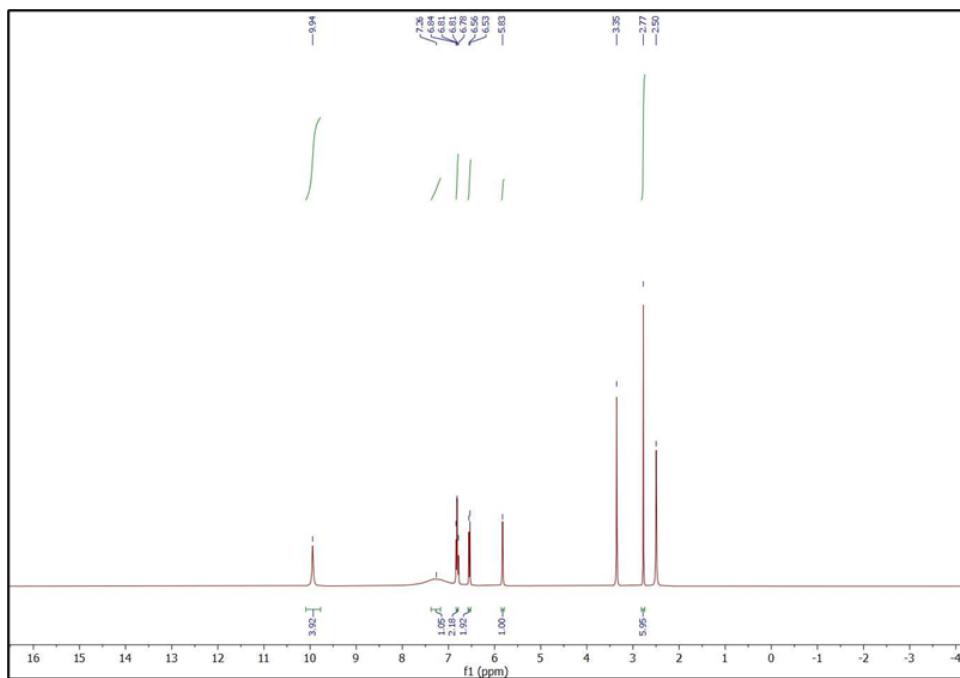
FT-IR of 5-(4-nitrophenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4c**)



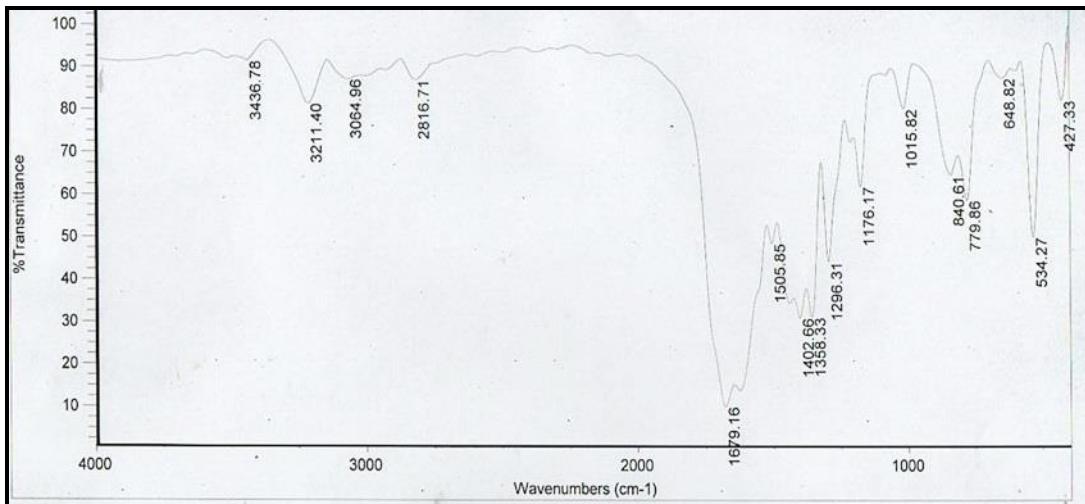
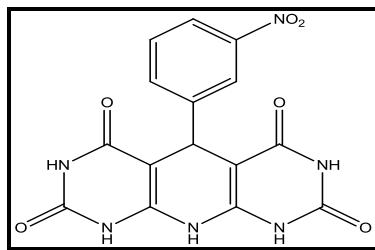
<sup>1</sup>H NMR of 5-(4-nitrophenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4c**)



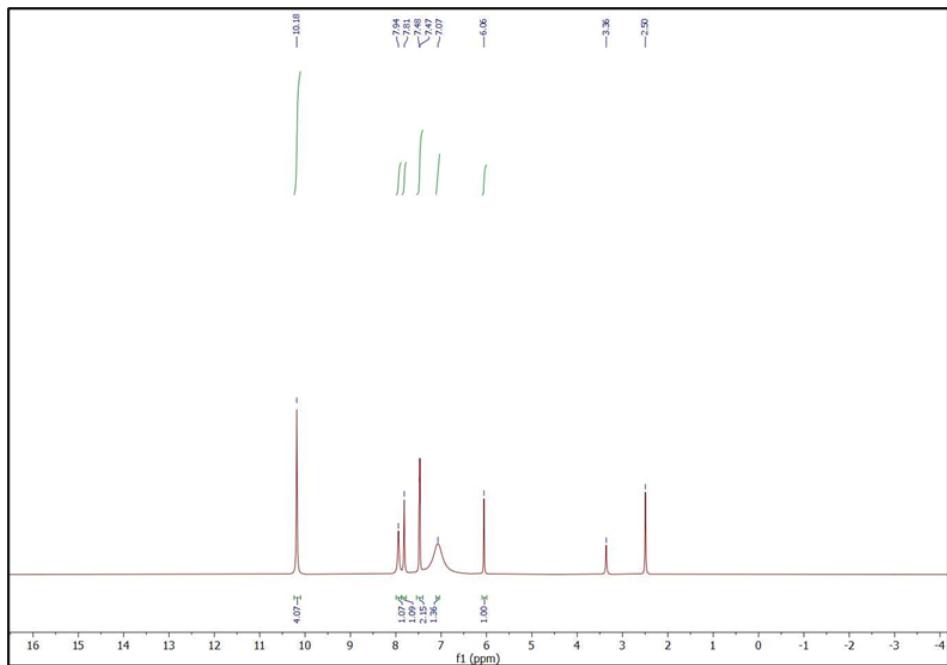
FT-IR of 5-(4-isopropylphenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4d**)



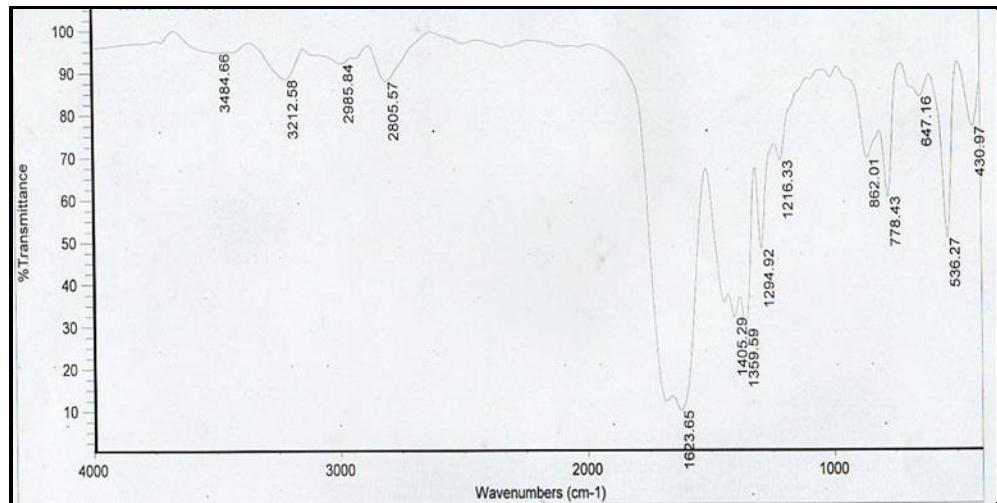
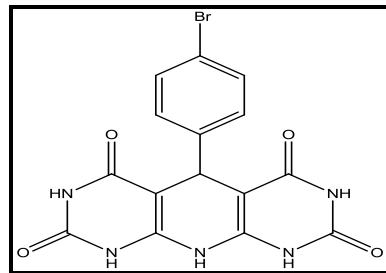
<sup>1</sup>H NMR of 5-(4-isopropylphenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4d**)



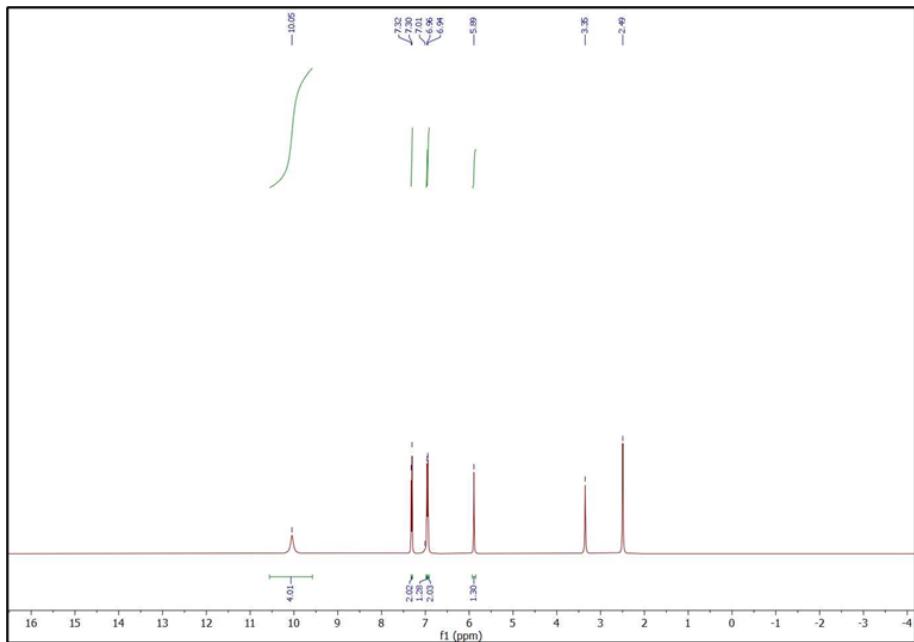
### FT-IR of 5-(3-nitrophenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4e**)



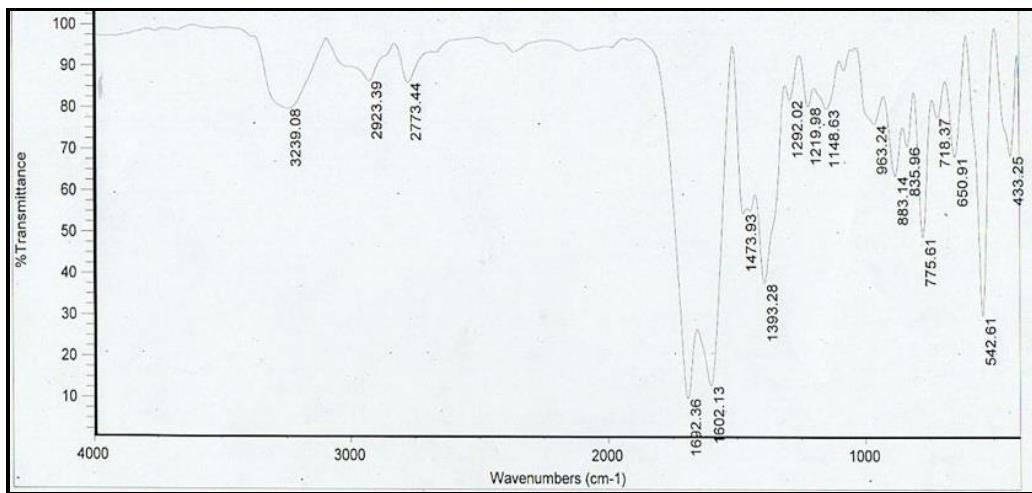
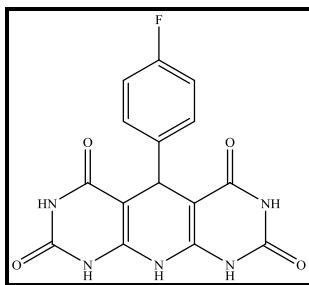
<sup>1</sup>H NMR of 5-(3-nitrophenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4e**)



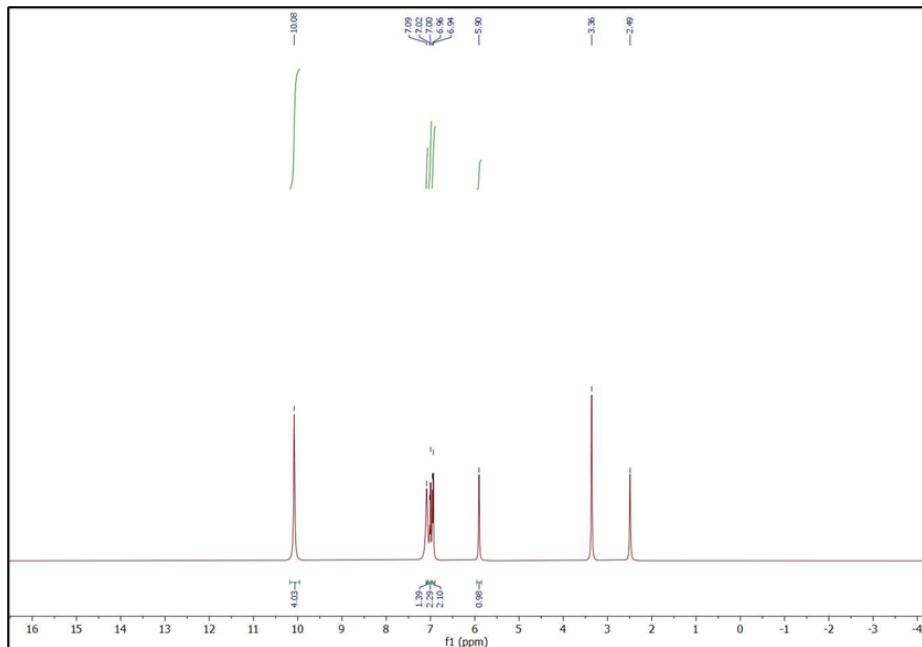
### FT-IR of 5-(4-bromophenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4f**)



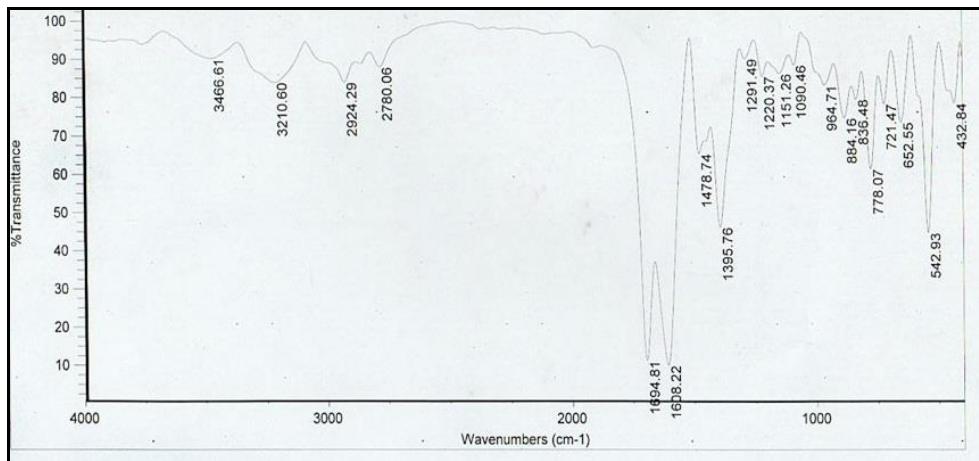
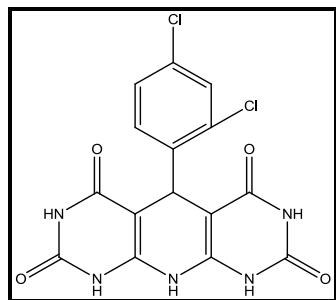
<sup>1</sup>H NMR of 5-(4-bromophenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4f**)



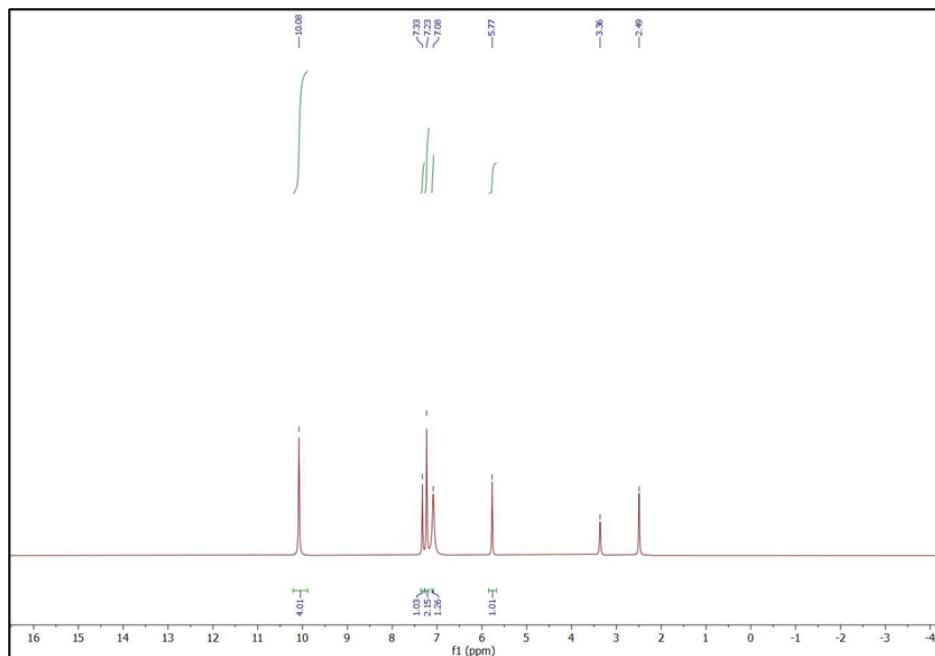
FT-IR of 5-(4-fluorophenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4g**)

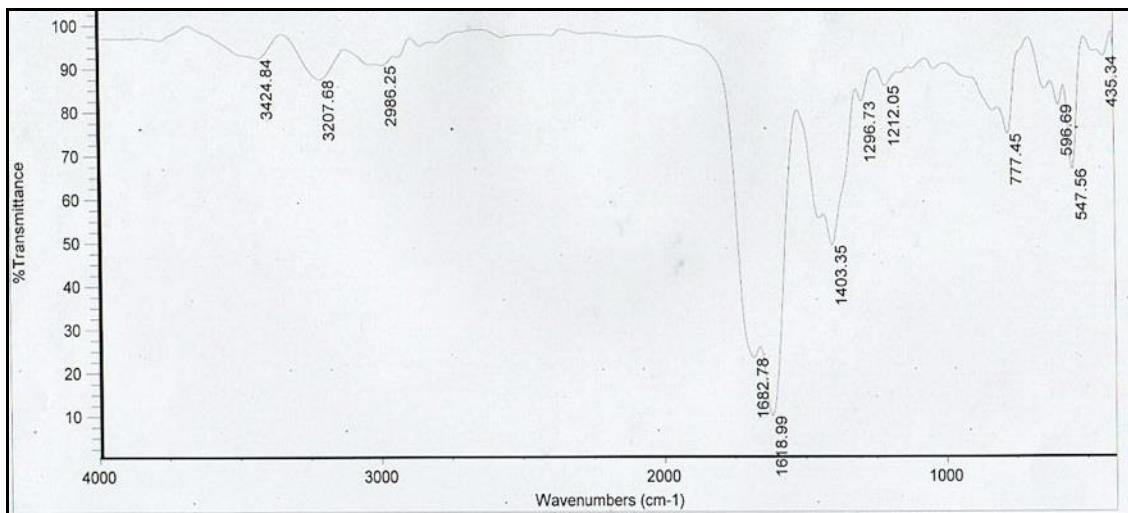
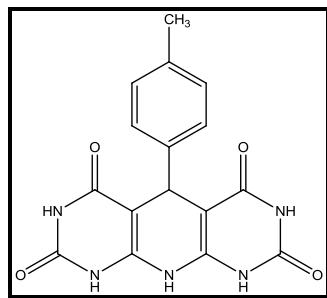


<sup>1</sup>H NMR of 5-(4-fluorophenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4g**)

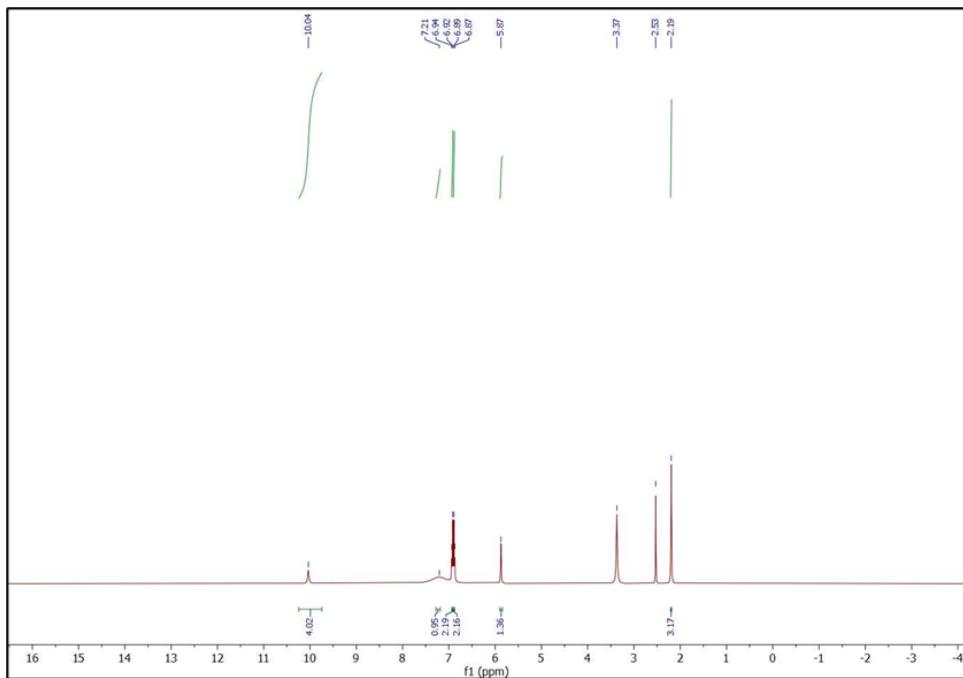


FT-IR of 5-(2,4-dichlorophenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4h**)

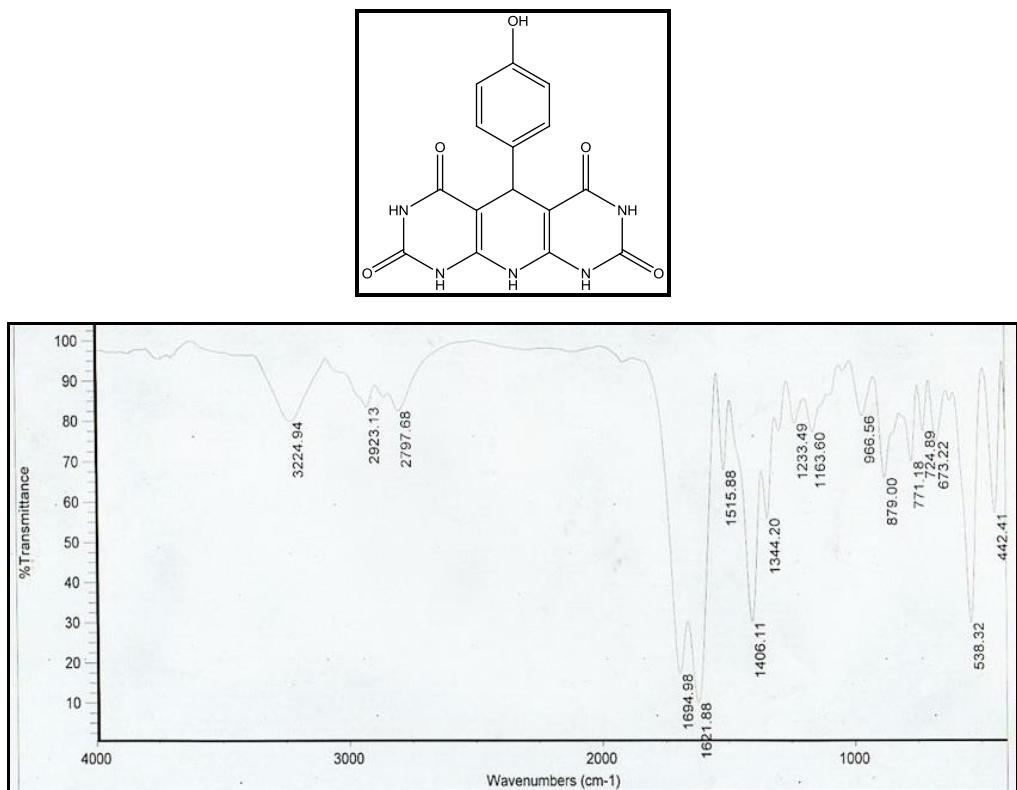




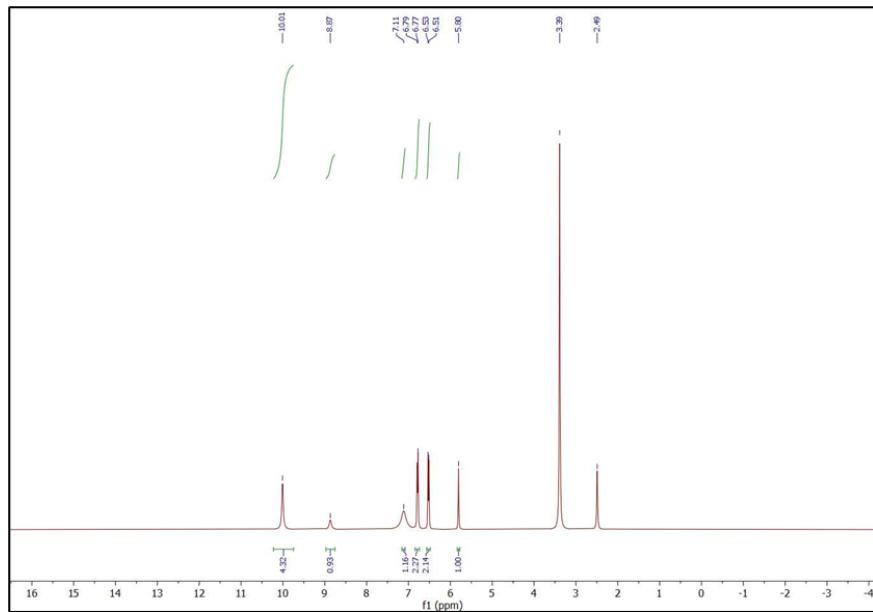
### FT-IR of 5-(p-tolyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4i**)



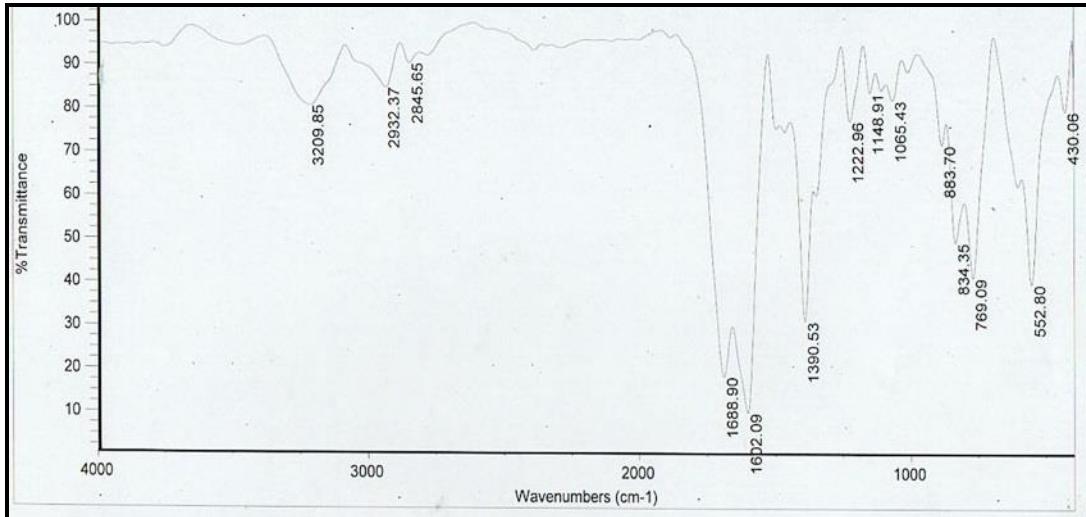
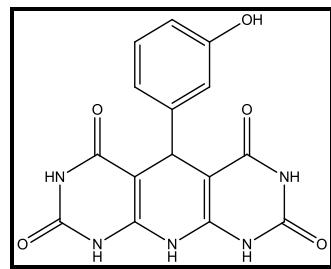
<sup>1</sup>H NMR of 5-(p-tolyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4i**)



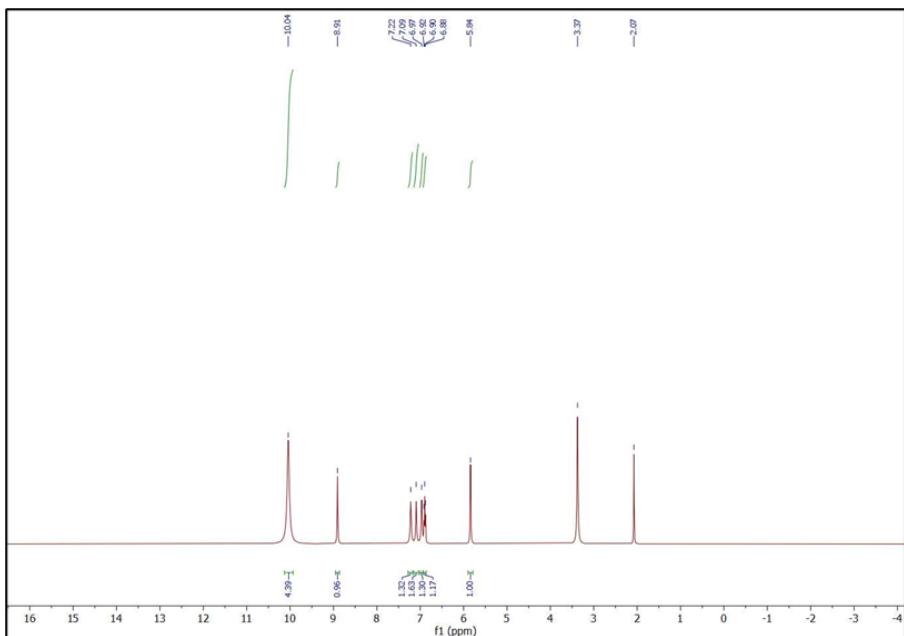
FT-IR of 5-(4-hydroxyphenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4j**)



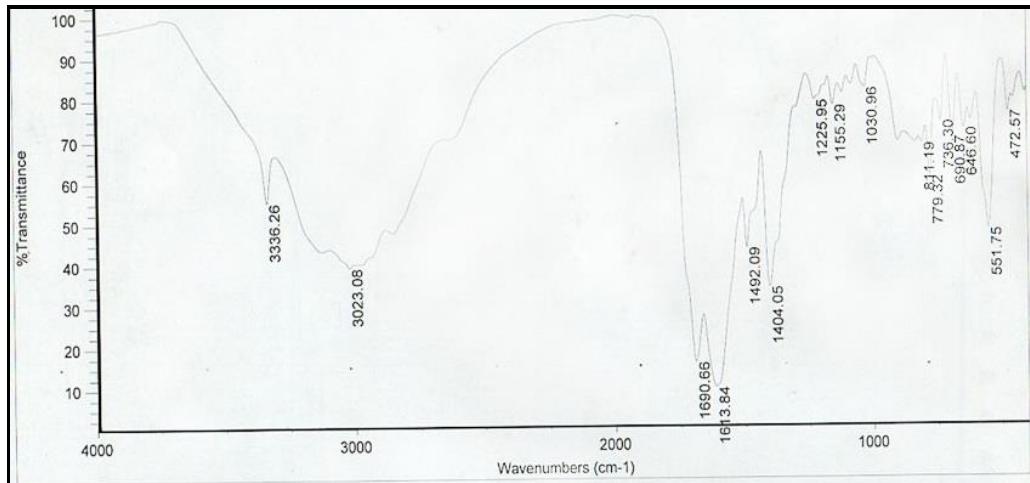
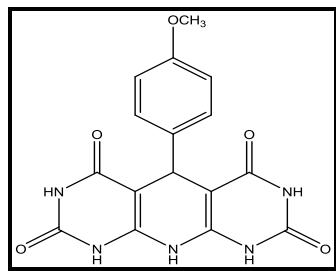
<sup>1</sup>H NMR of 5-(4-hydroxyphenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4j**)



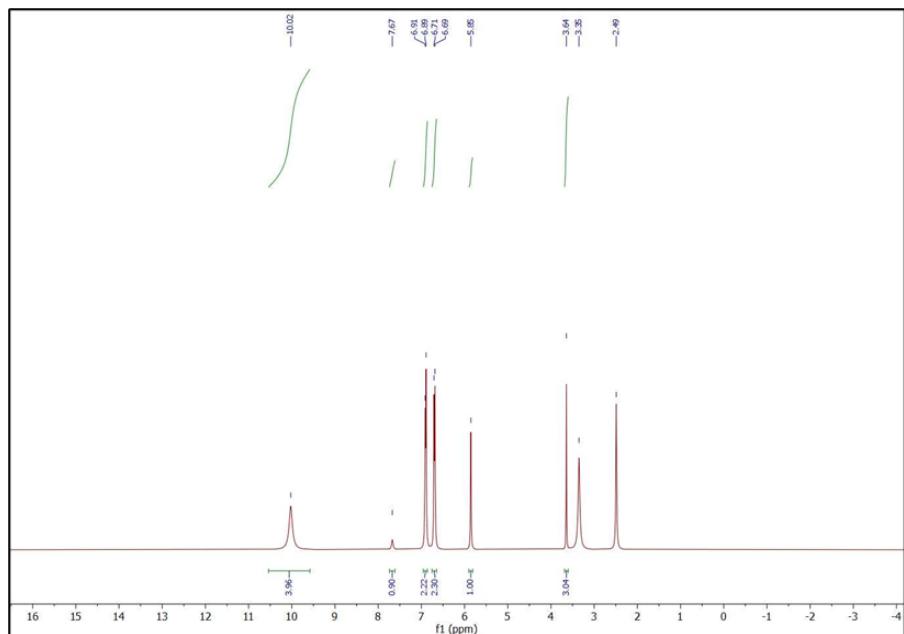
FT-IR of 5-(3-hydroxyphenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4k**)



<sup>1</sup>H NMR of 5-(3-hydroxyphenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4k**)



FT-IR of 5-(4-methoxyphenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4l**)



<sup>1</sup>H NMR of 5-(4-methoxyphenyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (**4l**)