**ABSTRACT**

Schiff’s base of indane-1,3-dione were synthesized from pyrimidine derivatives of indanedione. The structures of new compounds are confirmed by FTIR, 1H NMR and Mass spectral data. Schiff’s base and pyrimidine derivatives were evaluated for their analgesic, anti-inflammatory, anticancer, antibacterial and antifungal activity. The compound 2-(2-(4-methoxybenzylideneamino)-6-(2-nitrophenyl)pyrimidin-4-yl)-2Hindene- 1,3-dione and 2-(2-(4-methoxybenzylideneamino)-6-(4-nitrophenyl)pyrimidin-4- yl)-2H-indene-1,3-dione were found to have comparable activity with that of standards. Analyzing the pharmacological properties of both the pyrimidine and Schiff’s bases ofindane-1,3-dione it was found that Schiff’s bases were found to be more potent when compared to that of pyrimidine derivatives. Molecular docking was done by using Molegro Virtual Docker and 1CQ9M used as a PDB code. It shows good residualcontact and good Mol Dock score. 2D-QSAR was performed by using V-Life MDS and find out the correlation between actual and predicted activity.

**Keywords:** indane-1,3-dione, Schiff’s bases, Molecular docking and QSAR