**ABSTRACT**

In the present research work, the main motto was to develop new chemical entities as potential anticancer, anti-inflammatory, anthelmintic and antimicrobial agent. The design of anticancer agents was performed by molecular docking studies. 2-D QSAR studies of the newly synthesized compounds as (5a-5e) and (6a-6e) were performed. The starting material 3-methyl-1-substituted-1H-pyrazol-5(4H)-ones (1a-1b) were synthesized in high yieldsaccording to reported method using domestic microwave oven by the treatment of ethyl aetoacetate with appropriate 1-phenylhydrazine or 1-(2,4-dinitrophenyl)hydrazine. 4-acetyl- 3-methyl-1-substituted-1H-pyrazol-5(4H)-ones (2a-2b) were prepared by the acetylating of(1a-1b) with corresponding acid chloride following Jensen’s procedure. 4-(3- (substituted)acryloyl)-3-methyl-1-(substituted)-1H-pyrazol-5(4H)-ones as chalconederivatives (3a-3e) and (4a-4e) were prepared by reacting (2a-2b) with substituted aromatic aldehydes by using 70% sodium hydroxide in ethanol. 4-(2-amino-6-(substituted)pyrimidin- 4-yl)-3-methyl-1-(substituted)-1H-pyrazol-5(4H)-one (5a-5e) and (6a-6e) were prepared by reacting (3a-3e) and (4a-4e) with guanidine hydrochloride. Finally (5a-5e) and (6a-6e)reacted with different substituted aromatic aldehydes to give corresponding Schiff bases (7a- 7e) and (8a-8e) in very good yields. The structures of new compounds are characterized by TLC, FTIR, 1H NMR and Mass spectral data. The compounds (5a-5e) and (6a-6e) have been screened for their in vivo and in vitro anticancer, anti-inflammatory activities. The compounds (7a-7e) and (8a-8e) have been screened for their anthelmintic and antimicrobial activities.

**Keywords:** Molecular docking studies, 2-D QSAR, substituted pyrazolones, Schiff bases,

anticancer activity, anti-inflammatory activity.