AIM AND OBJECTIVE

AIM

- The main aim of this research work is to design, \textit{in silico} screening, synthesis, characterization and pharmacological activity of 3, 4 dihydro pyrimidones.

OBJECTIVES

The objectives of the present study are as follows

- To modify 3, 4 dihydro pyrimidones with different substitution and to create a library of compounds [24 compounds]. Synthesis those by conventional Biginelli's multicomponent reaction and characterisation of the lead molecule obtained.

- To utilize the various bioinformatics tool and software such as chemsketch, molegro Qikprop and glide software, to perform docking of the 24 new compounds against the selected proteins and ADMET properties.

- \textit{In vitro} studies were carried out to choose the lead molecule.

- In order to assess the underlying pathway of the inhibitory effect of these compounds on colon cancer, certain biochemical studies were carried out to throw some light on the antioxidant potential of these compounds.

- Propagative lipid per oxidation is a degenerative process that affects cell membranes and other lipid-containing structures under conditions of oxidative stress. Endogenous DNA adducts derived from oxidative stress, lipid per oxidation, or other endogenous processes have been proposed as contributors
to the etiology of human cancer. So, the level of hepatic and the colonic lipid per oxidation were assessed in order to evaluate the antioxidant activity of these compounds in the present investigation.

- Induction of GSTs, phase II enzymes that detoxify certain carcinogens, is regarded as a potential mechanism of blockade of the early stages of carcinogenesis. Moreover, GSTs, an intracellular non-seleno GSH-S-transferase have been implicated in lipid hydroperoxide detoxification. Hence, the modulatory influence of compounds on this xenobiotic detoxifying enzyme was assessed.

- Estimation of level of GOT and GPT in plasma to find out the function of liver.
Figure 10. Plan of work