SUMMARY

• Twenty four compounds were designed by changing the substitution in phenyl ring at fourth position and oxygen and sulfur in the dihydropyrimidone ring. Benzimidazole was substituted in the fifth position.

• All the compounds exhibit the safer result and good bioavailability. All the compounds obeyed these Lipinski’s five rule and Jorgensen’s rule of three.

• The docking studies were carried out for those twenty four compounds using Glide and Molegro software against cancer, tubercular and HIV target. All the compounds exhibited good binding energy and with hydrogen bonds. Few compounds exhibited more binding energy than the standard compounds.

• All the compounds were synthesized by conventional method. Synthesized compounds were first checked for its purity by melting points and Rf values. Compounds which were chosen as lead characterized by IR, NMR, 13C NMR and mass spectrum.

• In vitro antioxidant activity were carried out for eight compounds in that compound ITU, VTU and K exhibited IC50 values at 0.97 µg/ml, 7.81 µg/ml and 3.97 µg/ml.
• Compounds ITU, V and VTU exhibited MIC at very low concentration of 6.25, 1.56 and 3.13 µg/ml for luciferase reporter phage assay method. (In vitro antitubercular activity)

• Compounds ITU and VTU exhibit cytotoxic activity against the cell line HCT 116 and ITU exhibit growth inhibition factor at very low dose against HCT 116 and A549.

• Two compounds ITU and VTU were chosen as lead from in silico screening, ADMET and in vitro studies. Acute toxicity studies were carried out for those compounds using OECD 423 guidelines both were safe at the dose of 2000 mg/kg of body weight.

• Compound ITU enhanced the level of detoxifying enzyme (GST activity) with simultaneous decrease in lipid per oxidation levels in the treatment groups when compared to that of the carcinogen control group.
CONCLUSION

3, 4 dihydro pyrimidones were designed, in silico screening, synthesis, characterization, and pharmacological activities were carried out. Compound ITU possess antioxidant activities, inhibition against the *Mycobacterium tuberculosis* and enhance the level of detoxifying enzyme (GST activity) with simultaneous decrease in lipid per oxidation levels in the treatment groups when compared to that of the carcinogen control group.