Worked on various projects in my degree courses

- **Development and Repurposing of Triazine Dione as a chemotherapeutic agent**. (October 2019-April 2021)

The viral and bacterial infections are increasing at a greater rate nowadays. Cancer has now become a major killer disease worldwide. While there is large scale production and distribution of antiviral and antibacterial drugs, viruses are still a major cause of human disease. Usage of many antiviral and antibacterial agents has been suppressed due to drug resistance development and undesired side effects. Since the increase of emergence and reemergence of the viral epidemic, pressure has been created on the public health care community to find novel drugs which targets these viruses and bacteria. Synthesis and development of new drugs requires high costs and long time. The approval rate has been very low due to safety and pharmacodynamics properties of the drugs. Thus, drug repurposing (one drug two diseases) has been recently noted as cost effective and time consuming. A novel class of drugs called Triazine Dione because of its distinct structural features promises inhibiting various enzymes of different species. If a single drug acts on various targets, the possibility of recurrence reduces significantly.

Objectives-

To select a novel target which plays a key role in biosynthesis of essential enzymes required in various viruses, bacteria and cancer-causing agents.

To design such a molecule which acts on multiple targets of viruses and bacteria by using molecular docking technique and shortlist best molecules which have good docking scores in multiple targets.

Synthesis of those core molecules of Triazine Dione and its derivatives which may show promising activity.

There are 2 Methods

i. Computer Aided Drug design

It can be used to identify targets across the species and if these targets are deemed druggable then figuring out the ways to optimize the drug candidates. Molecular Docking can be used for this purpose. Similarly, to have an idea about the ADMET of identified candidates' online tools available for the purpose can be used.

ii. Synthesis of drug candidates

Following is a general route for synthesis

There are 2 schemes for synthesis of Triazine Dione derivatives – both are synthesized by proper stoichiometric chemistry.

The goal of the work was to identify if Triazine Dione scaffold may have multiple/ dual activity by inhibiting various enzymes in viruses, bacteria and cancer. These drugs should be well tolerated and should have good pharmacodynamics as well as pharmacokinetics profile. A secondary outcome may be to identify common and distinct substitutions to make them general or selective. Both the outcomes have been successfully met in this project.

- Worked and built a prototype of '**Stressometer' – a point of care diagnostics tool for rapid cortisol detection.** (September2020 -July 2021)

Stressometer® is a valid and reliable, computer-based mass screening tool for evaluation of stress level and sources of stress. Overall, Stressometer® (SOM) creates a robust measurement of stress and behavioral health that is likely culturally neutral and thus has universal applicability. A scale such as this one is ideal for use in the developing world to help bridge the treatment gap created and enhance behavioral health, especially in those suffering.

A simple portable, sensitive device which is made into a diagnostic device and meets the criteria for point of care diagnostics. This biosensor can be amalgamated with a flow channel for sample, a prism, gold nanoparticle, cortisol-aptamer, a solid metal platform and a light source of selected wavelength(p-polarized) which acts on blue gold nanoparticle and a detector to measure the light reflected, absorbed, refracted. Reflectivity parameter used for quantifying the amount of cortisol bound with aptamer and its biological interaction. Surface plasmon resonance acts on such system which allows real-time, label-free detection of biomolecular interactions

This Project got selected in 15th Inter-Collegiate/Institute/Department Avishkar Research Convention: 2020-21 in State level round of University of Mumbai.

- Masters project thesis – **Probing the Biology of Zinc Alpha 2 Glycoprotein for Cachexia** (December 2021- July 2022)

Zinc α2-Glycoprotein (ZAG) a protein released from white adipose tissue is a multidisciplinary protein with lot of metabolic functions has main role to play in cachexia of cancer. ZAG resembles MHC class-II protein in structure and ZAG has pocket which binds to ligand by hydrophobic linkage and thus can be novel ligand to treat cachexia. With the help of molecular biology techniques and docking we hypothesized the mechanism of ZAG and the Ligand which binds to it for muscle loss.