PANEL SESSION 3
3:30-4:30pm, Friday, October 2
https://meet.google.com/cfw-zuyn-cku

Panel Chair: **Stella Hadjiyanis '21**

Maya Lengvenis '22 – "Computationally Approaching Fragment-based Ligand Design"

Plasmodium Falciparum, the parasite that causes Malaria is increasingly becoming resistant to traditional drugs. PfGCN5, a protein used in epigenetic regulation is identified as a new drug target. A fragment-based approach is used to identify small organic molecule fragments that bind tightly to PfGCN5 and can be connected to form a single large molecule. A ZINC library of over 2.4 million potential drug fragments was screened for binding affinity with PfGCN5 in the hydrophobic pocket and the WPF shelf using Autodock Vina. The tightly binding fragments were screened for binding with human analogues of PfGCN5 with the goal of isolating the fragments that bind selectively.

Katya McDonald '22 – "Fungal Species and Fluconazole Resistance"

Fungal pathogens have immense medical importance, as they infect 4.9 million people globally a year. One type of fungal infection, Candidiasis, is caused by multiple different yet related species. Additionally, new species capable of causing this infection have emerged in the last ten years, showing the intensity of this problem. Species that are related to pathogenic species but are non-pathogenic themselves can represent a model system to examine how drug resistance develops in organisms without prior exposure. This includes several Brettanomyces species. This summer, we began by sequencing 23 different strains to determine their identity. Next, we selected 20 strains, which included seven different fungal species, to be screened for fluconazole resistance. This involved multiple replicates of minimum inhibitory concentration (MIC) assays. We found three isolates to be resistant, six to be have some degree of resistance, and one isolate to be sensitive to fluconazole. Other isolates were unable to be classified during our time. For three strains that were thought to be resistant, we sequenced ERG11, the specific gene that is the fluconazole drug target to see if mutations had occurred. We found that while two strains had no changes, one strain had two amino acid changes. For strains with some resistance, we investigated cross-resistance, and screened six strains for voriconazole and itraconazole. In the future, we would like to continue screening for cross-resistance in resistant strains and screening for fluconazole in unclassified strains, evolve nonresistant strains, and further sequence ERG11 in more strains.

Alexandru Florea '22 - "Comparison of Separation Factors Obtained Using Different Injection Approaches for High Performance Liquid Chromatography"

Conventional high performance liquid chromatography (HPLC) methods utilize a rotary valve to inject samples. While this is useful for the majority of HPLC experiments, trying to achieve millions of retention measurements in a relatively short period of time is not practical with this valve-based approach. This is because frequent switching of the rotary valve causes rapid deterioration of the rotor and stator in the valve, leading to frequent and high replacement costs. In this work we have developed a novel syringe-based injection method that takes advantage of a syringe pump to inject samples instead of the conventional rotary valve. This novel method significantly prolongs the life of autosampler components and eliminates the need to frequently replace valves. Using short (5mm) columns, analysis times can be reduced to less than 1 minute and thousands of retention data can be gathered in the span of a few hours. Preliminary work by our group has shown that differences in separation factors between syringe-based and valve-based injections are not practically significant, and this new approach looks promising as an alternative to valve-based injections.