



Analytical Chemistry Seminar

Tuesday, January 18, 2022

3:30 PM, WTHR 320

*“High Throughput Phenotypic Antibacterial Drug Screening
Using MALDI-TOF MS and Machine Learning”*



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Abstract

According to the World Health Organization, antibiotic resistance is one of the biggest threats to global health, food security, and development today. Unfortunately, around 90% of antibiotic drugs fail in the current pharmaceutical pipeline. One of the main reasons for this is that the most popular method, being a single target approach in biochemical assays, doesn't connect drug-target interactions to a realistic cellular environment. Other methods that do are generally slow, require high concentration of drug, or don't provide any information about the mechanism of action for a drug.

For this seminar we will examine a new high throughput label free method for phenotypic drug screening using matrix assisted laser desorption ionization time of flight mass spectrometry (MALDI-TOF MS) and machine learning. The motivation is to build a classification model that can accurately identify the mechanism of action in unknown drugs at very low concentrations.

References

van Oosten, Luuk N, and Christian D Klein. "Machine Learning in Mass Spectrometry: A MALDI-TOF MS Approach to Phenotypic Antibacterial Screening." *Journal of medicinal chemistry* vol. 63,16 (2020): 8849-8856. doi:10.1021/acs.jmedchem.0c00040

Seminar Time shared with Zachary McLeod