

Department of Chemistry & Biochemistry Seminar

Friday, April 9th, 2021

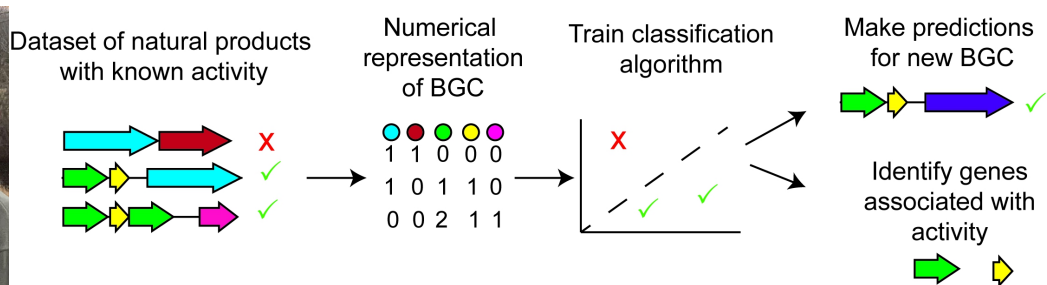
1:30pm – 2:45pm

Zoom ID: 960 452 0800

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A Machine Learning Tool for Predicting Natural Product Bioactivity

Speaker: Dr. Allison Walker, Harvard Medical School/Vanderbilt University



Abstract: We developed a machine learning-based bioinformatics tool that predicts natural product bioactivity using the natural product's biosynthetic gene cluster. We trained three commonly used classifiers, logistic regression, support vector machines, and random forests, on binary classification problems to predict the presence or absence of certain bioactivities. For this initial study we focused on different antimicrobial activities. All classifiers performed well, with balanced accuracies of at least 57% and as high as 79%. Our tool will allow researchers to take advantage of the increasing amount of genetic data to prioritize bacteria that are most likely to produce natural products with desirable activities. We also determined that some biosynthetic genes are highly associated with certain activities, linking molecular features to bioactivity.

Biography: Dr. Allison Walker is currently an NIH Ruth L. Kirschstein (F32) postdoctoral fellow in Dr. Jon Clardy's lab at Harvard Medical School. Allison will begin her independent career as an Assistant Professor of Chemistry and Biological Sciences at Vanderbilt University in the fall. Allison received her B.S. in Chemistry from Brown University and her Ph.D. in Chemistry from Yale University in the lab of Dr. Alanna Schepartz, where she studied computational

and experimental methods used to investigate allostery in biological macromolecules. Since completing her Ph.D., Allison has been working on developing a machine learning method for predicting natural product activities. Allison will continue this work and research on other applications of machine learning to chemical biology during her independent career at Vanderbilt.