



COLLEGE OF PHARMACY

MEDICINAL CHEMISTRY

UNIVERSITY OF MICHIGAN

## MedChem Remote Seminar



*"Computational Methods for  
Small Molecule Natural Product Discovery"*

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Thursday October 15, 2020 at 4:00 p.m.

**Meeting Link:**

<https://umich-health.zoom.us/j/97266142937>

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*“Computational methods for small molecule natural product discovery”*

Hosein Mohimani, PhD

Identification of small molecules is a critical task in various areas of life science. Recent advances in mass spectrometry have enabled the collection of tandem mass spectra of small molecules from hundreds of thousands of environments. To identify which molecules are present in a sample, one can search mass spectra collected from the sample against millions of molecular structures in small molecule databases. This is a challenging task as currently it is not clear how small molecules are fragmented in mass spectrometry. The existing approaches use the domain knowledge from chemistry to predict fragmentation of molecules. In this talk I overview our recently developed machine learning method for learning mass spectrometry fragmentation pattern of small molecules, and then highlight applications of this method for discovery of novel peptide natural products through genome mining.