Dissertation Defense - Krista J. Smith, PhD Bioinformatics and Computational Biology
November 15, 2021 12:00 - 2:00 PM

All are invited to attend the defense. For more information please contact Graduate Coordinator at dstgerma@gmu.edu

**Candidate:** Krista J. Smith  
**Program:** PhD, Bioinformatics and Computational Biology  
**Date:** Monday, November 15, 2021  
**Time:** 2:00 PM  
**Place:** Zoom Meeting Link: [https://gmu.zoom.us/j/99347825152?pwd=TkhRK0NtL1pxckVDK0MxbllWOVMvUT09](https://gmu.zoom.us/j/99347825152?pwd=TkhRK0NtL1pxckVDK0MxbllWOVMvUT09)  
**Title:** Sequence and Structure Based Classification and Prediction of Antimicrobial Peptides

**Committee Chair:** Dr. Iosif Vaisman  
**Committee Members:** Dr. Dmitri Klimov, Dr. Monique van Hoek

**ABSTRACT:**

In recent years pan-resistant microbes have begun to pose a significant risk, particularly in clinical settings. To combat this emerging threat new antimicrobial therapies are required. Antimicrobial peptides (AMPs) are a promising, and until recently, mostly underutilized resource. A large number of AMPs have been experimentally identified and predicted, very few of them are approved for clinical use, but thousands more may be hiding in plain sight in various databases. Machine learning offers a powerful technique to mine already available protein sequences for those with high potential to exhibit antimicrobial properties. This work is focused on creating and testing a novel set of descriptors based on reduced amino acid residue alphabets, structural, and topological properties of AMPs. These novel descriptors were used in the development of machine learning models capable of discriminating AMPs from non-AMPs. Such models may be used to screen proteins with known structures for potential antimicrobial activity.