

# CHEM5310 - Introduction to Programming and Machine Learning for Chemistry

[CHEM 5310](#) Introduction to Programming and Machine Learning for Chemistry (3 semester credit hours) This course will start by introducing chemistry students to basic computer programming concepts, with an emphasis on topics important for chemistry research such as the retrieval, processing, and analysis of chemistry data. The course will primarily use the Python language, due to its availability and current popularity in scientific programming, and a brief overview of other languages will also be included. Students will learn how to programmatically access online chemistry databases such as the Protein Data Bank and retrieve data, and use the numpy and scipy libraries to analyze chemical data sets. Finally, we will introduce the principles underlying machine-learning, including using the scikit-learn machine-learning libraries to train models to predict the properties of molecules and materials. Instructor consent required. (3-0) R