

Cheminformatics CHEM3351 Schedule Fall 2025

Week	OLCC topic	Tuesday	Thursday	Homework
August 18	Unit 0: OLCC Primer	Introduction, Overview of course, Nanohub, Request GitHub accounts	Introduction to python and jupyter notebooks Notebook: My python_basics.ipynb	My python_basics.ipynb due next class Tuesday? Reading Chapter 1 Weiss Text
August 25	Unit 0: Python Primer	Weiss Chapter 2 Intermediate python New notebook based on chapter	Weiss Chapter 3 Plotting with Matplotlib New notebook based on chapter	Reading Chapter 2 Weiss Text Reading Chapter 3 Weiss Text
September 1	Unit 0: Vibe Coding	Introduction to Vibe Coding set up of computers: WSL, VSCode, GitHub AI Notebook: New Vibe Coding notebook	Notebook: New Vibe Coding notebook continued	Start PubChem interactive tutorial ?
September 8	Unit 1: Introduction to Data Chemistry and Course Overview	Searching PubChem (and a few other public databases)	Notebooks: PubChemDataTypes Introduction to PUG REST API	PubChem tutorial due next class Tuesday? Reading PubChem tutorial (Current Protocols Paper) (https://doi.org/10.1002/cpz1.217)
September 15	Unit 2: Understanding Public Chemical Databases	PubChem tutorial (https://doi.org/10.1002/cpz1.217) Review of technical aspects of PubChem Jupyter notebooks (data visualization using PubChem Element data.) maybe look at the fair document	Oral Exam 1	

September 22	Unit 3: Chemical Representations	SMILES, InChI, mol files	New notebook based on my MCII_2025 notebook	
September 29	Unit 4: Advanced topics in PubChem search	New notebooks based on OLCC2019 lessons 2-5	New notebooks based on OLCC2019 lessons 2-5	
October 6	Midterm Exam	No Class Fall Break	Oral Exam 2	
October 13	Unit 7: QSAR/QSPR Unit 5: Exploratory data analysis of PubChem BioAssay data	My QSPR workbook	New notebook from Sunghwan?	QSPR homework due
October 20	Unit 8: Molecular Similarity	MS Notebooks: Part 1 and Part 2	Notebook: Part 3	
October 27	Unit 9: Computer-Aided Drug Discovery and Design	Notebooks: Introduction to Pandas Virtual Screening	Perform molecular docking experiment using autodock vina?	
November 3	Unit 13: Supervised Machine Learning	Notebook: Based on my MCII2025	Oral Exam 3	
November 10	Student Projects	Students create a supervised ML project with drug target of their choice		
November 17	Student Projects			

November 24	Student Projects	Final Presentations	No Class Thanksgiving Break	
December 1		Finals Week		