Cheminformatics CHEM3351 Schedule Fall 2025

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| 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](https://github.com/ebucholtz/Cheminformatics/blob/master/ehren_olcc2025/introduction/python_basics.ipynb) | [My python\_basics.ipynb](https://github.com/ebucholtz/Cheminformatics/blob/master/ehren_olcc2025/introduction/python_basics.ipynb) due next class Tuesday?  [Reading Chapter 1](https://weisscharlesj.github.io/SciCompforChemists/notebooks/chapter_01/chap_01_notebook.html) 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](https://weisscharlesj.github.io/SciCompforChemists/notebooks/chapter_02/chap_02_notebook.html) Weiss Text  [Reading Chapter 3](https://weisscharlesj.github.io/SciCompforChemists/notebooks/chapter_03/chap_03_notebook.html) 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](https://www.nlm.nih.gov/oet/ed/pubchem/tutorial/index.html) ? |
| September 8 | Unit 1: Introduction to Data Chemistry and Course Overview | Searching PubChem (and a few other public databases) | Notebooks:  [PubChemDataTypes](https://github.com/DivCHED-CCCE/DataChemistryOLCC/blob/main/module_development/01_Introduction/01-1_PubChemDataTypes.ipynb)  [Introduction to PUG REST API](https://github.com/ebucholtz/Cheminformatics/blob/master/ehren_olcc2025/01_Introduction/1.b-Introduction_PUG_REST.ipynb) | [PubChem tutorial](https://www.nlm.nih.gov/oet/ed/pubchem/tutorial/index.html) 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](https://github.com/ebucholtz/Cheminformatics/blob/master/ehren_olcc2025/QSPR_update_2025/QSPRUpdate2025.ipynb) | New notebook from Sunghwan? | QSPR homework due |
| October 20 | Unit 8: Molecular Similarity | MS Notebooks:  [Part 1](https://github.com/ebucholtz/Cheminformatics/blob/master/ehren_olcc2025/Molecular_similarity_2025/MS2025_part1.ipynb) and [Part 2](https://github.com/ebucholtz/Cheminformatics/blob/master/ehren_olcc2025/Molecular_similarity_2025/MS2025_part2.ipynb) | Notebook:  [Part 3](https://github.com/ebucholtz/Cheminformatics/blob/master/ehren_olcc2025/Molecular_similarity_2025/MS2025_part3.ipynb) |  |
| October 27 | Unit 9: Computer-Aided Drug Discovery and Design | Notebooks:  [Introduction to Pandas](https://github.com/ebucholtz/Cheminformatics/blob/master/ehren_olcc2025/9_virtual_screening/Pandas_introduction.ipynb)  [Virtual Screening](https://github.com/ebucholtz/Cheminformatics/blob/master/ehren_olcc2025/9_virtual_screening/virtual_screening_OLCC2025.ipynb) | 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 |  |  |