Computer Assisted Retrosynthesis Workshop Schedule

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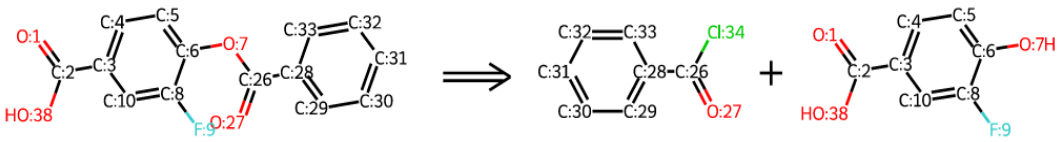

Overview

UA Libraries will be hosting a workshop series on open-source computer assisted retrosynthesis workflows. These workshops will use python programming and cheminformatics techniques for predicting retrosynthesis. Why attend?

- Enhance your chemical synthesis literature searching skills
- Learn how to use the cheminformatics toolkit, RDKit, for working with digital molecules and reactions
- Work through several open-source retrosynthesis workflows, including software and methods published by scientists at **MIT, AstraZeneca, and Eli Lilly**

Note

Registration Links: Registration is required – morning sessions: ua.libcal.com/calendar/instruction/morning_retro ; afternoon sessions: ua.libcal.com/calendar/instruction/afternoon_retro

Location: Rodgers Library Scholars' Station.

Time and Duration: All workshops will be offered twice on the date scheduled in order to accommodate schedules (see below). The morning session will start at **10:00 AM** and the afternoon session will start at **3:30 PM**; expected durations are about 1 hour.

Technology: We recommend bringing your own laptop; if you are using Windows, we recommend installing Windows Subsystem for Linux.

Additional Information: Prior programming experience is beneficial but not necessary. You will still learn how to get started, even if you don't fully understand all the code during the workshops.

Reusue and sharing: Code presented during the workshops is available here: github.com/ualibweb/retrosynthesis

Day	Date	Workshop Title	Notes
Day 1	Tues, Sept. 17	Workshop Overview and Python Programming Introduction	Intro to methods covered and retrosynthesis; environment setup; basic python programming.
Day 2	Wed, Sept. 18	RDKit/Cheminformatics Part 1	SMILES file format; reading and working with molecules; molecule depiction; canonicalization, identifiers, and hashes; chemical similarity and fingerprints; substructure search.
Day 3	Thurs, Sept. 19	RDKit/Cheminformatics Part 2	Descriptors; Reading and working with reactions; reaction depiction; reaction transformations; molecule and reaction standardization.
Day 4	Tues, Sept. 24	AiZynthFinder Retrosynthesis	Template based neural network model.
Day 5	Wed, Sept. 25	Retrosynthesis based on Similarity Ranking	Deterministic prediction model from start to finish.
Day 6	Thurs, Sept. 26	LillyMol Retrosynthesis	C++ command line based deterministic model.

Have questions? Interested but can't attend? Contact: vfscalfani@ua.edu