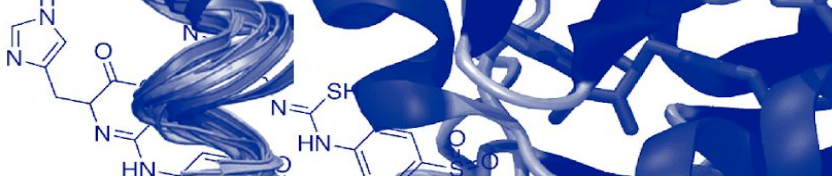
ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich



lwreg: lightweight chemical registration

Greg Landrum
2023 RDKit UGM
Mainz, Germany

lwreg: lightweight chemical registration for computational scientists[1]

What:

Simple, flexible, and powerful interface for tracking which compounds you've worked on

- Easily answer the question: "Have I looked at this compound before?"
- Configurable compound standardization
- Multiple levels for compound identity, e.g. tautomers, stereoisomers
- Can track conformers
- Simple to integrate in your workflow
- Easy integration with chemical search
- Easy to link with/store experimental data/metadata

1 It'll work for non-computational scientists too, but they aren't the target audience of this presentation.

“Demo”

https://github.com/rinikerlab/lightweight-registration/blob/main/demos/01_registration_basics.ipynb

lwreg: lightweight chemical registration for computational scientists[1]

Technical:

- https://github.com/rinikerlab/lightweight-registration
- MIT license
- RDKit based (of course)
- Python (of course)
- Python API and command-line tool
- Can use sqlite or PostgreSQL as a backend

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