Postdoctoral Scholar: Data Science and Machine Learning for Synthetic Organic Chemistry

Seeking postdoctoral researchers to join the data science projects in the Reisman group. Possible projects include (1) ligand design and optimization, (2) dataset design and automating data analysis workflows for HTE campaigns, and (3) implementation of synthesis planning and modeling workflows for total synthesis. Candidates should be interested in validating their modeling work through collaboration with experimentalists and comfortable operating across an active network of external collaborators in synthetic chemistry, computational chemistry, data science, and computer science.

Qualifications

1. Ph.D. in chemistry, cheminformatics, computer science, or a related discipline.
2. Experience in applied machine learning or data science, demonstrated through at least one first-author publication.
3. Ability to build, train, and rigorously evaluate machine learning models. Familiarity with ML-focused Python packages (e.g., scikit-learn, PyTorch, XGBoost) and standard cheminformatics packages (e.g., RDKit, Morfeus-ML, Chemprop, ASE, etc.) is expected.
4. Ability to use computational chemistry software for electronic property calculations, geometry optimizations, and conformer sampling. The candidate should be able to use software such as Gaussian, ORCA, xtb, or CREST, in addition to MLIPs, and to create Python scripts to build descriptor workflows executed at scale on HPC clusters.
5. Demonstrated fluency in Python programming, including version control (git) and reproducible, well-documented code intended for public release alongside publications.
6. Candidate should be highly motivated and independent, with strong written and verbal communication skills and the ability to explain ML concepts and results to synthetic chemists.

Experience with preparative synthetic organic chemistry is not required but would be beneficial; comfort reading a synthesis paper and reasoning about mechanism is expected.

Responsibilities

The postdoctoral scholar will:

1. Serve as the data science collaborator for experimentalists in the Reisman group and for external collaborations, scoping problems jointly and developing models to guide experimental campaigns.
2. Build and maintain descriptor generation pipelines, including conformer searching and DFT-derived steric/electronic parameterization of chiral ligand libraries. Release code and datasets openly alongside publications.
3. Mentor graduate students and undergraduates in Python, cheminformatics, and statistical practice, and help raise the group's baseline data literacy.
4. Prepare manuscripts, figures, and presentations; present at group meetings, collaborator meetings, and conferences. Contribute to grant proposal writing.

Representative projects

Anticipated directions build directly on the group's recent work:

- **Extending descriptor libraries beyond *N,N*-bidentate ligands.** Generalizing the BUNNY framework to expanded chiral ligand classes and testing whether descriptor sets and trained models transfer across Ni-catalyzed coupling manifolds, with the goal of prospective ligand selection for new asymmetric transformations.
- **Model-guided discovery of new catalytic reactions.** Applying and refining the data-science-guided workflow developed for transition-metal catalysis, including active learning and design-of-experiments approaches to reaction optimization.
- **Selectivity prediction on complex substrates.** Extending target-specific dataset design to site- and stereoselectivity problems in late-stage functionalization, including experimental data collection.
- **Analytical methods for HTE and/or multimodal structure determination as part of the ELECTRA PCL-Cloud Node.** Design innovative methods for reaction analysis and structure determination in collaboration with computer scientists and other partners within the ELECTRA Center.
- **Strategy-aware computer-aided synthesis planning.** Continue collaborative work on higher-level retrosynthetic strategy, including evaluation of CASP outputs against real synthetic campaigns in the group.

To apply

For full consideration, send the following materials to Tomomi Kano by October 15, 2026.

Requested materials. Cover letter with statement on research interests and relevant experience, Curriculum vitae, Research summary (2-3 pages), Names of three letter writers