

Tuesday, November 3, 2020

SOLICITATION FOR POSTDOCTORAL RESEARCH ASSOCIATE APPLICANTS
AT THE INTERFACE OF SYNTHETIC ORGANIC CHEMISTRY AND COMPUTER SCIENCE

The University of Illinois at Urbana-Champaign has recently established an NSF Funded Institute to merge synthetic chemistry with artificial intelligence, the Molecule Maker Lab Institute (MMLI). Our research groups have identified a need for an individual, formally trained in the area of synthetic organic chemistry, who is also interested in becoming proficient in chemoinformatics (programming, statistical analysis, modeling).

Suitable candidates should have the following qualifications:

1. Ph.D. in chemistry with extensive experience in organic synthesis including but not limited to total synthesis of natural products, methods development, mechanistic investigations, medicinal chemistry, organometallic chemistry.
2. Be proficient in multistep synthesis, have experience with anaerobic reaction techniques, have familiarity with catalytic transformations.
3. Have experience with different analytical techniques including HPLC, SFC, GC.
4. Be fluent in spectroscopic methods of structural analysis including multinuclear NMR, 2D NMR, variable temperature NMR, IR, mass spectrometry.

Furthermore, the candidate should be interested in learning and becoming proficient in the following areas of informatics/computer science. The following qualifications are not required but will be considered favorably:

1. Experienced in Python programming
2. Experience with Python packages such as SKlearn, Tensorflow, and Pytorch and cheminformatics-specific Python packages like RDKit.
3. Experience with basic computational chemistry software. Familiarity with conformational search algorithms and quantum chemistry packages
4. Experience with Schrodinger suite, Gaussian, Nwchem, and Openbabel

The postdoctoral research associate will report to Prof. Scott Denmark (Chemistry) and Prof. Saurabh Sinha (Computer Science), and have the following responsibilities:

1. Will be the experimentalist generating data for the groups and for some industrial and academic collaborations by:
 - a. Synthesizing training set members of catalysts
 - b. Executing catalytic reactions to generate data for computational modeling
 - c. Synthesizing new catalysts predicted by modeling efforts
 - d. Validating predictions and expanding reaction scope.
2. Will work closely with Artificial Intelligence (AI) researchers to develop training data sets usable in AI tools, and consulting with these researchers for development of such tools.
3. Will take over the management of our High Throughput Experimentation platforms including ChemSpeed and other capabilities.
4. Drafting manuscripts for publication and internal reports for the MMLI.

Individuals interested in being considered for this postdoctoral research opportunity should send their application materials (e-mail) to the address in the letterhead. The application should include:

- A cover letter stating:
 - educational and research background
 - long term career interests

- availability date
- A curriculum vita including
 - educational background
 - publications
 - presentations
 - awards
 - recommenders
- A brief description (2-3 pages) of graduate research projects
- Three letters of recommendation (sent separately) from individuals familiar with their research potential.

Thank you very much for your assistance.

Sincerely,



Scott E. Denmark
R. C. Fuson Professor of Chemistry



Saurabh Sinha
Founder Professor in Computer Science