Ryne C. Johnston

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Professional Experience

Schrödinger, Inc. — Portland, OR
Product Manager — Jun 2023 – Present

- Managed multiple products and directed teams to meet project goals and deadlines.
  - *Epik*: pK_a and protonation state predictor
  - *E-sol*: CNS permeability predictor
- Interacted with customers and provided software solutions to meet their needs.
- Interacted with marketing and sales teams to develop and execute product launch plans.

Principal Scientist/ Technical Lead — Jun 2021 – Jun 2023

- Developed and maintained best-in-class Python software to predict chemical properties through machine learning.
- Wrote scholarly articles and technical documents for public consumption.
- Wrote and maintained documentation and automated tests.
- Performed code reviews.

Senior Scientist — May 2017 – Jun 2021

- Developed software to enumerate and canonicalize different related chemical compounds.
- Maintained legacy chemistry C/C++ software.

Oak Ridge Nat'l Lab — Oak Ridge, TN
Postdoctoral Scholar — Jun 2015 – Feb 2017

- Effectively communicated progress to a large, cross-disciplinary group of researchers.
- Wrote scholarly articles and research project proposals.
- Awarded nearly $1M in research grant funds.

Education

2015 **Doctor of Philosophy**, Chemistry
Oregon State University

2010 **Bachelor of Science**, Chemistry
Henderson State University

Expertise

pK_a, tautomerism, chemical equilibria, homogenous catalysis, cheminformatics

Skills

- Python
- PyData
- PyTorch
- RDKit
- git/GitHub
- C++
- Fortran
- agile methodology
- productivity tools
- performance profilers
- computational chemistry packages
  - Schrödinger
  - ORCA

Scientific Communication

Recent Conferences: Oral presentation at the American Chemical Society National Meeting, Spring 2021

Selected Publication (from >25): Johnston, R. C. et al. Epik: pK_a and Protonation State Prediction through Machine Learning *Journal of Chemical Theory and Computation*, **2023**, *19*, 2380-2388, doi: 10.1021/acs.jctc.3c00044.

Interests

chemistry, geology, history, programming, hiking