

# Ryne C. Johnston

## 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/** Jun 2021 – Jun 2023  
**Technical Lead**

- 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.

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## EDUCATION

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

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

## EXPERTISE

$pK_a$ , tautomerism, chemical equilibria, homogeneous 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  
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.

*Selected Publication* (from >25)

## INTERESTS

chemistry, geology, history, programming, hiking