Ryne C. Johnston

Professional Experience

Schrödinger, Inc.

Product Manager

Portland, OR Jun 2023 – Present

- Managed multiple products and directed teams to meet project goals and deadlines.
 - Epik: p K_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.

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Peaverton, OR 97008

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
- PvData
- PyTorch
- RDKit
- git/GitHub
- C++
- Fortran

- agile methodology
- productivity tools
- performance profilers
- computational chemistry packages
 - Schrödinger
 - ORCA

SCIENTIFIC COMMUNICATION

 $\begin{array}{c} Recent \\ Conferences \end{array}$

Selected

Publication

(from > 25)

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.

Interests

chemistry, geology, history, programming, hiking