Ryne C. Johnston

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Professional Experience

Schrödinger, Inc. Portland, OR

Principal Scientist II/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*: Central nervous system 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 I/Technical Lead Jun 2021 – Jun 2023

- Developed and maintained best-in-class Python software to predict chemical properties through machine learning.
- Contributed to the development of a Python workflow for the rational design of homogenous catalysts to unlock previously unattainable reactivity.
- 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 National Laboratory Oak Ridge, TN

Postdoctoral Scholar Jun 2015 – Feb 2017

- Used quantum chemistry software to investigate environmentally relevant biogeochemical processes.
- Probed the mechanisms of how inorganic mercury is microbially assimilated into a bioaccumulative organic form and its later environmentally-mediated deposition back into its inorganic form.
- Developed methods for computing pK_a values of environmentally relevant functional groups and aqueous formation constants of metal complexes.
- Wrote scholarly articles and research project proposals.
- Awarded nearly $1M in research grant funds.

Projects

Epik

- I designed, developed, and now manage *Epik*, a Python software program for predicting aqueous the pK_a values and distribution of protonation states of small molecules. It leverages a machine learning model trained on 77k pK_a values for accurate predictions across broad chemical space.

E-sol

- I am the product manager of *E-sol*, a workflow using physics-based methods for calculating partition coefficients of small molecules with the aim of predicting their central nervous system permeability.

PetroSim

- As a passion side project, I created the open-source *PetroSim* Python package as a collection of the Python ports of the originally Visual Basic EC-(R)AFC petrological models for simulating the evolution of the geochemical composition of a magma body over time.

Education

2015 **Doctor of Philosophy**, Computational Chemistry — *Oregon State University*
2010 **Bachelor of Science**, Chemistry — *Henderson State University*

Publications

Skills

- Python
- NumPy
- scikit-learn
- pandas
- PyTorch
- RDKit
- version control (git/GitHub)
- C++
- Fortran
- agile methodology
- productivity tools
- performance profilers
- computational chemistry packages
  - Schrödinger
  - ORCA

Interests

- chemistry, geology, history, programming, hiking