

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 the aqueous 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 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	<i>Oregon State University</i>
2010	Bachelor of Science , Chemistry	<i>Henderson State University</i>

PUBLICATIONS

- (1) Li, M.; Scheeff, S.; Chen, J.; Johnston, R. C.; Rizzo, A.; Krenske, E. H.; Chiu, P. *Chem. Eur. J.* **2024**, *30*, DOI: [10.1002/chem.202401485](https://doi.org/10.1002/chem.202401485).
- (2) Johnston, R. C.; Yao, K.; Kaplan, Z.; Chelliah, M.; Leswing, K.; Seekins, S.; Watts, S.; Calkins, D.; Chief Elk, J.; Jerome, S. V.; Repasky, M. P.; Shelley, J. C. *J. Comp. Theory Comput.* **2023**, *19*, 2380–2388.
- (3) Watson, M. A.; Johnston, R. C.; Bochevarov, A. *J. Chem. Inf. Model.* **2023**, *63*, 5396–5399.
- (4) Lian, P.; Mou, Z.; Cooper, C. J.; Johnston, R. C.; Brooks, S. C.; Gu, B.; Govind, N.; Jonsson, S.; Parks, J. M. *J. Phys. Chem. A* **2021**, *125*, 5397–5405.
- (5) Cooper, C. J.; Alam, S.; de Paul N. Nziko, V.; Johnston, R. C.; Ivanov, A. S.; Mou, Z.; Turpin, D. B.; Rudie, A. W.; Elder, T. J.; Bozell, J. J.; Parks, J. M. *ACS Sustain. Chem. Eng.* **2020**, *8*, 7225–7234.
- (6) Dajnowicz, S.; Parks, J. M.; Hu, X.; Johnston, R. C.; Kovalevsky, A. Y.; Mueser, T. C. *ACS Catalysis* **2018**, *8*, 6733–6737.
- (7) Lian, P.; Johnston, R. C.; Parks, J. M.; Smith, J. C. *J. Phys. Chem. A* **2018**, *122*, 4366–4374.
- (8) Lombard, F. J.; Lepage, R. J.; Schwartz, B. D.; Johnston, R. C.; Healy, P. C.; Krenske, E. H.; Coster, M. J. *Org. Biomol. Chem.* **2018**, DOI: [10.1039/c7ob02123b](https://doi.org/10.1039/c7ob02123b).
- (9) Dajnowicz, S.; Johnston, R. C.; Parks, J. M.; Blakeley, M. P.; Keen, D. A.; Weiss, K. L.; Gerlits, O.; Kovalevsky, A.; Mueser, T. C. *Nature Commun.* **2017**, *8*, DOI: [10.1038/s41467-017-01060-y](https://doi.org/10.1038/s41467-017-01060-y).
- (10) Walden, D. M.; Jaworski, A. A.; Johnston, R. C.; Hovey, M. T.; Baker, H. V.; Meyer, M. P.; Scheidt, K. A.; Cheong, P. H.-Y. *J. Org. Chem.* **2017**, *82*, 7183–7189.
- (11) West, T. H.; Walden, D. M.; Taylor, J. E.; Brueckner, A. C.; Johnston, R. C.; Cheong, P. H.-Y.; Lloyd-Jones, G. C.; Smith, A. D. *J. Am. Chem. Soc.* **2017**, *139*, 4366–4375.
- (12) Chen, H.; Johnston, R. C.; Mann, B.; Chu, R. K.; Tolić, N.; Parks, J. M.; Gu, B. *Environ. Sci. Technol. Lett.* **2016**, DOI: [10.1021/acs.estlett.6b00460](https://doi.org/10.1021/acs.estlett.6b00460).
- (13) Johnston, R. C.; Zhou, J.; Smith, J. C.; Parks, J. M. *J. Phys. Chem. B* **2016**, *120*, 7307–7318.
- (14) Kang, J. Y.; Johnston, R. C.; Snyder, K. M.; Cheong, P. H.-Y.; Carter, R. G. *J. Org. Chem.* **2016**, *81*, 3629–3637.

- (15) Walden, D. M.; Ogba, O. M.; Johnston, R. C.; Cheong, P. H.-Y. *Acc. Chem. Res.* **2016**, DOI: [10.1021/acs.accounts.6b00204](https://doi.org/10.1021/acs.accounts.6b00204).
- (16) Challinor, V. L.; Johnston, R. C.; Bernhardt, P. V.; Lehmann, R. P.; Krenske, E. H.; Voss, J. J. D. *Chem. Sci.* **2015**, DOI: [10.1039/c5sc02056e](https://doi.org/10.1039/c5sc02056e).
- (17) Cohen, D. T.; Johnston, R. C.; Rosson, N. T.; Cheong, P. H.-Y.; Scheidt, K. A. *Chem. Commun.* **2015**, 51, 2690–2693.
- (18) Wang, X.-N.; Krenske, E. H.; Johnston, R. C.; Houk, K. N.; Hsung, R. P. *J. Am. Chem. Soc.* **2015**, 137, 5596–5601.
- (19) Gould, E.; Walden, D. M.; Kasten, K.; Johnston, R. C.; Wu, J.; Slawin, A. M. Z.; Mustard, T. J. L.; Johnston, B.; Davies, T.; Cheong, P. H.-Y.; Smith, A. D. *Chem. Sci.* **2014**, 5, 3651.
- (20) Jang, K. P.; Hutson, G. E.; Johnston, R. C.; McCusker, E. O.; Cheong, P. H.-Y.; Scheidt, K. A. *J. Am. Chem. Soc.* **2014**, 136, 76–79.
- (21) Johnston, R. C.; Cohen, D. T.; Eichman, C. C.; Scheidt, K. A.; Cheong, P. H.-Y. *Chem. Sci.* **2014**, 5, 1974.
- (22) Wang, X.-N.; Krenske, E. H.; Johnston, R. C.; Houk, K. N.; Hsung, R. P. *J. Am. Chem. Soc.* **2014**, 136, 9802–9805.
- (23) Johnston, R. C.; Cheong, P. H.-Y. *Org. Biomol. Chem.* **2013**, 11, 5057.
- (24) McGarraugh, P. G.; Johnston, R. C.; Martínez-Muñoz, A.; Cheong, P. H.-Y.; Brenner-Moyer, S. E. *Chem. Eur. J.* **2012**, 18, 10742–10752.
- (25) McIntosh, M. L.; Johnston, R. C.; Pattawong, O.; Ashburn, B. O.; Naffziger, M. R.; Cheong, P. H.-Y.; Carter, R. G. *J. Org. Chem.* **2012**, 77, 1101–1112.
- (26) Pattawong, O.; Mustard, T. J. L.; Johnston, R. C.; Cheong, P. H.-Y. *Angew. Chem.* **2012**, 125, 1460–1463.
- (27) Pierce, M. D.; Johnston, R. C.; Mahapatra, S.; Yang, H.; Carter, R. G.; Cheong, P. H.-Y. *J. Am. Chem. Soc.* **2012**, 134, 13624–13631.

SKILLS

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

INTERESTS

- chemistry, geology, history, programming, hiking