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

(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.

(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.

(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.

(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.

(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.

(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.

(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

- 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

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