William **Kumler**

Ph.D. Candidate

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Professional Summary

Chemical oceanographer with a data science specialization completing Ph.D. in July 2025. Expertise in automated and untargeted liquid chromatography mass spectrometry and experience developing computational tools for mass spectrometry data analysis and visualization. Fieldwork consisting of cruise planning, two months total ship time, and both wetlab and drylab operations onboard during the Simons Collaboration on Ocean Processes and Ecology (SCOPE) project.

Education

Ph.D. in Chemical Oceanography, University of Washington *2019 - 2025*

M.Sc. in Oceanography, University of Washington *2019 - 2023*

B.A. in Marine Science, University of California, Berkeley *2014 - 2018*

B.S. in Molecular and Environmental Biology, University of California, Berkeley *2014 - 2018*

Work Experience

Ph.D. student, Ingalls Lab, University of Washington, Seattle *2019 - 2025*

- Published papers on marine microbial metabolomics with a focus on untargeted methodologies
- Developed existing and novel mass spectrometry tools for analysis and visualization
- Fieldwork in the North Pacific Subtropical Gyre and California Current
- Mentored graduate and undergraduate students in metabolomics

Lab Manager, Koehl Lab, University of California, Berkeley *2018 - 2019*

- Maintained live cultures of choanoflagellates and protozoa
- Managed and organized lab members, materials, and safety protocols
- Assisted visiting researchers with statistical analyses
- Tutored undergraduates in ImageJ and R programming

Lab Manager, Edwards Lab, University of California, Berkeley *2018 - 2019*

- Performed HPLC-MS sample preparation and analysis using Thermo Fusion Lumos ID-X
- Developed and maintained a lipidomics pipeline for data handling and statistical analysis
- Educated undergraduates in R programming and SLURM cluster usage

Technical skills

- **Coding:** Ten years of experience in R. Expertise with full-pipeline construction including data ingestion, tidying, analysis, visualization, and sharing via reproducible documents, interactive web applications, and R packages published to both CRAN and Bioconductor. Three years of experience with Python largely centered around reverse-engineering mass-spectrometry file formats. Recent experience with database management systems and HTML/CSS. Extensive collaboration with international groups via Github.
- **Scientific analysis:** Univariate and multivariate statistics with a focus on permutational methods and machine learning (random forests, SOMs, autoencoders) resulting in four first-author papers and 12 national and international conference presentations.
- **Fieldwork and ship time:** Estimated 50 days at sea across both multi-week cruises and short-term time series sampling, one cruise as chief scientist. Experience with cruise planning, CTD operations, float deployments and recoveries, incubations, and real-time data ingestion and visualization. Two weeks of land-based fieldwork involving sample collection and small-volume chemostat-style mesocosms.

Technical Projects

- **MESOSCOPE visualization application**: Data aggregation and interactive visualization for three cruises during the 2015-2018 MESOSCOPE project (Microbial Ecology of the Surface Ocean - Simons Collaboration on Ocean Processes and Ecology). Used for multi-lab dataset overlap comparison and manuscript preparation at the 2022 SCOPE meeting in New York. Emphasis was placed on realtime data ingestion via APIs and web-scraping. Application deployed at `https://wkumler.shinyapps.io/mswebapp/`.
- **RaMS**: R package for reading and tidying mass-spectrometry data. Available on CRAN and GitHub.
- **pylgrams**: Python language gloss of the RaMS package. Available on PyPI and GitHub.
- **squallms**: R package for interactive multi-file annotation of chromatographic feature quality. Available on Bioconductor and GitHub.
- **planetan**: Personal project implementing a 3D multiplayer R Shiny game with a ruleset similar to Catan. Available on GitHub and as a live demo at `https://wkumler.shinyapps.io/planetan`. Will be submitted to the R Shiny Contest 2025.

Publications

- **W. Kumler**, W. Qin, R.A. Lundeen, B. Barone, L.T. Carlson & A.E. Ingalls (2024). Metabolites reflect variability introduced by mesoscale eddies in the North Pacific Subtropical Gyre. *Frontiers in Marine Science*, 11:1481409. DOI:10.3389/fmars.2024.1481409
- **Kumler, W.**, Hazelton, B.J. & Ingalls, A.E. (2023). Picky with peakpicking: assessing chromatographic peak quality with simple metrics in metabolomics. *BMC Bioinformatics*, 24:404. DOI:10.1186/s12859-023-05533-4
- **Kumler, W.** & Ingalls, A.E. (2022). Tidy data neatly resolves mass-spectrometry's ragged arrays. *R Journal*, 14(3), 193-202. DOI:10.32614/RJ-2022-050
- Boysen, A.K., Durham, B.P., **Kumler, W.**, et al. (2022). Glycine betaine uptake and metabolism in marine microbial communities. *Environmental Microbiology*, 24(5), 2380-2403. DOI:10.1111/1462-2920.16020
- **Kumler, W.E.**, Jorge, J., Kim, P.M., et al. (2020). Does formation of multicellular colonies by choanoflagellates affect their susceptibility to capture by passive protozoan predators? *Journal of Eukaryotic Microbiology*, 67(5), 555-565. DOI:10.1111/jeu.12808

In review:

- **W. Kumler**, S. LaRue & A.E. Ingalls (in review with *ACS Journal of Proteom Research*). Databases are an effective and efficient method for storage and access of mass-spectrometry data. Preprint available on GitHub.
- E.A. Seelen, S.J. Gleich, **W. Kumler**, H.S. Anderson, X. Bian, K.M. Bjorkman, D.A. Caron, S.T. Dyhrman, S. Ferrón, Z.V. Finkel, S.T. Haley, Y. Hy, A.E. Ingalls, A.J. Irwin, D.M. Karl, K.P. Kong, D. Lowenstein, A. Salazar Estrada, E. Townsend, J.C. Tracey, K. Turk-Kubo, B.A.S. Van Mooy & S.G. John (in review with *Nature Communications*). A tale of two nutrients: how nitrogen and phosphorus differentially control marine biomass production and stoichiometry.
- P. Louail, C. Brunius, M.G. Aloy, **W. Kumler**, N. Storz, J. Stanstrup, H. Treutler, P. Vangeenderhuysen, M. Witting, S. Neumann & J. Rainer (in review with *ACS Analytical Chemistry*). xcms at 20 and still in peak form.

Conference Proceedings

- **W. Kumler** & A.E. Ingalls. Databases are a speedy, small, and simple solution for mass-spectrometry data storage and access. Upcoming poster at the *2025 Annual International Conference of the Metabolomics Society*, Prague, Czechia.
- P. Louail, **W. Kumler**, P. Vangeenderhuysen, C. Brunius, M. Witting, S. Neumann, RforMassSpectrometry contributors & J. Rainer. xcms at 20 and still in peak form: Now anchoring a complete ecosystem for metabolomics data preprocessing and analysis. Upcoming presentation at the *2025 Annual International Conference of the Metabolomics Society*, Prague, Czechia.
- **W. Kumler**, L.T. Carlson & A.E. Ingalls plus the PARAGON team. Differences in 15N use by source during the PARAGON cruise in the NPSG. Presented as a poster at the *2024 Simons Collaboration on Ocean Processes and Ecology*, New York, NY.
- S. Garcia, F.X. Ferrer-González, J.S. Sacks, **W. Kumler**, L.T. Carlson, & A.E. Ingalls (2024). Characterizing the quality and quantity of metabolite production in phytoplankton cultures and the environment through endo-

and exometabolomics. Presented as a poster at the Gordon Research Conference on Marine Microbes, Les Diablerets, Switzerland. Poster #8.

- Y. Wang, **W. Kumler**, I. Kern, E. Seelen, S.G. John, & A.E. Ingalls (2023). Community metabolomes respond to nutrient supply in a mesocosm study in the North Pacific Subtropical Gyre. Presented as a poster at the *2023 Ocean Sciences Meeting*, New Orleans, LA. Poster #OB14B-0682.
- **W. Kumler**, L.T. Carlson, & A.E. Ingalls plus the PARAGON team (2023). Metabolic fate of dissolved nitrogen in the NPSG. Presented as a poster at the *2023 Ocean Sciences Meeting*, New Orleans, LA. Poster #OB14B-0702
- **W. Kumler** (2022). Unmasking the POC/Ness Monster: Depth and Mesoscale Features Drive Variability in Particulate Metabolite Profiles of the MESOSCOPE transect. Presented as a virtual poster at the *2022 Simons Collaboration on Ocean Processes and Ecology*, New York, NY.
- **W. Kumler** & A.E. Ingalls (2021). RaMS: R-based Access to Mass-Spectrometry Data. Presented as a poster at the *2021 Annual Conference of the Metabolomics Society (virtual)*. Poster #298.
- **W. Kumler**, H. Fredricks, J. Ossolinski, A. Allen, K. Thamatrakoln, K. Bidle, B. Van Mooy, & B. Edwards (2019). Sign of the times: the lipid signature of a collapsing phytoplankton bloom. Presented as a poster at the *2019 Aquatic Sciences Meeting*, San Juan, Puerto Rico. Poster #411.
- **W. Kumler** & M.A.R. Koehl (2018). Evolution of multicellularity: Capture of unicellular vs colonial choanoflagellates by a protozoan predator. Presented as a poster at the *2018 Society of Integrative and Comparative Biology Annual Meeting*, San Francisco, CA. Poster #P1-115.

Talks Given

- **Building a robust model of peak quality for untargeted mass-spectrometry** *2023*
  - Seminar given at UW's eScience Seminar (watch here)
  - Seminar given at UW's Quantitative Science Seminar
- **Data Visualization** *2022*
  - Workshop led at the Graduate Climate Conference
- **Profiling R code and identifying performance bottlenecks** *2019*
  - Invited speaker at FSH 507 (Super-advanced R)

Volunteer efforts

- eScience Institute Software Carpentries instructor *2023 - 2025*
  - Both R and Python tracks
  - Emphasis on teaching data access and visualization
- Data Science in Oceanography Summer Program *2022 - 2024*
  - Two-week in-person workshop for college students considering graduate school and interested in expanding their data science skills
  - Lectured on chemical oceanography and access to publicly available datasets
- SEAS Annual Aquatic Sciences Open House *2022 - 2025*
  - Organized booths for approximately 20+ individual labs
  - Facilitated media coverage and 1,000+ attendees from the greater Seattle area
  - Ran Marine Microbial Research Center booth with natural seawater visualization under a microscope
- Seattle Aquarium *2019 - 2025*
  - 100+ hours of engagement and interpretation at evening events
  - Particular emphasis on stewardship events such as Splash!, which brought in over half a million dollars from donors

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References

Dr. Anitra E. Ingalls, Ph.D. Advisor. `aingalls@uw.edu`, (206) 940-6755

Laura T. Carlson, Ingalls Lab Manager. `truxal@uw.edu`, (412) 554-5093