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Insights from Automated and Untargeted Marine Microbial Metabolomics

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**Abstract**

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Metabolomics is the study of small molecules that are the product of cellular metabolism. Most commonly done with mass spectrometry (MS), this field involves the characterization and quantification of the many small, bioactive molecules that serve as building blocks for life. In the marine environment, this gives us a powerful lens with which to view the forms of material and energy as well as the fluxes they undergo in a dynamic ecosystem dominated by microbial life. This dissertation applies metabolomics to the marine ecosystem to determine how the marketplace of metabolites is an integral part of the ocean's productivity. It also includes novel tools for metabolomics that were developed alongside these environmental analyses to streamline access to MS data because the existing frameworks were often fragile black boxes lacking reproducibility and scaling poorly across larger file sizes and sample sets. In Chapter 2, I developed an R package that reads the open-source mzML and mzXML file types into a tidy in-memory object for easy extraction and visualization of data subsets such as ion chromatograms. In Chapter 3 I extend this framework into the storage of MS data in on-disk databases to avoid the major memory constraints. I then contrast those databases with several alternative MS data storage methods and find that the simpler, on-disk methods result in performance improvements of 10-100x in query speed without much size penalty. In Chapter 4 I use this tool to improve the peak-picking performance of one of the most common untargeted mass-spectrometry tools and show that metabolites from the North Pacific Subtropical Gyre have a wide variety of patterns with depth in the ocean but most follow biomass. Chapter 5 expands upon this dataset by investigating how mesoscale eddy features affect the abundance of those same metabolites, with clear trends in metabolite abundance mirroring those in the biogeochemistry and community. Finally, in Chapter 6 I use isotope tracing to investigate how the open ocean euphotic community uses various forms of nitrogen. I determine that ammonia is highly bioavailable at the surface while nitrate's use is restricted to a subset of organisms. Organic nitrogen, on the other hand, is used slowly and steadily with equal utility at the surface and base of the euphotic zone. In sum, this thesis contains novel insights into marine metabolites with unprecedented detail through the use of new tools and provides a framework for future investigation into marine microbial ecosystems.