

**Laying the foundation for a potential future BioGeoSCAPES program:
Assessing needs and capabilities for studying controls on ocean metabolism through
integrated omics and biogeochemistry**

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A proposal for an OCB Scoping Workshop - October 16, 2019



Introduction

We seek funding in the amount of \$70,000 to conduct a 3-day workshop for 80 participants aimed at advancing US involvement and co-leadership towards the formation of an international program called BioGeoSCAPES. The program aims to improve our understanding of the functioning and regulation of ocean metabolism and its interactions with nutrient cycling, within the context of a hierarchical seascape perspective. The proposed workshop will be an open forum to bring US scientists together from across the country to present data, discuss the opportunities and challenges involved in such a global scale effort, and to develop a plan for coordinating national interests and objectives with the international momentum towards this exciting initiative.

With the rapid changes now apparent throughout the ocean, there is a pressing need to understand how biological diversity influences biogeochemical functions globally. Microbial communities are central to the biogeochemical processes that make Earth habitable, and a comprehensive understanding of Earth's biogeochemical cycles depends on understanding the complexity of their intrinsic biological-chemical connections. Historically, connecting the mechanistic underpinnings of biological processes to the influence on geochemical cycles has been a significant challenge. Yet with the technological improvements in 'omics approaches in recent decades (genomics, transcriptomics, proteomics, lipidomics and metabolomics) there are great opportunities in facilitating the interdisciplinary study of microbial biogeochemistry. It has been a decade since the OCB Molecular Biology of Biogeochemistry workshop (see below); with the maturation in 'omics methodologies as well as knowledge gained from the GEOTRACES program regarding inorganic micronutrients, the timing is right to envision and start planning a global microbial biogeochemistry program.

History

There has been growing interest in a large-scale coordinated global microbial biogeochemistry program for more than a decade, and OCB has played a key role in nurturing this development. Inspired by the WOCE and GEOTRACES programs that carried out physical and chemical characterization of the oceans through a sectional approach, as well as advances in the application of molecular tools to understand microbial taxonomy and physiology, a 2010 OCB Scoping Workshop entitled "Molecular Biology of Biogeochemistry: Using molecular methods to link ocean chemistry with biological activity" was organized in Los Angeles. This workshop explored the need for large-scale sectional surveys of microbial biogeography and concluded that coupling these with intercalibrated physical and chemical data would significantly advance understanding of connections between microbial diversity and activity and biogeochemistry. Yet, this idea proved somewhat ahead of its time; with the exception of a few large labs, the molecular biology community was not yet poised to handle the spatial scale and resulting sample volume necessary to fully integrate 'omics data with high resolution geochemical data.

Since this initial workshop, major advances in sequencing and bioinformatics technology, as well as laboratory automation, have pushed the molecular field forward to the point where a more complete integration of molecular biology and geochemistry can be undertaken in the ocean. The remarkable value of large scale genomics and transcriptomics surveys has been demonstrated by the GOS (Global Ocean Sampling), Tara Oceans, and Malaspina expeditions. Tara Oceans, in particular, involving 11 expeditions circumnavigating the globe between 2009-2013, produced an internally-consistent global dataset of genomic and transcriptomic transects. Even matched with a fairly modest suite of biogeochemical measurements, the community response to the dataset has been enormous; the initial papers have been cited >600 times in just the last four years [Sunagawa et al. 2015; de Vargas et al. 2015]. However, the limitations stemming from a lack of matching, intercalibrated chemical measurements have also become apparent [Caputi et al. 2019]. Moreover, all of these efforts thus far have focused on the euphotic zone with minimal depth resolution. Developing full depth ocean microbial maps characterizing genes and enzymes that could connect to biogeochemical processes remains an ambitious, exciting, and unrealized goal [Santoro 2019].

Efforts to integrate 'omics and biogeochemistry have been undertaken on smaller scales that further demonstrate the potential (and challenge) of this approach. Several groups have undertaken the collection and analysis of biological parameters (cyanobacteria genomics, proteomics, N-fixation gene abundance, cellular nutrient contents, photophysiology) on GEOTRACES expeditions, an effort termed BioGEOTRACES [e.g., Biller et al. 2018]. Similarly, NSF provided funding for GeoMICS (Global Scale Microbial Interactions across Chemical Surveys), a pilot study in 2012 to determine how, in practice, to integrate omics and chemical sampling across a biogeochemical gradient in the northeast Pacific Ocean. An OCB data synthesis workshop was held in Friday Harbor, WA in 2013 to coordinate project results, and discussions highlighted the challenge of meshing hypothesis-testing with exploratory discovery of omics datasets. Subsequent projects have shown the value of making data broadly available in a timely manner. Both TARA and GEOTRACES have coordinated release of curated data, even in advance of publications. This approach maximizes opportunities for community engagement and intellectual advances, and, combined with recent analytical and bioinformatic advances, will enable BioGeoSCAPES to successfully mesh complex, multi-disciplinary datasets.

Two other OCB workshops have further supported inter-disciplinary discussions and advanced community consensus about the value of combining detailed taxonomic, physiological, and chemical information to understand biogeochemistry. An OCB Scoping Workshop on "Improving predictive biogeochemical models through single cell-based analyses of marine plankton physiological plasticity, genetic diversity and evolutionary processes" was hosted at Bigelow Laboratory for Ocean Sciences in May 2014, focusing on understanding the need to include biological diversity in biogeochemical models. In 2016, OCB and GEOTRACES co-hosted a synthesis workshop on "Biogeochemical cycling of trace elements within the ocean" at which the value of 'omics characterizations of cell activities and stresses was highlighted. The intervening years have also seen individual research groups and collaborative teams undertake efforts to combine meta-omics with intercalibrated chemical measurements. These projects now provide a roadmap for how to mesh sampling, data analysis/synthesis, and hypothesis testing to address large-scale questions of ocean metabolism and biogeochemistry. Indeed, new community-scale programs such as EXPORTS are now incorporating meta-omics and state-of-the-art chemical

measurements. These previous efforts have demonstrated the value of closely integrated modeling efforts to synthesize data, place observations within the constraints of the physical environment, and enable future trends to be predicted [e.g., Coles et al. 2017].

Recognizing this progress, in November 2018 OCB, SCOR (Scientific Commission on Ocean Research), and the Gordon and Betty Moore Foundation supported a working group to explore a framework for an international program to assess global controls on ocean metabolism and nutrient cycling through coordinated, intercalibrated, 'omics and chemical measurements. The initial seeds of the BioGeoSCAPES program (www.biogeoscapes.org) were planted at that meeting, and a key outcome was the recognition that standardization and intercalibration efforts in the 'omics communities lagged behind those of the geochemistry community. As a result, two complementary OCB-supported 'omics intercalibration efforts have recently been launched. First, a metaproteomic intercalibration is being led by Mak Saito and Matt McIlvin that arose out of an EarthCube metaproteomic best practices workshop and publication [Saito et al., 2019]. For that effort, we have collected samples, completed metagenomic sequencing (needed for peptide-to-spectrum mapping), and will begin shipping samples shortly followed by a meeting in spring 2020. Second, a nucleic acids intercalibration effort, led by Bethany Jenkins, Andrew Allen, Paul Berube, Scott Gifford, Adrian Marchetti, and Alyson Santoro will be having a workshop entitled "Ocean nucleic acids 'omics intercalibration and standardization" in January of 2020 to identify a path towards "na'omics" standardization and intercalibration. An intercalibration exercise for metabolites and organic compounds has been discussed and is hoped to proceed in the near future.

There were several additional outcomes from the 2018 planning meeting described above. The name "BioGeoSCAPES" was chosen to represent this effort, building on the Seascales concept [Kavanaugh et al., 2016]. A workshop report was written and distributed through the biogeoscapes.org website and Twitter account (@biogeoscapes). Scientific aims were developed along with identification of the critical gaps in the current understanding of ocean metabolism that could be filled by such a program. Ocean metabolism is a useful organizing concept as it operates at an intracellular scale for each organism, which then collectively interact to shape net metabolism at the assemblage level across ocean biomes. Ultimately, ocean metabolism is at the heart of our planetary life support system, as it couples biochemical processes and ecosystem-scale cycling of carbon, oxygen and nutrients, especially during periods of environmental change. However, despite being central to our understanding of global biogeochemical cycling, ocean metabolism is only rudimentarily represented in global models due to the lack of mechanistic understanding of the dominant controls on these critical processes. Such an improved understanding is critical for robust future predictions of ocean function.

Meeting organizers felt there was broad international interest in pursuing a global microbial biogeochemistry program, and that national interest and community building would be a logical next step, with workshop participants acting as ambassadors to promote discussion and community building within their national communities. Specifically, national representatives were charged with engaging national chemical, biological and microbial oceanography, omics, physiology and modelling communities. National meetings should disseminate information, solicit feedback, develop preliminary research goals and vision, and build a national steering group. In this manner, a number of national meetings have already been or are being organized, including in Japan (September 2018), United Kingdom (January 2020), and Canada (October

2019). Presentations and discussion are also being organized at a range of professional meetings (e.g. 'Dawn of Biogeochemicals' session at 2018 Ocean Sciences Meeting, community discussion at 2019 Chemical Oceanography Gordon Research Conference, presentation at Kaplan Symposium in Israel in February 2019, presentation at Organic Biogeochemistry meeting in Delmenhorst, Germany 2019, 'Towards BioGeoSCAPES' session at 2020 Ocean Sciences Meeting) to grow awareness, solicit ideas, and build support.

Scoping Meeting Objectives

Understanding ocean metabolism on a changing planet is a complex and challenging problem that requires coordination across many different fields. We find ourselves finally at a point in time where international momentum has built and we are methodologically and intellectually poised to take on this challenge. Critically, we see the international community moving forward with this initiative and feel it is imperative that the US maintain its co-leadership role in the BioGeoSCAPES initiative. The proposed workshop would aim to achieve the goals described above and is well-aligned with the objectives of the OCB project office with regards to the study of carbon biogeochemistry and engaging with national and international science planning initiatives. Specifically, through presentations and discussions, the workshop would identify the key scientific questions that a coordinated microbial biogeochemistry program could address, and articulate how those would bridge disciplines (e.g. questions that are fundamentally biological, chemical, or both). Time would be devoted to discussing current technical capabilities available to enable the proposed studies and the current technical obstacles that would need to be addressed. Project scope would be discussed, with efforts made to develop consensus on how to focus the BioGeoSCAPES program within the broader fields of biological and chemical oceanography. The two ongoing intercalibration workshops/events would provide updates of their status and discussion of what further efforts will be needed for those domains. Furthermore, additional analytes that may be of scientific value may be identified as needing intercalibration efforts in order to create globally intercomparable values needed for a large-scale program.

For a preliminary schedule, we propose to begin with an introduction by the conveners, followed by several plenary talks to set the stage for the discussions, then having a combination of full group and break-out group discussions on topics. Discussion topics can include: identifying important scientific questions of interest (with break out groups by geographic region and depth), identifying analytes of interest and availability of intercalibration standards for ensuring accuracy in large scale sampling programs, discussing integration of sampling modes and their integration with scientific objectives (e.g. temporal and spatial) and the available and emerging sampling platforms, and discussing the challenges of data management and archival, synthesis, and modeling. An important aspect of the workshop will be using the discussion to develop a list of action items to enable the US program to further the progression towards a global scale microbial oceanography capability required for a BioGeoSCAPES program.

Expected Outputs:

- Defining the scope of the BioGeoSCAPES initiative (i.e. balance of field vs. lab measurements, section vs. process studies)
- Identification of most compelling microbial biogeochemistry science questions that could be addressed by US participants in such a program
- Identification of parameters of interest and evaluation of their technical readiness

- Identification of sampling modes of interest to the US community (spatial, temporal, locations, etc)
- Identification of data management challenges and opportunities
- Identification of potential funding sources and feasibility within the US system
- Community-building of a diverse group of national scientists with expertise in microbial biogeochemistry
- Discussion of mechanisms to facilitate international coordination
- Workshop report summarizing workshop findings and future action items

Meeting Participation: A key aspect of the workshop is the community building effort within the United States scientific community. As we expect a large amount of interest, having a meeting that is large enough to accommodate a broad and diverse group of scientists, and that is open to application for participation, will be a priority in the meeting design. In addition, if possible we will explore webcasting the meeting and incorporating remote feedback and questions in realtime. We recognize that in order for a BioGeoSCAPES program to become a reality, broad community input and support is essential. In addition, having an interdisciplinary focus, with expertise from microbiology and biological oceanography as well as biogeochemistry, including inorganic (trace metals), organic (e.g. metabolomics, lipidomics, vitamins), and macronutrient (N, P, Si) sub-disciplines, will be essential to producing a coherent scientific vision.

We will reserve a subset of workshop slots for community leaders in various areas of expertise, and have the remainder of workshop slots be available on an application basis in order to encourage a diverse attendance in terms of research backgrounds, career stages and demographics. Feedback from the OCB committee on this process in order to maximize fairness and inclusiveness is welcome. Representatives from the BCO-DMO (Biological and Chemical Data Management Office), which is mandated to manage data from all PIs funded by NSF Biological and Chemical Oceanography divisions, will be invited to the meeting to facilitate discussions regarding data management challenges. We will invite NSF program managers and additional experts that could contribute to the meeting; for example, Bob Anderson, the US leader of the GEOTRACES program, would be ideal in order to share his wisdom regarding the development of international programs, and several representatives involved with developing BioGeoSCAPES initiatives internationally in order to facilitate communication (e.g. European Union, Canada).

Logistics: A meeting would be held at a site to be determined, based on cost effectiveness to maximize participation in the time window of Fall 2020 to Spring 2021. We propose a 3 day meeting and request \$70,000 with the aim of 80 participants; we will maximize participation if additional funding can be obtained or costs can be economized. Scoping costs based on Woods Hole off season rates are used here for preliminary budgeting, with estimated lodging costs of \$75 per person per day at negotiated rate (\$18,000), food and catering costs (per diem \$71, 4 days, \$21,300) and partial travel support with the remaining funds (\$30,700, or \$383 per person). Venue space will be provided free of charge from the sponsoring institution. Applicants will be asked if they are able to contribute to their own airplane or ground transport, and any funds saved would enable those without travel support to attend. Offseason Woods Hole is used as an economical option here, but other venues will be considered during the planning process. We will work with the OCB project office in organizing and promoting the meeting, including building a workshop website, holding town hall meetings at national meetings (such as Ocean Sciences), and promoting it through email, the OCB newsletter, and social media.

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