SCOR Working Group Proposal

Title: Developing resources for the study of Methylated Sulfur compound cycling PROcesses in the ocean **Acronym:** DMS-PRO

1. Abstract

Organic methylated sulfur compounds (MSCs) play key roles in planktonic food webs as important carbon and sulfur substrates and also as infochemicals that facilitate biological interactions. In addition, the oceanic emission of biogenic volatile MSCs (dimethylsulfide and methanethiol) to the atmosphere acts as a source of aerosols, which impact cloud formation and properties, and hence climate. Understanding the role of MSCs in the Earth system requires accurate rate measurements to capture the rapid biotic and abiotic cycling processes responsible for the turnover of MSCs in the surface ocean. However, we currently lack both standardized protocols for the analytical determination, and a quality-controlled database for process rate measurements of MSCs. Therefore, the DMS-PRO SCOR working group proposes to address these knowledge gaps by compiling a comprehensive, open-access database of quality-controlled, existing and future MSC cycling rates; and publishing standardized operating practices on analytical procedures involved in the determination of MSCs rates. The overarching goal of this proposal is to stimulate research on the oceanic MSCs cycle, building capacity, and sharing knowledge and skills with the oceanographic and Earth system science communities. The resulting work will actively engage diverse perspectives which will critically expand our current understanding of MSCs and our ability to predict their roles in a future changing ocean.

2. Scientific Background and Rationale

2.1 Role of methylated sulfur compounds (MSCs) in upper-ocean biogeochemistry and climate

Sulfur (S) is an essential element for life and a major component of organic matter. The microorganisms that form the base of open-ocean food webs typically have a carbon:sulfur (C:S) molar ratio \leq 100, meaning that S is at least as abundant as phosphorus in marine biomass^{1,2}. S-containing molecules play central roles in key redox reactions, metabolic processes, and biological interactions that shape the functioning of the marine ecosystem and drive vital biogeochemical fluxes.

A salient feature of the marine S cycle is that a large proportion of the inorganic S assimilated by organisms is routed to the production of a unique compound: dimethylsulfoniopropionate (DMSP)^{1,3}. This multifunctional compound is synthesized mainly by marine phytoplankton, but also by corals and their algal symbionts, heterotrophic bacteria, macroalgae, seagrasses, and brackish-water plants. Current understanding posits that DMSP is primarily an osmolyte that helps organisms cope with salinity stress, but it can serve additional functions that protect cells against other physiological stressors. Moreover, DMSP acts as a powerful chemical cue that shapes biological interactions⁴.

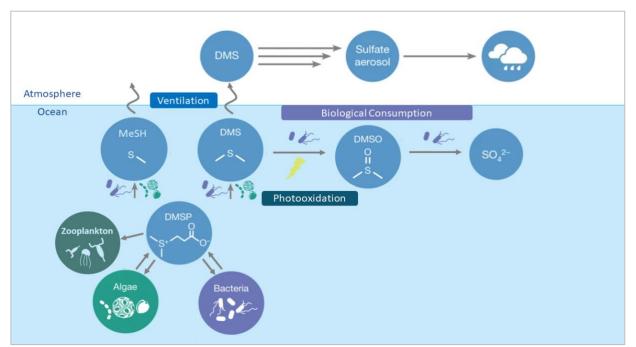


Figure 1. Simplified scheme of MSC cycling in the upper ocean and lower atmosphere. Adapted from Thume et al. (2018) <u>doi.org/10.1038/s41586-018-0675-0</u>.

The biogeochemical cycling pathways and rates of DMSP and its derivative MSCs are best known in the upper ocean ecosystem. Globally, phytoplankton invest around half of their S assimilation and ~5% of their carbon fixation into DMSP synthesis^{1,5}, conferring to this compound a prominent role in energy transfer up the marine food web. Research conducted over the past decades has identified DMSP as the most significant single bacterioplankton substrate and as a major source of S and C to other microbes and zooplankton^{1,3,4,6}. Marine microorganisms have evolved several pathways to metabolize DMSP^{1,6}, which result in either S assimilation into biomass or release. Globally, around 15% of DMSP breakdown by bacterial and algal enzymes is released to seawater in the form of dimethylsulfide (DMS)⁵, a climatically active gas^{7,8}.

The dominant fate of the DMS dissolved in seawater is its oxidation to less-reactive organic compounds, and ultimately inorganic sulfate. Oxidation proceeds through several competing biotic and abiotic pathways including bacterial consumption, photochemistry, and reaction with halogenated compounds⁹. Consequently, only around 10% of the DMS produced in the upper ocean can be vented to the atmosphere globally⁵, despite DMS being supersaturated in surface seawater.

Biogeochemical cycling of DMSP and DMS produces other organosulfur compounds in significant amounts¹, including highly reactive volatiles like methanethiol (MeSH, a by-product of DMSP-S assimilation into biomass) and potentially methane. Dimethylsulfoxide (DMSO) is a major product of biotic and abiotic DMS oxidation and can also be reduced back to DMS by microbes. In comparison to DMSP and DMS, the cycling mechanisms and rates of these and other MSCs remain poorly understood.

Oceanic emission of DMS (20–30 Tg S yr⁻¹) and MeSH (~5 Tg S yr⁻¹) is the largest natural source of S to the atmosphere¹⁰. Currently, these fluxes represent around 30% of the total S emissions, only exceeded by anthropogenic S emission. In the vast and relatively unpolluted marine atmosphere, oxidation of these reactive gases contributes to the formation and growth of aerosols. These aerosols scatter incoming sunlight and can act as cloud condensation nuclei, which makes clouds brighter, thus cooling the Earth's surface. Biogenic MSCs are, therefore, key climatic agents^{7,8}.

2.2 Need and timeliness for a SCOR Working Group

The first measurements of biological and photochemical MSC cycling rates in seawater were published in the late 1980s³. Since then, important progress has been made in the development of techniques for the determination of MSC cycling rates under *in situ* conditions. Recent compilations of DMSP and DMS cycling rates in the ocean^{5,11,12}, as well as model intercomparison exercises^{13,14}, have identified important research gaps and evidenced the need for a renewed community wide effort. Here we propose to establish standard methods and a public database of MSC cycling rates in the pelagic ocean, accompanied by several capacity building activities that will leverage MSC research. The proposed activities are urgently needed to address, at least, three grand challenges:

1) *Establishing standard methods and enabling systematic methodological comparisons*: Currently, several processes can be measured with more than one technique. For example, microbial DMS removal rates can be measured through seawater incubation with either inhibitor compounds or trace additions of isotopic labels⁵. The existence of methodological alternatives is desirable because (i) it can be used to detect and correct systematic biases, enabling more realistic quantification of methodological uncertainty and increasing the overall robustness of the data, and (ii) it can make measurements accessible to laboratories with economic and logistic limitations. Our efforts will lead to the establishment of detailed protocols or standard operating practices (SOP), along with recommendations about the suitability of each method depending on the questions being addressed. This exercise can also prompt targeted intercomparison exercises (which are not included in this proposal).

2) Fostering coordination and integration between measurements of MSC cycling rates and stocks and their biotic and abiotic drivers: MSC cycling rates are regulated by the physicochemical environment (temperature, salinity, nutrients, light, pH, oxygen) and its interplay with a wide range of biological processes and their underlying molecular drivers (e.g., gene abundance and expression). A coordinated effort is needed to encourage interdisciplinary work and concurrent sampling of MSC cycling rates and stocks along with their known or hypothesized drivers, setting the stage for an improved understanding of their interrelationships. This effort is also essential to (i) establish a baseline against which to compare future measurements made under the increasing influence of environmental stressors (ocean

stratification, warming, acidification, deoxygenation, etc.) and (ii) enable evaluation of the modeled response of MSC cycling to these stressors, from genes to ecosystems.

3) *Improving the translation of knowledge on MSC cycling rates into predictive models*: Previous studies found a mismatch between measured key parameters and the values used in numerical models, negatively affecting model realism and accuracy⁵. Spatiotemporal patterns in sea-surface DMS concentration predictions vary widely between current numerical models and also with respect to the sea-surface DMS climatology¹⁴, an observational benchmark, despite such climatologies being available since 1999¹⁰. Moreover, the four DMS models included in the last Climate Model Intercomparison Project phase 6 (CMIP6), which informs the IPCC report, produce divergent projections of DMS emission in response to climate change¹³. These large uncertainties hamper the assessment of the role of volatile MSCs in future climate. The database and recommendations issued from our activities will enhance mechanistic understanding and predictive capacity and are therefore urgently needed to build a new generation of MSC cycling models for upcoming CMIP exercises (e.g., CMIP7).

In summary, DMSP and DMS are among the best-known planktonic and microbial metabolites, and their study has yielded deep insights into the functioning of the marine ecosystem at the molecular, biogeochemical, and ecological scales. The activities proposed herewith will be crucial to systematize and consolidate the knowledge and data amassed during the previous decades, identify knowledge gaps and spark new research on MSCs, inform methodological recommendations and modelling activities, and ultimately contribute to answering pressing scientific and societal questions.

3. Terms of Reference (T)

Our proposed WG will work to achieve the following objectives:

- **T1.** To develop community consensus on the measurement of MSC cycling rates, evaluate the suitability of available methods, and recommend standard operating practices (SOP).
- **T2.** To compile a comprehensive database of MSC cycling rates in the ocean and to freely disseminate the database and related documentation according to the FAIR (Findability, Accessibility, Interoperability, and Reusability) principles¹⁵.
- **T3.** To develop a framework for the quality assessment and control, standardization, and curation of MSC cycling datasets.
- **T4.** To analyze and summarize the patterns of MSC cycling rates in the global ocean in relation to their abiotic and biotic environment.
- **T5.** To provide expert guidance on the use of the MSC cycling database for model development and evaluation.
- **T6.** To improve the coordination between measurements of MSC cycling rates and stocks, and foster interdisciplinary research by relating these to other biogeochemical variables and molecular and 'omics data.
- **T7.** To establish an international community of practice focused on research, capacity development, and oceanographic multidisciplinary collaboration in the topic of oceanic S cycle.

Terms of reference T1 –T3 correspond to the WG's core activities and will result in Deliverables D1–D3 (section 5); T4–T5 rely upon the core activities and will result in Deliverables D4–D6; T6–T7 are

crosscutting objectives that will be achieved through the completion of T1–T5 and by placing strong emphasis on capacity building activities.

4. Working plan

The internal organization of the WG will rely on the following items to ensure that our goals are met:

- <u>Plenary group meetings</u> (hybrid: in-person + online) will be convened to discuss with the entire WG the direction and organization of our activities. These meetings (M) will be scheduled with at least annual frequency simultaneously with larger conferences and workshops. Additional <u>online group meetings</u> will be scheduled on demand.
- <u>Internal communication</u> will make frequent use of email, chat, and videoconference platforms that are internationally accessible to ensure continuous progress and smooth coordination.
- <u>Thematic teams</u> will be defined during the kick-off meeting (M1) and assigned specific tasks according to their members' expertise.

The activities in order to achieve the **specific Terms of Reference** T1–T5 are described below, and the detailed timeline is summarized in a Gantt Chart (Figure 2).

Discussion on relevant measurement methods and publication of the SOP – T1

We will review and discuss the set of measurements necessary to build a relevant and informative database of MSC cycling. Our effort will focus on the pelagic coastal and open ocean environments, but the database could include other marine environments such as sediments and sea ice in the future as more data become available. The WG will fully evaluate the analytical procedures and uncertainties in the quantification of MSC cycling rates and will synthesize findings and recommendations on SOP. Critical assessments of the methods employed for MSC cycling rates are needed to ensure intercomparability and to quantify limitations. Drafting of the SOP will be committed to the corresponding writing team after M3, reviewed and agreed by the whole WG, and posted on the <u>Ocean Best Practices</u> repository for public consultation during the second year (D1). This exercise will guide the design of the content and structure of the database as well as set the necessary quality control standards.

Data compilation, database design and assembly, public release of database and software – T2 and T3

To fulfill T2, we will compile all available MSC cycling rates and accompanying variables, sourcing peer reviewed publications and unpublished data. After the initial call for data contributions from the entire community, planned for year 1, reminders will be sent regularly until the end of year 2, the deadline for contributions to the first version of the database. A Data Management Plan will be prepared by the database and software team and submitted for approval by the entire WG during M2. This document will specify the procedures for long-term management and periodic update of the database.

In parallel to data collection, the database and software team will work on the design and implementation of the software used to assemble the database (T3) following the guidelines resulting from WG meetings and open workshop W1. The database will be hosted at the Institut de Ciències del Mar (CSIC, Spain), taking advantage of its <u>Data Science Service</u>, and distributed through <u>ERDDAP</u>, an open-source data server developed by NOAA that is used by over 90 organizations from several countries to distribute over 200 oceanographic databases. ERDDAP was recently adopted by the <u>Global</u>. <u>Surface Seawater DMS(P) Database</u> and brings important advantages, including seamless access and subsetting of data from DMS-PRO and related oceanographic databases and data export in several standard formats. Scripts used in data processing will be posted on a repository and encapsulated in a

well-documented software package, ensuring a transparent and reproducible workflow. Beta versions of the database (D2) and software (D3) will be released during year 3. After an interim review period, the final release of DMS-PRO_v1 along with the data paper (D4) is planned for the second half of year 3.

Data analysis and peer reviewed publications – T4 and T5

This activity encompasses the analysis of the compiled data to address specific objectives and the subsequent preparation of three peer-reviewed papers with complementary scopes. All papers will be submitted to open-access journals and posted as pre-prints before submission.

- The *database description paper* (D4) will be designed during M3, after which a writing team will produce an initial draft that will be reviewed by the entire WG and submitted on year 3. A citable version of DMS-PRO_v1 will be deposited in a public repository upon paper submission.
- The *modeling guidelines paper* (D5) will benefit from recommendations made by both the WG members, during M3, and the wider community and especially modelers, who will be invited to provide their feedback during an open workshop (W2, year 3) and to act as co-authors. Submission is planned for the beginning of year 4.
- The *perspective paper* (D6) will be conceived during a meeting (M5) scheduled after a large international meeting. Two dedicated teams will be tasked, respectively, with the analysis of patterns in MSC cycling rates in relation to the biogeochemical environment and their underlying molecular bases across ocean biomes. An assigned writing group will collect these results and the feedback from the wider scientific community to identify knowledge gaps and make recommendations for future research.

The **overarching Terms of Reference (T6–T7)** comprise activities that span the entire duration of the project and rely to a large extent on communication and capacity building activities (section 6). A communication team will be setup during M1 and tasked with the setup of a website and social media accounts (Twitter, Facebook, ResearchGate), where we will post news about the activities of the WG. The website will also be a gateway to the DMS-PRO database, SOP, and related resources and serve as a forum for exchanging useful information. To reach all potential data contributors and users, we will use our communication channels as well as those from several international organizations (section 6.1). Temporary working teams will be tasked with the organization of at least one conference session (S), three workshops (W), and several targeted training events, further engaging DMS-PRO users in our community of practice.

Figure 2. Timeline of the WG activities	he WG a	ctivities														
ltem		Year 1	Year 1 (2023)			Year 2 (2024)	(2024)			Year 3 (2025)	(2025)			Year 4 (2026)	(2026)	
	1	2	с	4	1	2	e	4	1	2	с	4	1	2	с	4
Terms of Reference (T). Overarching T6 and T7 not included	Verarchin	. Bud T6 and	T7 not incl	uded												
T1. Methods review & discussion		•	•		•		*									
T2. Database compilation		•	×													
T3. Software repository & package			•													
T4. Data analysis, discussion					-				*	•						
T5. Guidelines for modelers										•						
Deliverables (section 5)							1D		D2	D3	ħQ		D5			D6
Milestones																
Plenary WG meetings	M1	M2			M3				M4		M5					
Open workshops, sessions		W1							W2					W3		S1
Trainings (hybrid)			гa				T				Т				ъ	
Conferences		ASM ^b EGU ^c		AGUd	OSM ^e	EGU ^c	DMSP ^f	AGUd	ASM ^b	EGU ^c	osc ^d	AGU ^d		EGU ^c		AGU ^d
Calls for data contributions		×		×		×		×								
^a Tentative dates of the SOLAS Summer School	SOLAS Su	mmer Sc	hool			-	-									

^b Aquatic Sciences Meeting (ASLO —Association for the Sciences of Limnology and Oceanography) ^c European Geosciences Union annual assembly (April)

 d American Geophysical Union annual meeting (December) e Ocean Sciences Meeting (ASLO, AGU and TOS —The Oceanography Society) f Tentative date of the 7th DMSP Symposium

^g Open Science Conference (SOLAS, Surface Ocean - Lower Atmosphere Study)

5. Deliverables

(With related Terms of Reference in parentheses)

- **D1.** Publication of Standard Operating Practices (T1): Compilation of available methodologies for measuring MSC cycling rates, recommendations for their use, and critical assessments as to their limitations and inter-comparability.
- **D2. Database and web portal** (T2): Quality-controlled database of MSC cycling rates and web portal providing access to the data and related software repositories and documentation, including a Data Management Plan.
- **D3. Software repository and package** (T3): Well-documented software package written in a highlevel open-source programming language (R or Python), including scripts used for (i) data preprocessing prior to submission to the database, e.g. application of quality control criteria, standardization of measurement units, time frames, and uncertainty metrics; (ii) data postprocessing, allowing users to reproduce the statistical descriptors and visualizations displayed in the peer-reviewed documents and SOP.
- **D4. Database description paper** (T1–T4): Presentation of the rationale behind the database, technical description of the quality control and data processing procedures, basic statistical description of the database.
- **D5. Modeling guidelines paper** (T5): Expert guidance on the use of the database for model development and evaluation and for uncertainty assessments, agreed on with the modelling community. Will include a comparison between key MSC cycling processes and parameters, compiled in DMS-PRO, and their representation in models.
- **D6. Perspective paper** (relates to T1–T7): Community paper that will provide an overview of current knowledge on MSC cycling and identify knowledge gaps and priorities for future research, from the molecular to the ecosystem scale.

6. Capacity Building (CB)

6.1 Strategy overview

The fundamental objective of DMS-PRO is to develop open resources that consolidate and re-energize MSC research and expand the global community of practice (**T6, T7**). The DMS-PRO database, SOP, and related documentation and software are major assets of our CB strategy, and will be placed in the public domain and will follow the FAIR principles to guarantee maximum utility and ensure equal access. SOP will be submitted for inclusion to the <u>Ocean Best Practices repository</u>, a permanent, open access, digital repository maintained by the International Oceanographic Data and Information Exchange (IODE) of the UNESCO-IOC. The publication of SOP will expand and diversify the group currently obtaining MSC rates data by providing access in one single document to standardized and community-agreed protocols.

A non-exhaustive survey of the MSC literature indicates that the authors of scientific papers in this domain are overwhelmingly associated to institutions based in developed countries at the time of their contribution. Hence, the MSC community is in special need for inclusion of members from developing countries to build capacity for MSC-related research in these countries. To embed potential CB from the very start of the project, our WG includes members from countries usually classified as emerging/developing economies (e.g., India, Argentina), as well as early-career researchers.

Possible reasons for the geographic imbalance in MSC cycling research are (i) the relatively small size and high specialization of the research community, (ii) the economic costs associated to the acquisition of MSC data and maintenance of the related infrastructure (ship time, instrumentation) and qualified personnel, and (iii) the tendency of MSC studies to focus on open-ocean regions relevant to global climate, rather than on the nations' exclusive economic zones (which usually center the research efforts in developing countries owing to their more immediate economic return).

Consistent with this diagnosis, the CB activities proposed by our WG will emphasize training of scientists in the use of the DMS-PRO resources, for both data analysis and modelling purposes, by means of online or hybrid events (see 6.3). These events will be advertised by our communication team using our website and social media, email dissemination lists and newsletters from international organizations (SCOR, SOLAS, POGO, ICES, ASLO, AGU, EGU, etc.) and also through the <u>Community of Practice on</u> <u>Capacity Development (COP11)</u> promoted by the UN's <u>Decade of Ocean Science for Sustainable</u> <u>Development</u>.

The adoption of online or hybrid formats will guarantee inclusion of different geographic, economic, and gender perspectives, while minimizing the environmental impacts caused by travel. We will take additional inclusion measures such as recording events to facilitate access by scientists with family duties, setting up text chats during live events for participants who are not comfortable with oral communication in English, and providing captions in recorded webinars. The trainings will combine teaching of domain-specific content and generic knowledge and tools (e.g., data analysis, molecular biology techniques), ensuring that the participants develop transferable skills that can enhance their careers beyond MSC research and/or outside academia. Feedback from participants will be routinely collected to ensure that the trainings fulfill the participants' needs.

6.2 Complementary funding

Acquisition of complementary funding is a critical aspect of our CB strategy. The WG will actively help build capacity by seeking funding and taking advantage of existing programs within WG member's institutions, as well as from national and international programs and philanthropic initiatives.

A survey among our members has already identified programs from their institutions that could provide funding to engage researchers, prioritizing those from developing countries and/or at their early career stage. Examples include the <u>Isblue</u> initiative accessible through the Brest University (E. Bucciarelli, associate member) and the Severo Ochoa Visiting Scholars program currently running at the Institut de Ciències del Mar, CSIC (M. Galí, co-chair). These programs could fund student and technician internships and attendance to DMS-PRO trainings.

The WG members have committed to align the objectives of their future project proposals with the terms of reference of DMS-PRO, thus providing further opportunities for building capacity in MSC research. Moreover, we foresee that DMS-PRO will act as a catalyzer for interdisciplinary collaboration and will encourage the preparation of new project proposals with a strong CB component. An example is the <u>Doctoral Networks</u> program, which is funded by the Marie Skłodowska-Curie Actions of the European Commission and can be joined by organizations from any country in the world.

In addition to supporting CB activities, the complementary funding obtained by DMS-PRO members can be used to cover publication fees in open access journals, travel, and long-term maintenance of the DMS-PRO database. The latter aspect is especially important to ensure a permanent legacy of the DMS-

PRO WG. Therefore, a strategy for long-term funding of database maintenance will be discussed during M1 and subsequently implemented and periodically reviewed in plenary WG meetings.

6.3 Specific CB activities

The Working Group activities will provide global CB towards present and future production and use of MSC cycling rates, while ensuring the wide and early adoption of the database, software package and SOP. To this end, we envision a variety of approaches to engage researchers with diverse profiles, as detailed in the sections below:

Forum: In conjunction with the database web portal, we will provide a platform for a forum to improve dialogue within our community and beyond, facilitate collaboration and mentoring and maximize utilization of complementary funding from other institutions. We will use this platform to advertise opportunities for lab stays, participation in research cruises and mesocosm experiments, fellowship opportunities, etc. By promoting such exchanges, we will foster coordination of MSC cycling measurements with complementary data (**T6**) and increase the MSC producer and user base (**T7**).

Online training events and tutorials: The DMS-PRO database will be accompanied by tutorials in the form of recorded webinars, which will span from imparting a basic understanding of the marine S cycle, to more complex tutorials on the use of the database and the software package. Complementary to the online tutorials, the WG will contact the <u>SOLAS Summer School</u> and the Partnership for Observation of the Global Oceans, <u>POGO</u>, to inquire about the possibility of adding the DMS-PRO tutorials and procedures to their portfolio of education activities.

Hybrid training events: Taking advantage of the interdisciplinary composition of the WG, we will organize several hands-on training events covering various aspects of MSC cycling research, from the analysis and modelling of MSC cycling rates and their budgets, to the molecular monitoring of microbial MSC cycling and the exploration of MSC cycling genes in genomic databases. These hybrid events will be scheduled during large conferences (Figure 2) or in partnership with courses such as the SOLAS Summer School, the Helmholtz School for Marine Data Science (MarDATA), and the Masters' program on <u>Ocean</u>, <u>Atmosphere and Climate</u> (University of Galway and SOLAS). Trainings making use of genomic databases may also benefit from the collaboration with <u>TARA Oceans</u> and <u>Malaspina</u> project coordinators (S. Acinas and J.M. Gasol) from the same institution as M. Galí (co-chair).

Open workshops and conference sessions: At least three DMS-PRO workshops are planned (Figure 2) to discuss about the design of the DMS-PRO database and SOP (W1), the translation of measurements in numerical models (W2), and the perspectives in MSC research from molecular to ecosystem scales (W3). These events will run in hybrid mode and be open to all scientists with interest in MSC, allowing them to shape DMS-PRO deliverables. The WG will also support actively the organization of the 7th edition of the DMSP Symposium. This international meeting series had 4-year periodicity until the 6th edition held in 2014, and resuming it is a priority of our WG. Finally, the WG will propose a conference session focused on promotion of the DMS-PRO resources during a large international conference on year 4.

DMS-PRO network: In addition to our WG members, several renowned scientists have already expressed interest in contributing to the WG objectives by providing feedback on DMS-PRO activities and documents and engaging in the organization of CB activities. These colleagues currently include Thomas Bell (Plymouth Marine Laboratory, UK, and SOLAS Steering Committee), David Kieber (State University of New York, USA), Maurice Levasseur (Laval University, Canada), Naomi Levine (University of Southern California, USA), Mary-Ann Moran (University of Georgia and NSF C-CoMP, USA) and Rafel

Simó (Institut de Ciències del Mar, CSIC, Spain). The WG will promote mentorship of early career researchers, including technicians, by its members and the larger DMS-PRO network. Through the proactive identification of talented individuals and the emphasis on personal ties and high-quality training, this crosscutting activity will ensure that DMS-PRO has long-lasting impacts.

7. Working Group composition

Our WG will be comprised of 10 Full and 10 Associate members with complementary expertise in the fields of chemical and microbial oceanography, molecular microbiology, photochemistry, sea-air exchange, and biogeochemical modelling, as well as cross-cutting skills such as data analysis, scientific writing, and fundraising. Our WG also includes an expert in database management and other members with previous experience in database setup. The diversity of perspectives and interdisciplinary skills ensures that the WG will significantly advance the understanding of MSC cycling processes and will produce impactful science of interest to a wide community.

Geographical spread: The 20 members originate from 14 countries in Asia, North and South America, Oceania, and Europe. Our Full members represent 7 different countries, including 2 countries usually classified as emerging/developing economies with upper-middle income (Argentina, China). Similarly, our Associate members are based in 9 different countries, including countries with emerging/developing economies with low (India) and upper-middle (China) income.

Participation of early-career researchers: ECRs are well represented in our working group, with 3 ECRs among the Full members (Galí, Hayashida, and McParland), including one Co-chair (Galí), and 3 ECRs among the Associate members (Deschaseaux, Zárate, and Zhang).

Gender balance: Our WG is comprised of 4 female and 6 male Full members, and 4 female and 6 male Associate members. Three out of 6 ECRs are female. Overall, 40% of members are female, hence slightly imbalanced but well above the average percentage of females in postdoc (35%) and senior (20%) career stages in Earth Sciences¹⁶.

Name	Gender	Place of work	Expertise relevant to proposal
1. Martí Galí (Co-chair)	М	Spain	MSC cycling rates, remote
			sensing, modelling
2. Daniela del Valle (Co-	F	Argentina	MSC cycling rates, microbial
chair)			ecology
3. Steve Archer	М	USA	MSC cycling rates, modelling
4. José González	М	Spain	Genomics of marine bacteria
			and MSC transformations
5. Hakase Hayashida	М	Japan	Modelling of MSCs in the ocean
			and sea-ice
6. Frances Hopkins	F	UK	Marine biogeochemistry of
			MSCs
7. Sohiko Kameyama	М	Japan	High resolution measurements
			of MSCs in seawater

7.1 Full Members

8. Erin McParland	F	USA	DMSP production, community
			composition, environmental
			drivers, 'omics
9. Jacqueline Stefels	F	Netherlands	MSC biogeochemistry in
			seawater and ice ecosystems,
			phytoplankton ecophysiology
10. Marcos Zárate	М	Argentina	Database management,
			biodiversity informatics

7.2 Associate Members

Name	Gender	Place of work	Expertise relevant to proposal
11. Hermann Bange	М	Germany	MSC quantification, database management
12. Eva Bucciarelli	F	France	Synthesis and uptake of MSCs by phytoplankton
13. Elisabeth Deschaseaux	F	Australia	DMS and other VOCs emissions from coral reefs and other tropical ecosystems
14. Ki-Tae Park	М	South Korea	MSCs in seawater and atmosphere, polar oceans
15. Damodar Shenoy	Μ	India	MSC biogeochemistry in coastal and open ocean, low-oxygen conditions
16. Jon Todd	М	UK	Molecular microbiological analysis of MSC cycling
17. Philippe Tortell	Μ	Canada	Analytical measurements and stable isotope tracer studies of MSCs
18. Lenny Winkel	F	Switzerland	Coupling between MSC cycling and halogens
19. Gui-Peng Yang	М	China	Marine biogeochemistry of MSCs
20. Miming Zhang	F	China	MSC measurement and cycling in polar oceans

8. Working Group contributions

Terms of Reference (T) each full member can contribute more to are indicated.

Martí Galí made the most comprehensive compilations of biological (Galí and Simó 2015) and photochemical (Galí et al., 2016) cycling rates of DMS(P) published to date, laying the ground for the current proposal (T1–T4). He has wide experience in the measurement and modeling of DMS budgets (Royer, Galí et al., 2016) (T5).

Daniela del Valle has key expertise in the analytical determination of cycling rates of MSCs and a thorough understanding of the oceanic biogeochemical cycling of these compounds. Her expertise will be critical for the quality control and curation of the data, as well as the preparation of a SOP (T1–T4).

Stephen Archer has extensive experience in quantifying the process rates that govern DMS(P) production and fate (T1) and in incorporating those into mechanistic models (T3–T5). Recently, he has been investigating the influence of ocean acidification on DMS-climate feedbacks (T6).

José González is an expert on bioinformatics methods and the identification of genes involved in S transformations in oceanic environments (Buchan et al., 2014; González et al., 2019), bringing key expertise in database design in connection with molecular data (T2, T4, T6).

Hakase Hayashida has experience in developing sea-ice and ocean biogeochemical models including DMS at local, regional, and global scales (T5). His modelling and large-scale expertise will contribute to the development and management of the global DMS database proposed (T2–T4, T6).

Frances Hopkins is an expert in the measurement of MSC cycling rates in the surface oceans (Dixon, Hopkins et al. 2020). Her research has tackled diverse angles of this topic, including the influence of ocean acidification (e.g., Hopkins and Archer 2014, Hopkins et al. 2020) and the role of corals.

Sohiko Kameyama is a specialist in measurements of DMS(P) in seawater with high accuracy and resolution (T1, T3, T4). He applied cutting-edge technology to optimize analytical methods (Li et al., 2020) including high-resolution measurements (Kameyama et al., 2009; 2013).

Erin McParland has expert knowledge in the study of DMSP production by marine phytoplankton in relation to their diversity (McParland and Levine 2019) including the upscaling of observations with modeling (T1, T4, T5). She is also knowledgeable in the utilization of molecular biology techniques (T6).

Jacqueline Stefels has expertise in the ecophysiology of pelagic and sea-ice algae in relation to the S cycle. She developed new methods using stable isotopes to measure DMSP production (Stefels et al. 2009) and has built up a database on MSC conversion rates in polar ecosystems (e.g. Stefels et al. 2018) (T1–T4).

Marcos Zárate is a data scientist with experience in data management and publication in oceanography and marine biodiversity following the FAIR principles. His expertise will be key to designing and implementing the data management plan and the software package (T2, T3, T5, T6).

9. Relationship to other international programs and SCOR Working groups

The objectives of DMS-PRO are well aligned with those of the international <u>Surface Ocean - Lower</u> <u>Atmosphere Study</u> (SOLAS) project, especially with its core themes #4 (Interconnections between marine ecosystems, aerosols, and clouds) and #5 (Ocean biogeochemical control on atmospheric chemistry). Intense collaboration with SOLAS is a key element in our capacity building and communication strategy. The SOLAS Scientific Steering Committee and Executive Director were informed of the preparation of our WG proposal, which they support, and Thomas G. Bell accepted to act as our main contact point within the SOLAS Scientific Steering Committee. To officialize these relationships we will request endorsement of DMS-PRO by SOLAS.

Our proposed WG will also make relevant and timely contributions towards addressing the challenges of the UN's <u>Decade of Ocean Science for Sustainable Development</u> (#5: Unlock ocean-based solutions to climate change; #7: Expand the Global Ocean Observing System; #9: Skills, knowledge and technology for all). Hence, we will seek endorsement of our project and specific activities by this program and

related ones sponsored by UNESCO-IOC, e.g. the <u>Global Ocean Observing System (GOOS</u>). We will also liaise with several UN's Ocean Decade Communities of Practice according to our shared goals.

Coordination with the managers of the existing Global Surface Seawater DMS(P) Database, hosted by NOAA's <u>Pacific Marine Environmental Laboratory</u> (PMEL), is another key element of our strategy. We have established fruitful contact with Tim Bates, James Johnson and Derek Coffman at PMEL, which has led us to the adoption of a common data server, ERDDAP, to distribute these related databases.

Our WG will benefit from the experience of our members in past working groups, which led to the setup of the MEMENTO N_2O and CH_4 database (WG #143), the production of SOP (WG #143, #156), and the organization of several successful capacity building activities. The ties of our WG with other WGs, both in thematic and membership terms, are listed below:

#140, 2011. Biogeochemical Exchange Processes at the Sea-Ice Interfaces (BEPSII). Co-chaired by J. Stefels (full member in DMS-PRO) and N. Steiner (expert in MSC modelling).

#141, 2012. Sea-Surface Microlayers. Included G.P. Yang (associate member in DMS-PRO).

#143, 2013: Dissolved N_2O and CH_4 measurements: Working towards a global network of ocean time series measurements of N_2O and CH_4 . Co-chaired by H. Bange, included P. Tortell (associate members in DMS-PRO).

#155, 2017. Eastern boundary upwelling systems (EBUS): diversity, coupled dynamics and sensitivity to climate change. Included D. Shenoy (associate member in DMS-PRO).

#156, 2018. Active Chlorophyll fluorescence for autonomous measurements of global marine primary productivity. Co-chaired by P. Tortell (associate member in DMS-PRO).

#162, 2020. Developing an Observing Air-Sea Interactions Strategy (OASIS). Co-chaired by C. Marandino (expert in air-sea gas exchange, including DMS).

#163, 2021. Coupling of ocean-ice-atmosphere processes: from sea-Ice biogeochemistry to aerosols and Clouds (Clce2Clouds). Co-chaired by N. Steiner (expert in MSC modelling), included H. Hayashida (full member in DMS-PRO).

10. Key References

(WG members underlined)

- 1. Moran, M. A. & Durham, B. P. (2019). Sulfur metabolites in the pelagic ocean. *Nat. Rev. Microbiol.* 17, 665–678, <u>doi.org/10.1038/s41579-019-0250-1</u>
- 2. Ksionzek, K. B. *et al.* (2016). Dissolved organic sulfur in the ocean : Biogeochemistry of a petagram inventory. *Science* 354, 456–459, <u>doi.og/10.1126/science.aaf7796</u>
- 3. <u>Stefels, J.</u>, Steinke, M., Turner, S. M., Malin, G., Belviso, S. (2007) Environmental constraints on the production and removal of the climatically active gas dimethylsulphide (DMS) and implications for ecosystem modelling. *Biogeochemistry* 83, 245–275, <u>doi.org/10.1007/s10533-007-9091-5</u>
- Seymour, J. R., Simó, R., Ahmed, T., Stocker, R. (2010). Chemoattraction to dimethylsulfoniopropionate throughout the marine microbial food web. *Science* 329, 342–345, <u>doi.org/10.1126/science.1188418</u>
- 5. <u>Galí, M.</u> & Simó, R. (2015). A meta-analysis of oceanic DMS and DMSP cycling processes:

Disentangling the summer paradox. *Global Biogeochem. Cycles* 29, 496–515, doi.org/0.1002/2014GB004940

- 6. Kiene, R. P., Linn, L., Bruton, J. (2000). New and important roles for DMSP in marine microbial communities. *J. Sea Res.* 43, 209–224, <u>doi.org/10.1016/S1385-1101(00)00023-X</u>
- 7. Charlson, R. J., Lovelock, J. E., Andreae, M. O., Warren, S. G. (1987). Oceanic phytoplankton, atmospheric sulphur, cloud albedo and climate. *Nature* 326, 655–661, doi.org/10.1038/326655a0
- 8. Carslaw, K. S. *et al.* (2013). Large contribution of natural aerosols to uncertainty in indirect forcing. *Nature* **503**, 67–71, <u>doi.org/10.1038/nature12674</u>
- Müller, E., von Gunten, U., Bouchet, S., Droz, B., <u>Winkel, L. H. E</u>. Hypobromous acid as an unaccounted sink for marine dimethyl sulfide? *Environ. Sci. Technol.* 53, 13146–13157 (2019), <u>doi.org/10.1021/acs.est.9b04310</u>
- 10. Lana, A. *et al.* (2011). An updated climatology of surface dimethlysulfide concentrations and emission fluxes in the global ocean. *Global Biogeochem. Cycles* 25, GB1004, doi.org/10.1029/2010GB003850
- 11. <u>Galí, M</u>. *et al.* (2016). CDOM sources and photobleaching control quantum yields for oceanic DMS photolysis. *Environ. Sci. Technol.* 50, 13361–13370, <u>doi.org/10.1021/acs.est.6b04278</u>
- 12. <u>Hopkins, F</u>. *et al.* (2020). A meta-analysis of microcosm experiments shows that dimethyl sulfide (DMS) production in polar waters is insensitive to ocean acidification. *Biogeosciences* 17, 163–186, <u>doi.org/10.5194/bg-17-163-2020</u>
- 13. Bock, J. *et al.* (2021). Evaluation of ocean dimethylsulfide concentration and emission in CMIP6 models. *Biogeosciences* 18, 3823–3860, <u>doi.org/10.5194/bg-18-3823-2021</u>
- 14. Tesdal, J. E., Christian, J. R., Monahan, A. H., Von Salzen, K. (2016). Sensitivity of modelled sulfate aerosol and its radiative effect on climate to ocean DMS concentration and air-sea flux. *Atmos. Chem. Phys.* 16, 10847–10864, <u>doi.org/10.1071/EN14255</u>
- 15. Wilkinson, M. D. *et al.* (2016). Comment: The FAIR Guiding Principles for scientific data management and stewardship. *Sci. Data* 3, Article number: 160018, doi.org/10.1038/sdata.2016.18
- 16. Popp, A. L., Lutz, S. R., Khatami, S., van Emmerik, T. H. M., Knoben, W. J. M. (2019). A Global survey on the perceptions and impacts of gender inequality in the Earth and space sciences. *Earth Sp. Sci.* 6, 1460–1468, doi.org/10.1029/2019EA000706

<u>Appendix</u>

Five key publications related to the proposal are indicated for each Full Member. Publications are sorted in order of relevance. Underlining is used to highlight the name of each WG member within her/his list of publications. If a member of the WG is co-author on a publication listed by another member, her/his name is also underlined to highlight previous collaborations among WG members. There are no duplicated publications.

Martí Galí (Co-chair)

<u>Galí, M.</u>, Simó, R. (2015). A meta-analysis of oceanic DMS and DMSP cycling processes: Disentangling the summer paradox. *Global Biogeochemical Cycles*, *29*(4), 496-515, <u>doi.org/10.1002/2014GB004940</u>

<u>Galí, M.</u>, Kieber, D. J., Romera-Castillo, C., Kinsey, J. D., Devred, E., Pérez, G. L., Westby, G. R., Marrasé, C., Babin, M., Levasseur, M., Duarte, C. M., Agustí, S., Simó, R. (2016). CDOM sources and photobleaching control quantum yields for oceanic DMS photolysis. *Environmental Science & Technology*, *50*(24), 13361-13370, <u>doi.org/10.1021/acs.est.6b04278</u>

Royer, S. J., <u>Galí, M.</u>, Mahajan, A. S., Ross, O. N., Pérez, G. L., Saltzman, E. S., Simó, R. (2016). A high-resolution time-depth view of dimethylsulphide cycling in the surface sea. *Sci Rep* 6, 32325 (2016), <u>doi.org/10.1038/srep32325</u>

<u>Galí, M.</u>, Simó, R. (2010). Occurrence and cycling of dimethylated sulfur compounds in the Arctic during summer receding of the ice edge. *Marine Chemistry*, *122*(1-4), 105-117, doi.org/10.1016/j.marchem.2010.07.003

<u>Galí, M.</u>, Levasseur, M., Devred, E., Simó, R., Babin, M. (2018). Sea-surface dimethylsulfide (DMS) concentration from satellite data at global and regional scales. *Biogeosciences*, *15*(11), 3497-3519, doi.org/10.5194/bg-15-3497-2018

Daniela del Valle (Co-chair)

<u>del Valle, D. A.</u>, Kieber, D. J., Kiene, R. P. (2009). Biological consumption of dimethylsulfide (DMS) and its importance in DMS dynamics in the Ross Sea, Antarctica. *Limnology and Oceanography*, 54: 785-798, doi.org/10.4319/lo.2009.54.3.0785

<u>del Valle, D. A.</u>, Kieber, D. J., Toole, D. A., Bisgrove, J., Slezak, D., Kiene, R. P. (2009). Dissolved DMSO production via biological and photochemical oxidation of dissolved DMS in the Ross Sea, Antarctica. *Deep-Sea Research I*, 56: 166-177, <u>doi.org/10.1016/j.dsr.2008.09.005</u>

<u>del Valle, D. A.</u>, Martínez-García, S., Sañudo-Wilhelmy, S., Kiene, R. P., Karl, D. M. (2015). Methionine and dimethylsulfoniopropionate as sources of sulfur to the microbial community of the North Pacific Subtropical Gyre. *Aquatic Microbial Ecology*, 75:103-116, <u>doi.org/10.3354/ame01750</u>

<u>del Valle, D. A</u>., Kieber, D. J., Kiene, R. P. (2007). Depth-dependent fate of biologically-consumed dimethylsulfide in the Sargasso Sea. *Marine Chemistry*, 103: 197-208, doi.org/10.1016/j.marchem.2006.07.005

<u>del Valle, D. A.</u>, Kieber, D. J., Bisgrove, J., Kiene, R. P. (2007). Light-stimulated production of dissolved DMSO by a particle-associated process in the Ross Sea, Antarctica. *Limnology and Oceanography*, 52: 2456-2466, <u>doi.org/10.4319/lo.2007.52.6.2456</u>

Stephen Archer

<u>Archer, S. D.</u>, Suffrian, K., Posman, K., Bach, L. T., Matrai, P. A., Countway, P. D., Ludwig, A., Riebesell, U. (2018). Processes that drive decreased dimethyl sulfide production in response to ocean acidification in subtropical waters. *Frontiers in Marine Science*, 5, Article 245, <u>doi.org/10.3389/fmars.2018.00245</u>

<u>Archer, S. D.</u>, <u>Stefels, J.</u>, Airs, R. L., Lawton, T., Smyth, T. J., Rees, A. P., Geider, R. J. (2018). Limitation of DMSP synthesis at high irradiance in natural phytoplankton communities. *Limnology and Oceanography*, 63: 227-242, <u>doi.org/10.1002/lno.10625</u>

<u>Archer, S. D.</u>, Stelfox-Widdicombe, C. E., Burkill, P. H., Malin, G. (2001) A dilution approach to quantify the production of dissolved dimethylsulphoniopropionate and dimethyl sulphide due to microzooplankton herbivory. *Aquatic Microbial Ecology*, 23:131-145, <u>doi.org/10.3354/ame023131</u>

<u>Archer, S. D.</u>, Tarran, G. A., Stephens, J. A., Butcher, L. J., Kimmance, S. A. (2011). Combining flow sorting with gas chromatography to determine phytoplankton group-specific intracellular content of dimethylsulphoniopropionate (DMSP). *Aquatic Microbial Ecology*, 62 (2) 109-121, <u>doi.org/10.3354/ame01464</u>

<u>Archer, S. D.</u>, Gilbert, F. J., Allen, J. I., Blackford, J., Nightingale, P.D. (2004). Modelling of the seasonal patterns of dimethylsulphide production and fate during 1989 at a site in the North Sea. *Canadian Journal of Fisheries and Aquatic Sciences*, 61:765-787, <u>doi.org/10.1139/f04-028</u>

José González

<u>González, J. M.</u>, Hernández, L., Manzano, I., Pedrós-Alió, C. (2019). Functional annotation of orthologs in metagenomes: a case study of genes for the transformation of oceanic dimethylsulfoniopropionate. The ISME journal, 13(5), 1183-1197, <u>doi.org/10.1038/s41396-019-0347-6</u>

Buchan, A., LeCleir, G. R., Gulvik, C. A., <u>González, J. M.</u> (2014). Master recyclers: features and functions of bacteria associated with phytoplankton blooms. *Nature Reviews Microbiology*, 12(10), 686-698, <u>doi.org/10.1038/nrmicro3326</u>

González, J. M., Kiene, R. P., Moran, M. A. (1999). Transformation of sulfur compounds by an abundant lineage of marine bacteria in the α -subclass of the class Proteobacteria. *Applied and environmental microbiology*, 65(9), 3810-3819, <u>doi.org/10.1128/aem.65.9.3810-3819.1999</u>

Howard, E. C., Henriksen, J. R., Buchan, A., Reisch, C. R., Bürgmann, H., Welsh, R., Ye, W., <u>González, J.</u> <u>M.</u>, Mace, K., <u>Joye, S. B.</u>, Kiene, R. P., <u>Whitman, W. B.</u>, Moran, M. A. (2006). Bacterial taxa that limit sulfur flux from the ocean. *Science*, *314*(5799), 649-652, <u>doi.org/10.1126/science.1130657</u>

Alonso-Sáez, L., Morán, X. A. G., <u>González, J. M.</u> (2020). Transcriptional patterns of biogeochemically relevant marker genes by temperate marine bacteria. *Frontiers in microbiology*, 11, 465, <u>doi.org/10.3389/fmicb.2020.00465</u>

Hakase Hayashida

<u>Hayashida, H.</u>, Carnat, G., <u>Galí, M.</u>, Monahan, A. H., Mortenson, E., Sou, T., Steiner, N. S. (2020). Spatiotemporal variability in modelled bottom-ice and sea-surface dimethylsulfide concentrations and fluxes in the Arctic during 1979-2015. *Global Biogeochemical Cycles*, 34(10), e2019GB006456, <u>doi.org/10.1029/2019GB006456</u> <u>Hayashida, H.</u>, Christian, J. R., Holdsworth, A. M., Hu, X., Monahan, A. H., Mortenson, E., Myers, P. G., Riche, O. G. J., Sou, T., Steiner, N. S. (2019). CSIB v1 (Canadian Sea-ice Biogeochemistry): a sea-ice biogeochemical model for the NEMO community ocean modelling framework. *Geoscientific Model Development*, 12(5), 1965-1990, doi.org/10.5194/gmd-12-1965-2019

<u>Hayashida, H.</u>, Steiner, N., Monahan, A., Galindo, V., Lizotte, M., Levasseur, M. (2017). Implications of sea-ice biogeochemistry for oceanic production and emissions of dimethyl sulfide in the Arctic. *Biogeosciences*, *14*(12), 3129-3155, <u>doi.org/10.5194/bg-14-3129-2017</u>

Abbatt, J. P. D., Leaitch, W. R., Aliabadi, A. A., Bertram, A. K., Blanchet, J.-P., Boivin-Rioux, A., Bozem, H., Burkart, J., Chang, R. Y. W., Charette, J., Chaubey, J. P., Christensen, R. J., Cirisan, A., Collins, D. B., Croft, B., Dionne, J., Evans, G. J., Fletcher, C. G., Ghahremaninezhad, R., Girard, E., Gong, W., Gosselin, M., Gourdal, M., Hanna, S. J., <u>Hayashida, H.</u>, Herber, A. B., Hesaraki, S., Hoor, P., Huang, L., Hussherr, R., Irish, V. E., Keita, S. A., Kodros, J. K., Köllner, F., Kolonjari, F., Kunkel, D., Ladino, L. A., Law, K., Levasseur, M., Libois, Q., Liggio, J., Lizotte, M., Macdonald, K. M., Mahmood, R., Martin, R. V., Mason, R. H., Miller, L. A., Moravek, A., Mortenson, E., Mungall, E. L., Murphy, J. G., Namazi, M., Norman, A.-L., O'Neill, N. T., Pierce, J. R., Russell, L. M., Schneider, J., Schulz, H., Sharma, S., Si, M., Staebler, R. M., Steiner, N. S., <u>Galí,</u> <u>M.</u>, Thomas, J. L., von Salzen, K., Wentzell, J. J. B., Willis, M. D., Wentworth, G. R., Xu, J.-W., Yakobi-Hancock, J. D. (2019). New insights into aerosol and climate in the Arctic. *Atmospheric Chemistry and Physics*, 19, 2527–2560, <u>doi.org/10.5194/acp-19-2527-2019</u>

<u>Hayashida, H.</u>, Jin, M., Steiner, N., Swart, N., Watanabe, E., Fiedler, R., Hogg, A., Kiss, A., Matear, R., and Strutton, P. (2021). Ice Algae Model Intercomparison Project phase 2 (IAMIP2). *Geoscientific Model Development*, 14, 6847–6861, <u>doi.org/10.5194/gmd-14-6847-2021</u>

Frances Hopkins

<u>Hopkins, F. E.</u>, Nightingale, P. D., Stephens, J. A., Moore, C. M., Richier, S., Cripps, G. L., <u>Archer, S. D.</u> (2020). A meta-analysis of microcosm experiments shows that dimethyl sulfide (DMS) production in polar waters is insensitive to ocean acidification. *Biogeosciences*, 17(1), 163-186, <u>doi.org/10.5194/bg-17-163-2020</u>

Dixon, J. L., <u>Hopkins, F. E.</u>, Stephens, J. A., Schäfer, H. (2020). Seasonal changes in microbial dissolved organic sulfur transformations in coastal waters. *Microorganisms*, 8(3), 337, <u>doi.org/10.3390/microorganisms8030337</u>

<u>Hopkins, F. E.</u>, <u>Archer, S. D.</u> (2014). Consistent increase in dimethyl sulfide (DMS) in response to high CO 2 in five shipboard bioassays from contrasting NW European waters. *Biogeosciences*, 11(18), 4925-4940, doi.org/10.5194/bg-11-4925-2014

<u>Archer, S. D.</u>, Kimmance, S. A., Stephens, J. A., <u>Hopkins, F. E.</u>, Bellerby, R. G. J., Schulz, K. G., Piontek, J., Engel, A. (2013). Contrasting responses of DMS and DMSP to ocean acidification in Arctic waters. *Biogeosciences*, 10(3), 1893-1908, <u>doi.org/10.5194/bg-10-1893-2013</u>

<u>Hopkins, F. E.</u>, Bell, T. G., Yang, M., Suggett, D. J., Steinke, M. (2016). Air exposure of coral is a significant source of dimethylsulfide (DMS) to the atmosphere. *Scientific Reports*, *6*(1), 1-11, <u>doi.org/10.1038/srep36031</u>

Sohiko Kameyama

<u>Kameyama, S.</u>, Tanimoto H., Inomata S., Tsunogai U., Ooki, A., Yokouchi, Y., Takeda S., Obata H., and M. Uematsu (2009). Equilibrator inlet-proton transfer reaction-mass spectrometry (EI-PTR-MS) for

sensitive, high-resolution measurement of dimethyl sulfide dissolved in seawater. *Analytical Chemistry*, 81(21), 9021-9026, <u>doi.org/10.1021/ac901630h</u>

<u>Kameyama, S.</u>, Tanimoto, H., Inomata, S., Yoshikawa-Inoue, H., Tsunogai, U., Tsuda, A., Uematsu, M., Ishii, M., Sasano, D., Suzuki, K., Nosaka, Y. (2013). Strong relationship between dimethyl sulfide and net community production in the western subarctic Pacific. *Geophysical Research Letters*, 40, 3986-3990, doi.org/10.1002/grl.50654

<u>Kameyama, S.</u>, Otomaru M., McMinn A., and Suzuki K. (2020). Ice melting can change DMSP production and photosynthetic activity of the haptophyte *Phaeocystis antarctica*. *Journal of Phycology*, 56(3) 761-774, <u>doi.org/10.1111/jpy.12985</u>

Li, J.-L., <u>Kameyama, S.</u>, and Yang, G.-P. (2020). In-situ measurement of trace isoprene and dimethyl sulfide in seawater and oceanic atmosphere based on room temperature adsorption-thermal desorption. *Marine Chemistry*, 222, <u>doi.org/10.1016/j.marchem.2020.103787</u>

<u>Kameyama, S.</u>, Tanimoto, H., Inomata, S., Suzuki, K., Komatsu, D. D., Hirota, A., Konno, U., Tsunogai, U. (2011). Application of PTR-MS to incubation experiments of the marine diatom *Thalassiosira pseudonana*. *Geochemical Journal*, 45, 355-363, <u>doi.org/10.2343/geochemj.1.0127</u>

Erin McParland

<u>McParland, E.</u>, Levine, N. (2019). The role of differential DMSP production and community composition in predicting variability of global surface DMSP concentrations. *Limnology & Oceanography*, <u>doi.org/10.1002/lno.11076</u>

<u>McParland, E.</u>, Lee, M., Webb, E., Alexander, H., Levine, N. (2021). DMSP synthesis genes distinguish two types of DMSP producer phenotypes. *Environmental Microbiology*, <u>doi.org/10.1111/1462-</u> 2920.15393

<u>McParland, E.</u>, Wright, A., Art, K., He, M., Levine, N. (2020). Evidence for contrasting roles of DMSP production in *Emiliania huxleyi* and *Thalassiosira oceanica*. *New Phytologist*, doi.org/10.1111/nph.16374

O'Brien, J., <u>McParland, E.</u>, Bramucci, A., Siboni, N., Ostrowski, M., Kalkhe, T., Levine, N., Brown, M., Van De Kamp, J., Bodrossy, L., Messer, L., Petrou, K., Seymour, J. (2022). Biogeographical and seasonal dynamics of the marine Roseobacter community and ecological links to DMSP-producing phytoplankton. *ISME Communications*. <u>doi.org/10.1038/s43705-022-00099-3</u>

Jackson, R., Matrai, P., Woodhouse, M., Cropp, R., Jones, G., <u>Deschaseaux, E.</u>, Omori, Y., <u>McParland, E.</u>, Swan, H., Tanimoto, H. (2021). Parameterizing the impact of seawater temperature and irradiance on dimethylsulfide (DMS) in the Great Barrier Reef and the contribution of coral reefs to the global sulfur cycle. *JGR Oceans*, <u>doi.org/10.1029/2020jc016783</u>

Jacqueline Stefels

Webb, A. L., van Leeuwe, M. A., den Os, D., Meredith, M. P., Venables H., <u>Stefels, J.</u> (2019) Extreme spikes in DMS flux double estimates of biogenic sulfur export from the Antarctic coastal zone to the atmosphere. *Scientific Reports* 9:2233, <u>doi.org/10.1038/s41598-019-38714-4</u>

<u>Stefels, J.</u>, van Leeuwe, M. A., Jones, E. M., Meredith, M. P., Venables, H. J., Webb, A. L., Henley, S. F. (2018). Impact of sea-ice melt on dimethyl sulfide (sulfoniopropionate) inventories in surface waters of

Marguerite Bay, West Antarctic Peninsula. *Phil. Trans. R. Soc.* A 376: 20170169, doi.org/10.1098/rsta.2017.0169

<u>Stefels, J.</u>, Carnat, G., Dacey, J. W. H., Goossens, T., Elzenga, J. T. M., Tison, J-L. (2012). The analysis of dimethylsulfide and dimethylsulphoniopropionate in sea ice: dry-crushing and melting using stable isotope additions. *Marine Chemistry* 128-129:34-43, doi.org/10.1016/j.marchem.2011.09.007

<u>Stefels, J.</u>, Dacey J. W. H., Elzenga, J. T. M. (2009). In vivo DMSP-biosynthesis measurements using stable-isotope incorporation and proton-transfer-reaction mass spectrometry (PTR-MS). *Limnology and Oceanography: Methods* 7:595-611, <u>doi.org/10.4319/lom.2009.7.595</u>

<u>Stefels, J.</u>, Steinke, M., Turner, S., Malin, G., Belviso, S. (2007). Environmental constraints on the production and removal of the climatically active gas dimethylsulphide (DMS) and implications for ecosystem modelling. *Biogeochemistry* 83:245–275, <u>doi.org/10.4319/lom.2009.7.595</u>

Marcos Zárate

Snowden, D., Tsontos, V. M., Handegard, N. O., <u>Zarate, M.</u>, O'Brien, K., Casey, K. S., Smith, N., Sagen, H., Bailey, K., Lewis, M.N., Arms, S. C. (2019). Data interoperability between elements of the global ocean observing system. *Frontiers in Marine Science*, 6, 442, <u>doi.org/10.3389/fmars.2019.00442</u>

Zárate, M., Braun, G., Lewis, M., Fillottrani, P. (2022). Observational/Hydrographic data of the South Atlantic Ocean published as LOD. *Semantic Web*, 13(2), 133-145, <u>doi.org/10.3233/SW-210426</u>

Zárate, M., Braun, G., Fillottrani, P., Delrieux, C., Lewis, M. (2020). BiGe-Onto: an ontology-based system for managing biodiversity and biogeography data. *Applied Ontology*, 15(4), 411-437, doi.org/10.3233/AO-200228

<u>Zárate, M.</u>, Rosales, P., Braun, G., Lewis, M., Fillottrani, P. R., Delrieux, C. (2019). OceanGraph: some initial steps toward a oceanographic knowledge graph. In *Iberoamerican Knowledge Graphs and Semantic Web Conference*, 1029, 33-40, Springer, Cham, <u>doi.org/10.1007/978-3-030-21395-4_3</u>

Zárate, M., Buckle, C. (2021). LOBD: Linked Data Dashboard for Marine Biodiversity. In *Conference on Cloud Computing, Big Data & Emerging Topics*, 1444, 151-164, Springer, Cham, <u>doi.org/10.1007/978-3-030-84825-5_11</u>