Dissolved B vitamin and vitamer concentrations in surface seawater collected during the Malaspina Circumnavigation Expedition from December 2010 to July 2011

Website: https://www.bco-dmo.org/dataset/954686
Data Type: Cruise Results
Version: 1
Version Date: 2025-02-27

Project
» Putting B-vitamins on the map: to what extent do they shape phytoplankton dynamics and biogeography in the global ocean? (VitaMaps)

Contributors	Affiliation	Role
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Abstract
This dataset includes dissolved B vitamin and vitamer concentrations in surface seawater collected during the Malaspina Circumnavigation Expedition. The samples were collected aboard the Hesperides between dates 2010-12-16 and 2011-7-9 in the Atlantic, Pacific, and Indian Oceans. Seawater samples were collected using Niskin bottles attached to a rosette equipped with a CTD. The different B vitamins were analyzed using a triple quadrupole mass spectrometer coupled to a liquid chromatography system after a solid-phase extraction with a C18 resin. Understanding the global distribution of vitamins is helping us to determine the impact of dissolved B vitamins' availability in microbial species biogeography.

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Coverage

Location: Pacific and Indian Oceans
Spatial Extent: **N**:35.161876 **E**:-179.5331244 **S**:-39.841384 **W**:150.9605738
Temporal Extent: 2010-12-16 - 2011-07-09

Methods & Sampling

Sampling protocol:
Samples were collected using a Teflon tow-fish sampling system deployed at approximately 3-meters (m) depth utilizing established trace metal-clean techniques. After sample collection, seawater was filtered on board through acid-washed 0.2-micrometer (µm) filter cartridges and frozen until analysis.

Preconcentration protocol:
Samples for dissolved vitamin analysis were preconcentrated as previously described (Okbamichael and Sañudo-Wilhelmy, 2004; Okbamichael and Sañudo-Wilhelmy, 2005; Sañudo-Wilhelmy et al., 2012; Suffridge et al., 2017). Briefly, preconcentration columns were prepared by pouring 1:1 MeOH: C18 resin (HF Bondesil (Agilent Technologies)) slurry into Poly-Prep Columns (Biorad). The resin was allowed to settle, and the excess MeOH was drained, leaving 7 milliliters (ml) of resin. Thawed samples were adjusted to pH 6.5 using dilute HCl and passed over the preconcentration column at 1 ml per minute. The residual salt was rinsed off the resin using 30 ml of LC/MS grade water. The target analytes were then eluted from the resin using 12 ml of LC/MS grade methanol into methanol-rinsed 15 ml conical centrifuge tubes. Eluted samples were then further concentrated via evaporation in a nitrogen dryer using 5-20 PSI compressed N2 gas, in a dark, at room temperature. Samples were allowed to evaporate until 250 microliters (µl) remained, and then stored at -20 degrees Celsius (°C) until LC/MS analysis, which occurred within 24 hours. Prior to LC/MS analysis, samples were adjusted to pH 6.5 using 10 µl of dilute NaOH.

LC/MS Analysis:
Quantification of vitamin B7 (biotin); four different chemical forms of vitamin B12 ((adenosyl (AB12)-cyano (CB12)-hydroxy (HB12), and methyl (MB12) B12; vitamin B1 (thiamin); two of its precursors (HMP,(4-Amino-5-hydroxymethyl-2-methylpyrimidine) and cHET (5-(2-Hydroxyethyl)-4-methyl-1,3-thiazole-2-carboxylic acid) as well as HET (4-Methyl-5-thiazoleethanol), precursor of cHET and AmMP (4-amino-5-aminomethyl-2-methylpyrimidine), a salvage compound for the HMP synthesis, was carried out with a Thermo TSQ Altis Plus triple quadrupole mass spectrometer, coupled to a Vanquish Flex UHPLC system. The LC system used a stable-bond C18 reversed-phase column (Discovery HS C18 10cm x 2.1mm, 5µm column, Supelco Analytical) with a 50 µl sample loop. The computer software Trace Finder General 5.2 Quan and TSQ Altis Plus 3.4 Tune (Thermo Scientific) were used for data acquisition and analysis. A 12-minute gradient flow was used with mobile phases of methanol (MeOH) and LC/MS grade water, both buffered to pH 4 with 0.5% acetic acid. The flow rate was set at 230 microliters per minute (µl/min) throughout the run, with a gradient starting at 93% LC/MS water: 7% MeOH for two minutes, changing to 100% MeOH by seven minutes, and continuing at 100% MeOH until nine minutes and returning to initial conditions until the gradient completes at twelve minutes. All peaks were identified using standards dissolved in LC/MS grade water. The mass spectrometer was run in Selected Reaction Monitoring (SRM) mode with positive polarity with a well time of 100 milliseconds (ms) per transition. The resolution of the mass filters used for quadrupoles 1 and 2 were 0.7 and 0.1 m/z, respectively. The ESI spray voltage was 4000V, sheath gas (N2) pressure was 30 PSI, the auxiliary gas (Ar) pressure was 3 PSI, the capillary temperature was 269°C, and the collision pressure was 2.1 torr. B vitamin and vitamer values reported as 0.00 should be interpreted as "non-detectable".

Data Processing Description

The computer software Trace Finder General 5.2 Quan and TSQ Altis Plus 3.4 Tune (Thermo Scientific) were used for data acquisition and analysis.

BCO-DMO Processing Description

- Imported original file "Dataset_MH_B-vitamin concentrations_Final data set_20241206.xlsx" into the BCO-DMO system.
- Renamed fields to comply with BCO-DMO naming conventions.
- Converted date field to YYYY-MM-DD format.
- Saved the final file as "954686_v1_dissolved_b_vitamins_and_vitamers.csv".

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Related Publications

Okbamichael, M., & Sañudo-Wilhelmy, S. A. (2004). A new method for the determination of Vitamin B12 in seawater. Analytica Chimica Acta, 517(1–2), 33–38. https://doi.org/10.1016/j.aca.2004.05.020
Methods

Okbamichael, M., & Sañudo-Wilhelmy, S. A. (2005). Direct determination of vitamin B1in seawater by solid-phase extraction and high-performance liquid chromatography quantification. Limnology and Oceanography: Methods, 3(5), 241–246. Portico. https://doi.org/10.4319/lom.2005.3.241
Methods

Sanudo-Wilhelmy, S. A., Cutter, L. S., Durazo, R., Smail, E. A., Gomez-Consarnau, L., Webb, E. A., … Karl, D. M. (2012). Multiple B-vitamin depletion in large areas of the coastal ocean. Proceedings of the National Academy of Sciences, 109(35), 14041–14045. doi:10.1073/pnas.1208755109
Methods

Suffridge, C., Cutter, L., & Sañudo-Wilhelmy, S. A. (2017). A New Analytical Method for Direct Measurement of Particulate and Dissolved B-vitamins and Their Congeners in Seawater. Frontiers in Marine Science, 4. doi:10.3389/fmars.2017.00011
Methods

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Parameters

Parameter	Description	Units
Cruise	Cruise name	unitless
Sample_ID	Sample ID	unitless
Station	Station number	unitless
Date	Date of sampling	unitless
Longitude	Longitude of sampling; negative values = West	decimal degrees
Latitude	Latitude of sampling; negative values = South	decimal degrees
Depth_m	Sample depth	meters (m)
HMP_pM	4-aminio-5-hydroxymethyl-2-methylpyrimidine concentration	picomoles per liter (pico mol L-1)
AmMP_pM	4-amino-5-aminomethyl-2-methylpyrimidine concentration	picomoles per liter (pico mol L-1)
B1_pM	Thiamin concentration	picomoles per liter (pico mol L-1)
HET_pM	4-methyl-5-thiazoleethanol concentration	picomoles per liter (pico mol L-1)
Thiazole_pM	Thiazole concentration	picomoles per liter (pico mol L-1)
cHET_pM	5-(2-Hydroxyethy)-4-Methyl-1,3-Thiazole-2-Carboxylic Acid concentration	picomoles per liter (pico mol L-1)
B7_pM	Biotin concentration	picomoles per liter (pico mol L-1)
HB12_pM	Hydroxycobalamin concentration	picomoles per liter (pico mol L-1)
CB12_pM	Cyanocobalamin concentration	picomoles per liter (pico mol L-1)
AB12_pM	Adenosylobalamin concentration	picomoles per liter (pico mol L-1)
MB12_pM	Methylcobalamin concentration	picomoles per liter (pico mol L-1)

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Instruments

Dataset-specific Instrument Name	Thermo TSQ Altis Plus triple quadrupole mass spectrometer
Generic Instrument Name	Quadrupole Mass Spectrometer
Dataset-specific Description	Thermo TSQ Altis Plus triple quadrupole mass spectrometer, coupled to a Vanquish Flex UHPLC system
Generic Instrument Description	A piece of apparatus that consists of an ion source, a mass-to-charge analyser, a detector and a vacuum system and is used to measure mass spectra. The detector is a quadrupole mass-to-charge analyser, which holds the ions in a stable orbit by an electric field generated by four parallel electrodes.

Dataset-specific Instrument Name	Teflon tow-fish sampling system
Generic Instrument Name	towed unmanned submersible
Dataset-specific Description	a Teflon tow-fish sampling system deployed at approximately 3m depth utilizing established trace metal-clean techniques
Generic Instrument Description	A vehicle towed by rigid cable through the water column at fixed or varying depth with no propulsion and no human operator (e.g. Towfish, Scanfish, UOR, SeaSoar).

Dataset-specific Instrument Name	Vanquish Flex UHPLC system
Generic Instrument Name	Ultra high-performance liquid chromatography
Dataset-specific Description	Thermo TSQ Altis Plus triple quadrupole mass spectrometer, coupled to a Vanquish Flex UHPLC system
Generic Instrument Description	Ultra high-performance liquid chromatography: Column chromatography where the mobile phase is a liquid, the stationary phase consists of very small (< 2 microm) particles and the inlet pressure is relatively high.

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Deployments

Malaspina_2010_Hesperides

Website	https://www.bco-dmo.org/deployment/911265
Platform	R/V Hespérides
Start Date	2010-12-16
End Date	2011-07-10
Description	The Malaspina circumnavigation of 2010 was an interdisciplinary research project whose main objectives were to evaluate the impact of global change on the ocean as well as to explore its biodiversity. It began in December 2010 with the departure from Cádiz of the oceanographic research vessel Hespérides operated by the Spanish Navy. After a voyage passing through Rio de Janeiro, Cape Town, Perth, Sydney, Auckland, Honolulu, Cartagena de Indias and Panama, it returned to Spain in July 2011. At the same time, the ship Sarmiento de Gamboa, operated by the Spanish National Research Council (CSIC), worked in parallel between Las Palmas de Gran Canaria, Santo Domingo and Vigo. In this way, for seven months, over 250 scientists aboard the two ships carried out an expedition combining cutting-edge scientific research with the training of young researchers, and the promotion of marine science and scientific culture in society. (description from: https://sandrarebok.net/malaspina-2010)

Malaspina_2010_Gamboa

Website	https://www.bco-dmo.org/deployment/911261
Platform	R/V Sarmiento de Gamboa
Start Date	2010-12-16
End Date	2011-07-10
Description	The Malaspina circumnavigation of 2010 was an interdisciplinary research project whose main objectives were to evaluate the impact of global change on the ocean as well as to explore its biodiversity. It began in December 2010 with the departure from Cádiz of the oceanographic research vessel Hespérides operated by the Spanish Navy. After a voyage passing through Rio de Janeiro, Cape Town, Perth, Sydney, Auckland, Honolulu, Cartagena de Indias and Panama, it returned to Spain in July 2011. At the same time, the ship Sarmiento de Gamboa, operated by the Spanish National Research Council (CSIC), worked in parallel between Las Palmas de Gran Canaria, Santo Domingo and Vigo. In this way, for seven months, over 250 scientists aboard the two ships carried out an expedition combining cutting-edge scientific research with the training of young researchers, and the promotion of marine science and scientific culture in society. (description from: https://sandrarebok.net/malaspina-2010)

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Project Information

Putting B-vitamins on the map: to what extent do they shape phytoplankton dynamics and biogeography in the global ocean? (VitaMaps)

NSF Award Abstract:
B-vitamins (thiamin, B1; biotin B7; cobalamin, B12) are organic molecules necessary for all the biological transformations of the chemical elements that support life on Earth. Without the activity of those molecules, the chemistry of life on Earth—as we know it—would end. In marine systems, the availability of B-vitamins also affects food web dynamics by controlling both bacterial and phytoplankton growth and species diversity. Because many organisms that can make several B-vitamins lack the ability to synthesize others, their vitamin needs and environmental accessibility could define which, when, and where specific phytoplankton species flourish. As a result, planktonic communities in nature need to constantly share B-vitamins in a complex mosaic of interdependencies. Despite the early discovery of their relevance in the 1940s, most current marine vitamin research is still based on laboratory experiments or studies focusing on the biological responses of B-vitamin additions on algae and bacteria. Yet, vitamin distributions in the world ocean are mostly unknown, as they have only been measured in a few marine basins. Thus, the actual effect of their natural distributions in

phytoplankton communities is still a mystery today. The main goal of this project is to elucidate the effects of B-vitamins availability on the spatial distributions of different phytoplankton species in surface waters of the world ocean. These data are needed to start untangling the rules by which members of the microbial plankton are interconnected through vitamin exchange and to determine how these essential interrelations may control surface ocean ecosystem functioning, such as phytoplankton and bacterial growth. Ultimately understanding these controls and their dynamics is critical to predicting future changes in the marine environment. In the future greenhouse world, the ocean is expected to be of paramount importance, providing the required protein to nurture future human populations and to reduce the levels of human-produced atmospheric CO2 through its uptake by photosynthetic organisms with different vitamin requirements.

This study is to establish the first global map of B-vitamin distributions in surface waters of the world ocean collected during the Malaspina circumnavigation expedition. This global map of vitamins is being used to determine their importance on phytoplankton species biogeography, a still unresolved ecological riddle. Another objective of the study is to establish how ambient vitamin concentrations, combined with bioactive trace elements and macronutrients, promote changes in the relative abundance of different eukaryotic and prokaryotic plankton species on the surface ocean. Overall, this is the first global study on the role of B-vitamins on ecosystem functioning and species composition in subtropical and tropical open ocean environments including the ocean gyres. The investigators are carrying out targeted metagenomic analyses to identify B-vitamins synthesizers and consumers within the planktonic community at several globally distributed stations across the Atlantic, Pacific, and Indian oceans. The extensive datasets already generated by the hundreds of participants of the Malaspina expedition is fully available to interpret the vitamin results. This study allows us to expand our understanding of B-vitamin distributions on a global scale and further investigate how surface ocean’s plankton community dynamics are intertwined with ambient B-vitamin pools.

This award reflects NSF's statutory mission and has been deemed worthy of support through evaluation using the Foundation's intellectual merit and broader impacts review criteria.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-2220546

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