# Ross Sea metaproteome peptide spectral counts searched against Phaeocystis strain transcriptome from net tows during RVIB Nathaniel B. Palmer cruise NBP0601 in December of 2015

Website: https://www.bco-dmo.org/dataset/768259 Data Type: Cruise Results Version: 2 Version Date: 2024-05-24

### Project

» Controls of Ross Sea Algal Community Structure (CORSACS)

#### Program

» Ocean Carbon and Biogeochemistry (OCB)

Contributors	Affiliation	Role
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#### Abstract

A net tow metaproteome of a Phaeocystis antarctica bloom in the Ross Sea, mapped here to Phaeocystis metatranscriptomes analyzed by 2D LCMS, in units of peptide spectral counts.

# **Table of Contents**

- <u>Coverage</u>
- <u>Dataset Description</u>
  - <u>Methods & Sampling</u>
  - Data Processing Description
  - BCO-DMO Processing Description
- Data Files
- <u>Related Publications</u>
- <u>Related Datasets</u>
- <u>Parameters</u>
- Instruments
- <u>Deployments</u>
- <u>Project Information</u>
- Program Information
- Funding

## Coverage

Location: Ross Sea Spatial Extent: Lat:-76.82 Lon:170.76 Temporal Extent: 2005-12-30

## **Dataset Description**

These data are part of the Ocean Protein Portal "Ross Sea Net Tow (Bender)" dataset version 1 (<u>https://proteinportal.whoi.edu/;</u> Saito et al., 2019).

Sampling was conducted with a 20 micron plankton net on 12/30/2005 at about 1am (local time), near station 137, was extracted for total protein using an SDS detergent method followed by tube gel purification, reduction, alkylation, and tryptic digestion and analyzed on a Thermo Orbitrap Fusion using 2-dimensional separation scheme to maximize metaproteome depth. Detailed methods available in Bender et al. 2018.

Organism identifier (LifeSciences Identifier, LSID): Phaeocystis antarctica, urn:lsid:marinespecies.org:taxname:341585

#### **Data Processing Description**

Mass spectra from 2D LC-MS was peptide-to-spectrum matched using the SEQUEST algorithm within Proteome Discoverer software, followed by spectral counting with Proteome Software's Scaffold software using the FASTA sequence file generated from Phaeocystis culture transcriptome study. Data processing documented in Bender et al. 2018.

### **BCO-DMO Processing Description**

Data version 1: 2024-04-29

\* Data file "peptides\_V2.csv" was imported into the BCO-DMO data system for this dataset. This was the file imported into Ocean Protein Portal version 1 of the Bender Ross Sea dataset.

\*\* Missing data values are displayed differently based on the file format you download. They are blank in csv files, "NaN" in MatLab files, etc.

\* Column name "absolute\_unites\_fmol\_L" corrected to "absolute\_units\_fmol\_L"

\* Date converted to ISO 8601 format

\* several columns ( median\_retention\_time,total\_precursor\_intensity,TIC,absolute\_units\_fmol\_L) contain no values but were not removed since these are named columns in the Ocean Protein Portal template, though optional columns.

Data version 2: 2024-05-24 fixes issue in version 1 peptide data where the Z was removed from timestamp values.

This version 2 matches the data at the Ocean Protein Portal "Ross Sea Net Tow (Bender)" dataset version 1 (<u>https://proteinportal.whoi.edu/;</u> Saito et al., 2019).

[ table of contents | back to top ]

## Data Files

File

768259\_v2\_bender-ross-sea-peptides.csv

(Comma Separated Values (.csv), 1.09 MB) MD5:48b12c83f351f9b14f5a2142dc533fb5

Primary data file for dataset ID 768259, version 2. Corresponds to Ocean Protein Portal Bender-Ross Sea data (version 1) .

[ table of contents | back to top ]

## **Related Publications**

Bender, S. J., Moran, D. M., McIlvin, M. R., Zheng, H., McCrow, J. P., Badger, J., ... Saito, M. A. (2018). Colony formation in Phaeocystis antarctica connecting molecular mechanisms with iron biogeochemistry. Biogeosciences, 15(16), 4923–4942. doi:<u>10.5194/bg-15-4923-2018</u> *Results* 

Saito, M. A., Bertrand, E. M., Duffy, M. E., Gaylord, D. A., Held, N. A., Hervey, W. J., Hettich, R. L., Jagtap, P. D., Janech, M. G., Kinkade, D. B., Leary, D. H., McIlvin, M. R., Moore, E. K., Morris, R. M., Neely, B. A., Nunn, B. L.,

Saunders, J. K., Shepherd, A. I., Symmonds, N. I., & Walsh, D. A. (2019). Progress and Challenges in Ocean Metaproteomics and Proposed Best Practices for Data Sharing. Journal of Proteome Research, 18(4), 1461–1476. https://doi.org/<u>10.1021/acs.jproteome.8b00761</u> *Methods* 

[ table of contents | back to top ]

# **Related Datasets**

### IsRelatedTo

Saito, M. A. (2024) **FASTA file of protein identifications from net tows during RVIB Nathaniel B. Palmer cruise NBP0601 in December of 2015.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2019-05-17 doi:10.26008/1912/bco-dmo.769266.1 [view at BCO-DMO]

Relationship Description: Generated from the same sampling event and methodology. These data are part of the same dataset "Ross Sea Net Tow (Bender)" version 1 at the Ocean Protein Portal (https://proteinportal.whoi.edu/).

Saito, M. A. (2024) **Ross Sea metaproteome protein spectral counts searched against Phaeocystis strain transcriptome from net tows during RVIB Nathaniel B. Palmer cruise NBP0601 in December of 2015.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 1) Version Date 2024-04-29 doi:10.26008/1912/bco-dmo.768237.1 [view at BCO-DMO] Relationship Description: Generated from the same sampling event and methodology. These data are part of the same dataset "Ross Sea Net Tow (Bender)" version 1 at the Ocean Protein Portal (https://proteinportal.whoi.edu/).

[ table of contents | back to top ]

Parameters

Parameter	Description	Units
sample_id	Sample identifier. Identifies the sample associated with this annotation	unitless
cruise_id	Cruise identifier	unitless
station_id	Station identifier where sample was taken	unitless
latitude_dd	Station latitude	decimal degrees (DD)
longitude_dd	Station longitude	decimal degrees (DD)
depth_m	Sample depth	meters (m)
date_local	Date (local) of sample collection in format YYYY-mm-dd. Time zone is Antarctica/McMurdo (NZST/NZDT, UTC+12/UTC+13)	unitless
time_local	Time (local) of sample collection in format HH:MM:SS. Time zone is Antarctica/McMurdo (NZST/NZDT, UTC+12/UTC+13)	unitless
minimum_filter_size_microns	Minimum size of the collection filter	microns (um)
maximum_filter_size_microns	Maximum size of the collection filter	microns (um)
peptide_sequence	Peptide genomic sequence	unitless
peptide_start_index	Start location of peptide within protein sequence	unitless
peptide_stop_index	Stop location of peptide within protein sequence	unitless
protein_molecular_weight_kDa	Molecular weight in kilo-Daltons of the related protein	kilo-Daltons (kDa)
protein_id	Identification parameter for protein sequence, typically shared with metagenomic database	unitless
spectral_count_sum	Sum of spectral counts (+2, +3, +4 ions)	unitless
other_protein_ids	Additional IDs from similar proteins that share peptide sequences	unitless
best_protein_id_probability	A percentage identifying the quality of the protein identification	unitless
best_sequest_DCn_score	Sequest DCn score	unitless
best_sequest_Xcorr_score	Sequest Xcorr	unitless
plus2H_spectra_count	Spectral counts of +2 ions	unitless
plus3H_spectra_count	Spectral counts of +3 ions	unitless
plus4H_spectra_count	Spectral counts of +4 ions	unitless
median_retention_time	Median retention time of peptide	unitless
total_precursor_intensity	Total precursor intensity (ms1) of peptide	unitless
TIC	Total ion current (TIC) value of peptide	unitless
absolute_units_fmol_L	Concentration of peptide in calibrated absolute units (fmol / L)	femtomoles per liter (fmol/L)
ISO_DateTime_UTC	Timestamp (UTC) in standard ISO 8601:2004(E) format YYYY- mm-ddTHH:MM:SSZ	unitless

[ table of contents | back to top ]

Instruments

Dataset- specific Instrument Name	Thermo Scientific Q-Exactive Orbitrap mass spectrometer with a Michrom Advance CaptiveSpray source
Generic Instrument Name	Mass Spectrometer
Generic Instrument Description	General term for instruments used to measure the mass-to-charge ratio of ions; generally used to find the composition of a sample by generating a mass spectrum representing the masses of sample components.

### [ table of contents | back to top ]

# Deployments

### NBP0601

Website	https://www.bco-dmo.org/deployment/57985	
Platform	RVIB Nathaniel B. Palmer	
Report	http://data.bco-dmo.org/CORSACS/cruises/Dunbar_Hydrography_report_NBP0601.pdf	
Start Date	2005-12-17	
End Date	2006-01-30	
Description	This was the first of two Controls of Ross Sea Algal Community Structure (CORSACS) project cruises and was funded by the NSF Office of Polar Programs. The NBP0601 cruise was conducted in the Ross Sea in December 2005 and January 2006, Ross Sea, ca. 65.21°S-78.65°S, 164.98°E-164.70°W, and supported by NSF research grant, OPP-0338097. The 'Science Pan and Project Description' document includes details of the cruise sampling strategy. Related Files: Science Plan and Project Descriptions (PDF file)Cruise track map (PDF file)Photo of Ice Breaker Nathaniel B. Palmer on station near Beaufort Island (JPG image) Related Sites: MGDS catalog: <a href="http://www.marine-geo.org/tools/search/entry.php?id=NBP0601">http://www.marine-geo.org/tools/search/entry.php?id=NBP0601</a>	

### [ table of contents | back to top ]

## **Project Information**

### Controls of Ross Sea Algal Community Structure (CORSACS)

Website: http://www.whoi.edu/sites/corsacs

**Coverage**: Ross Sea Southern Ocean

## **Project summary**

The Controls of Ross Sea Algal Community Structure (CORSACS) project was funded by the NSF Office of Polar Programs as "Collaborative Research: Interactive Effects of Iron, Light and Carbon Dioxide on Phytoplankton Community Dynamics in the Ross Sea". Two cruises were completed in 2006 to investigate the interactions between the primary productivity of the Ross Sea and pCO2, iron and other trace elements. Data sets of carbon, nutrient, metal, and biological measurements will be reported.

The main objective in the proposed research was to investigate the relative importance and potential interactive effects of iron, light and CO2 levels in structuring algal assemblages and growth rates in the Ross Sea. The investigators hypothesized that the interaction of these three variables largely determines the bottom-up control on these two dominant Southern Ocean phytoplankton taxa. While grazing and other loss processes

are important variables in determining the relative dominance of these two taxa, the CORSACS research project was designed to focus on the bottom-up control mechanisms. It is important to understand such environmentally-driven taxonomic shifts in primary production, since they are expected to impact the fixation and export of carbon and nutrients, and the production of DMS, thus potentially providing both positive and negative feedbacks on climate.

The CORSACS investigators considered a range of ambient iron, light and pCO2 levels that span those typically observed in the Ross Sea during the growing season. That is, dissolved iron ranging from ~0.1 nM (low iron) to greater than 1 nM (high iron) (Fitzwater et al. 2000; Sedwick et al. 2000); mean irradiance (resulting from vertical mixing/self shading) ranging from less than 10% Io (low light) to greater than 40% (high light) (Arrigo et al., 1998, 1999), possibly adjusted based on field observations during the CORSACS cruises; and pCO2 ranging (Sweeney et al. 2001) from ~150 ppm (low CO2) to the probable higher levels of pCO2 - 750 ppm as a conservative estimate - that are likely to be attained later this century due to anthropogenic perturbation of the global carbon cycle (IPCC, 2001).

From the information previously available from both field observations and experiments, the investigators formulated the following specific hypotheses regarding the interactive role of iron, light and CO2 in regulating algal composition in the Ross Sea: diatoms bloom in the southern Ross Sea only under optimum conditions of high iron, light and pCO2; colonial Phaeocystis dominate under conditions of high iron with either (or both) low light or low pCO2; and solitary Phaeocystis are predominant under conditions of low iron with either (or both) low light or low pCO2.

### **References:**

Fitzwater, S.E., K.S. Johnson, R.M. Gordon, K.H. Coale, and W.O. Smith, Jr. (2000). Trace metal concentrations in the Ross Sea and their relationship with nutrients and growth. Deep-Sea Research II, 47: 3159-3179.

Martin JH, Gordon RM, Fitzwater SE. Iron in Antarctic waters. Nature 1990 ;345(6271):156-158. Martin JH. 1990. Glacial-interglacial CO2 change: The iron hypothesis. Paleoceanography 5(1):1-13

P. N. Sedwick, G. R. DiTullio, and D. J. Mackey, Iron and manganese in the Ross Sea, Antarctica: Seasonal iron limitation in Antarctic shelf waters, Journal of Geophysical Research, 105 (C5), 11,321-11,336, 2000.

Sweeney, C. K. Arrigo, and G. van Gijken (2001). Prediction of seasonal changes in surface pCO2 in the Ross Sea, Antarctica using ocean color satellite data. 2001 Annual AGU meeting, San Fransisco, CA Dec. 10-15.

IPCC, 2001: Climate Change 2001: Synthesis Report. A Contribution of Working Groups I, II, and III to the Third Assessment Report of theIntegovernmental Panel on Climate Change [Watson, R.T. and the Core Writing Team (eds.)]. Cambridge University Press, Cambridge,United Kingdom, and New York, NY, USA, 398 pp.

### Publications

Saito, M. A., Goepfert, T. J., Noble, A. E., Bertrand, E. M., Sedwick, P. N., and DiTullio, G. R.: A seasonal study of dissolved cobalt in the Ross Sea, Antarctica: micronutrient behavior, absence of scavenging, and relationships with Zn, Cd, and P, Biogeosciences, 7, 4059-4082, doi:10.5194/bg-7-4059-2010, 2010 (http://www.biogeosciences.net/7/4059/2010/bg-7-4059-2010.html)

Bertrand EM, Saito MA, Lee PA, Dunbar RB, Sedwick PN and DiTullio GR (2011) Iron limitation of a springtime bacterial and phytoplankton community in the Ross Sea: implications for vitamin B12 nutrition. Front. Microbio. 2:160. doi: 10.3389/fmicb.2011.00160 (http://www.frontiersin.org/Aquatic Microbiology/10.3389/fmicb.2011.00160/abstract)

[ table of contents | back to top ]

### **Program Information**

### Ocean Carbon and Biogeochemistry (OCB)

Website: http://us-ocb.org/

Coverage: Global

The Ocean Carbon and Biogeochemistry (OCB) program focuses on the ocean's role as a component of the global Earth system, bringing together research in geochemistry, ocean physics, and ecology that inform on and advance our understanding of ocean biogeochemistry. The overall program goals are to promote, plan, and coordinate collaborative, multidisciplinary research opportunities within the U.S. research community and with international partners. Important OCB-related activities currently include: the Ocean Carbon and Climate Change (OCCC) and the North American Carbon Program (NACP); U.S. contributions to IMBER, SOLAS, CARBOOCEAN; and numerous U.S. single-investigator and medium-size research projects funded by U.S. federal agencies including NASA, NOAA, and NSF.

The scientific mission of OCB is to study the evolving role of the ocean in the global carbon cycle, in the face of environmental variability and change through studies of marine biogeochemical cycles and associated ecosystems.

The overarching OCB science themes include improved understanding and prediction of: 1) oceanic uptake and release of atmospheric CO2 and other greenhouse gases and 2) environmental sensitivities of biogeochemical cycles, marine ecosystems, and interactions between the two.

The OCB Research Priorities (updated January 2012) include: ocean acidification; terrestrial/coastal carbon fluxes and exchanges; climate sensitivities of and change in ecosystem structure and associated impacts on biogeochemical cycles; mesopelagic ecological and biogeochemical interactions; benthic-pelagic feedbacks on biogeochemical cycles; ocean carbon uptake and storage; and expanding low-oxygen conditions in the coastal and open oceans.

### [ table of contents | back to top ]

### Funding

Funding Source	Award
NSF Office of Polar Programs (formerly NSF PLR) (NSF OPP)	<u>OPP-0338097</u>

[ table of contents | back to top ]