## Total spectral counts of peptides from the R/V Falkor cruise 160115 in the Central Pacific for the ProteOMZ expedition in 2016.

Website: https://www.bco-dmo.org/dataset/737596 Data Type: Cruise Results Version: 1 Version Date: 2018-05-25

#### Project

» <u>The ProteOMZ Expedition: Investigating Life Without Oxygen in the Pacific Ocean</u> (ProteOMZ (Proteomics in an Oxygen Minimum Zone))

Contributors	Affiliation	Role
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#### Abstract

Relative protein abundance data of the upper 1000m water column from the ProteOMZ R/V Falkor expedition. There are 109952 unique peptides, each with spectral counts associated with each of the 103 samples, for 10 million data points.

## **Table of Contents**

- <u>Coverage</u>
- Dataset Description
  - Data Processing Description
  - BCO-DMO Processing Description
- <u>Related Datasets</u>
- Parameters
- Instruments
- Deployments
- Project Information
- Funding

#### Coverage

**Spatial Extent**: N:17.4465 **E**:-139.1089 **S**:-0.4708 **W**:-157.3022 **Temporal Extent**: 2016-01-19 - 2016-01-28

## **Dataset Description**

These data are part of the Ocean Protein Portal "ProteOMZ" dataset (<u>https://proteinportal.whoi.edu/;</u> Saito et al., 2019).

#### **Data Processing Description**

The raw mass spectra files were searched against SEQUEST within Proteome Discoverer v2.2 software. Processed files were then loaded into Proteome Software and protein and peptide reports as well as and fasta files were exported. The files were modified slightly to map to the Protein Portal data model for submission to BCO-DMO. The peptide report was too large to work with within Excel and was modified in Pandas/Python to produce a CSV file.

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

-Date, time, filter min, filter max, lat, lon, and cruise columns added based on information from the Falkor 160115 Event log and CTD log. -Column names reformatted to comply with BCO-DMO standards.

[ table of contents | back to top ]

## **Related Datasets**

#### IsSupplementTo

Saito, M. A. (2018) **Total spectral count of proteins from R/V Falkor cruise 160115 for the ProteOMZ expedition in the Central Pacific in 2016.** Biological and Chemical Oceanography Data Management Office (BCO-DMO). (Version 3) Version Date 2018-12-10 http://lod.bcodmo.org/id/dataset/737620 [view at BCO-DMO]

[ table of contents | back to top ]

#### **Parameters**

Parameter	Description	Units
cruise	Cruise deployment ID	unitless
station	Station number	unitless
Depth	Depth of sampling	meters
date	Date of sampling; yyyy/mm/dd	unitless
time	Time of sampling; hh:mm	unitless
lon	Longitude	decimal degrees
lat	Latitude	decimal degrees
min_filter_size	Minimum filter size	microns
max_filter_size	Maximum filter size	microns
MS_MS_sample_name	RAW file name; crossreferences to proteomexchange or OPP repository	unitless
Protein_ID	Metagenome ID; needed to map to protein IDs.	unitless
Protein_accession_numbers	Duplicate of Protein ID but can contain multiple entries.	unitless
Protein_molecular_weight	Protein molecular weight	kDa
Peptide_sequence	Unique Peptide sequence; this is the most unique identifier	unitless
Best_Peptide_identification_probability	Metric of peptide quality	unitless
Best_SEQUEST_XCorr_score	Metric of peptide quality	unitless
Best_SEQUEST_DCn_score	Metric of peptide quality	unitless
Number_of_identified_2H_spectra	Count of +2H spectra	count
Number_of_identified_3H_spectra	Count of +3H spectra	count
Number_of_identified_4H_spectra	Count of +4H spectra	count
SUM_Spectral_Counts	Sum of +2 +3 +4 data = total unnormalized spectral counts; Quantitative Value	count
Median_Retention_Time	Median retention time	minutes
Total_Precursor_Intensity	Quantitative Value (2 of 3)	unitless
Total_TIC	Quantitative Value (3 of 3)	unitless
Peptide_start_index	Data useful in creating peptide coverage map for WHO page	unitless
Peptide_stop_index	Data useful in creating peptide coverage map for WHO page	unitless
ISO_DateTime_UTC	DateTime UTC ISO formatted	unitless

[ table of contents | back to top ]

## Instruments

Dataset- specific Instrument Name	Alpkem Autosampler
Generic Instrument Name	Alpkem RFA300
Dataset- specific Description	Used in nutrient analysis
	A rapid flow analyser (RFA) that may be used to measure nutrient concentrations in seawater. It is an air-segmented, continuous flow instrument comprising a sampler, a peristaltic pump which simultaneously pumps samples, reagents and air bubbles through the system, analytical cartridge, heating bath, colorimeter, data station, and printer. The RFA-300 was a precursor to the smaller Alpkem RFA/2 (also RFA II or RFA-2).

Dataset- specific Instrument Name	SeaBird SBE19 CTD
Generic Instrument Name	CTD Sea-Bird
Dataset- specific Description	Used for water sampling
Generic Instrument Description	Conductivity, Temperature, Depth (CTD) sensor package from SeaBird Electronics, no specific unit identified. This instrument designation is used when specific make and model are not known. See also other SeaBird instruments listed under CTD. More information from Sea-Bird Electronics.

Dataset- specific Instrument Name	Technicon AutoAnalyzer II
Generic Instrument Name	Technicon AutoAnalyzer II
Dataset- specific Description	Used to measure phosphate and ammonium
Generic Instrument Description	A rapid flow analyzer that may be used to measure nutrient concentrations in seawater. It is a continuous segmented flow instrument consisting of a sampler, peristaltic pump, analytical cartridge, heating bath, and colorimeter. See more information about this instrument from the manufacturer.

Dataset-specific Instrument Name	Trace Metal Rosette
Generic Instrument Name	Trace Metal Bottle
<b>Dataset-specific Description</b>	Used for nutrient sampling
Generic Instrument Description	Trace metal (TM) clean rosette bottle used for collecting trace metal clean seawater samples.

## Deployments

#### FK160115

Website	https://www.bco-dmo.org/deployment/708387
Platform	R/V Falkor
Report	https://service.rvdata.us/data/cruise/FK160115/doc/FK160115_OfficialCruiseReport_Saito_v3.pdf
Start Date	2016-01-16
End Date	2016-02-11
Description	Project: Using Proteomics to Understand Oxygen Minimum Zones (ProteOMZ) More information is available from the ship operator at <u>https://schmidtocean.org/cruise/investigating-life-without- oxygen-in-the</u> Additional cruise information is available from the Rolling Deck to Repository (R2R): <u>https://www.rvdata.us/search/cruise/FK160115</u>

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

## **Project Information**

# The ProteOMZ Expedition: Investigating Life Without Oxygen in the Pacific Ocean (ProteOMZ (Proteomics in an Oxygen Minimum Zone))

Website: <u>https://schmidtocean.org/cruise/investigating-life-without-oxygen-in-the-tropical-pacific/#team</u>

Coverage: Central Pacific Ocean (Hawaii to Tahiti)

From Schmidt Ocean Institute's ProteOMZ Project page:

Rising temperatures, ocean acidification, and overfishing have now gained widespread notoriety as humancaused phenomena that are changing our seas. In recent years, scientists have increasingly recognized that there is yet another ingredient in that deleterious mix: a process called deoxygenation that results in less oxygen available in our seas.

Large-scale ocean circulation naturally results in low-oxygen areas of the ocean called oxygen deficient zones (ODZs). The cycling of carbon and nutrients – the foundation of marine life, called biogeochemistry – is fundamentally different in ODZs than in oxygen-rich areas. Because researchers think deoxygenation will greatly expand the total area of ODZs over the next 100 years, studying how these areas function now is important in predicting and understanding the oceans of the future. This first expedition of 2016 led by Dr. Mak Saito from the Woods Hole Oceanographic Institution (WHOI) along with scientists from University of Maryland Center for Environmental Science, University of California Santa Cruz, and University of Washington aimed to do just that, investigate ODZs.

During the 28 day voyage named "ProteOMZ," researchers aboard R/V *Falkor* traveled from Honolulu, Hawaii to Tahiti to describe the biogeochemical processes that occur within this particular swath of the ocean's ODZs. By doing so, they contributed to our greater understanding of ODZs, gathered a database of baseline measurements to which future measurements can be compared, and established a new methodology that could be used in future research on these expanding ODZs.

[ table of contents | back to top ]

## Funding

Funding Source	Award
Gordon and Betty Moore Foundation: Marine Microbiology Initiative (MMI)	<u>GBMF3782</u>
Schmidt Ocean Institute (SOI)	<u>R/V Falkor 160115 SOI ProteOMZ</u> Expedition

[ table of contents | back to top ]