

# Proteomic data of dilution series of bacteria and diatoms using MS.

**Website:** <https://www.bco-dmo.org/dataset/719080>

**Data Type:** experimental

**Version:**

**Version Date:** 2017-11-13

## Project

» [Collaborative Research: Proteins as functional biomarkers: integrating organic characterization with proteomics to track routes for carbon and nitrogen recycling and preservation](#) (Proteins as Biomarkers)

Contributors	Affiliation	Role
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## Dataset Description

To mimic a complex marine sample, a dilution series of *R. pomeroyi* and *T. pseudonana* was created at different cellular ratios. These mixtures were filtered and proteins were extracted from the filter for tryptic digestion and LC-MS/MS analysis.

Biological fractions were lysed, digested and analyzed using proteomic mass spectrometry.

Data are available for download at the EBI PRIDE Archive.

Homepage: <https://www.ebi.ac.uk/pride/archive>

Project URL: <https://www.ebi.ac.uk/pride/archive/projects/PXD004758>

Data URL: <https://www.ebi.ac.uk/pride/archive/projects/PXD004758/files>

## Methods & Sampling

Peptide samples were spiked with a quality control mix of PRTC-BSA peptides and 2 ul containing 1 ug of protein was injected on a 27 cm column (C18 beads) and 3 cm trap (C18). Data were collected in 4 m/z isolation width windows in 125 m/z ranges (400-525, 525-650, 650-775, 775-900). For each method, a gradient of 5-80% acetonitrile over 90 minutes was applied for peptide spectra acquisition on a Q-Exactive-HF.

Instrument(s): QExactive Thermo Finnegan

## Data Processing Description

In order to generate spectral libraries for targeted method development, Peptide Centric Analysis was completed with the software PECAN (Ting et al., 2015). Input files included the list of peptides generated for targeted proteomics and the mzML files generated from raw DIA files using MSConvert. PECAN correlates a list of peptide sequences of interest with the acquired DIA spectra in order to locate the peptide-specific spectra within the acquired DIA dataset. The PECAN .blib output file was then imported into Skyline daily for targeted method development. The selected reaction monitoring dataset is published in PeptideAtlas under Accession number PASS00917.

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## Data Files

File
<b>Bacterial_detection_Timmins.csv</b> (Comma Separated Values (.csv), 193 bytes) MD5:71ff326f3478ae0fb4a045d4bd1ebb17
Primary data file for dataset ID 719080

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## Parameters

Parameter	Description	Units
Repository	Name of database where data are currently served	unitless
Project	Unique project identifier for the database where data are currently served	unitless
Project_URL	Link to project page at the database where data are currently served	unitless

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## Instruments

<b>Dataset-specific Instrument Name</b>	QExactive Thermo Finnegan
<b>Generic Instrument Name</b>	Mass Spectrometer
<b>Generic Instrument Description</b>	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.

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## Project Information

## **Collaborative Research: Proteins as functional biomarkers: integrating organic characterization with proteomics to track routes for carbon and nitrogen recycling and preservation (Proteins as Biomarkers)**

**Coverage:** Multiple locations: Canadian and US Beaufort Sea

### NSF Award Abstract:

Proteins are a major contributor to organic carbon and nitrogen in the ocean and their amino acid building blocks comprise a major fraction of the total nitrogen identified in coastal and oceanic waters and sediments. Over the last decade, tandem mass spectrometry methods developed for the analysis of peptides and protein reconstruction together with informatics developments have re-assembled the amino acid signatures and unlocked the information inherent in the proteins they represent. This interdisciplinary research team has the combined expertise in marine organic biogeochemistry, proteomics, and bioinformatics to help determine the fate of individual proteins during degradation and likely mechanisms for their preservation. This research aims to identify and quantify the proteins responsible for chemical transformations of organic matter in the ocean, thereby exposing how microbial communities control and contribute to the carbon and nitrogen cycle and to organic matter preservation. This project has the potential to trigger a fundamental change in how we view, analyze, and model microbial degradation processes.

Recent findings from microbial ecologists show that bacteria with broad responses to various nutrients (i.e. the generalists) can fine-tune the gene expression of various proteins as a reflection of substrate availability; the proponents of this project have observed a suite of bacterial proteins present during organic matter recycling and that this protein expression changes as degradation proceeds. These observations hint that bacterial proteins have potential as organic biomarkers to reflect the taxonomic distribution of the functioning catalysts in degradation processes. The investigators propose to build on these results to investigate the potential for organic matter preservation to be linked to proteomic expression of the microbial community that drive carbon and nitrogen cycling. The project objectives are: 1) to address the relationship between marine organic matter composition and protein expression by the bacterial community (metaproteome) which act as catalysts for degradation; 2) to detail protein expression in the context of detailed organic matter characterization and 3) to distinguish how proteins present in oceanic sediments derived from different kingdoms of life (e.g. eukaryotic or bacterial) reflect the complex process of organic matter preservation. The overall goal is to capture proteins as critical markers of both presence and process in marine systems. The investigators will link the rapid advances in protein identification to track bacterial proteins to act as "functional biomarkers" and indicators of carbon and nitrogen utilization.

The project would provide multiple opportunities for interdisciplinary student training in marine geochemistry and proteomics, and address the goal of disseminating results and tools to a broad audience. In the more traditional role, the project will expand the career for a female research faculty member in marine proteomics and support both graduate and undergraduate student research at each participating institution. On the broader community level, both Harvey and Nunn are also heavily involved in high school outreach programs.

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## **Funding**

<b>Funding Source</b>	<b>Award</b>
<a href="#">NSF Division of Ocean Sciences (NSF OCE)</a>	<a href="#">OCE-1633939</a>

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