Nutrients, targeted proteomics, and pigments from the METZYME cruise (KM1128)

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Data Type: Cruise Results
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Project
» Connecting Trace Elements and Metalloenzymes Across Marine Biogeochemical Gradients (GPc03) (MetZyme)

Program
» U.S. GEOTRACES (U.S. GEOTRACES)

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Coverage

Spatial Extent: **N**:17 **E**:205.6 **S**:-15 **W**:185.5
Temporal Extent: 2011-10-03 - 2011-10-24

Dataset Description

This dataset includes data from 3 sampling systems:
- Macronutrients from the trace metal rosette (TMR); analyzed by Joe Jennings at OSU.
- Targeted metaproteomics from the McLane pumps; analyzed by triple quadrupole mass spectrometry calibrated with stable isotope labeled peptides.
- Pigments from a combination of CTD and TMR samples; determined by HPLC; analyzed by Jack DiTullio, University of Charleston. Note that pigments were collected by both CTD and TMR due to a loss of the CTD as station 2/3.

Samples were collected during the KM1128 METZYME research expedition (Metals and Enzymes in the Pacific) on the R/V *Kilo Moana* October 1-25, 2011 from Oahu, Hawaii to Apia, Samoa.

01 Aug 2017: dataset was revised to include columns for date/time and cast numbers for each sampling system.

Related publications:

Saito, M. A., M. R. McIlvin, D. M. Moran, T. J. Goepfert, G. R. DiTullio, A. F. Post, and C. H. Lamborg. 2014. Multiple nutrient stresses at intersecting Pacific Ocean biomes detected by protein biomarkers. *Science* 345:1173-1177. DOI: 10.1126/science.1256450

Saito, M. A.; Dorsk, A.; Post, A. F.; McIlvin, M.; Rappé, M. S.; DiTullio, G.; Moran, D. 2015. Needles in the Blue Sea: Sub-Species Specificity in Targeted Protein Biomarker Analyses Within the Vast Oceanic Microbial Metaproteome. *Proteomics.* DOI: 10.1002/pmic.201400630

Methods & Sampling

The methods are provided in the supplemental from the Saito et al., 2014 paper. Relevant sections are duplicated here:

Research Expedition and Sample Collection

Samples were collected during the KM1128 METZYME research expedition (Metals and Enzymes in the Pacific) on the R/V *Kilo Moana* October 1-25, 2011 from Oahu, Hawaii to Apia, Samoa, with Carl Lamborg and Mak Saito as Chief Scientists. Microbial biomass for protein analyses was collected on vertical profiles using *in situ* high volume particle filtration pumps with a focus on the North Pacific and Equatorial regions (Table S1). Specifically, the protein samples were collected by a suite of 4 L/min and 8 L/min McLane Pumps (WTS-LV; McLane Research Laboratories Inc., Falmouth MA, USA) outfitted with custom Mini-MULVS multiple filter head systems. The 0.2-3.0 micron size fraction was collected on 142 mm filters (Supor, Pall Corp.) for analyses used in this study. The volume of water was pumped until a minimal flow rate was achieved or the allotted cast time period expired, typically ~300-500 L. Filters were sectioned immediately after pump retrieval, and protein samples (¼ filter) were stored in RNAlater reagent (Ambion, Life Technologies), which has been shown to be an effective preservative for cyanobacterial biomass (Saito et al. 2011a), frozen at -80 degrees C, transported back to the laboratory on dry ice, and stored at -80 degrees C until analysis.

Dissolved trace metal samples (iron and cobalt) were collected by an internally programmed standard SBE Rosette (Seabird Electronics Inc.) user-modified to serve as a trace metal clean system with 12 8 L X-Niskin bottles (Ocean Test Equipment), 12 X-Niskin bottles were attached to the rosette per deployment) with minimal exposed metal surfaces using 5000 m of non-metallic non-conducting line. Temperature, oxygen and conductivity sensor data were collected using a SBE19*plus*V2 system (Seabird Electronics Inc.) attached to a CTD extension stand on the Trace Metal Rosette. All sensors were factory calibrated immediately prior to the expedition. X-Niskins were pressurized with ultra-high purity nitrogen gas and seawater was filtered through cleaned 47 mm 0.2 micron Supor membrane filters within a HEPA filtered cleanroom space aboard the ship. The volume filtered was calculated (X-Niskin volume minus small unfiltered samples) and the filters were stored in cleaned tubes and frozen for particulate metal analysis (see below).

Protein Extraction

Total microbial protein (0.2-3.0 um fraction) was extracted using detergent-based methods, described below. Total protein showed enhanced concentrations in the photic zone, particularly in the Equatorial and South Pacific portions of the transect (Fig. S1F). For protein extraction, samples were thawed and the filter and RNAlater preservative (Ambion Life Technologies) were separated. The removed preservative was spin-concentrated by a 5K MWCO membrane (Sartorius Stedim Biotech 6 mL, 5 K MWCO Vivaspin units; Goettingen, Germany), and rinsed with 0.1M Tris buffer to recover, desalt, and concentrate any suspended material. The sample filter was unfolded and placed in a larger tube to which 1% SDS extraction buffer (1% SDS, 0.1M Tris/HCL pH 7.5, 10mM EDTA) and the rinsed/desalted RNAlater fraction was added back. Each sample was incubated at room temperature for 15 minutes, heated at 95 degrees C for 10 minutes, and shaken at room temperature for 350 rpm for 1 h. The protein extract was decanted and placed in a new tube and centrifuged for 30 min x 3220 g at room temperature. The supernatants were removed and filtered through a 5 um low protein binding syringe filter (Fisher Scientific), and the filter rinsed with extraction buffer. The extracts were concentrated by 5 kD membrane centrifugation to a small volume, washed with extraction buffer, and concentrated again. Each sample was precipitated with cold 50% methanol (MeOH) 50% acetone 0.5 mM HCL for 3 days at –20 degrees C, centrifuged at 14100 x g (14500 rpm) for 30 m at 4 degrees C, decanted and dried by vacuum concentration (Thermo Savant Speedvac) for 10 min or until dry. Pellets were resuspended in 1% SDS extraction buffer and left at room temperature (RT) for 1 h to redissolve. Total protein was quantified (Bio-Rad DC protein assay, Hercules, CA) with BSA as a standard.

Extracted proteins were purified from SDS detergent, reduced, alkylated, and trypsin digested, while embedded within a polyacrylamide tube gel, using a modified protocol from a previously published method (Lu et al. 2005). The tube gel approach allowed all proteins including membrane proteins to be solubilized by detergent and purified while immobilized in the gel matrix. A gel premix was made by combining 1 M Tris HCL (pH 7.5) and 40% Bis-acrylimide L 29:1 (Acros Organics) at a ratio of 1:3. The premix (103 ul) was combined with an extracted protein sample (usually 25 ug-200 ug), TE, 7 ul 1% APS and 3 ul of TEMED (Acros Organics) to a final volume of 200 ul. After 1 h of polymerization at RT, 200 ul of gel fix solution (50% ETOH, 10% acetic

acid in LC/MS grade water) was added to the top of the gel and incubated at RT for 20 minutes. Liquid was then removed and the tube gel was transferred into a new 1.5 mL microtube containing 1.2 mL of gel fix solution then incubated at room temperature, 350 rpm in a Thermomixer R (Eppendorf) for 1 h. Gel fix solution was then removed and replaced with 1.2 mL destain solution (50% MeOH, 10% acetic acid in H2O) and incubated at 350 rpm, RT for 2 h. Liquid was then removed, gel cut up into 1 mm cubes and then added back to tubes containing 1 mL of 50:50 acetonitrile:25 mM ammonium bicarbonate (ambic) incubated for 1 h, 350 rpm, and at RT. Liquid was removed and replaced with fresh 50:50 acetonitrile:ambic and incubated at 16 degrees C and 350 rpm overnight. The step was repeated for 1h the following morning. Gel pieces were then dehydrated twice in 800 ul of acetonitrile for 10 min at RT and dried for 10 min in a ThermoSavant DNA110 speedvac after removing solvent. 600 ul of 10 mM DTT in 25 mM ambic was added to reduce proteins incubating at 56 degrees C, 350 rpm for 1 h. Unabsorbed DTT solution was then removed with volume measured. Gel pieces were washed with 25 mM ambic and 600 ul of 55 mM iodacetamide was added to alkylate proteins at RT, 350 rpm for 1 h. Gel cubes were then washed with 1 mL ambic for 20 minutes, 350 rpm at RT. Acetonitrile dehydrations and speedvac drying were repeated as above. Trypsin (Promega #V5280) was added in appropriate volume of 25 mM ambic to rehydrate and submerse gel pieces at a concentration of 1:20 ug trypsin:protein. Proteins were digested overnight at 350 rpm 37 degrees C. Unabsorbed solution was removed and transferred to a new tube. 50 ul of peptide extraction buffer (50% acetonitrile, 5% formic acid in water) was added to gels, incubated for 20 min at RT then centrifuged at 14,100 x g for 2 min. Supernatant was collected and combined with unabsorbed solution. The above peptide extraction step was repeated combining all supernatants. Combined protein extracts were centrifuged at 14,100 x g for 20 minutes, and supernatants transferred into a new tube and dehydrated down to approximately 10 ul-20 ul in the speedvac. Concentrated peptides were then diluted in 2% acetonitrile 0.1% formic acid in water for storage until analysis. All water used in the tube gel digestion protocol was LC/MS grade, and all plastic microtubes were ethanol rinsed and dried prior to use.

Targeted Protein Analyses

Biomarkers selected for this study focused on trypsin-digested peptide fragments of the proteins (tryptic peptides) that were frequently identified in metaproteome analyses with reproducible mass spectra fragmentation patterns to allow for targeted analyses by triple quadrupole mass spectrometry (Fig. S3-4). The specificity of these tryptic peptide biomarkers was determined by searching for their sequences within sequenced microbial genomes and gene databases (Fig. S9-S14). Absolute quantitation of proteins was conducted by triple quadrupole mass spectrometry using a Thermo Vantage mass spectrometer and synthetic isotope labeled peptide standards as described previously (Bertrand et al. 2013; Saito et al. 2011b). Selected peptides were chosen with an effort to minimize presence of methionines and cysteines both of which can be oxidized and create variability in analyses (Lange et al. 2008, Stahl-Zeng et al. 2007). However, in some cases tryptic peptides were identified in the metaproteome than included these amino acid residues (Peptides IDs 31and 144) with few alternatives peptides corresponding to the protein of interest. Mass spectrometry conditions were optimized for each peptide (collision energy and S-lens), and analyzed using chromatographic scheduling to increase the multiplexing capabilities and resolution for each peptide analyte. These peptide sequences and optimization conditions are presented in Table S3 (PDF). Peptide abundances were calculated as a peak ratio of the corresponding isotopically labeled internal standard. Each internal standard was examined for its linear performance on the mass spectrometer using standard curves (Figure S17). Isotopically labeled standards were obtained from JPT Peptide Technologies, which contain a C-terminal peptide tag. The tag was released by tryptic digestion prior to analysis following the manufacturer's protocol. Chromatographic separation and mass spectrometry were performed using a Paradigm MS4 HPLC (Michrom Bioresources) coupled to a Thermo Vantage TSQ mass spectrometer (Thermo Scientific) via an Advance capillary electrospray source (Michrom Bioresources). Samples were loaded on a peptide CapTrap prior to separation on a Magic C18AQ column (0.2 x 50 mm, 3 mm particle size, 200 Å pore size, Michrom Bioresources). Chromatographic separation was done with a 45 min gradient of 5% to 35% buffer B (where buffer A was 0.1% formic acid in water, Fisher Optima and buffer B was 0.1% formic acid in acetonitrile, Fisher Optima) at 4 mL/min. Examples of methodological precision are shown in Figure S18 for triplicate analyses of two Station 6 samples.

Pigment and Nutrient Analyses

Nutrient analyses were conducted by nutrient autoanalyzer by Joe Jennings at Oregon State University as previously described (Noble et al. 2012). HPLC: Seawater samples (4 L) were filtered onto glass fibre filters (Whatman GF/F) and stored in liquid nitrogen until analysis. Samples were analyzed on an Agilent 1100 HPLC (High Performance Liquid Chromatography) system with diode array and fluorescence detection. Elution gradient and protocols were described in detail elsewhere (DiTullio et al. 2003).

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Data Processing Description

For targeted protein values, protein concentrations in fmol / microgram total protein were converted to fmol / liter seawater filtered by multiplying by the total protein extraction and dividing by the McLane pump volume filtered (per ¼ filter extracted).

BCO-DMO Processing:
- modified parameter names to conform with BCO-DMO naming conventions;
- replaced #N/A and blanks (missing data) with "nd" ("no data");
- corrected year from 0011 to 2011 in original Excel file;
- 01 Aug 2017: dataset was revised to include columns for date/time and cast numbers for each sampling system; names of the targeted metaproteomics were changed to conform with the recommended BioGeotraces naming conventions.
- 24 May 2018: made correction to a parameter name; changed "PEP_NEAVENDLIVDNK_UDP_sulfoquin_Pro_PUMP" to "PEP_NEAVE0LIVDNK_UDP_sulfoquin_Pro_PUMP" per request of PI.

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Data Files

File	
nutrients_metaproteome.csv	(Comma Separated Values (.csv), 71.00 KB) MD5:365fabfeb49ffe373b2d3897fbeb6526
Primary data file for dataset ID 646115	

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Parameters

Parameter	Description	Units
cruise	Cruise identifier.	unitless
station	Station identifier.	unitless
lon	Longitude in decimal degrees east.	decimal degrees
lat	Latitude in decimal degrees; negative values indicate south.	decimal degrees
depth	Sampling depth.	meters
Nuts_TMR_cast	Trace metal rosette (TMR) cast number; nutrients came from TMR samples.	unitless
Nuts_TMR_time_local	Date and time of the Nuts_TMR_cast; formatted as yyyy-mm-ddTHH:MM (where T indicates the start of the time string); times are reported in the local time zone.	unitless
McLane_cast	McLane pump cast number; proteins came from McLane samples.	unitless
McLane_time_local	Date and time of the McLane_cast; formatted as yyyy-mm-ddTHH:MM (where T indicates the start of the time string); times are reported in the local time zone.	unitless
Pigment_cast	Cast number identifying the cast from which pigments were sampled (either CTD or TMR)	unitless
Pigment_time_local	Date and time of the Pigment_cast; formatted as yyyy-mm-ddTHH:MM (where T indicates the start of the time string); times are reported in the local time zone.	unitless
PO4	Phosphate (PO4).	micromoles per liter (uM)

NO2_NO3	Nitrite + nitrate (NO2 + NO3).	micromoles per liter (uM)
silicate	Silicate.	micromoles per liter (uM)
NO2	Nitrite (NO2).	micromoles per liter (uM)
NH4	Ammonium (NH4).	micromoles per liter (uM)
O2	Oxygen (O2).	micromles per kilogram (umol / kg)
NO3	Nitrate (NO3).	micromoles per liter (uM)
protein	Total extracted protein 0.2 - 3.0 micron size fraction.	micrograms per liter (ug/L)
PEP_VAAEAVLSMTK_NiSOD_ProSyn_PUMP	Targeted peptide biomarker: Nickel-containing superoxide dismutase [Synechococcus sp. WH 8102]. The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named NiSOD_25 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_SPYNQSLVANQIVNK_IdiA_Pro_PUMP	Targeted peptide biomarker: Iron ABC transporter, substrate binding protein (IdiA) [Prochlorococcus marinus MIT 9515]. The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named idiA_27 in earlier version of this dataset).	femtomoles per liter (fmol/L)

PEP_LHNFISSAESPK_Fld_Pro_PUMP	Targeted peptide biomarker: Flavodoxin [Prochlorococcus marinus MIT 9515]. The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named Fld_30 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_AGADMVGYVDK_Fld_Pro_PUMP	Targeted peptide biomarker: Flavodoxin [Prochlorococcus marinus MIT 9515]. The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named Fld_31 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_TVGIYYATTTGK_Fld_Pro_PUMP	Targeted peptide biomarker: Flavodoxin [Prochlorococcus marinus MIT 9515]. The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named Fld_32 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_VNSVIDAIAEAAK_P_II_glnB_glnK_Pro_PUMP	Targeted peptide biomarker: Nitrogen Regulatory Protein P-II glnB glnK. The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named NRP_34 in earlier version of this dataset.)	femtomoles per liter (fmol/L)

PEP_LSHQAIAEAIGSTR_NtcA_Cyano_PUMP	Targeted peptide biomarker: Nitrogen Regulatory Protein NtcA. The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named NtcA_35 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_SKLEDDPANPELILTAR_PhoP_Syn_PUMP	Targeted peptide biomarker: Two Component Phosphate Regulator PhoP [Synechococcus WH8109] (45% Identity to Bacillus subtilis PY79 PhoP). The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named PhoP_38 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_LIDQDGVPVVFGGWTSASR_UreaTran_Pro_PUMP	Targeted peptide biomarker: Urea ABC transporter, substrate binding protein [Prochlorococcus marinus MIT 9215].The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named UreaT_39 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_VVGEDYLPLGNTEVAPIISK_UreaTran_Pro_PUMP	Targeted peptide biomarker: Urea ABC transporter, substrate binding protein [Prochlorococcus marinus MIT 9215]. The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named UreaT_41 in earlier version of this dataset.)	femtomoles per liter (fmol/L)

PEP_IEYIVEDGASDWPTFAEK_UreaTran_ProSyn_PUMP	Targeted peptide biomarker: Urea ABC transporter (Pro and Syn). The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named UreaT_42 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_IPEDIAFAESR_UreC_Pro_PUMP	Targeted peptide biomarker: Urease Alpha subunit UreC (Prochlorococcus). The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named UreaA_118 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_VGVAGPVGSGK_UreG_Pro_PUMP	Targeted peptide biomarker: Urease UreG (Prochlorococcus). The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named UreG_122 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_FDYDGDYGTVLNR_UDP_sulfoquin_m_taxa_PUMP	Targeted peptide biomarker: sulfolipid (UDP-sulfoquinovose). The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named Sulfo_132 in earlier version of this dataset.)	femtomoles per liter (fmol/L)

PEP_NEAVE0LIVDNK_UDP_sulfoquin_Pro_PUMP	Targeted peptide biomarker: sulfolipid (UDP-sulfoquinovose). The letters correspond to abbreviations while the numbers are unique internal identifiers to differentiate sequences. Refer to Table S3 for more information, including the sequence. (Parameter named Sulfo_134 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_EAYPDFASAK_NH4_transporter_Pro_PUMP	Targeted peptide biomarker: Ammonium transporter [Prochlorococcus MIT9312]. The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named NH4_T_135 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_FDSLINSADNVMTYK_Glut_synt_Pro_PUMP	Targeted peptide biomarker: Glutamine synthetase, glutamate--ammonia ligase [Prochlorococcus marinus MIT 9215]. The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named GS_144 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_EGYFPVSPNDTAQDIR_Glut_synt_Pro_PUMP	Targeted peptide biomarker: Glutamine synthetase, glutamate--ammonia ligase [Prochlorococcus marinus MIT 9215]. The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named GS_145 in earlier version of this dataset.)	femtomoles per liter (fmol/L)

PEP_HAPSFLAFTNPTTNSYK_Glut_synt_ProSyn_PUMP	Targeted peptide biomarker: Glutamine synthetase, glutamate--ammonia ligase [Synechococcus sp. RS9916]. The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named GS_Syn_146 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PEP_VASLTGADINYLPNPR_UDP_sulfoquin_Pro_PUMP	Targeted peptide biomarker: sulfolipid (UDP-sulfoquinovose). The 5-part naming convention is as follows: (1) analysis type (e.g. PEP); (2) peptide sequence; (3) targeted peptide sequence name; (4) Targeted peptide within specified genus/species (note that this is only specified in some targeted peptides); (5) sampling system (e.g. PUMP). (Parameter named Sulfo_171 in earlier version of this dataset.)	femtomoles per liter (fmol/L)
PigStn	Pigment station number.	unitless
PigDepth	Pigment depth.	meters (m)
chl_a	Chlorophyll-a determined by HPLC.	nanograms per liter (ng/L)
dv_chl_a	Divinyl chlorophyll-a determined by HPLC.	nanograms per liter (ng/L)
fuco	Fucoxanthin determined by HPLC.	nanograms per liter (ng/L)
zeax	Zeaxanthin determined by HPLC.	nanograms per liter (ng/L)
MgDVP	Mg-2,4-divinyl pheoporphyrin determined by HPLC.	nanograms per liter (ng/L)
chl_c2	Chlorophyll c2 determined by HPLC.	nanograms per liter (ng/L)
peridinin	Peridinin determined by HPLC.	nanograms per liter (ng/L)
but19	19-prime-butanoyloxyfucoxanthin determined by HPLC.	nanograms per liter (ng/L)

hex19	19-prime-hexanoyloxyfucoxanthin determined by HPLC.	nanograms per liter (ng/L)
DD	Diadinox determined by HPLC.	nanograms per liter (ng/L)

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Instruments

Dataset-specific Instrument Name	SBE19plusV2
Generic Instrument Name	CTD Sea-Bird SBE SEACAT 19plus
Dataset-specific Description	Temperature, oxygen and conductivity sensor data were collected using a SBE19plusV2 system (Seabird Electronics Inc.) attached to a CTD extension stand on the Trace Metal Rosette.
Generic Instrument Description	Self contained self powered CTD profiler. Measures conductivity, temperature and pressure in both profiling (samples at 4 scans/sec) and moored (sample rates of once every 5 seconds to once every 9 hours) mode. Available in plastic or titanium housing with depth ranges of 600m and 7000m respectively. Minature submersible pump provides water to conductivity cell.

Dataset-specific Instrument Name	Paradigm MS4 HPLC
Generic Instrument Name	High-Performance Liquid Chromatograph
Dataset-specific Description	Chromatographic separation and mass spectrometry were performed using a Paradigm MS4 HPLC (Michrom Bioresources) coupled to a Thermo Vantage TSQ mass spectrometer (Thermo Scientific). Pigments were determined using an Agilent 1100 HPLC (High Performance Liquid Chromatography) system with diode array and fluorescence detection.
Generic Instrument Description	A High-performance liquid chromatograph (HPLC) is a type of liquid chromatography used to separate compounds that are dissolved in solution. HPLC instruments consist of a reservoir of the mobile phase, a pump, an injector, a separation column, and a detector. Compounds are separated by high pressure pumping of the sample mixture onto a column packed with microspheres coated with the stationary phase. The different components in the mixture pass through the column at different rates due to differences in their partitioning behavior between the mobile liquid phase and the stationary phase.

Dataset-specific Instrument Name	Thermo Vantage mass spectrometer
Generic Instrument Name	Mass Spectrometer
Dataset-specific Description	Absolute quantitation of proteins was conducted by triple quadrupole mass spectrometry using a Thermo Vantage mass spectrometer. Chromatographic separation and mass spectrometry were performed using a Paradigm MS4 HPLC (Michrom Bioresources) coupled to a Thermo Vantage TSQ mass spectrometer (Thermo Scientific).
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.

Dataset-specific Instrument Name	McLane Pumps WTS-LV
Generic Instrument Name	McLane Large Volume Pumping System WTS-LV
Dataset-specific Description	The protein samples were collected by a suite of 4 L/min and 8 L/min McLane Pumps (WTS-LV; McLane Research Laboratories Inc., Falmouth MA, USA) outfitted with custom Mini-MULVS multiple filter head systems.
Generic Instrument Description	The WTS-LV is a Water Transfer System (WTS) Large Volume (LV) pumping instrument designed and manufactured by McLane Research Labs (Falmouth, MA, USA). It is a large-volume, single-event sampler that collects suspended and dissolved particulate samples in situ. Ambient water is drawn through a modular filter holder onto a 142-millimeter (mm) membrane without passing through the pump. The standard two-tier filter holder provides prefiltering and size fractioning. Collection targets include chlorophyll maximum, particulate trace metals, and phytoplankton. It features different flow rates and filter porosity to support a range of specimen collection. Sampling can be programmed to start at a scheduled time or begin with a countdown delay. It also features a dynamic pump speed algorithm that adjusts flow to protect the sample as material accumulates on the filter. Several pump options range from 0.5 to 30 liters per minute, with a max volume of 2,500 to 36,000 liters depending on the pump and battery pack used. The standard model is depth rated to 5,500 meters, with a deeper 7,000-meter option available. The operating temperature is -4 to 35 degrees Celsius. The WTS-LV is available in four different configurations: Standard, Upright, Bore Hole, and Dual Filter Sampler. The high-capacity upright WTS-LV model provides three times the battery life of the standard model. The Bore-Hole WTS-LV is designed to fit through a narrow opening such as a 30-centimeter borehole. The dual filter WTS-LV features two vertical intake 142 mm filter holders to allow simultaneous filtering using two different porosities.

Dataset-specific Instrument Name	X-Niskin bottles (Ocean Test Equipment)
Generic Instrument Name	Niskin bottle
Dataset-specific Description	Dissolved trace metal samples (iron and cobalt) were collected by an internally programmed standard SBE Rosette (Seabird Electronics Inc.) user-modified to serve as a trace metal clean system with 12 8 L X-Niskin bottles (Ocean Test Equipment)
Generic Instrument Description	A Niskin bottle (a next generation water sampler based on the Nansen bottle) is a cylindrical, non-metallic water collection device with stoppers at both ends. The bottles can be attached individually on a hydrowire or deployed in 12, 24, or 36 bottle Rosette systems mounted on a frame and combined with a CTD. Niskin bottles are used to collect discrete water samples for a range of measurements including pigments, nutrients, plankton, etc.

Dataset-specific Instrument Name	nutrient autoanalyzer
Generic Instrument Name	Nutrient Autoanalyzer
Dataset-specific Description	Nutrient analyses were conducted by nutrient autoanalyzer by Joe Jennings at Oregon State University.
Generic Instrument Description	Nutrient Autoanalyzer is a generic term used when specific type, make and model were not specified. In general, a Nutrient Autoanalyzer is an automated flow-thru system for doing nutrient analysis (nitrate, ammonium, orthophosphate, and silicate) on seawater samples.

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Deployments

KM1128

Website	https://www.bco-dmo.org/deployment/59053
Platform	R/V Kilo Moana
Start Date	2011-10-01
End Date	2011-10-25
Description	This is a MetZyme project cruise. The original cruise data are available from the NSF R2R data catalog.

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Project Information

Connecting Trace Elements and Metalloenzymes Across Marine Biogeochemical Gradients (GPc03) (MetZyme)

Coverage: Tropical North Pacific along 150 degrees West from 18 degrees North to the equator

MetZyme project researchers will determine the role of enzymatic activity in the cycling of trace metals. Specifically the research will address the following questions: (1) degradation of sinking particulate organic material in the Tropical North Pacific can be influenced by the ability of microbes to synthesize zinc proteases, which in turn is controlled by the abundance or availability of zinc, and (2) methylation of mercury is controlled, in part, by the activity of cobalt-containing enzymes, and therefore the supply of labile cobalt to the corrinoid-containing enzymes or co-factors responsible for methylation. To attain their goal, they will collect dissolved and particulate samples for trace metals and metalloenzymes from three stations along a biogeochemical gradient in the Tropical North Pacific (along 150 degrees West from 18 degrees North to the equator). Sinking particles from metal clean sediment traps will also be obtained. The samples will also be used to carry out shipboard incubation experiments using amendments of metals, metal-chelators, B12, and proteases to examine the sensitivity and metal limitation of heterotrophic, enzymatic degradation of organic matter within the oceanic "Twilight Zone" (100-500 m). This study will result in a novel metaproteomic/metalloenzyme datasets that should provide insights into the biogeochemical cycling of metals, as well as co-limitation of primary productivity and controls on the export of carbon from the photic zone. In addition to the final data being contributed to BCO-DMO, an online metaproteomic data server will be created so the community has access to the raw data files generated by this research.

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Program Information

U.S. GEOTRACES (U.S. GEOTRACES)

Website: http://www.geotraces.org/

Coverage: Global

GEOTRACES is a SCOR sponsored program; and funding for program infrastructure development is provided by the U.S. National Science Foundation.

GEOTRACES gained momentum following a special symposium, S02: Biogeochemical cycling of trace elements and isotopes in the ocean and applications to constrain contemporary marine processes (GEOSECS II), at a 2003 Goldschmidt meeting convened in Japan. The GEOSECS II acronym referred to the Geochemical Ocean Section Studies To determine full water column distributions of selected trace elements and isotopes, including their concentration, chemical speciation, and physical form, along a sufficient number of sections in each ocean basin to establish the principal relationships between these distributions and with more traditional hydrographic parameters;

* To evaluate the sources, sinks, and internal cycling of these species and thereby characterize more completely the physical, chemical and biological processes regulating their distributions, and the sensitivity of these processes to global change; and

* To understand the processes that control the concentrations of geochemical species used for proxies of the past environment, both in the water column and in the substrates that reflect the water column.

GEOTRACES will be global in scope, consisting of ocean sections complemented by regional process studies. Sections and process studies will combine fieldwork, laboratory experiments and modelling. Beyond realizing the scientific objectives identified above, a natural outcome of this work will be to build a community of marine scientists who understand the processes regulating trace element cycles sufficiently well to exploit this knowledge reliably in future interdisciplinary studies.

Expand "Projects" below for information about and data resulting from individual US GEOTRACES research projects.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1031271
NSF Division of Ocean Sciences (NSF OCE)	OCE-1337780
Gordon and Betty Moore Foundation: Marine Microbiology Initiative (MMI)	GBMF3934
Gordon and Betty Moore Foundation: Marine Microbiology Initiative (MMI)	GBMF3782

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