Data Management Plan.

The proposed research project will generate iron-binding organic ligand data and siderophore characterization data from the analysis of field survey and shipboard experimental samples collected on the U.S. GEOTRACES GP17-OCE and GP17-ANT cruise sections in project years 1 and 2. Additional iron-binding organic ligand data and siderophore characterization data will be generated from the proposed laboratory experiments. A summary of the data that will be collected is provided in Table 1 below. All field samples will be collected by the U.S. GEOTRACES GP17 sampling teams (assembled by the GP17 cruise management teams) following the protocols recommended by the international GEOTRACES program to ensure that results generated by this work are compatible with all GEOTRACES studies of the same parameters. Altogether, GEOTRACES protocols for sample collection, processing, and analysis will be followed in the collection of the proposed datasets for this project.

Iron-binding organic ligand data and siderophore characterization data generated from the cruise will be submitted by project PIs to the Biological and Chemical Oceanography Data Management Office (BCO-DMO) for management and archiving. These data sets will be made available online from the BCO-DMO data system within two years, following standard NSF requirements. Within the BCO-DMO system, this data will additionally be linked to previous data generated from the GEOTRACES program using standardized parameter naming formats; Buck has contributed similar data sets to BCO-DMO from previous projects. Raw mass spectrometry data will be posted on the Global Natural Products Social Molecular Networking (GNPS) and R code for processing the mass spectrometry data will be made available through PI Bundy's GitHub site with corresponding descriptions of how to use the processing code. The proposed inter-lab intercalibration activities will facilitate synthesis of project datasets across project PIs, as well as with previous and future GEOTRACES efforts. All project data will also be submitted for inclusion in GEOTRACES International Data Products.

Table 1. Data to be generated from the proposed research.

Sample type	Sample resolution	Parameters measured	Method employed
Water column (depth profile) samples from U.S. GEOTRACES GP17-OCE and GP17-ANT cruises	All stations (super, full, demi)	Dissolved (<0.2 μm) Fe-binding organic ligand concentrations, conditional stability constants, resulting Fe′ concentrations	CLE-AdCSV, single analytical window, 25 μM SA
Water column (depth profile) samples from U.S. GEOTRACES GP17-OCE and GP17-ANT cruises	Super only	Dissolved (<0.2 μm) Fe-binding organic ligand concentrations, conditional stability constants, resulting Fe′ concentrations	CLE-AdCSV, intercalibration analytical window, 5 μM SA
Water column samples from U.S. GEOTRACES GP17-OCE and GP17-ANT cruises	Surface towfish of all stations	Dissolved (<0.2 μm) siderophore concentrations and identities	Solid phase extraction, ICP-MS and ESI-MS analysis
Pore water samples from U.S. GEOTRACES GP17-OCE and GP17-ANT provided by S. Severmann (see letter of collaboration)	Select multi-corer	Dissolved (<0.2 μm) Fe-binding organic ligand concentrations, conditional stability constants, resulting Fe′ concentrations	CLE-AdCSV, single analytical window, 25 μM SA

Pore water samples from U.S. GEOTRACES GP17-OCE and GP17-ANT provided by S. Severmann (see letter of collaboration)	Select multi-corer	Dissolved (<0.2 μm) siderophore concentrations and identities	Solid phase extraction, ICP-MS and ESI-MS analysis
Size-fractionated water column samples from U.S. GEOTRACES GP17-OCE and GP17-ANT provided by J. Fitzsimmons (see letter of collaboration)	Select super	Soluble (<0.02 μm) Fe-binding organic ligand concentrations, conditional stability constants, resulting Fe′ concentrations	CLE-AdCSV, single analytical window, 25 μM SA
Size-fractionated water column samples from U.S. GEOTRACES GP17-OCE and GP17-ANT provided by J. Fitzsimmons (see letter of collaboration)	Select super	Soluble (<0.02 μm) siderophore concentrations and identities	Solid phase extraction, ICP-MS and ESI-MS analysis
Photochemistry experimental samples provided by R. Boiteau (see letter of collaboration)	GP17-ANT shipboard photochemistry experiments	Dissolved (<0.2 μm) Fe-binding organic ligand concentrations, conditional stability constants, resulting Fe′ concentrations	CLE-AdCSV, single analytical window, 25 μM SA
Model ligand experimental samples	Laboratory-based model ligand experiments	Dissolved (<0.2 μm) Fe-binding organic ligand concentrations, conditional stability constants, resulting Fe′ concentrations	CLE-AdCSV, single analytical window, 25 μM SA
Model ligand experimental samples	Laboratory-based model ligand experiments	Dissolved (<0.2 μm) siderophore concentrations and identities	Solid phase extraction, ICP-MS and ESI-MS analysis