This is a readme for Metabolomics Workbench data deposition

Project Title: Metabolite flux from temperature-acclimated diatom strains

Project Summary: The temperature increase occurring in the surface ocean has fundamental implications for physiological rates and processes of marine microbes. Here we asked whether the temperature at which a marine diatom strain is acclimated affects carbon transfer to a co-cultured heterotrophic bacterium. Model systems were established in which the diatom *Thalassiosira pseudonana* was acclimated for three months at temperatures below (14°C), equal to (20°C), and above (28°C) the temperature of optimal growth, and then inoculated with the heterotrophic bacterium *Ruegeria pomeroyi*. This deposition is for the results of diatom endometabolites obtained from the main experiment of this study.

\* mwTab file name: (Automatically assigned)

\* Name of archive file to be uploaded: UGA\_ temp\_Oct2023\_main\_zip

\* Data type being submitted: NMR

\* Protocol methods filename(s):

2\_Collection protocol\_UGA\_temp\_Oct2023\_main.docx

3\_Treatment protocol\_UGA\_temp\_Oct2023\_main.docx

4\_Sample preparation protocol\_UGA\_temp\_Oct2023\_main.docx

5\_Analysis protocol\_UGA\_temp\_Oct2023\_main.docx

\* MS/NMR instrument manufacturer: Bruker

\* MS/NMR instrument model: Bruker AVANCE lll

\* Binary data format: .ser

\* Open source text formats: .csv

\* Multi-part study: No

\* Embargo: No

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UGA\_ temp\_Oct2023\_main \_zip contains:

File: 1\_Study design\_UGA\_temp\_Oct2023\_main.xlsx

File: 2\_Collection protocol\_UGA\_temp\_Oct2023\_main.docx

File: 3\_Treatment protocol\_UGA\_temp\_Oct2023\_main.docx

File: 4\_Sample preparation protocol\_UGA\_temp\_Oct2023\_main.docx

File: 5\_Analysis protocol\_UGA\_temp\_Oct2023\_main.docx

File: 6\_Acquisition and processing parameters\_UGA\_temp\_Oct2023\_main.xlsx

Folder: Spectra

Folder: Data\_analysis

Note: We excluded the pooled sample and extraction and buffer blanks from ‘MW\_tab\_data.txt’ to create a metadata sheet in the Metabolomics Workbench system because those samples can’t have required factors. Although those samples are not in the metadata sheet, they are still included in the deposited file package. Files: HSQC for annotation, ‘/Annotation/3’; HSQC-TOCYS for annotation ‘/Annotation/4’; Media blank, ‘rawFiles/4’; Extraction blank-1, ‘rawFiles/104’; Extraction blank-2, ‘rawFiles/108’.