DATA TITLE: Gulf of Maine bulk and amino acid nitrogen isotope data from 1783-2010 PROJECT TITLE: Paired bulk organic and individual amino acid δ^{15} N analyses of bivalve shell periostracum: A palaeoceanographic proxy for water source variability and nitrogen cycling processes

DATA ABSTRACT: The data presented here are bulk and amino acid nitrogen isotopes and amino acid concentrations measured in *Arctica islandica* shells collected from the Gulf of Maine between 2009 and 2014. The samples are dated between 1783 and 2010 C.E. using cross-dating techniques. Three different tissue types were analyzed: periostracum, calcium carbonate shell, and adductor muscle. Carbon isotopes of periostracum are also presented. Isotope data were analyzed using an isotope ratio mass spectrometer coupled with a Gas Chromatograph and an Elemental Analyzer for amino acid and bulk analyses, respectively. Amino acid concentration data were analyzed using a Flame Ionization Detector and concentration curves. Trophic position of *Arctica islandica* through time was determined using a trophic position equation gleaned from the literature.

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ASSOCIATED PUBLICATIONS:

Whitney N. M., Johnson B. J., Dostie P. T., Luzier K. and Wanamaker A. D. (2019) Paired bulk organic and individual amino acid δ^{15} N analyses of bivalve shell periostracum: A paleoceanographic proxy for water source variability and nitrogen cycling processes. *Geochim. Cosmochim. Acta* 254, 67-85. https://doi.org/10.1016/j.gca.2019.03.019 COLLECTION INFORMATION: Time period(s): Collection occurred 2009-2014 SITE INFORMATION Site name: Seguin Island, Jonesport, Cobscook Bay, Isle au Haut, Damariscotta Estuary, Darling Marine Center Location: Gulf of Maine Country: United States Northernmost latitude (decimal degree, South negative, WGS84): 44.9 Southernmost latitude (decimal degree, South negative, WGS84): 43.7 Easternmost longitude (decimal degree, West negative, WGS84): -67.1 Westernmost longitude (decimal degree, West negative, WGS84): -69.7

Elevation (m), below sea level negative: -38 meters to -80 meters

----- FILE DIRECTORY -----

----- FILE LIST-----

A. Gulf of Maine bulk and amino acid nitrogen isotope data as taken from *Arctica islandica* samples from 1783-2010 - These are the data used to make the figures published in "Paired bulk organic and individual amino acid δ^{15} N analyses of bivalve shell periostracum: A paleoceanographic proxy for water source variability and nitrogen cycling processes"

A.a. [Figure 2] - Nitrogen and carbon isotope data from periostracum material as displayed in Figure 2 of the manuscript

A.b. [Figure 3] - Nitrogen isotope data from periostracum and carbonate as displayed in Figure 3 of the manuscript

A.c. [Figure 4] – Bulk nitrogen isotope data from periostracum, carbonate, and adductor muscle as displayed in Figure 4 of the manuscript

A.d. [Figure 5] - Nitrogen isotope data from bulk and phenylalanine material from periostracum as displayed in Figure 5 of the manuscript

A.e. [Figure 6] - Amino acid concentration data from periostracum, carbonate, and adductor muscle as displayed in Figure 6 of the manuscript

A.f. [Figure 7] - Nitrogen isotope of amino acid data from periostracum, carbonate, and adductor muscle as displayed in Figure 7 of the manuscript

A.g. [Figure 8] – Calculated trophic position of from nitrogen isotopes of amino acids measured in periostracum as displayed in Figure 8 of the manuscript

A.h. [Supplementary Figure 2] - Amino acid concentration data from periostracum as displayed in Supplementary Figure 2 of the manuscript

----- VARIABLES -----

Please see the datasheets for specific descriptions of the variables. Missing data (i.e. no data is available for that year/increment number etc.) is denoted by -999.

----- METHODS AND MATERIALS -----

----- DATA COLLECTION METHODS -----

Arctica islandica shells were collected from several different locations in the Gulf of Maine. Shells were collected from 38 meters water depth near Seguin Island, 80 meters water depth near Jonesport and 31 meters water depth near Isle au Haut using scallop dredges. Shells were also collected from 10 meters water depth in Cobscook Bay by divers. Most shells were shipped on dry ice to the Stable Isotope Lab at Iowa State University, although several shells were put in tanks in the Darling Marine Center in Walpole, Maine or in cages in the Damariscotta River estuary for 29 weeks.

----- DATA PROCESSING METHODS -----

Periostracum were removed from shells using a razor blade and treated with HCl to remove any remaining carbonate powder. Carbonate powder was collected from shells using a Dremel hand mill or a micromill. Adductor muscle was removed, cleaned with DI water and frozen for 24 hours before freeze drying.

Bulk nitrogen and carbon isotopes were Costech Elemental Analyzer connected to a Finnegan Delta Plus XL mass spectrometer in continuous flow mode at Iowa State University. Results were corrected using a regression method and 4 different reference standards: Caffeine (IAEA-600), IAEA-N2, Cellulose (IAEA-CH-3), and Acetanilide (laboratory standard). All nitrogen isotope values were standardized relative to Air (atmospheric N₂) and all carbon isotope values were standardized relative to VPDB (Vienna Pee Dee Belemnite).

For compound specific amino acid analyses, samples were hydrolyzed at Bates College and then derivatized to TFAA derivatives. The n-TFAA amino acid derivatives were analyzed by gas chromatography flame ionization detection (GC-FID) using an Agilent 6890 N equipped with a HP-ULTRA 1 column. An amino acid standard mixture was created from 17 L-amino acid analytical standards (Sigma Aldrich). Calibration curves were created by analyzing 4 different dilutions of the 17 amino acid standards. These curves were used to convert the peak areas of each amino acid to concentration. For nitrogen isotope analysis of amino acids, samples were analyzed using a HP ULTRA 1 column in a Trace Gas Chromatograph interfaced to a Thermo Delta V Advantage stable isotope ratio mass spectrometer via the GC column interface III with a liquid nitrogen trap. A laboratory standard was made using 14 L-amino acid analytical standards from Sigma Aldrich added in concentrations similar to amino acid concentrations in periostracum. Aliquots of this laboratory standard were derivatized and analyzed with each batch of 6 samples processed. Different dilutions of the laboratory standard were used to correct for linearity issues with the CSIA-AA analyses. Each sample was run at least 3 times, with δ^{15} N values averaged over all runs, unless any individual run was deemed unusable.

Trophic position was calculated using the equation TP = [$(\delta^{15}N_{\text{proline}} - \delta^{15}N_{\text{phenylalanine}} - 2.8)/6.3$]+1.

----- Licensing ------

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