Metadata for datasets of *L&O-Letters* articles

**Table 1.** Description of the fields needed to describe the creation of your dataset.

|  |  |
| --- | --- |
| **Title of dataset** | *Initial-hydrolysis-ms* |
| **URL of dataset** | *https://github.com/shutingliu/initial-hydrolysis-ms.git* |
| **Abstract** | *This study is to use peptide hydrolysis data to investigate initial peptide hydrolysis that occurred in short-time scale (1-2 h) and the roles of free vs. attached enzymes in peptide initial hydrolysis in coastal seawater.* |
| **Keywords** | *Initial hydrolysis, AVFA, fragments* |
| **Dataset lead author** | *Shuting Liu* |
| **Position of data author** | *graduate student, current post-doctoral researcher* |
| **Address of data author** | *Marine Science Institute, The University of Texas at Austin, Port Aransas, TX 78373*  *Current address: Marine Science Institute, Department of Ecology, Evolution, and Marine Biology, University of California, Santa Barabra, CA 93117* |
| **Email address of data author** | *shutingliu@utexas.edu* |
| **Primary contact person for dataset** | *Shuting Liu* |
| **Position of primary contact person** | *graduate student, current post-doctoral researcher* |
| **Address of primary contact person** | *Marine Science Institute, Department of Ecology, Evolution, and Marine Biology, University of California, Santa Barabra, CA 93117* |
| **Email address of primary contact person** | *shutingliu@utexas.edu* |
| **Organization associated with the data** | *Marine Science Institute, The University of Texas at Austin, Port Aransas, TX 78373* |
| **Usage Rights** | *publicly available and free to use* |
| **Geographic region** | *Port Aransas, TX, US; Gulf of Mexico; Atlantic Ocean* |
| **Geographic coverage** | *26-32°N, 78-98°W* |
| **Temporal coverage - Begin date** | *Oct 2011* |
| **Temporal coverage - End date** | *Apr 2015* |
| **General study design** | *Ship channel in Port Aransas, TX, located in the western Gulf of Mexico; and coastal stations in the northern Gulf of Mexico or N. Atlantic Ocean* |
| **Methods description** | *To study peptide hydrolysis in the seawater, we collected seawater from different coastal stations, and incubate peptide in seawater under dark. Aliquots were filtered through 0.2 m filters at various time intervals during incubations for peptides and amino acid analyses.* |
| **Laboratory, field, or other analytical methods** | *AVFA and the hydrolyzed fragments were measured with either high performance liquid chromatography (HPLC, Shimadzu Prominence) equipped with a photo diode array detector or HPLC-mass spectrometry. Amino acids were analyzed by HPLC after o-phthaldialdehyde (OPA) derivatization.*  *To estimate the degree of T0 hydrolysis, we summarized the concentration percentage of hydrolysis products (peptide fragments and amino acids) at T0 with respect to amended AVFA. As diverse peptide fragments and amino acids were produced during peptide hydrolysis, we use all fragments containing a respective identical amino acid for mass balance calculations. For example, we use all hydrolysis fragments of AVFA with amino acid F, including AVF, VFA, VF, FA, and F to calculate the percent of hydrolysis.* |
| **Quality control** | *Duplicate samples were analyzed to make sure reproducibility. Incubations were conducted in 34 cases at different sites and different seasons to generalize pattern.* |
| **Additional information** | *Datasets were mostly plot in Sigmaplot.* |

**Table 2.** Description of the variables (i.e., columns) in EACH dataset in sufficient detail for another user to understand and use the data. If there are 10 variables (i.e., columns) in the dataset, then there should be 10 rows in this column that describe each column.

Dataset filename: \_\_\_\_\_\_\_map.m\_\_\_\_\_\_\_\_\_\_\_\_

|  |  |  |
| --- | --- | --- |
| **Column name** | **Definition** | **Units** |
| *coordinates* | *Coordinates for map generation were included in the matlab code.* | *°N, °W* |

Dataset filename: \_\_\_\_\_Fig. 2 AVFA conc vs initial hydrolysis percentage\_\_\_\_\_\_\_\_\_\_\_\_\_\_

|  |  |  |
| --- | --- | --- |
| **Column name** | **Definition** | **Units** |
| *AVFA concentration* | *Amended AVFA concentrations in 34 studied cases.* | *mol L-1* |
| Initial hydrolysis percentage | Concentration percentage of hydrolyzed fragments vs. amended AVFA concentrations. | % |

Dataset filename: \_\_\_\_\_\_\_Fig. 3a initial exp-AVFA \_\_\_\_\_\_\_\_\_\_\_\_

|  |  |  |
| --- | --- | --- |
| **Column name** | **Definition** | **Units** |
| *time* | *Incubation time.* | *min* |
| AVFA concentration | AVFA concentration at different time points during incubation. | *mol L-1* |

Dataset filename: \_\_\_\_\_\_\_Fig. 3b initial exp-VFA \_\_\_\_\_\_\_\_\_\_\_\_

|  |  |  |
| --- | --- | --- |
| **Column name** | **Definition** | **Units** |
| *time* | *Incubation time.* | *min* |
| VFA concentration | Produced VFA concentration at different time points during incubation. | *mol L-1* |

Dataset filename: \_\_\_\_\_\_\_Fig. 3c initial exp-FA \_\_\_\_\_\_\_\_\_\_\_\_

|  |  |  |
| --- | --- | --- |
| **Column name** | **Definition** | **Units** |
| *time* | *Incubation time.* | *min* |
| FA concentration | Produced FA concentration at different time points during incubation. | *mol L-1* |

Dataset filename: \_\_\_\_\_\_\_Fig. 3d initial exp-VF \_\_\_\_\_\_\_\_\_\_\_\_

|  |  |  |
| --- | --- | --- |
| **Column name** | **Definition** | **Units** |
| *time* | *Incubation time.* | *min* |
| VF concentration | Produced VF concentration at different time points during incubation. | *mol L-1* |

Dataset filename: \_\_\_\_\_\_\_Fig. 3e initial exp-AV \_\_\_\_\_\_\_\_\_\_\_\_

|  |  |  |
| --- | --- | --- |
| **Column name** | **Definition** | **Units** |
| *time* | *Incubation time.* | *min* |
| AV concentration | Produced AV concentration at different time points during incubation. | *mol L-1* |

Dataset filename: \_\_\_\_\_\_\_Fig. 3f initial exp-Ala \_\_\_\_\_\_\_\_\_\_\_\_

|  |  |  |
| --- | --- | --- |
| **Column name** | **Definition** | **Units** |
| *time* | *Incubation time.* | *min* |
| Ala concentration | Produced Ala (A) concentration at different time points during incubation. | *mol L-1* |

Dataset filename: \_\_\_\_\_\_\_Fig. 3g initial exp-Val \_\_\_\_\_\_\_\_\_\_\_\_

|  |  |  |
| --- | --- | --- |
| **Column name** | **Definition** | **Units** |
| *time* | *Incubation time.* | *min* |
| Val concentration | Produced Val (V) concentration at different time points during incubation. | *mol L-1* |

Dataset filename: \_\_\_\_\_\_\_Fig. 3h initial exp-Phe \_\_\_\_\_\_\_\_\_\_\_\_

|  |  |  |
| --- | --- | --- |
| **Column name** | **Definition** | **Units** |
| *time* | *Incubation time.* | *min* |
| Phe concentration | Produced Phe (F) concentration at different time points during incubation. | *mol L-1* |

Dataset filename: \_\_\_\_\_\_\_Fig. 4 freezer test AVFA and fragments \_\_\_\_\_\_\_\_\_\_\_\_

|  |  |  |
| --- | --- | --- |
| **Column name** | **Definition** | **Units** |
| *time* | *Incubation time.* | *min* |
| AVFA concentration | AVFA concentration at different time points during incubation. | *mol L-1* |
| Fragments concentration | Fragments concentration (sum of AVF, VFA and FA) at different time points during incubation. | *mol L-1* |