Raw LCMS data files from study of metabolomics of blue crab urine inducing fear in prey

Website: https://www.bco-dmo.org/dataset/720684
Data Type: experimental
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Project
» The role of the sensory environment and predator chemical signal properties in determining NCE strength in cascading interactions on oyster reefs (SensoryNCE)

Contributors	Affiliation	Role
Weissburg, Marc	Georgia Institute of Technology (GA Tech)	Principal Investigator
Kubanek, Julia	Georgia Institute of Technology (GA Tech)	Co-Principal Investigator
Gaul, David	Georgia Institute of Technology (GA Tech)	Contact
Rauch, Shannon	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

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Dataset Description

This dataset includes the following files, packaged in a .zip file:

- "LCMS negative mode" = contains MS1 negative mode files.
- "LCMS positive mode" = contains MS1 positive mode files.
- LCMS File Summary.docx = document describing the files.
- METADATA_CrabUrine.xlsx = metadata describing the study and the files.

MS data files are also publicly available on the NIH Metabolomics Workbench (doi: 10.21228/M86M4G).

The following PNAS paper contains the analyses of the processed data:
Poulin RX, Lavoie S, Siegel K, Gaul D, Weissburg M, Kubanek J (2018) Chemical encoding of risk perception and predator detection among estuarine invertebrates. Proceedings of the National Academy of Sciences. 115:662-667; doi:10.1073/pnas.1713901115

Methods & Sampling

MS data were aligned with an adaptive curve and metabolic features (retention time (Rt), m/z pairs) were detected after removal of isotopes and adducts in Compound Discoverer. Background peaks were removed from the dataset using a sample blank. Fill gaps and normalization by constant sum was applied to the data. Select features with a fold change greater or equal to 2 in urine from blue crabs fed mud crabs when compared to urine from blue crabs fed oysters and relative standard deviation of less than 30 were used to build an un-supervised PCA model with leave-one-out cross-validation using MATLAB R2012b (Version 8.0.0.783 The MathWorks, Inc.) and the PLS Toolbox (v.6.71, Eigenvector Research, Inc.). Data were preprocessed by auto-scaling the features' peak areas across the samples.

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Data Files

File	
Chemical_encoding_of_risk_perception_MS_metabolomics_dataset.zip	(ZIP Archive (ZIP), 2.00 GB) MD5:05e026002eb7da9e64974c584bd96f50
LCMS Raw data	

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Parameters

Parameters for this dataset have not yet been identified

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Instruments

Dataset-specific Instrument Name	
Generic Instrument Name	Mass Spectrometer
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.

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Project Information

The role of the sensory environment and predator chemical signal properties in determining NCE strength in cascading interactions on oyster reefs (SensoryNCE)

Coverage: Intertidal and subtidal oyster reefs in Wassaw Sound, Georgia, US

Extracted from the NSF award abstract:

In this project, the investigators will examine the ability of top blue crab predators to indirectly benefit the abundance of basal oyster prey by reducing the density (consumptive effects, CEs) and suppressing foraging (non-consumptive effects, NCEs) of intermediate mud crab predators. These NCEs are mediated by chemical perception of aversive cues in blue crab urine and produce a behaviorally mediated trophic cascade. Through a series of manipulative experiments, the investigators will examine how the strength of this behaviorally-mediated trophic cascade is modulated and factors that influence perceptive range such as predator diet and intake rate, and the flow environment. The investigators will also determine the chemical identity, concentration and release rate of chemical cues.

Identifying the quantitative and molecular aspects of aversive cues, and linking them to behavioral responses that produce trophic cascades establishes the chemical basis of risk perception by prey and how this

translates into cascading ecological effects. The use of perceptive range as a framework for evaluating the effects of both chemistry and environment provides an integrated view of processes affecting chemically-mediated NCEs. The use of a water borne predator-prey signaling system to test ideas on the strength of NCEs should have broad applications.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1234449

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