NMR spectral files from study of metabolomics of blue crab urine inducing fear in prey

Website: https://www.bco-dmo.org/dataset/720697
Data Type: experimental
Version: 19 December 2017
Version Date: 2017-12-19

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, Contact
Poulin, Remington	Max Planck Institute for Chemical Ecology (MPI CE)	Student
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:

- archived_pca_spectra.zip = unprocessed ^{1}H NMR spectral data files underlying PCA analysis in the publication "Chemical encoding of risk perception and predator detection among estuarine invertebrates."
- archived_pls-r_spectra.zip = unprocessed ^{1}H NMR spectral data files underlying PLS-R analysis in the publication "Chemical encoding of risk perception and predator detection among estuarine invertebrates."
- README_ArchivedSpectraDataset (1).doc = readme file describing the files.
- spectral_labels_for_pls-r_dataset.xlsx = spreadsheet containing spectral labels.

Poulin et al (2018) contains the analyses of the processed data. These NMR data files are also available from the Georgia Tech database, SMARTech at http://hdl.handle.net/1853/59056

Methods & Sampling

1H NMR spectra were processed in MATLAB, version 8.1.0.604, using NMRLab. Spectra were manually phased, baseline corrected, aligned, and the following regions excluded to remove contaminants from statistical analysis: TMSP (-0.5 to 0.5 ppm), water (4.6-5.2 ppm), residual methanol (3.2-3.4 ppm), and excess area (9.0-12.4 ppm) that contained no spectroscopic features. Spectroscopic features were clustered into 0.005 ppm bins, probabilistic quotient normalized to remove dilution bias, and generalized log (glog) transformed to avoid bias towards high concentration metabolites without affecting between-sample variation. Glog optimization values, λ, were generated from five technical replicates that consisted of equal parts from a single bulk urine sample using the methods above. For urine samples collected at Skidaway Institute of Oceanography, λ = 2.9359×10^{-7} and for urine samples at Georgia Tech λ = 8.2585×10^{-9}.

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Data Files

File
NMR_metabolomics.csv (Comma Separated Values (.csv), 223 bytes) MD5:5591dd1bb900f4e114d31d77288f2e24 Primary data file for dataset ID 720697

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Related Publications

Poulin, R. X., Lavoie, S., Siegel, K., Gaul, D. A., Weissburg, M. J., & Kubanek, J. (2018). Chemical encoding of risk perception and predator detection among estuarine invertebrates. Proceedings of the National Academy of Sciences, 115(4), 662–667. doi:10.1073/pnas.1713901115
Results

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Related Datasets

Different Version

Poulin, R. X., Lavoie, S., Siegel, K., Gaul, D. A., Weissburg, M. J., & Kubanek, J. (2017). Chemical encoding of risk perception and predator detection among estuarine invertebrates dataset. https://hdl.handle.net/1853/59056

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Parameters

Parameter	Description	Units
description	Description of the file package	dimensionless
file_size	Approximate file size	megabytes (MB)
download_link	Link to download the file	dimensionless

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Instruments

Dataset-specific Instrument Name	
Generic Instrument Name	Nuclear Magnetic Resonance Spectrometers
Generic Instrument Description	Instruments that identify and quantify magnetically active chemical entities by subjecting a sample to orthogonal magnetic and electrical fields.

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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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