

MS-based polar metabolomics on diatom response to allelopathic chemicals from red tide dinoflagellate (*Karenia brevis*)

Website: <https://www.bco-dmo.org/dataset/537359>

Data Type: Cruise Results

Version: 21 March 2018

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Project

» [Waterborne chemical cues in the plankton: a systems biology approach](#) (Plankton Chemical Cues)

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Dataset Description

These mass spec data files are in Thermo-Finnigan .raw format. Vendor software can be used to view these files, and there are free viewers that can also be used (one example is [PVIEW](#)). The files can also be converted to mzXML files using MSconvert.

Note: Data files in .raw format are also available from the Chorus repository (<https://chorusproject.org>) under project ID number 650 (project name: "Diatom response to allelopathy"), experiment ID number 848. See: <https://chorusproject.org/anonymous/download/experiment/8464697144662088343>

Methods & Sampling

Field assemblages of plankton were sampled during two cruises (EN496 and EN509), and shipboard experiments were conducted to test the community-level effects of *Karenia brevis* allelopathy on Gulf of Mexico plankton. The sampling and shipboard experiments are described fully in: Poulson-Ellestad et al. 2014. Are offshore phytoplankton susceptible to *Karenia brevis* allelopathy? J. Plankton Res. 36:1344-1356. doi: [10.1093/plankt/fbu064](https://doi.org/10.1093/plankt/fbu064)

See related publication:

Poulson-Ellestad, K.L., Jones, C.M., Roy, J., Viant, M.R., Fernandez, F.M., Kubaneck, J., & Nunn, B.L. 2014. Metabolomics and proteomics reveal impacts of chemically mediated competition on marine plankton. PNAS Proc Natl Acad Sci USA, 111(24): 9009-14. doi:[10.1073/pnas.1402130111](https://doi.org/10.1073/pnas.1402130111)

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Data Files

File
MS-based_polar_metabolomics_on_diatom_response.zip (ZIP Archive (ZIP), 3.73 GB) MD5:96a009fce767a982f1c0e6ed33f110aa

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Parameters

Parameters for this dataset have not yet been identified

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Instruments

Dataset-specific Instrument Name	Xevo G2 QTOF Mass Spectrometer
Generic Instrument Name	Mass Spectrometer
Dataset-specific Description	A Xevo G2 QTOF Mass Spectrometer was used.
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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Deployments

EN496

Website	https://www.bco-dmo.org/deployment/58932
Platform	R/V Endeavor
Start Date	2011-07-02
End Date	2011-07-27
Description	Original data are available from the NSF R2R data catalog

EN509

Website	https://www.bco-dmo.org/deployment/58933
Platform	R/V Endeavor
Start Date	2012-05-25
End Date	2012-06-20
Description	Original data are available from the NSF R2R data catalog

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Project Information

Waterborne chemical cues in the plankton: a systems biology approach (Plankton Chemical Cues)

Website: <http://devwp.kubanek.biology.gatech.edu/red-tide-competition-and-metabolomics/>

Coverage: Gulf of Mexico

Description from NSF award abstract:

Competition is a major force structuring communities, including the marine plankton. The release of compounds that inhibit competitors, a process known as allelopathy, is hypothesized to be important among phytoplankton, especially for species that compete poorly for resources yet form dense blooms. Ecological interactions involving the toxic red tide dinoflagellate *Karenia brevis* present an ideal system for understanding chemically mediated interactions. Blooms of this species occur frequently in accessible coastal areas of the Gulf of Mexico, causing massive fish kills and contaminating shellfish. The dramatic consequences of these blooms motivate the following questions. What strategies does this harmful alga use in competition with other phytoplankton? What lethal and sub-lethal effects are experienced by competitors? How do phytoplankton respond, resist, and detoxify their surroundings? What roles do chemical cues play in these interactions? How are different phytoplankton communities affected by allelopathy?

Previous studies have shown that *K. brevis* is allelopathic to several naturally co-occurring phytoplankton species, but compounds other than the known neurotoxic brevetoxins produced by *K. brevis* generally were responsible. This species produces allelopathic mixtures of unstable, 500-1000 Da organic compounds which cause reduced photosystem II activity and disrupt cell membranes of sensitive species, whereas some other competitors remain unaffected. Moreover, natural blooms of *K. brevis* were allelopathic to the competing diatom *Skeletonema grethae*. This species, in turn, appeared to influence the chemistry of *K. brevis*, reducing its allelopathic effects. Death is a rare outcome of *K. brevis* allelopathy; more subtle, non-lethal responses have predominated. Overall, environmental context may be critical for predicting what ecologically important chemical mediators are released into marine systems and the consequences of these compounds to plankton communities.

The project will:

- 1) Characterize the exudate metabolome among *K. brevis* samples of varying allelopathic potency. Exudates of *K. brevis* strains and natural bloom samples will be studied by mass spectrometry (MS) and nuclear magnetic resonance (NMR) metabolomics to pinpoint candidate chemical cues involved in competition. *Karenia brevis* protein expression will be examined by MS proteomics to test whether *K. brevis* up- or down-regulates key proteins involved in pathway networks in response to challenges by competitors.

- 2) Seek to understand sub-lethal metabolic impacts of exposure to allelopathy on target phytoplankton, by studying responses of phytoplankton to *K. brevis* allelopathy by MS-based metabolomics and proteomics. This work will provide an unbiased approach to determining molecular targets of allelopathy and allow testing of whether sub-lethal responses to allelopathy include suppressed fundamental cellular functioning and up-regulated pathways related to stress and detoxification.

- 3) Relate allelopathic sensitivity to metabolic responses in target phytoplankton, by comparing metabolomic and proteomic changes of sensitive versus resistant competitors to *K. brevis* allelopathy. The expectation is that more resistant species experience enhancement of detoxification pathways and more robust, unaffected

cellular function relative to competitors most sensitive to allelopathy.

4) Determine how estuarine and off-shore phytoplankton differ in their physiological responses to allelopathy, because allelopathy may be more important for maintaining dense blooms in near-shore waters than in the initiation of blooms off-shore.

Phytoplankton blooms can be devastating to local economies and pose human health risks. The discovery of new chemically mediated interactions and metabolic responses in the marine plankton could eventually lead to prediction and control strategies to alleviate the harmful consequences of these blooms. Continued effort to characterize mixtures of allelopathic compounds and determine their effects on competing species could lead to biodegradable treatments for reducing phytoplankton or microbial growth in aquatic and terrestrial environments. This study builds on past successes, applying lessons learned from chemistry about ecological processes and using ecological insights to discover unique natural products with important biological functions.

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1060300

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