Raman spectra from several different bivalve species; analysed in the North lab at UMCES HPL from 2012-2014 (Raman Spec Bivalves project)

Website: https://www.bco-dmo.org/dataset/536864
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Project
» Can Raman spectroscopy be used as a high-accuracy method to identify bivalve larvae? (Raman Spec Bivalves)

Contributors	Affiliation	Role
North, Elizabeth	University of Maryland Center for Environmental Science (UMCES/HPL)	Principal Investigator
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Dataset Description

This data set contains Raman spectra of the following species: *Argopecten irradians, Crassostrea gigas, Crassostrea virginica, Gemma gemma, Geukensia demissa, Ischadium recurvum, Macoma mitchelli, Mercenaria mercenaria, Mulinia lateralis, Mya arenaria, Mytilopsis leucophaeata, Ostrea lurida, Rangia cuneata, Tagelus plebeius, Spisula solidissma, Panopea generosa*. Detailed information on the source and preparation of larvae can be found in Thompson et al. (*in prep*). All spectra were acquired by Adam Schlenger and Christine Thompson.

Methods & Sampling

Detailed information on the source and preparation of larvae can be found in Thompson et al. (*in prep*). All spectra were acquired by Adam Schlenger and Christine Thompson. The following information on the acquisition and processing of the spectra that comprise this dataset was quoted from Thompson et al. (*in prep*):

"Raman spectra were acquired with an XploRA confocal Raman microscope by Horiba Jobin Yvon, Inc. The system includes a flat field spectrograph with a multichannel air cooled CCD detector and color camera optically coupled to an Olympus BX41 microscope. We used three lasers: a 532 nm 25 mW solid-state laser, a 638 nm 25 mW laser diode, and a 785 nm 25 mW laser diode. The lasers ran through a 100x objective using a 1200 grove mm-1 grating and hole and slit size of 300 µm and 100 µm, respectively. Spectra were recorded in the range of 200-2000 cm-1. Spectra were acquired from 20 larval shells for each sample by averaging 3 accumulations with an exposure time of 10 s. For one shell in each sample, three spectra were taken from

different positions on the shell. Spectral acquisition was controlled using Horiba's LabSpec software (version 6). Wavelength calibration was performed on the XploRA system using a neon light source that was calibrated daily with a silicon wafer.

All spectra were first pre-processed to remove noise and other variability. Immediately after acquisition, noise was removed using a smoothing function in LabSpec. Baseline correction was then performed using a freely-available integrated software system for processing Raman spectra (Reisner et al. 2011) implemented in MATLAB (v. R2011a). Next, all wavenumbers were shifted to ensure the aragonite peak for all spectra fell at 1085 cm-1 and then spectra were standardized to the intensity of the aragonite peak on a scale of 0 to 1."

The two columns of numbers in each file correspond to *wavenumber* with units of cm-1 (first column) and *relative intensity* which is unitless (second column).

References:
Reisner, L.A., Cao, A., & Pandya, A.K. 2011. An integrated software system for processing, analyzing, and classifying Raman spectra. Chemom Intell Lab Syst 105:83–90. doi: 10.1016/j.chemolab.2010.09.011

Thompson, C.M., North, E.W., Kennedy, V.S., & White, S.N. *In prep*. Classifying bivalve larvae using shell pigments identified by Raman spectra. Analytical and Bioanalytical Chemistry.

Data Processing Description

BCO-DMO downloaded the original data files from the DropBox URL provided by Dr. E. North. BCO-DMO created additional data columns for serving based on the file name conventions and metadata. See the original metadata form describing the file name conventions: Metadata_for_Raman_Spectra_of_Bivalve_Larvae (PDF file).

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Data Files

File
raman_spectra.csv (Comma Separated Values (.csv), 851.97 MB) MD5:7e79980f6cfa1384e5c98313e9797ee0 Primary data file for dataset ID 536864

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Parameters

Parameter	Description	Units
wavelength	Wavelength of the laser light source used (532, 638, or 785).	nanometers (nm)
species_name	Name of the species.	text
species_code	Unique species code.	text
year	4-digit year of spawning.	YYYY
loc_code	Unique sample location code.	text
location	Sample location.	text
city	City of the sample location.	text
state	2-letter abbreviation for the state of the sample location.	text
day	Age of larvae in days in the format DX where X = how many days old the larva was*. For specimens where age was unclear: DS = d-stage; VE = veliger; PV = pedi-veliger larvae (unclear how old); R = larvae released from brood (for brooding species); H = larvae at time of harvest (for brooding species). *For RCSL samples, day 13 is written as 13D	number of days
loc_additional	Additional location marker for some samples of Mytilopsis leucophaeata; Mulinia lateralis; and Macoma mitchelli. CT = Choptank River (Maryland USA). nd = not applicable/no additional location code.	text
shell_num	Shell number in the format SXX where XX = number shell (1-20 usually).	alphanumeric
position	Position number in the format PX where X = position (some shells had multiple positions for spectra).	alphanumeric
file_name	Name of the original spectra file containing the wavenumber and relative_intensity. Notes: sd = standardized to aragonite 1085 peak; pp = post-processed (flattened, noise reduction).	text
wavenumber	Wavenumber.	per centimeter (cm-1)
relative_intensity	Relative intensity.	unitless

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Instruments

Dataset-specific Instrument Name	XploRA confocal Raman microscope
Generic Instrument Name	Raman Microscope
Dataset-specific Description	Raman spectra were acquired with an XploRA confocal Raman microscope by Horiba Jobin Yvon, Inc. The system includes a flat field spectrograph with a multichannel air cooled CCD detector and color camera optically coupled to an Olympus BX41 microscope. The investigators used three lasers: a 532 nm 25 mW solid-state laser, a 638 nm 25 mW laser diode, and a 785 nm 25 mW laser diode. See more information about the Raman microscope on the UMCES website.
Generic Instrument Description	The Raman microscope is a laser-based microscopic device used to perform Raman spectroscopy. The Raman microscope begins with a standard optical microscope, and adds an excitation laser, laser rejection filters, a spectrometer or monochromator, and an optical sensitive detector such as a charge-coupled device (CCD), or photomultiplier tube, (PMT). One example is the XploRA confocal Raman microscope (information from the manufacturer).

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Deployments

lab_North_Raman_Spectra

Website	https://www.bco-dmo.org/deployment/537938
Platform	UMCES_HPL_labs
Start Date	2012-07-01
End Date	2014-06-01
Description	Laboratory-based research was conducted as part of the project titled "Can Raman spectroscopy be used as a high-accuracy method to identify bivalve larvae?" at: University of Maryland Center for Environmental Science, Horn Point Laboratory 2020 Horns Point Rd., Cambridge, MD

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Project Information

Can Raman spectroscopy be used as a high-accuracy method to identify bivalve larvae? (Raman Spec Bivalves)

Identification of bivalve larvae is notoriously difficult and time consuming; currently no ‘gold standard’ method exists for distinguishing larvae collected in the field. We proposed to determine if Raman spectroscopy could be used to identify species of bivalve larvae. Raman spectroscopy is a non-destructive method that uses a focused laser to produce a spectrum, a graph with peaks that indicate the presence of different molecules like calcium carbonate and organic pigments. Previous work exploring the use of Raman spectroscopy on shells of bivalve larvae revealed that larval shells of the eastern oyster (*Crassostrea virginica*) exhibit a unique spectrum at one wavelength which was distinguishable from those of six other bivalve species. The objective of this

research was to analyze additional species of larvae and to determine if spectra collected at three different wavelengths could be used to distinguish the larvae. We collected Raman spectra at three wavelengths from 25 samples of bivalve larvae representing 16 species and four taxonomic Orders. Use of the Raman spectra with three wavelengths enabled classification of larvae into Order/Family groups with accuracies ≥ 92% (Thompson et al. *in prep*). This study indicates that continued evaluation of this approach would be a fruitful line of research which could advance knowledge of shellfish biology and ecology.

(Project description provided by Dr. Elizabeth North.)

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1240266

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