Metadata for Raman Spectra of Bivalve Larvae

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Data set 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. 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.
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> 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."

Each spectra is stored in an individual .txt file. The files are formatted so that can be read into the freely-available integrated software system for processing Raman spectra (Reisner et al. 2011) implemented in MATLAB (The MathWorks, Natick, MA). The file nomenclature is described below. 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).

File name nomenclature

The name of each file in this data set provides information on the spectra type, species, sample location, year of spawning, age of larvae in days, shell number, position of laser on shell, and the wavelength of the laser. The key for file names is below:

Spectra:
sd = standardized to aragonite 1085 peak
pp = post-processed (flattened, noise reduction)

Species name:
AI = *Argopecten irradians*
CG = *Crassostrea gigas*
CV = *Crassostrea virginica*
GG = *Gemma gemma*
GD = *Geukensia demissa*
IR = *Ischadium recurvum*
MT = *Macoma mitchelli*
MM = *Mercenaria mercenaria*
ML = *Mulinia lateralis*
MA = *Mya arenaria*
DF = *Mytilopsis leucophaeata*
OL = *Ostrea lurida*
RC = *Rangia cuneata*
TP = *Tagelus plebeius*
SS = *Spisula solidissma*
PG = *Panopea generosa*

Sample location:
ARC = Aquaculture Research Corp. Dennis, MA
ME = University of Maine, Machias, ME
HI = University of Hawaii, Hilo, HI
AK = Alutiiqu Pride Shellfish Hatchery, Seward, AK
RCSL = Rutgers Cape Shore Lab, Cape May, NJ
WC = Whiskey Creek Shellfish Hatchery, Tilamook, OR
NL = North Lab, Cambridge, MD
HPL = Horn Point Lab Oyster Hatchery, Cambridge, MD
VIMS = Virginia Institute of Marine Science, Gloucester Point, VA
WHOI = Woods Hole Oceanographic Inst., Woods Hole, MA

Additional locations for some *Mytilopsis leucophaeata*, *Mulinia lateralis,* and *Macoma mitchelli:*
CT = Choptank River (Maryland, USA)

Year:
08 = 2008
09 = 2009
10 = 2010
11 = 2011

12 = 2012
13 = 2013

Day:
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

Shell number:
SXX where XX = number shell (1-20 usually)

Position number:
PX where X = position (some shells had multiple positions for spectra)

Wavelength:
532, 638, or 785 corresponds to laser light source used

Acknowledgements

Funding for this research was provided by the National Science Foundation (OCE-1240266).

Literature cited

Reisner LA, Cao A, Pandya AK (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., E. W. North, V. S. Kennedy, and S. N. White. *In prep*. Classifying bivalve larvae using shell pigments identified by Raman spectra. Analytical and Bioanalytical Chemistry.