

FEATURE ARTICLE

High resolution chemical contaminant characterization using optically-based methods

By: Grace Chang, Ph.D., Frank Spada, and Todd Martin, P.E.
Integral Consulting Inc.

The OPTICS (OPTically-based In-situ Characterization System; U.S. Patent No. 11079368) tool integrates commercial, off-the-shelf, in situ optical and water quality sensors, periodic discrete surface water sampling, and a multi-parameter statistical prediction model to provide high-resolution characterization of surface water chemicals of concern (COCs) (Chang et al. 2018a, b). The OPTICS methodology is suitable for addressing a wide range of questions at contaminated sediment and surface water sites (e.g., Blake et al. 2007; Bridges et al. 2008), including, but not limited to:

- Where are COCs coming from and where are they going?
- Could erosion of the sediment bed lead to the exposure of buried contamination?
- Will sediment transport and water movement lead to the redistribution of contamination within the site, or movement of contamination off site?
- Will natural processes lead to the burial and isolation of contamination by relatively clean sediment?
- If a site is actively remediated, could sediment transport lead to the recontamination?
- Are control measures effective at reducing contaminant transport?

The novel use of optically-based in situ monitoring for high-resolution, robust derivation of chemical properties allows for quantification of surface water COC concentrations over unprecedented temporal and spatial scales.

The principle behind OPTICS is based on the relationship between optical properties and the nature of particles and dissolved material in the water column. Chemical contaminants such as PCBs and heavy metals are hydrophobic in nature and tend to sorb to materials in the water column, which have unique optical signatures (e.g., Agrawal and Pottsmith 2000; Boss et al. 2001a, b; Twardowski et al. 2001; Babin et al. 2003; Coble et al. 2004; Sullivan et al. 2005; Chang et al. 2006; Briggs et al. 2013; Slade and Boss 2015). Further, chemical-associated material often covaries with a system's biophysical processes, which can be assessed using commercially available optical and water quality sensors. In situ optical and water quality measurements can thus be related to measured dissolved and particulate concentrations of contaminants in the water column through statistical modeling techniques. OPTICS is analogous to the empirical derivation of total suspended solids concentration (TSS) from optical turbidity using traditional linear regression (e.g., Rasmussen et al. 2009).

President's Corner



Maggie Stack

Hello SoCal SETAC! I hope everyone's year has started off strong, with much to look forward to in 2024. Just like so many people, I find the start of the new year to be a productive time to reflect on my goals – for both career and life – and that reflection can lead to reinvigoration about research and experiences. We can think about incorporating new changes and tools into our research, asking new questions, and pushing our field forward. I'm excited to see

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(Clickable links)

FEATURE ARTICLE (continued)

However, rather than deriving one response variable (TSS) from one predictor variable (turbidity), OPTICS involves derivation of one response variable (e.g., PCB concentration) from a suite of predictor variables (e.g., turbidity, temperature, salinity, and fluorescence of dissolved organic matter) using multi-parameter statistical regression).

Several OPTICS studies have been conducted by U.S. Geological Survey (USGS) scientists and Integral Consulting Inc. (Integral). USGS researchers, Bergamaschi et al. (2011; 2012a, b), assessed heavy metal dynamics in a tidal wetland in the San Francisco Bay Delta, California, as well as in a mangrove dominated estuary in the Everglades, Florida. Integral performed OPTICS studies at multiple lacustrine, riverine, estuarine, and coastal contaminated sites.

The Berry's Creek Study Area (BCSA; New Jersey) OPTICS study was conducted to understand COC sources and transport mechanisms to develop an effective remediation strategy. OPTICS successfully extended periodic discrete surface water samples to continuous, high-resolution measurements of PCBs, mercury, and methylmercury to elucidate COC sources and transport throughout the BCSA tidal estuary system (Chang et al. 2018b). OPTICS provided data at resolution sufficient to investigate COC variability in the context of physical processes (Figure 1).

The results facilitated focused and effective site remediation and management decisions that could not be determined based on periodic discrete surface water samples to continuous, high-resolution measurements of PCBs, mercury, and methylmercury to elucidate COC sources and transport throughout the BCSA tidal estuary system (Chang et al. 2018b). OPTICS provided data at resolution sufficient to investigate COC variability in the context of physical processes (Figure 1). The results facilitated focused and effective site remediation and management decisions that could not be determined based on periodic discrete samples alone, despite over seven years of monitoring at different locations throughout the system over a range of different seasons, tidal phases, and environmental conditions.

OPTICS was applied at the South

River (Virginia) to quantify sources of legacy mercury in the system that are contributing to recontamination and continued elevated mercury concentrations in fish tissue.

OPTICS provided information necessary to identify mechanisms for COC redistribution and to quantify the relative contribution of each mechanism to total mass transport of mercury and methylmercury in the system. Continuous, high-resolution COC data afforded by OPTICS helped resolve baseflow daily cycling that had never before been observed at the South River, and provided data at temporal resolution necessary to verify storm-induced particle-bound COC resuspension and mobilization through bank interaction (Chang et al. 2018a) (Figure 2). Daily cycling is hypothesized to be the result of nocturnal bioturbation, potentially from crayfish feeding activities.

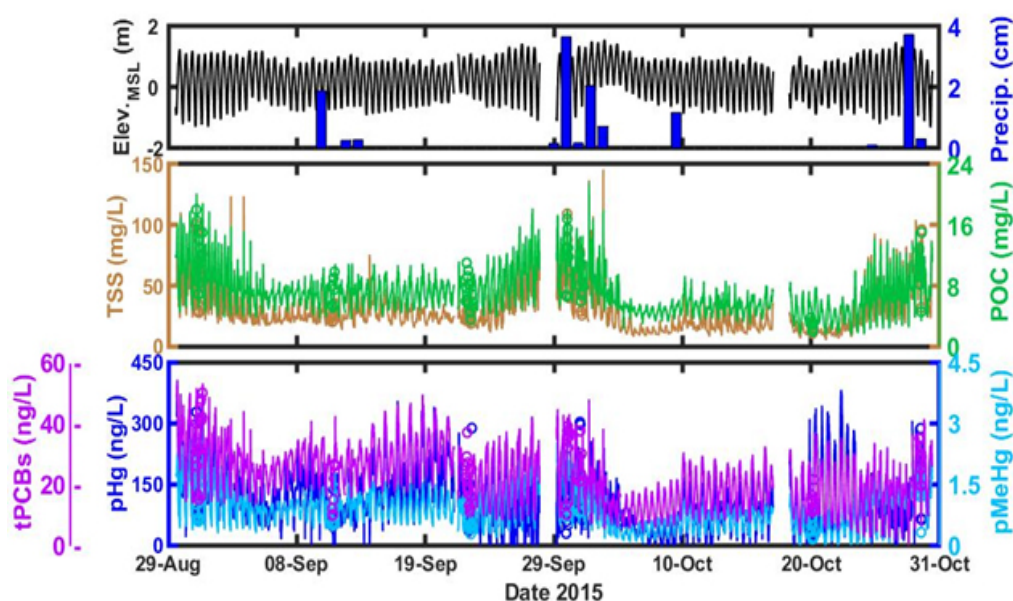


Figure 1. High temporal resolution COCs and solids concentration derived using OPTICS in the context of environmental processes at the Berry's Creek Study Area. Top: Water level and

FEATURE ARTICLE (continued)

In addition to high temporal resolution studies, Integral has used OPTICS to monitor stormwater plumes and solids and residuals impacts associated with environmental dredging operations (Chang et al. 2013; USEPA 2016). Results from these studies included accurate mapping and characterization of the spatial extent, concentration, and volume of COCs in plume waters (Figure 3), as well as quantification of the mass of residuals generated during dredging.

These and other successful studies yielded high temporal and spatial determinations of COC concentrations, including for PCBs, mercury, copper, lead, DDx (dichlorodiphenyl-trichloroethane, -dichloroethylene, and -dichloroethane), and TCDDs (2,3,7,8-Tetrachlorodibenzo-p-dioxin), and enabled evaluation and characterization of COC dynamics, transport, and loading into and throughout surface waters at multiple contaminated sediment sites. These successful deployments provide confidence in OPTICS to provide cost-effective monitoring at sites impacted by a wide variety of chemical contaminants, to support site baselining, source control investigation and monitoring, remedial action evaluation, and monitoring of remedy effectiveness.

(References available upon request)

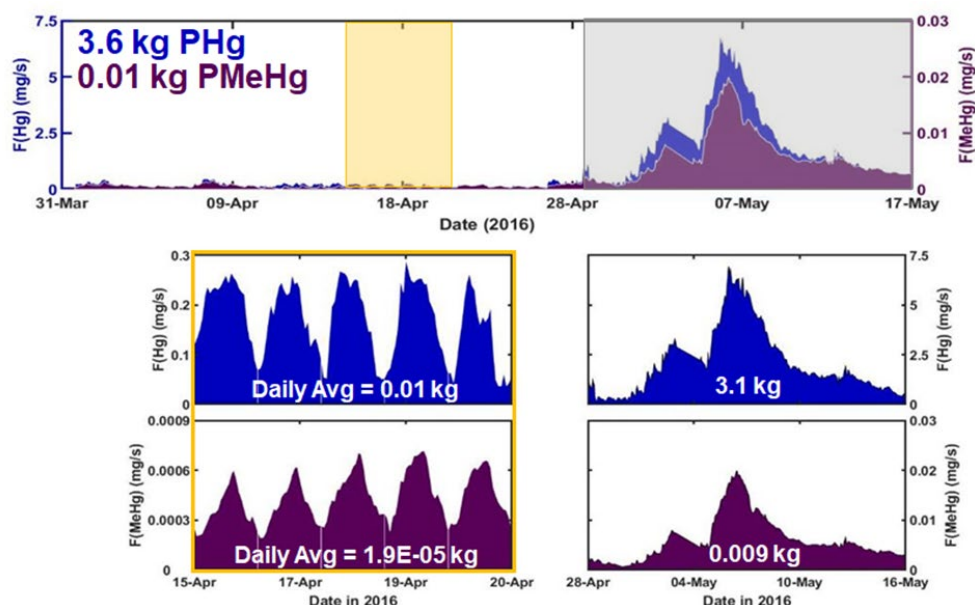


Figure 2. Flux (mass transport rate) of mercury and methylmercury, $F(\text{Hg})$ and $F(\text{MeHg})$, derived using OPTICS methods at South River during the 6-week monitoring period (top), baseflow daily cycling (lower left), and a storm event (lower right). The storm resulted in mass transport of 3.1 kg and 0.009 kg Hg and MeHg (87% and 84% of the total over the 6-week monitoring period). The average baseflow daily cycling mass transport was 0.01 kg and 1.9×10^{-5} kg Hg and MeHg. However, assuming daily cycling is continuous over the year, this could amount to 3.7 kg and 0.007 kg – comparable to the storm event.

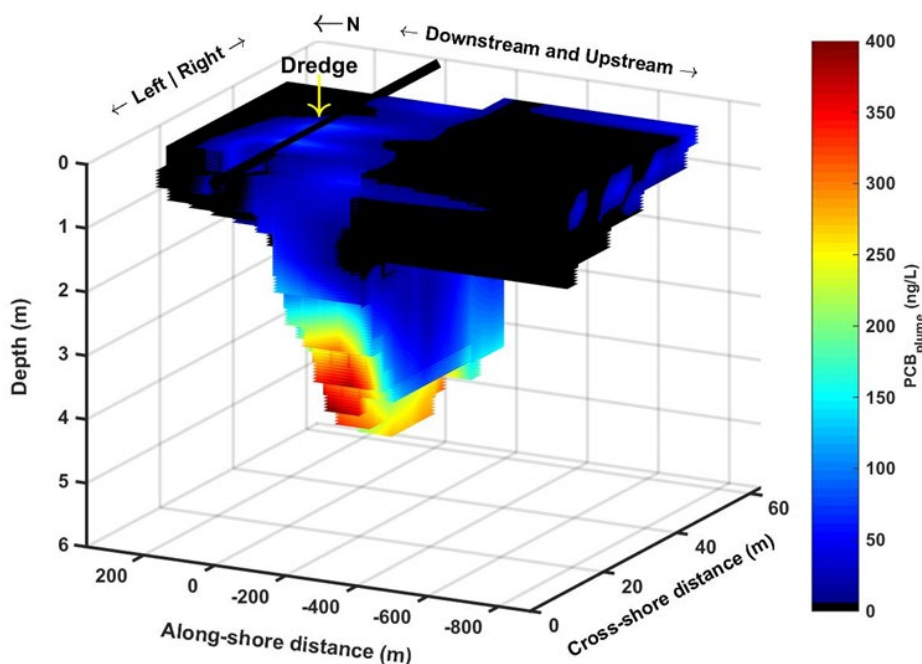


Figure 3. Spatially-resolved, OPTICS-derived unfiltered PCBs generated during environmental dredging. From data sets like this, the dredge plume can be characterized in terms of dredge plume volume, mass of residual COCs generated during dredging activities, and spatial extent of impact.

President's Corner, con.

what progress and changes we can make this year!

As evidenced in this quarter's newsletter, the SoCal SETAC community is consistently pushing forward to new developments in environmental science and chemistry. In our feature article, we hear from Integral Consulting Inc. about their OPTically-based In-situ Characterization System (OPTICS) tool. This technology can be used for optical and water quality monitoring to characterize chemicals of concern. They've developed the tool to address both long-term and very acute timescales, making it a powerful method for resolving daily water quality trends. But the new developments from the SoCal SETAC community don't stop there! In one of our Paper Highlights, we hear from one of our own student board members, Evan Tjeerdema. His team at UCSD/Scripps Institution of Oceanography has been working to update the urchin bioassay so that it can be used at the same level as zebrafish and other model organisms that are important for toxicologists. Through stable genetics and machine learning, his group showed that urchins can be used for high-throughput toxicology screening. It's exciting to see how new technology can help us to answer questions by providing better, more resolved data.

Not only is the new year a good time to integrate new technology and methods to our work, but it's also a time to consider how we can work together and collaborate to better answer questions. In our second Paper Highlight, we hear from SoCal SETAC member Chris Sayers about his work on mercury monitoring in neotropical birds. His work was a collaboration between 22 institutions and community partners. The findings were critical for understanding the effects of gold mining on neotropical birds, some of which are endangered. Collaboration in science can help us to answer questions more effectively and more efficiently. With so many environmental issues arising in today's world – climate change, the plastics problem, water scarcity – it's important to work together toward solutions.

Finally, one of the best things about the new year is that we have our SoCal SETAC Annual Meeting to look forward to once more! This year, we will be returning to the beautiful Lake Arrowhead for our 2-day conference from April 21-23. Keep an eye out for the call for abstracts and registration. And, if you or your organization are interested in becoming a sponsor for the Annual Meeting, you can find more information on our website. We can't wait to hear about the progress and research you've all been making over the past year. As always, thank you for your continued support of our community and we can't wait to see you in April!

Join us March 17, 2024 for our Spring Dinner Meeting in Carlsbad, CA!

We are excited to host an evening event as students present 5-minute lightning talks on their work and to provide a venue for networking opportunities.



Additional details and registration:

[Spring 2024 Dinner Meeting | socal-setac](https://www.socal-setac.org/Spring2024DinnerMeeting)



MEET THE BOARD

Sean Anderson, PhD

**Professor of Environmental Science and
Resource Management, CSU Channel Islands
Director, PIRatE Lab**



Some of SoCal SETAC Board Member Sean Anderson's first experiences in science swirled around toxicological challenges and projects. He cut his teeth as an undergrad on efforts to monitor in situ impacts of produced water from offshore oil wells in the Santa Barbara Channel. From SCUBA-based sampling of infaunal communities to running Mussel Watch stations and laboratory analyses, toxicology informed much of his early thinking and training at UC Santa Barbara. As he transitioned to graduate school at UC Los Angeles, he kept an active foot in the ecotoxicology world. All of this was supported by the now-defunct University of California Toxic (UCTSRTP) Substances Research and Teaching Program, a program funded directly from the state legislature to make sure we always had a cadre of toxicology experts on hand should the state have an emergency needs to assure California was positioning researchers to better understand/explore emerging toxicity challenges across the state.

Soon after starting his current faculty position at CSU Channel Islands, Sean started a new long-term project in New Orleans and coastal Louisiana, restoring bottomland hardwood forest wetland and food systems in the wake of Hurricane Katrina. That brought him to a celebration of a program funneling money into large-scale wetland restoration efforts in the lower Mississippi delta a mere 100 km from the Macondo Prospect Wellhead in Mississippi Canyon Block 252 and 30 hours before the start explosion that initiated the largest marine oil spill in U.S. History. As he crafted a national working group to help inform the toxicological understanding of the spill, he drew heavily upon his California ecotoxicology training. Many of the agency folks tasked to spill response (mostly from non-toxicology focused units in the Department of the Interior or Commerce) had been trained in California by the very same UCTSRTP and were no strangers to SETAC. That Deepwater Horizon Oil Spill Ecotoxicology working group was instrumental in helping contextualize the spill and assure key sampling was happening at the correct locations to better understand oil spill impacts.

Much of Sean's current ecotox efforts are focused on microplastics and on environmental justice components of pollution exposures. His colleagues and students and CSU Channel Islands have been documenting environmental concentrations and composition of microplastics in sediments, coastal waterbodies, air masses, and beer for the last decade. His newest line of research, inspired by pandemic lockdowns, has been a very long-term and very deep dive in cocktails. As with most things he has studied over the years, the toxicology of cocktails appears to be all about the dose-response curve; he is hunting for an appropriate journal to publish this earth-shattering revelation!



(Top) Sean Anderson counting Lost Island duck nests.

(Left) Sean showing his colors during restoration efforts in New Orleans, LA.

Paper Highlights

Our “Paper Highlights” showcase recent publications by Chapter members. This quarter, we share highlights from Chris Sayers from the Tingley Lab at UCLA and recent graduate student scholarship awardee; and Evan Tjeerdema of the Hamdoun Lab at SIO UCSD, and a SoCal SETAC board member.

Mercury in Neotropical birds: a synthesis and prospectus on 13 years of exposure data

By Chris Sayers

Paper link: <https://link.springer.com/article/10.1007/s10646-023-02706-7>

Mercury is a persistent environmental pollutant that poses a significant threat to human health and biological diversity on a global scale. While there has been a great deal of geopolitical progress to reduce mercury emissions across the Global North, emissions have skyrocketed throughout the Global South in recent decades due to mercury’s use in artisanal and small-scale gold mining. Following the 2008–2009 global financial crisis and subsequent market shifts, gold mining has rapidly expanded as a promising economic opportunity for developing nations, but can compromise human welfare and biodiversity conservation across the tropics as the largest anthropogenic source of mercury pollution. The Neotropics, in particular, produce over 40% of all mercury emissions from gold mining, while supporting 60% of all terrestrial species. Despite this problematic overlap, there has been little investment to study the biotic consequences of this industry, nor how mercury could contribute to ongoing biodiversity losses. Due to their global distribution and sensitivity to pollution, birds provide a valuable opportunity as bioindicators to begin resolving these knowledge gaps.

We assembled and synthesized the largest database on Neotropical bird Hg concentrations ($n = 2,316$) and established exposure baselines for 322 bird species spanning nine countries across Central America, South America, and the West Indies. By quantifying Hg prevalence and variation across bird species and functional traits, this research provides critical baseline knowledge for terrestrial Hg biomagnification in the Neotropics. Importantly, our study highlights alarming mercury bioaccumulation at gold mining sites—a wake-up call for tropical bird conservation—and identifies high priority taxa that should serve as bioindicators in future monitoring efforts.



A Black-spotted Bare-eye (*Phlegopsis nigromaculata*) captured next to an artisanal gold mine in Madre de Dios, Peru. © Chris Sayers

This study would not have been possible without a collaborative research network of 36 scientists spanning 22 institutions and seven countries, the Tropical Research for Avian Conservation and Ecotoxicology (TRACE) Initiative. Through sharing of expertise, funding, resources, data, and authorship among collaborators, TRACE can: (1) produce, provide unified access to, and disseminate emerging Pantropical data on biotic contamination to better inform bird conservation, and (2) generate crucial research capacity and leadership opportunities in tropical nations. For more information about how to contribute to TRACE, please visit: <https://briwildlife.org/TRACE/>.

This publication contributes to a special issue on global mercury exposure to biodiversity in Ecotoxicology, which will directly inform UN Secretariats as they improve the efficacy of the Minamata Convention on Mercury and Convention on Biological Diversity.



A typical artisanal gold mining operation in Madre de Dios, Peru. © Chris Sayers

PAPER HIGHLIGHTS (continued)

Semi-automated, high-content imaging of drug transporter knockout sea urchin (*Lytechinus pictus*) embryos

By: Evan Tjeerdema

Paper link: <https://onlinelibrary.wiley.com/doi/10.1002/jez.b.23231>

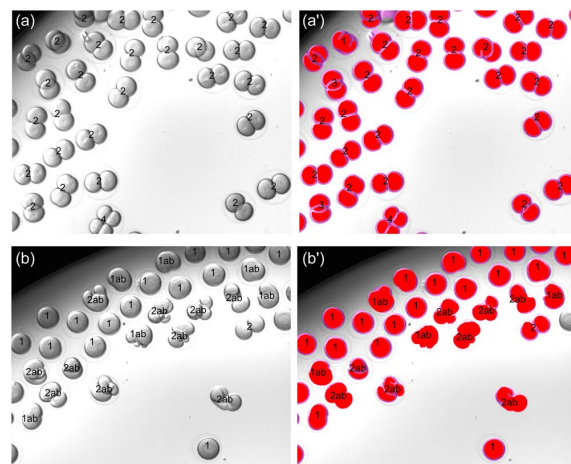
A defining feature of sea urchins is their extreme fecundity. Urchins produce millions of transparent, synchronously developing embryos, ideal for spatial and temporal analysis of development. This biological feature has long made them a key model organism for obtaining ensemble measurement of biochemical changes and the impacts of environmental pollutants on developing larvae. Indeed, EPA-approved sea urchin bioassays are standard in the repertoire of aquatic toxicologists. However, aquatic toxicology has not adopted the key developments of automation and stable genetics that have been transformative for other toxicological models, including zebrafish and rodents. Sea urchin bioassays are typically conducted by hand with wild-caught organisms of undefined genetic background. Together, these serve to bottleneck the utility of urchin bioassays by reducing the number of samples which can be processed and introducing variation in unknown genetic histories.

To address these gaps, we developed an “update” to the classical urchin bioassays, leveraging recent innovations in laboratory husbandry practices, stable genetics, and a semi-automated pipeline for conducting and assessing toxicant exposure on sea urchin embryos. Recent successes in our lab in growing a local sea urchin species, *Lytechinus pictus*, through multiple generations have resulted in the implementation of stable genetics in this organism via CRISPR/Cas9 mutagenesis. Following the creation of a sea urchin *ABCB1* (aka P-glycoprotein) knockout line, we developed a high-throughput assay to probe the role of this xenobiotic transporter in urchin embryos. We used high content imaging to rapidly acquire images of chemical-exposed embryos from which we could compare accumulation and toxicity of canonical substrates and inhibitors of the transporter, including fluorescent molecules and antimetabolic cancer drugs. This approach generated a high volume of imaging data, with over 5000 images of knockout and wildtype embryos acquired over the course of the study.

To measure responses from the resulting image data, we used a machine learning-based image analysis approach. This approach was characterized by nesting several convolutional neural networks, which rapidly classified embryos according to fluorescence or cell division. Our machine learning approach identified sea urchin embryos with 99.8% accuracy and determined two-cell and aberrant embryos with 96.3% and 89.1% accuracy, respectively. The results revealed that

ABCB1 knockout embryos accumulated the transporter substrate calcein 3.09 times faster than wildtypes. Similarly, knockouts were 4.71 and 3.07 times more sensitive to the mitotic poisons vinblastine and taxol, and EC50 values derived from machine learning did not significantly differ from those derived from manual assessment of embryos. Therefore, our novel urchin embryo bioassay pipeline was validated for control compounds, providing an example of how stable genetics, high content imaging, and machine learning-based image analysis can be used to exploit the fecundity and synchrony of sea urchins in imaging-based drug and toxicant screens.

As new toxicants of human environmental concern are continuously emerging, this update to the classical approach to urchin bioassays fits quite nicely within the arsenal of tools available for the aquatic toxicologist. The volume of samples which may be processed in our automated system outpaces manual approaches by at least an order of magnitude, dramatically increasing the number of compounds and concentrations which can be assessed, all the while reducing potential error introduced by the human scientist. Significantly, the introduction of stable genetics in this organism strengthens toxicity data by reducing noise and variation between animals (for sea urchin this can be as high as 5% allelic variation between individuals). The advent of sea urchin knockout lines for genes of human concern, like the xenobiotic transporter *ABCB1*, is poised to reveal targets of toxicity for novel environmental compounds and increase the depth of urchin toxicity beyond live/dead by targeting phenotypes associated with specific genes, molecular pathways, or mechanisms of action. Overall, the urchin bioassay pipeline described here represents a broadening of the horizons for aquatic toxicology in the volume of samples which can be assessed and the power of insights which can be derived from this classic toxicology model.



Examples of embryo phenotypes scored by the machine learning model. Annotations made by humans (a, b) are comparable to those achieved through our machine learning approach (a', b'). (adapted from Tjeerdema et al. 2023)

2024 Southern California Regional Chapter of the Society of Environmental Toxicology and Chemistry Annual Meeting

Mark your calendars! The SoCal SETAC Annual Meeting is back this April 21-23, 2024 at Lake Arrowhead, CA. Meeting registrations covers all fees, meals*, non-alcoholic beverages, beer and wine.

Deadlines to remember:

March 18: Abstract submission due

March 18: Early registration ends

April 5: Meeting registration closes

April 7: Reservations for UCLA Lake Arrowhead Lodge closes

More information can be found at: [2024 Annual Meeting | Registration \(socal-setac.org\)](https://socal-setac.org)

*Sunday includes dinner only; Monday includes breakfast, lunch, and dinner; Tuesday includes breakfast and lunch.

Training Courses!!

On Sunday, 21 April 2024, we will be offering two training courses.

Attend one or both and learn from world experts in our Chapter!

Sign up during the Annual Meeting Registration.

Course Titles:

- I. "The microplastics policy and regulation landscape: how to navigate it" (1:30-3:30 PM)
- II. "Spectroscopy fundamentals and best practices for analysis and reporting of microplastics data" (4:00-6:00 PM)

Instructors:

- Dr. Win Cowger, The Moore Institute for Plastic Pollution Research

Cost:

- Students:
1 session \$40;
both sessions \$70
- Non-student:
1 session \$60;
both sessions \$100



Register [Here!](https://socal-setac.org)

Meeting/Training Registration:



Abstract Submission:



CALENDAR OF EVENTS**March 2024**

March 11 - 14

39th Annual WasteReuse Symposium. Denver, CO, USA

[WasteReuse Association](#)

March 10 - 14

Society of Toxicology (SOT) 62nd Annual Meeting and ToxExpo. Salt Lake City, UT, USA [2024 SOT Annual Meeting and ToxExpo \(toxicology.org\)](#)

March 17 - 21

American Chemical Society (ACS): Many Flavors of Chemistry. New Orleans, Louisiana, USA (Hybrid)

[ACS Spring - American Chemical Society](#)

March 18 - 21

33rd Annual International Conference on Soil, Water, Energy, and Air. San Diego, CA, USA

[West Coast Conference | AEHS \(aehsfoundation.org\)](#)

March 24 - 27

Association of Environmental Professionals, Anaheim, CA, USA

[2024 AEP Conference - California Association of Environmental Professionals \(califaep.org\)](#)

March 17

SoCal SETAC Spring Dinner Meeting. Tortilla Mia, Carlsbad, CA, USA.

[Spring 2024 Dinner Meeting | social-setac](#)

April 2023

April 16 - 18

National Environmental Justice Conference and Training Program, Washington DC, USA

[National Environmental Justice Conference and Training Program \(thenejc.org\)](#)

April 21 - 23

Southern California Regional Chapter of the Society of Environmental Toxicology and Chemistry Annual Meeting (SoCal SETAC). Lake Arrowhead, CA, USA

[2024 Annual Meeting | Registration \(social-setac.org\)](#)



Don't forget to follow our LinkedIn page!

Connect with us to stay up-to-date on all events, job opportunities, grants, and more!

Southern California SETAC: <https://www.linkedin.com/company/southern-california-setac/>



May 2024

May 5 - 9

SETAC Europe 34th Meeting, Seville, Spain

[SETAC Europe Annual Meeting](#)

June 2024

June 2 - 6

Society for Freshwater Science Annual Meeting, Philadelphia, PA, USA

[SFS Annual Meeting](#) | [Society for Freshwater Science](#)

September 2024

September 18 - 22

SETAC Asia-Pacific 14th Biennial Meeting, Tianjin, China

[SETAC Asia-Pacific 14th Biennial Meeting](#)

October 2024

October 21 - 23

California Stormwater Quality Association (CASQA) 20th Annual Conference, Sacramento, CA, USA

[Annual Conference](#) | [California Stormwater Quality Association \(casqa.org\)](#)

October 20 - 24

SETAC North America 45th Annual Meeting, Fort Worth, TX, USA

[SETAC North America 45th Annual Meeting](#)

Have you checked out the Student Resources Page on the SoCal SETAC Website?

This page is available to help students find resources that will assist them in continuing to learn and engage with community and prepare for the next steps. Check it out and please email Leslie Nanninga, lnanninga@sandiego.gov if you have any additional resources or tips to share!

<https://www.socal-setac.org/student-resources>



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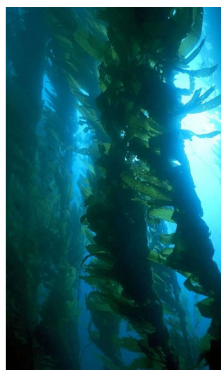
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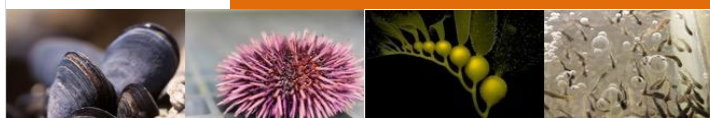


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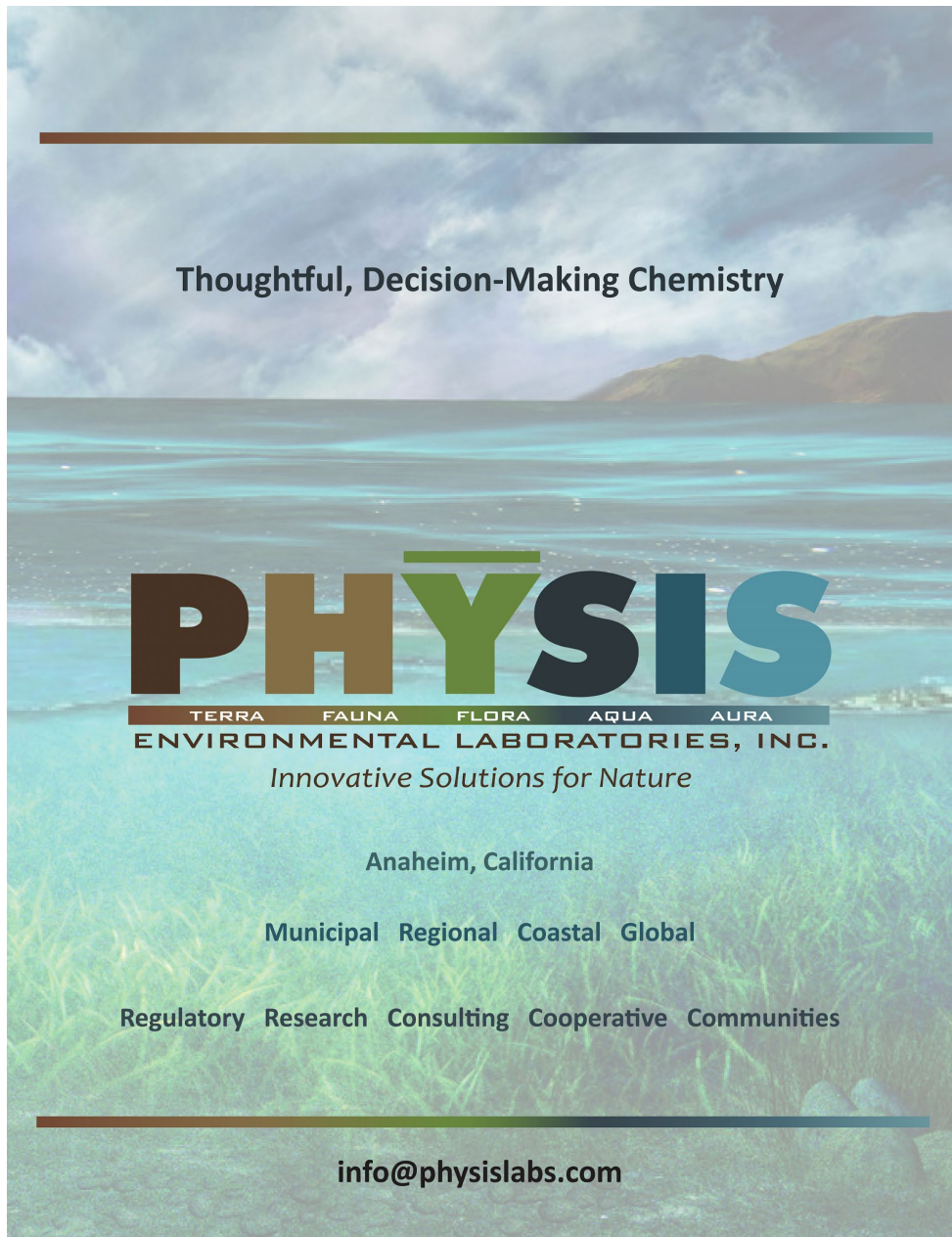
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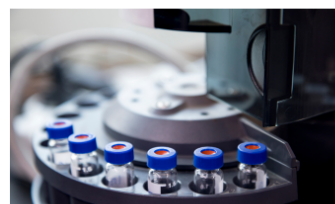
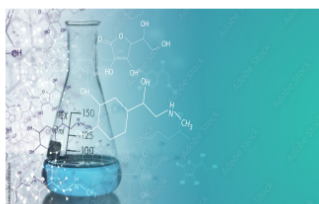
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