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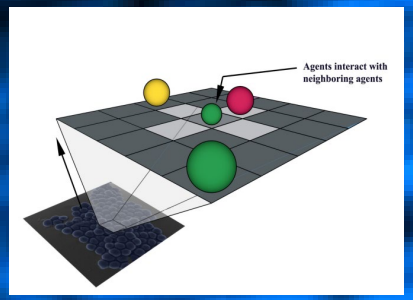
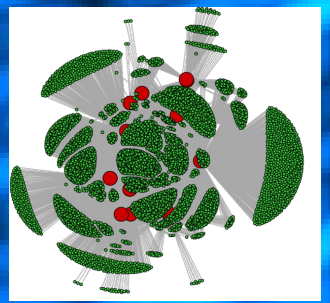
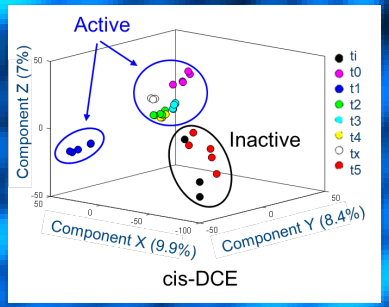
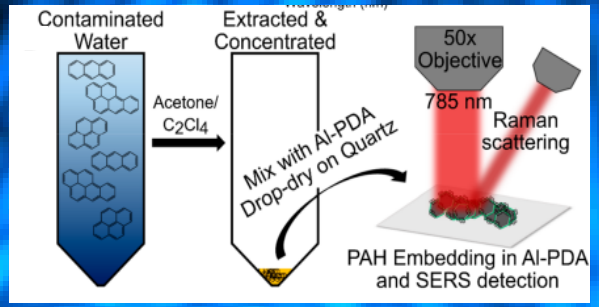
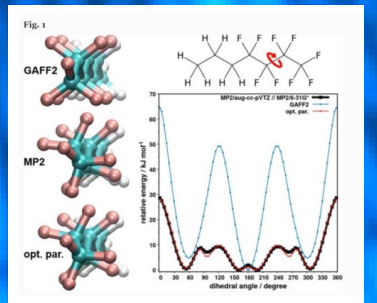
NIEHS Superfund Research Program (SRP) Machine Learning and Artificial Intelligence Activities

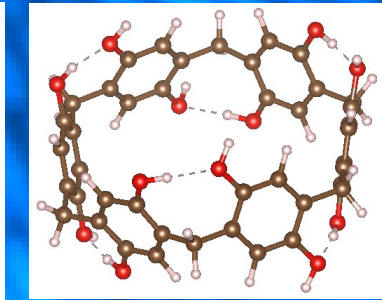












Heather Henry, Ph.D.
Health Scientist Administrator

Superfund Research Program
National Institute of Environmental Health Sciences (NIEHS)

National Institutes of Health • U.S. Department of Health and Human Services

Superfund Research Program Mandates

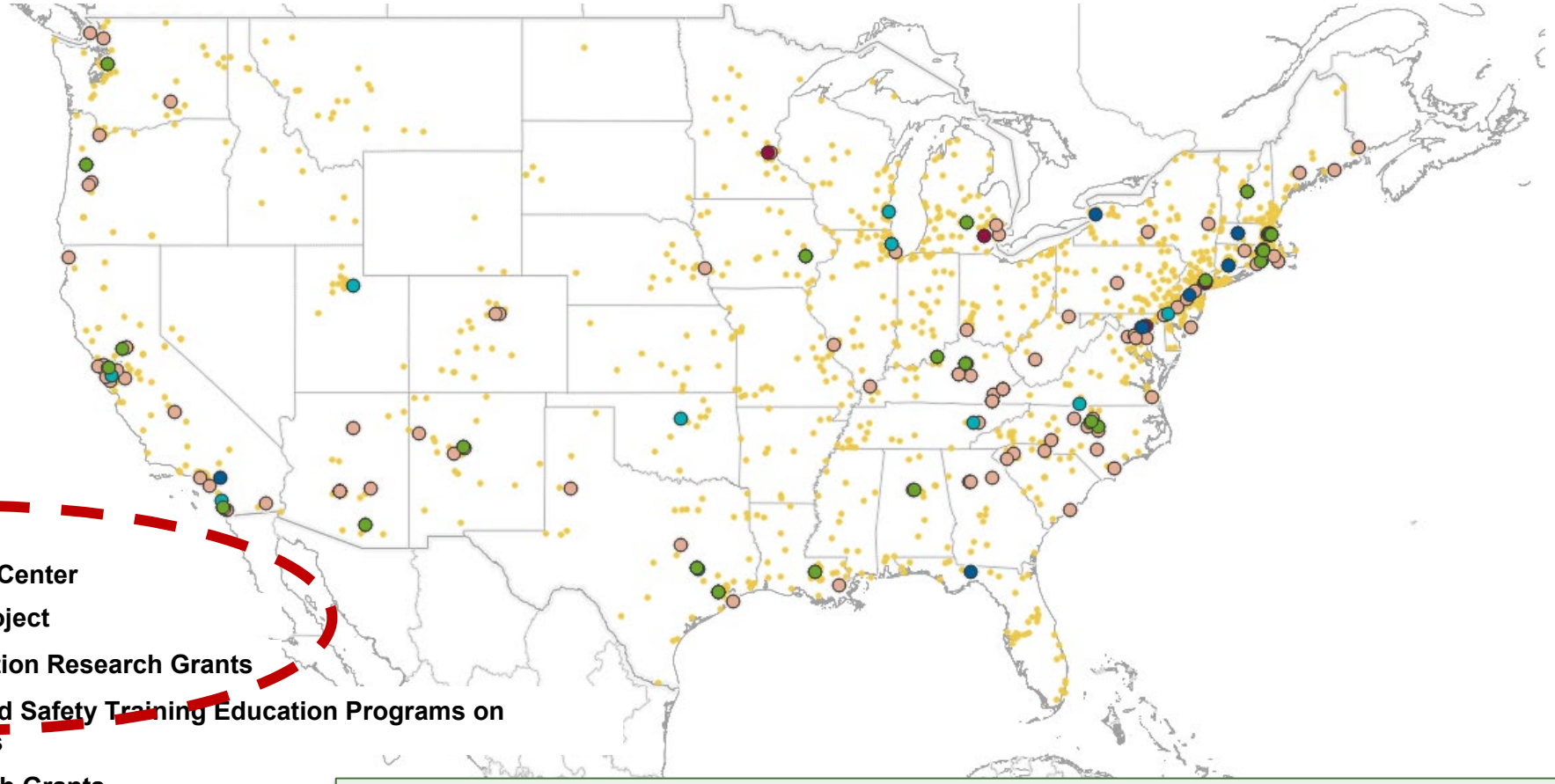
Integrating Health and Environmental/Engineering Sciences with Research Translation, Community Engagement, Data Science and Training

Health Effects	• Advanced techniques for the detection, assessment, and evaluation of the human health effects of hazardous substances
Assessing Risk	• Methods to assess the risks to human health presented by hazardous substances
Detection	• Methods and technologies to detect hazardous substances in the environment
Remediation	• Basic biological, chemical, and physical methods to reduce the amount and toxicity of hazardous substances

Artificial Intelligence and Machine Learning

- Contaminant Detection
- Gene/Enzyme Discovery
- Materials Design Optimization
- Geospatial/Ecosystem-level Information

Superfund Research Program



- Multi-project Research Center
- Individual Research Project
- Small Business Innovation Research Grants
- Occupational Health and Safety Training Education Programs on Emerging Technologies
- Time-Sensitive Research Grants
- Institutions that Partner with SRP Grantees
- Superfund Sites

Link to Map:
https://tools.niehs.nih.gov/srp/sites/www.cfm

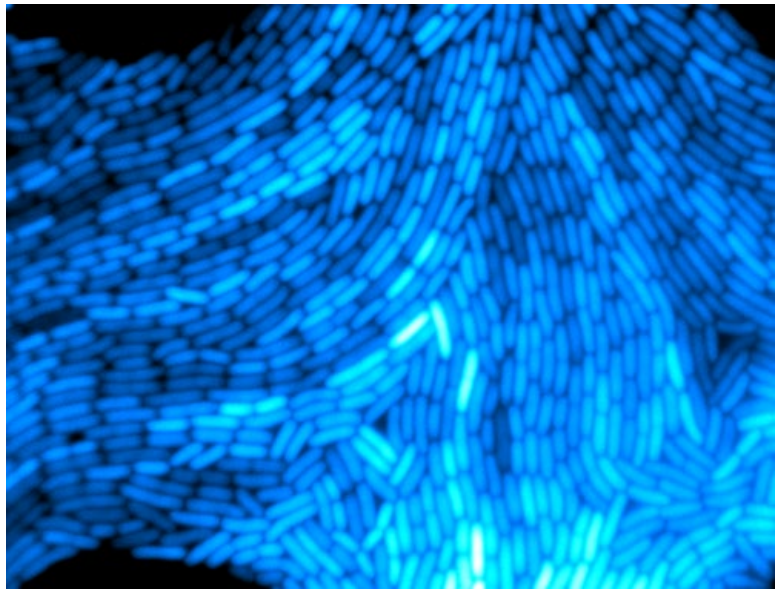
SRP Grantees: https://tools.niehs.nih.gov/srp/programs/index.cfm
SRP Funding Opportunities:
https://www.niehs.nih.gov/research/supported/centers/srp/funding/index.cfm

Quantitative Biosciences (QBiSci)

A Customizable Real-Time Biosensor for Continuous Monitoring of Water Contaminants

Scott Cookson, R43ES028993

- Developing "Qube" a customizable online biosensor microfluidic platform
  - Sensitive "sensor strains" (e.g. *E. coli*) customized to fluoresce when a specific target is present
  - Customized optics and image processing platform converts signal into concentration information
  - Process uses **machine learning** algorithm trained to recognize the type and amount of each contaminant present in continuous water stream, as well as sudden pulses and subtly varying concentrations.



QBiSci's "Qube" uses spatially-isolated microbial strains that fluoresce in presence of specific water contaminants

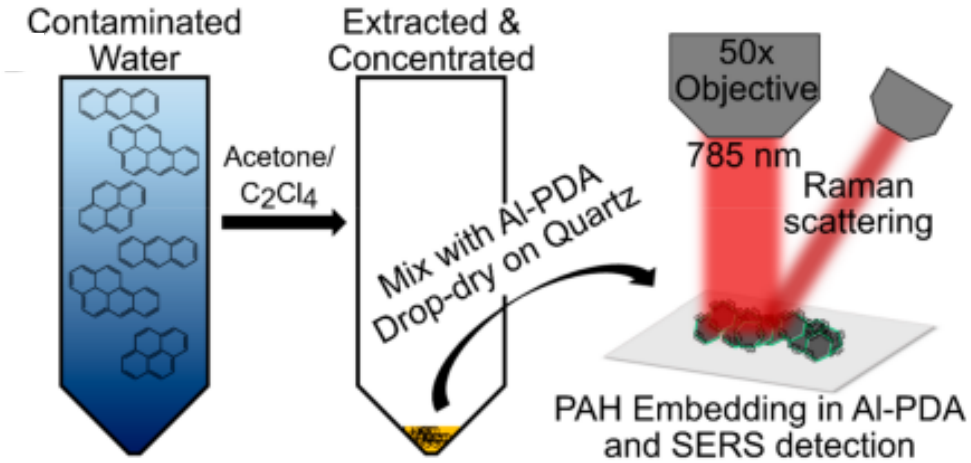
Phase 1 results (ppb): Arsenic (5), Cadmium (2), Uranium (300), Mercury (1), Lead (30), Nitrate (25), Nitrite (250), Ammonium (250), Phosphate (25). (See Progress Report 2020: https://tools.niehs.nih.gov/srp/programs/progress_report.cfm?Project_ID=R43ES028993)

Baylor College of Medicine

Streamlined Identification of PAHs/PACs in Environmental Samples Using Ultracompact Spectroscopy Platforms and Machine Learning Strategies

Naomi Halas (Rice University), Peter Nordlander (Co-PI, Rice University), Ankit Patel (Co-PI), P42ES027725

- Aluminum nanoengineered substrates for streamlined ultrasensitive PAH and PAC detection
  - Polydopamine (biomimetic polymer) selectively extracts and adsorbs PAH and PAC molecules onto the nanosensing platform
  - Uses **machine learning** to analyze Surface Enhanced Raman Spectroscopy (SERS) and Surface Enhanced Infrared Absorption (SEIRA) spectra signals
  - Ultracompact, ultrasensitive chemical analysis, identifies multiple analytes in a single sample, no need for separation and purification steps



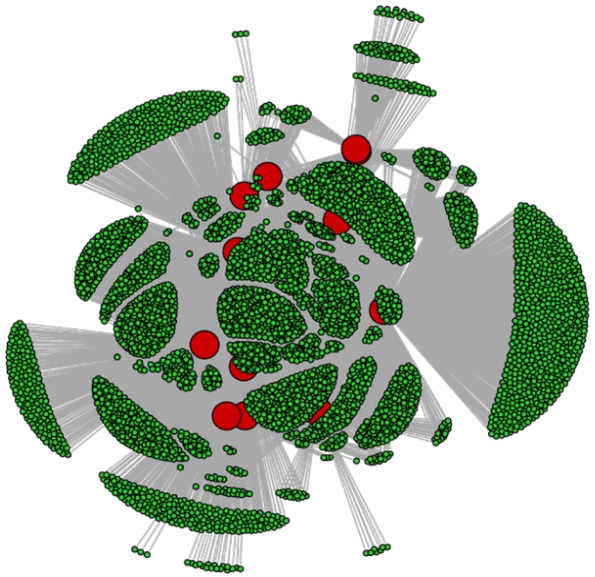
Renard et al., ACS Nano, 2019

Biomimetic polydopamine polymer inspired by mussel adhesive proteins

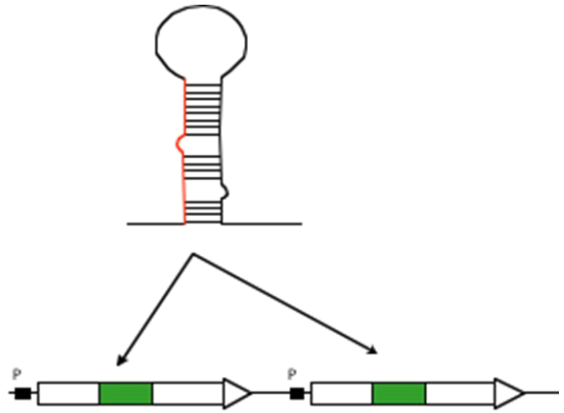
University of California, San Diego

Molecular Mechanisms of Heavy Metal Detoxification and Engineering Accumulation in Plants

Julian Schroeder, P42ES010337



- Machine Learning Approaches
  - New powerful screen to identify new genes, gene families, and network principles that function in **heavy metal** and **arsenic** resistance (Zhang et al., Nat Commun, 2018; Xie et al., Plant Cell Environ, 2021)
  - Developed genome-wide artificial microRNA libraries that can identify the genes, signal transduction pathways, and mechanisms underlying heavy metal(loid) accumulation in plants (Hauser et al., Plant Cell, 2013; Hauser et al., J Exp Bot, 2019)
  - Screened for genes involved in cadmium hyperaccumulation (Yu et al., Planta, 2021)
  - The UCSD artificial microRNA database is available online at: http://phantomdb.ucsd.edu/

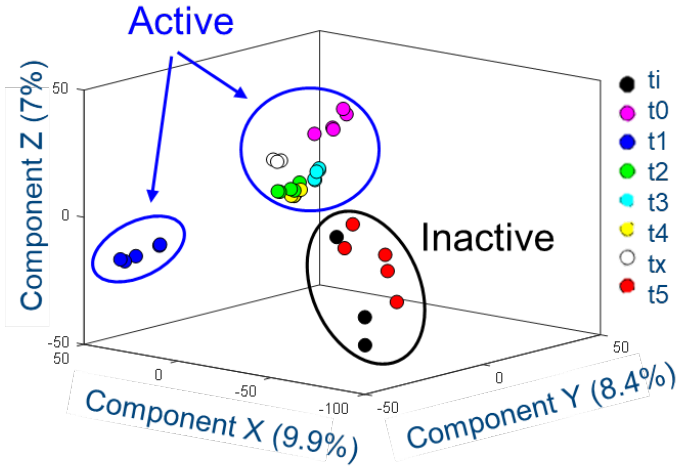


Microbial Insights

Expanding the Tool Box: Environmental Metabolomics Improves Decision Making and Management of Contaminated (Superfund) Sites

Dora Taggart, R43ES030669

- Sampling metabolomes from the environment and comparing profiles from different contaminated sites
- Identification of 80 – 100 known compounds in samples; thousands of unknown compounds
- Comparison of the overall metabolic profile of samples from different known conditions
- Use statistical analysis and pattern recognition to predict and understand activity of key degraders



cis-DCE

microbialinsights

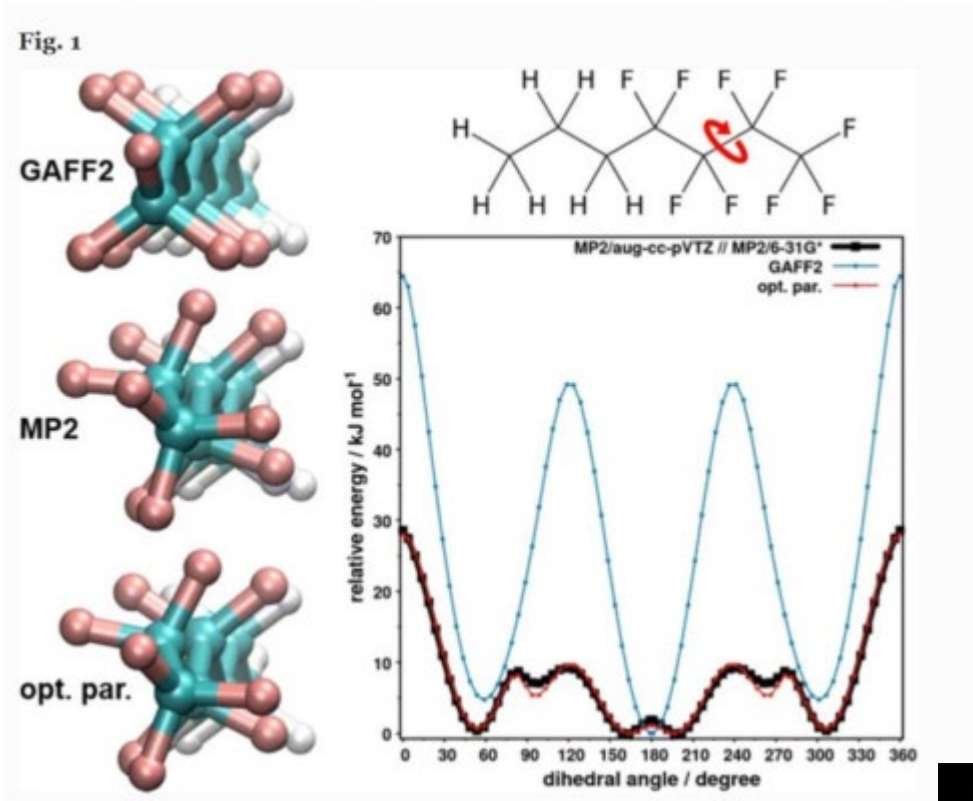
Commercializing technology: https://www.niehs.nih.gov/research/supported/centers/srp/news/2020news/monitoring_tools/index.cfm

Individual Research: SUNY at Buffalo

Model-aided Design and Integration of Functionalized Hybrid Nanomaterials for Enhanced Bioremediation of Per-and Polyfluoroalkyl Substances (PFASs)

Diana S. Aga, Ian Bradley, Nirupam Aich, Carla A. Ng (University of Pittsburgh), R01ES032717

- PFAS biodegradation using enriched microbial communities combined with catalytic hybrid nanomaterial pre-treatment.
- Using molecular modeling and quantum chemistry simulations to bring mechanistic insight into specific PFAS-surface and PFAS-enzyme interactions.
- Screening for enzymes capable of degrading structurally diverse PFAS.

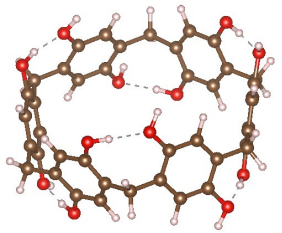


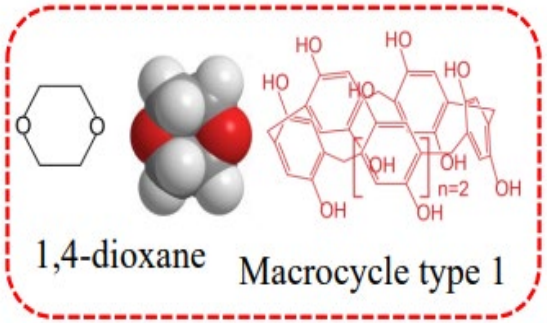
Florida State University

Enhancing Bioremediation of Groundwater Co-contaminated by Chlorinated Volatile Organic Compounds and 1,4-Dioxane Using Novel Macrocyclic Materials

Youneng Tang, Yuexiao Shen (Texas Tech University), R01ES032692

- Synthesizing macrocyclic materials to enhance bioremediation of CVOCs and 1,4-dioxane.
- Developing mathematical models of macrocyclic sorbents and using computational approaches to gain insight into binding mechanisms.
- Using 1,4-dioxane-metabolizing culture for bioremediation that is more effective at low, environmentally relevant concentrations.



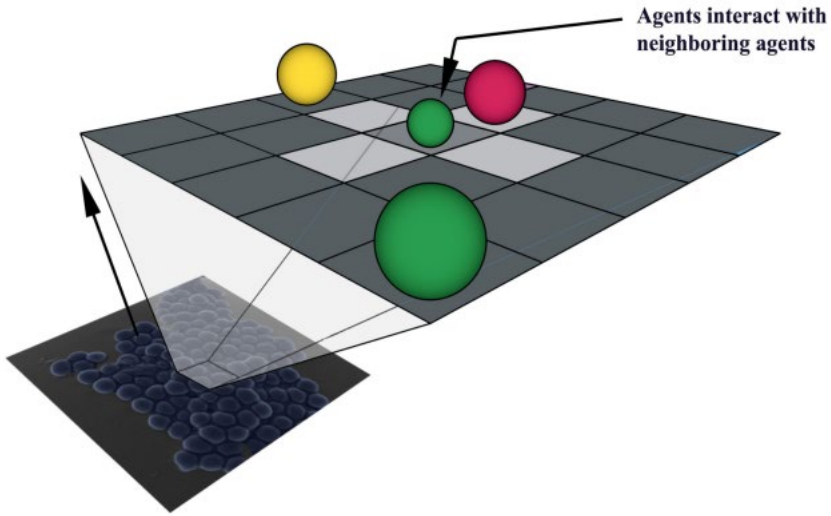


Small Business: Microvi Biotechnologies, Inc.

An Agent-Based Modeling Platform for Environmental Biotechnology

Fatemeh Shirazi, R44ES026541

- Developed EnviroABM, an agent-based modeling platform that predicts interactions between microbial ecosystems and hazardous groundwater contaminants.
- Integrating publicly available databases with machine learning to develop tailored microbiomes for degrading mixtures of polyfluorinated compounds (PFCs), volatile organic compounds (VOCs), and heavy metals separately.
- Developing a continuous-flow, lab scale prototype for real-world bioremediation using Microvi's Multi-Zone MicroNiche Engineering (MZ-MNE) platform, which uses biological organisms to degrade organic compounds into harmless by-products.



Northeastern University

Effect of Extreme Weather on Potential Exposure of Contaminant Mixtures in Karst Water Systems

Ingrid Y. Padilla (University of Puerto Rico at Mayaguez)
Co-Investigators: Damian E. Helbling (Cornell University), Philip Larese-Casanova, Raul Macchiavelli (University of Puerto Rico at Mayaguez), Dorothy Vesper (West Virginia University) **P42ES017198**

- Geospatial **artificial intelligence and machine learning** to discover patterns in groundwater flow and contaminant transport in karst systems in Puerto Rico
- Construct predictive models of the fate and transport of contaminants in groundwater, and aims at classifying damage after disasters, including near Superfund sites after Hurricane Maria
- Part of a KC Donnelly award to Luisa Feliciano for collaboration with Geospatial Research Laboratory, Engineering Research and Development Center, US Army Corps of Engineers

Luisa Feliciano, KC Donnelly award winner using ML/AI to study impacts of Hurricane Maria with US ACE

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Questions: Heather Henry
heather.henry@nih.gov

Special thanks to Megan Boland, MDB, Inc.

SRP Webpage:
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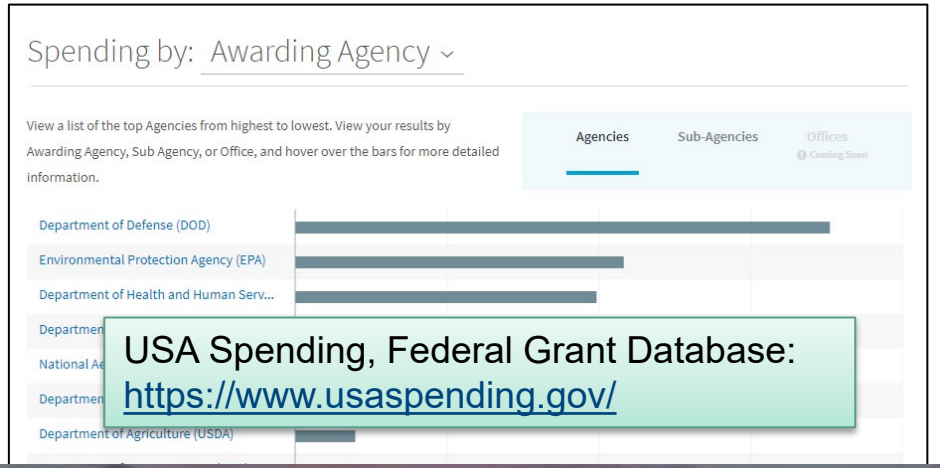
SRP Funding Opportunities:
https://www.niehs.nih.gov/research/supported/centers/srp/funding/index.cfm

Ongoing NIEHS Solicitations

Small Business Innovative Research Grants with new initiatives on Climate Change

Mechanism for Time-Sensitive Research Opportunities in Environmental Health Sciences (R21) Monthly receipt dates



USA Spending, Federal Grant Database:
https://www.usaspending.gov/

SRP 35th Anniversary Annual Meeting

System AppRoAches for Innovative and Inclusive Environmental Health Solutions

December 14 – 16, 2022 Raleigh, NC

Current SRP Funding Mechanisms

Multi-Project Centers (P42)	• Designed for integration across disciplines: Biomedical and Non-Biomedical Research; Community Engagement, Research Translation, and Training. Basic and application-oriented.
Individual Research Projects (R01)	• Designed to address specific issues to complement the multi-project research program; tackle issues of emerging concern for Superfund.
Small Business Research Grants (SBIR) (R43-44)	• Foster the commercialization of technologies, relevant to hazardous substance clean-up and monitoring.
Time-Sensitive Grants (R21)	• Research on unpredictable events with a limited window to collect samples or data.
Conference Grants (R13)	• Provides funding for conferences related to SRP mandates.
Supplement Awards	• Trainee externships/work exchanges, technology transfer opportunities.

SRP Grantees: https://tools.niehs.nih.gov/srp/programs/index.cfm
SRP Funding Opportunities: https://www.niehs.nih.gov/research/supported/centers/srp/funding/index.cfm