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The quest for average water:


Determining Representative Surface Water Concentrations for Chemical Risk Assessment Prioritization

1: Center for Computational Toxicology and Exposure, U.S. Environmental Protection Agency;

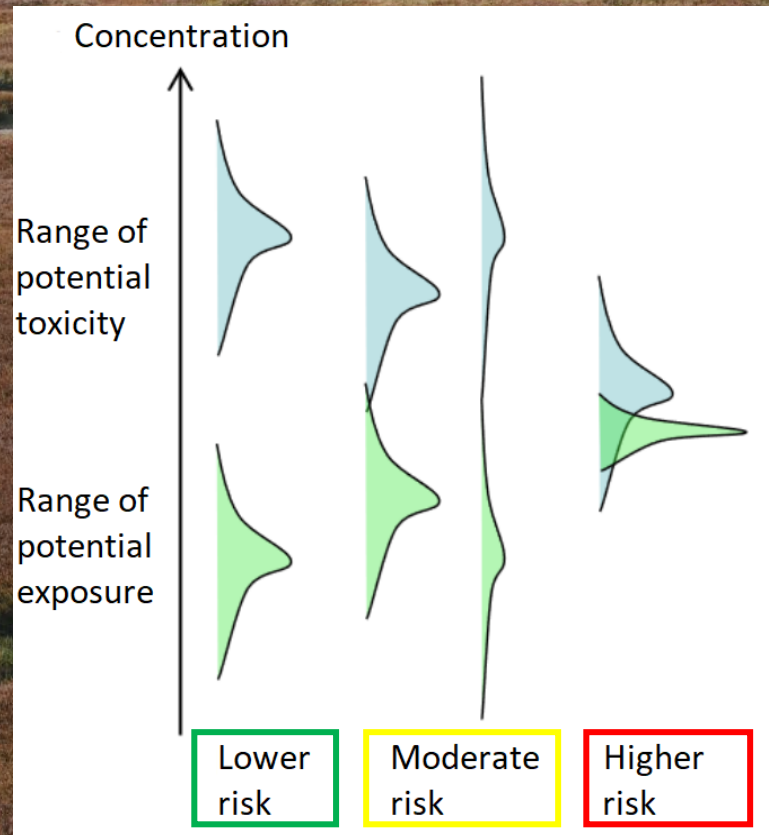
2: Department of Environmental Sciences and Engineering, UNC Chapel Hill; 3: Oak Ridge

Institute for Science and Education, Oak Ridge, Tennessee; *Emeritus

This presentation does not necessarily reflect U.S. EPA policy.

An aerial photograph of a vast, flat landscape, likely a wetland or marsh. The terrain is covered in dense, low-lying vegetation that appears brownish-green, suggesting a dry or autumnal season. A narrow, winding river or stream flows through the center of the landscape, creating a meandering path. The water in the stream is a light, silty grey color. The overall scene is one of a remote, natural environment.

Why do I want to find
average water?



Even a highly uncertain estimate can provide enough information to rank chemicals for risk prioritization.

Risk prioritization:

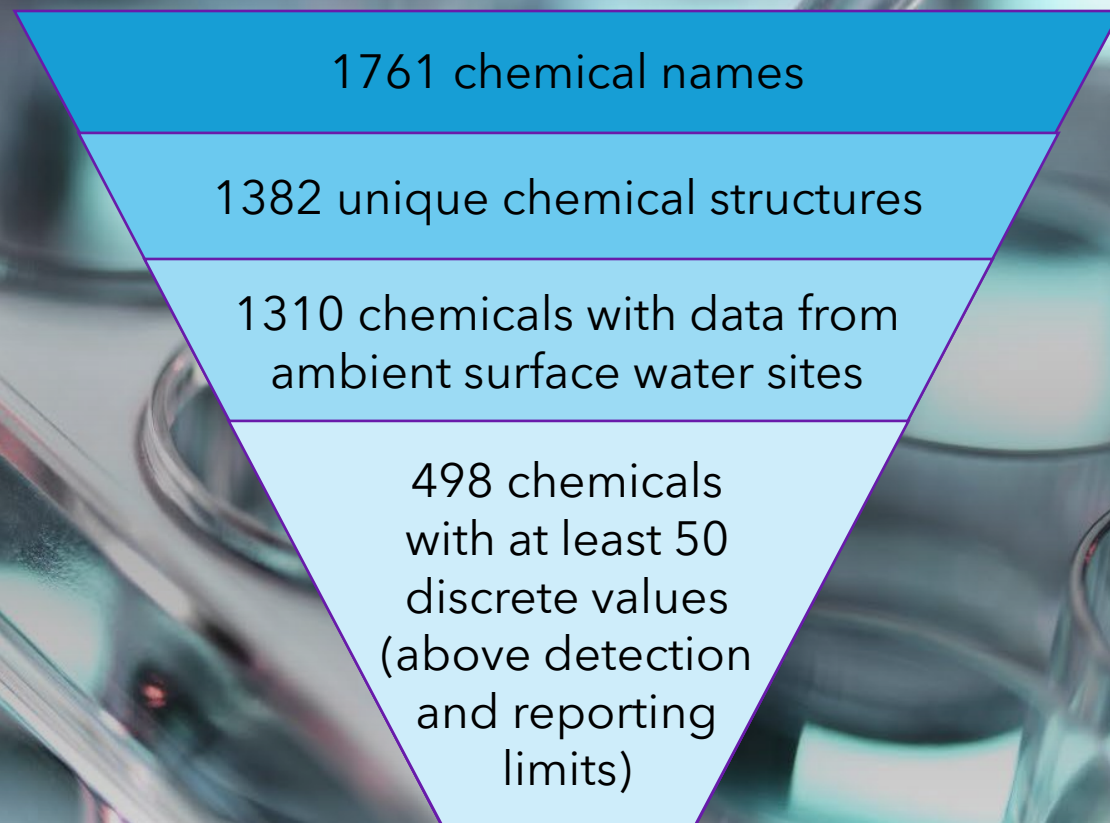
National average surface water concentrations of anthropogenic chemicals can be used to estimate one type of potential **exposure**: a component needed to identify the most important chemicals for a thorough risk evaluation.



What data will help me find
average water?

Representative samples:

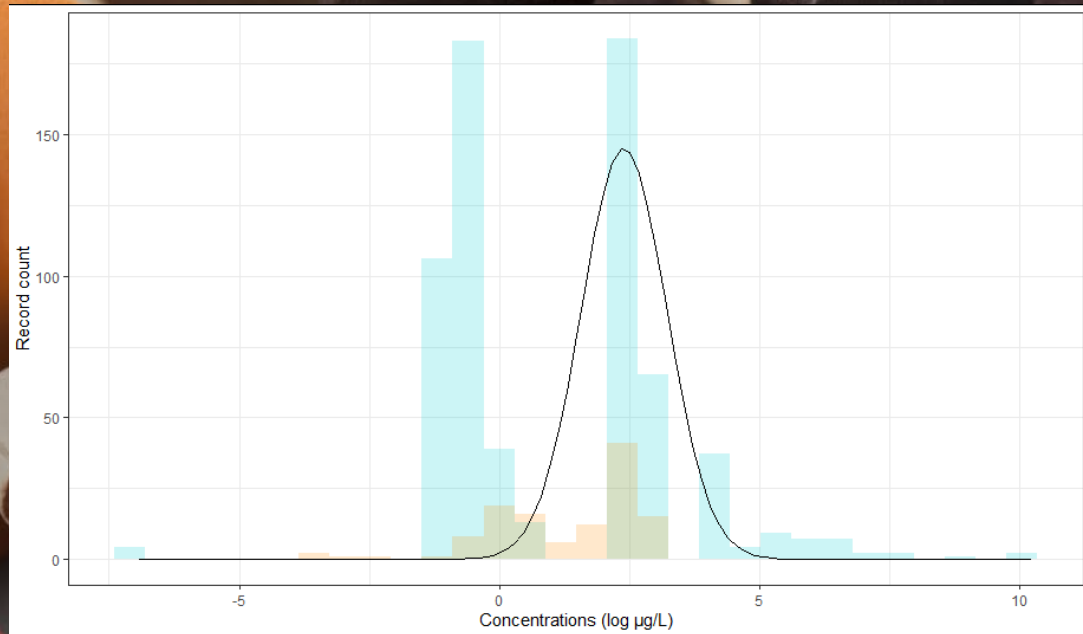
I designed an automated workflow to pull and clean National Water Quality Portal records from 2008-2018 for all organic chemicals from sites or activities that would yield ambient concentrations from across the U.S.



The number of chemicals for which estimates could be made decreased with each data cleaning step.



How will I get representative
values from my data?



Estimated representative distribution for 1,4-Dioxane, with histogram showing censored (aqua) and uncensored (orange) data

Mean of the lognormal maximum likelihood estimate:

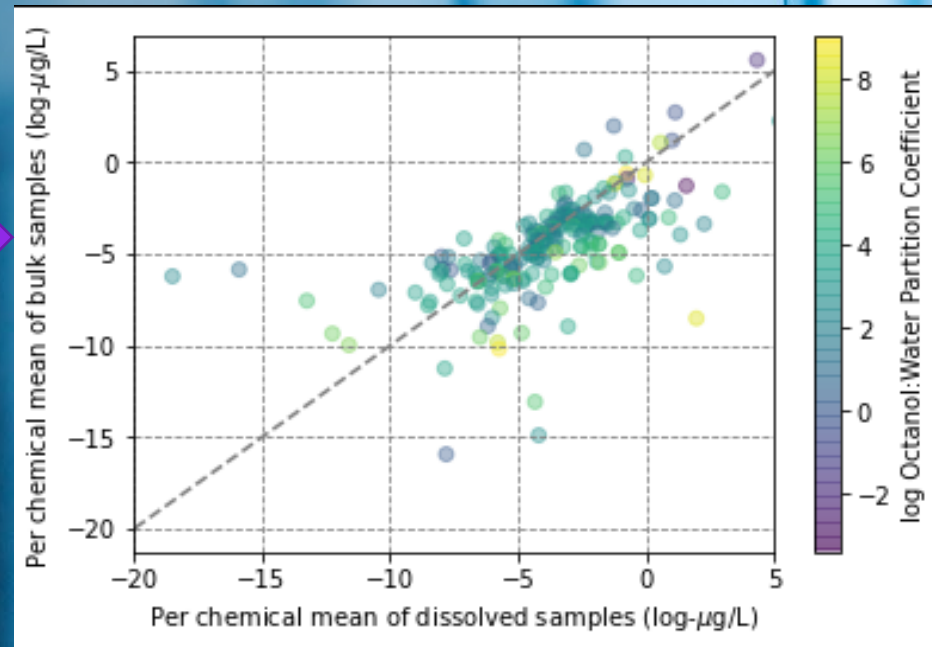
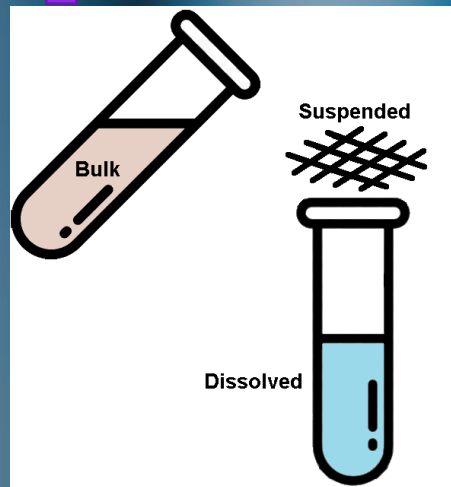
Records for most chemicals were over 80% censored (below a detection or reporting limit).

We needed a method that could incorporate knowledge from both discrete values and left-censoring limits.

The image shows a laboratory setting with several glass test tubes. In the foreground, a test tube is tilted at an angle, containing a vibrant red liquid. The background is filled with other test tubes, some containing clear liquids and others with darker substances, all slightly out of focus. The overall color palette is dominated by blues and greys, with the red liquid providing a strong contrast.

Do different sample types
change the average?

Different sample types had similar averages



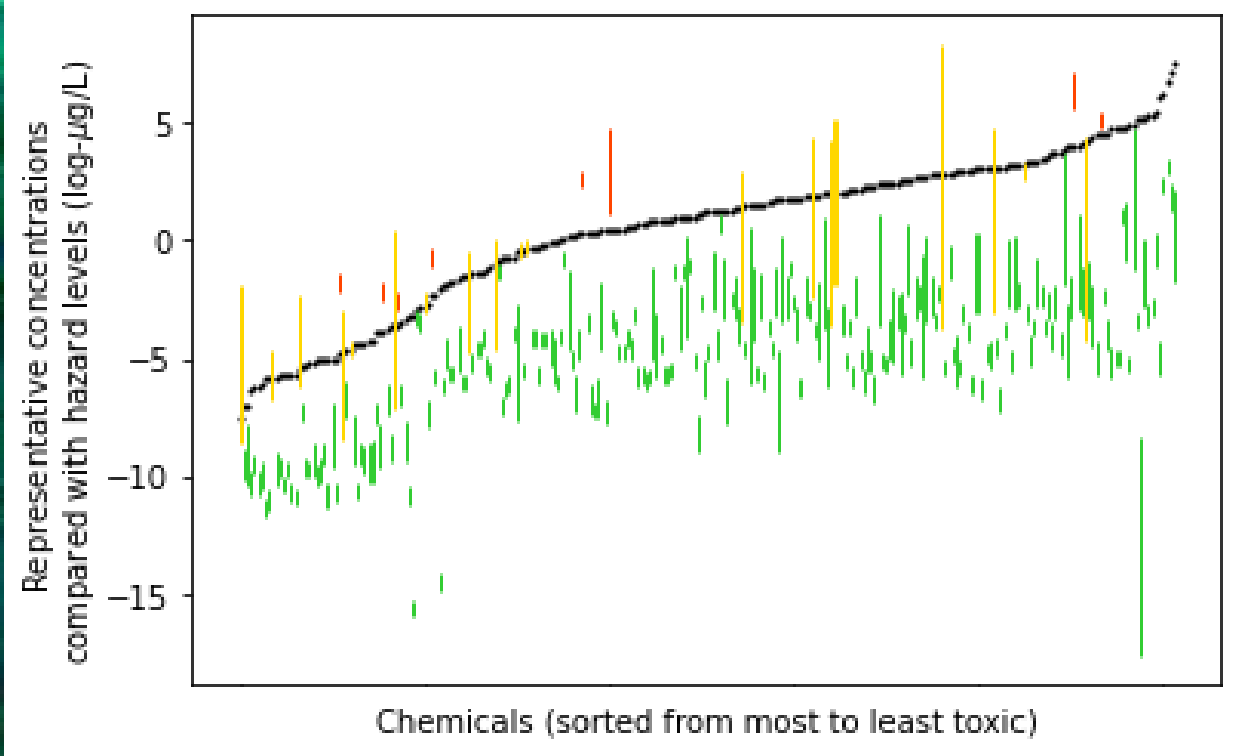
For most chemicals, the mean bulk concentration is similar to the mean dissolved concentration, regardless of the chemical's affinity for organic matter.



Are my representative ranges
informative enough for risk
prioritization?

Representative ranges overlap hazard concentrations in *Daphnia* for some chemicals

The uncertainty in the mean + standard deviation is less than the range of toxicities and can help prioritize risk to *Daphnia*, a sensitive organism.



Chemicals where the estimated average exceeds the toxic level are the highest priority (red). The most toxic chemicals are not always the highest priority, due to low exposures.



Thank you!