



# **Sunscreens and UV Blockers: Aquatic Source to Receptor Approach For Evaluating Complex Chemical Mixtures**

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*The National  
Academies of*

SCIENCES  
ENGINEERING  
MEDICINE

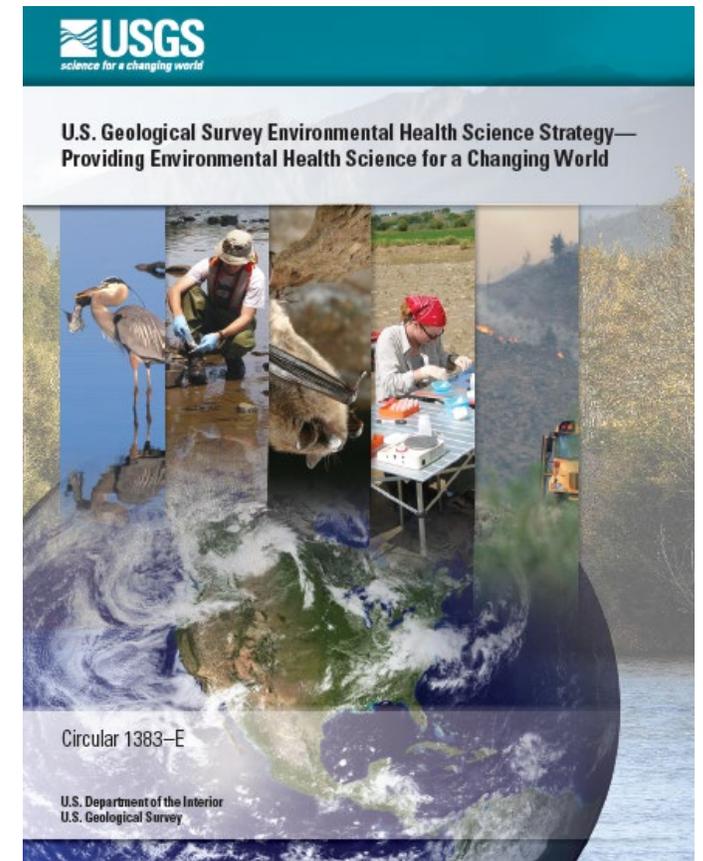
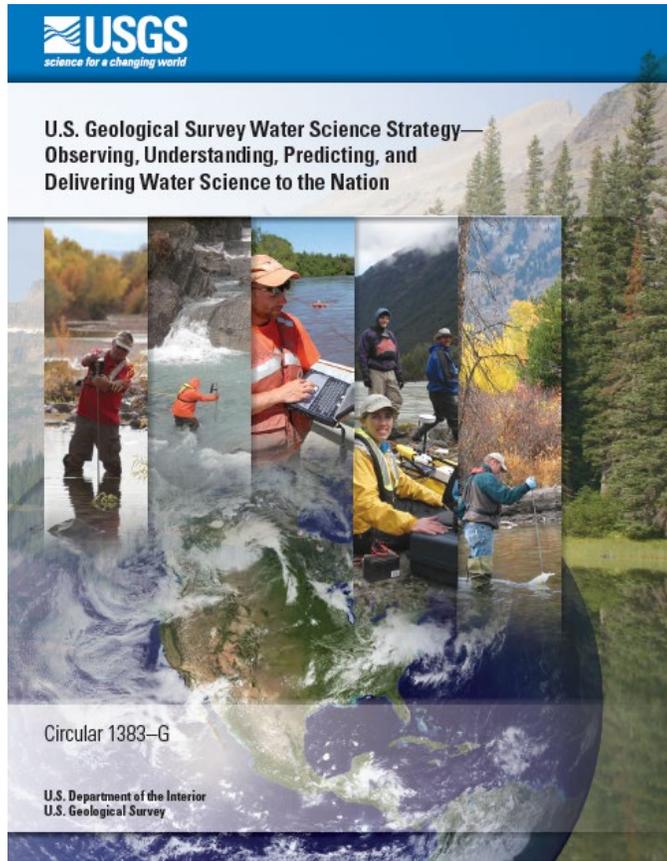
**Environmental Impact of Currently Marketed Sunscreens and  
Potential Human Impacts of Changes in Sunscreen Usage**

May 28, 2021

# Science for a Changing World

## Department of Interior

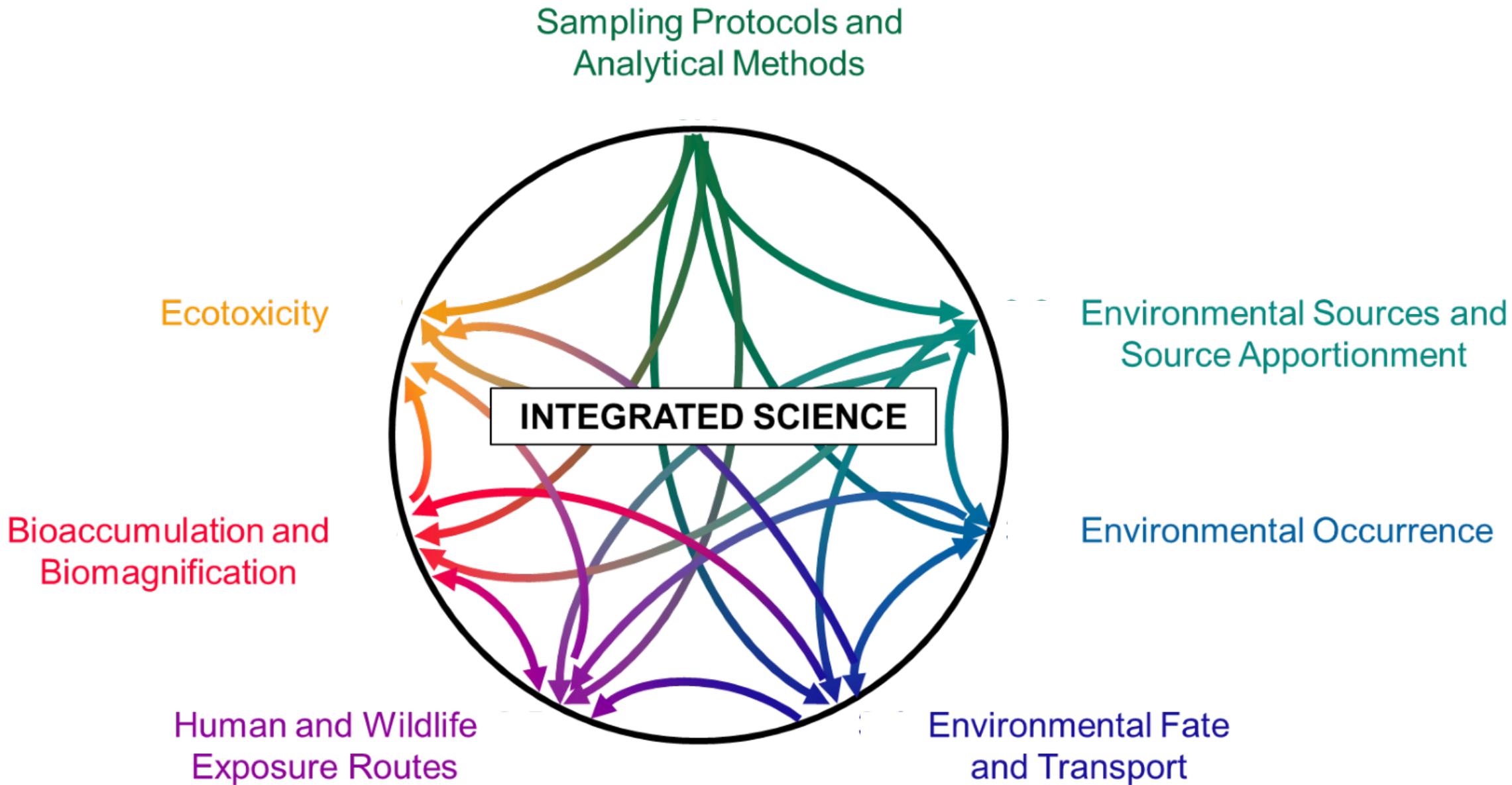
*U.S. Geological Survey*  
Water Mission Area  
Water Resource Availability Program  
Ecosystems Mission Area  
Environmental Health Program



- Amount and quality of water
- Processes that determine availability
- Changes due to environmental dynamics
- Emergencies and conflicts

- Contaminants of emerging concern
- Impact on the environment
- Exposure and effects
- Natural and anthropogenic disasters

# Source to Receptor Integrated Science



# Contaminants of Emerging Concern (CECs) in US Streams



Kolpin et al., 2002, Environ. Sci. Technol.

139 Streams in 30 States  
62 Intense AFO Activities  
52 Intense Urbanization  
17 Mixed Land Use  
8 Minimally Developed  
22 Antibiotics  
14 Prescription Drugs  
5 Nonprescription Drugs  
15 Hormones and Steroids  
39 Household and Industrial

- Widespread occurrence
- Complex mixtures
- Biologically active compounds

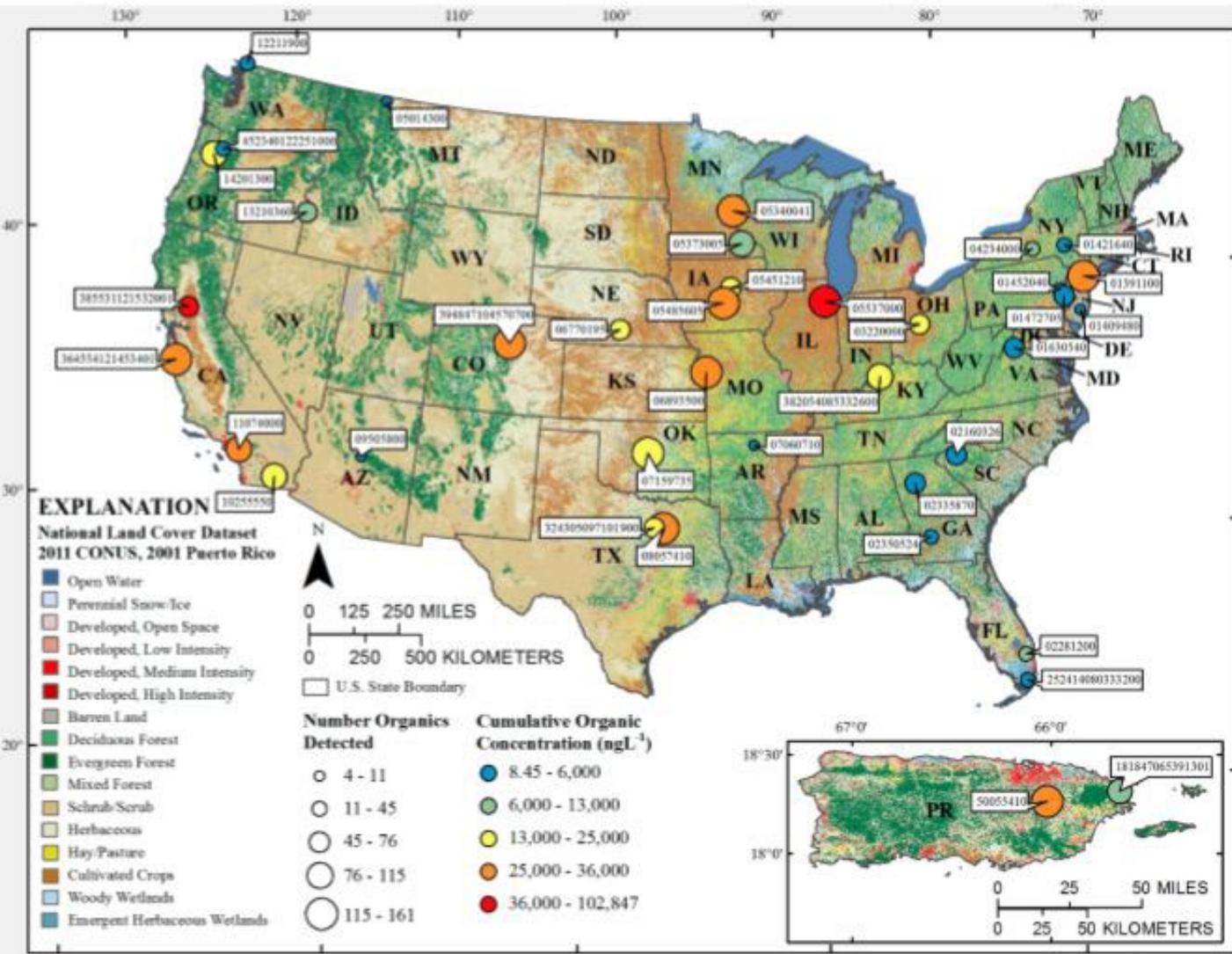
**Sunscreens and UV Blockers  
not measured**

# 20 Year Follow-Up National Study Showed CECs Everywhere

## New Analytical and Modeling Tools

- Sampled 38 streams in 30 states
- 719 compounds analyzed
- 406 compounds detected
- 100% of streams had detections
- Complex chemical mixtures
- 57% of chemicals bioactive by design

**Sunscreens and UV blockers  
not measured**



Bradley et al., 2017, Environ. Sci. Technol.

# Sunscreens and UV Blockers are Complex CEC Mixtures

## Terminology Smorgasboard



Sunscreen = formulation

UV blocker = photoreactive/reflective molecule

UV blockers have multiple uses beyond sunscreens

## Mineral UV Blockers

- Zinc and titanium oxide nanoparticles
- Coated and dispersed to improve performance
- No skin penetration
- No degradation
- High SPF on their own

## Organic UV Blockers

- Fossil fuel derived
- Environmental impacts
- Skin penetration (metabolism)
- Degradation
- Cocktails required to achieve high SPF

# Sunscreen Drug Products for Over-The-Counter-Human Use

Aminobenzoic acid\*\*

Avobenzene\*\*\*

Cinoxate\*\*\*

Dioxybenzone\*\*\*

Homosalate\*\*\*

Meradimate\*\*\*

Octocrylene\*\*\*

Octinoxate\*\*\*

Octisalate\*\*\*

Oxybenzone\*\*\*

Padimate O\*\*\*

Ensulizole \*\*\*

Sulisobenzene\*\*\*

Titanium dioxide\*

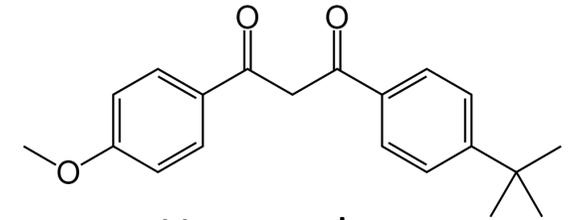
Trolamine salicylate\*\*

Zinc oxide\*

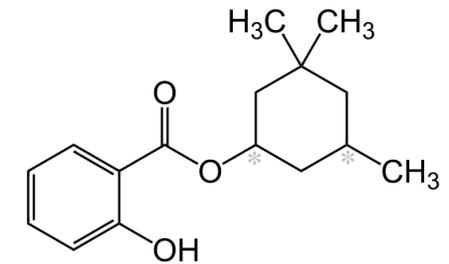
## UV Blockers



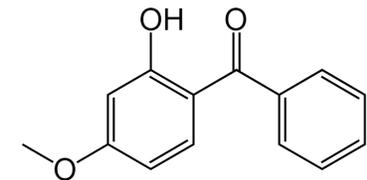
Avobenzene



Homosalate



Oxybenzone



\* Generally recognized as safe and effective

\*\* Not currently used

\*\*\* Insufficient data

# Formulations Consist of Active and Inactive Ingredients

## Sunscreen Lotion

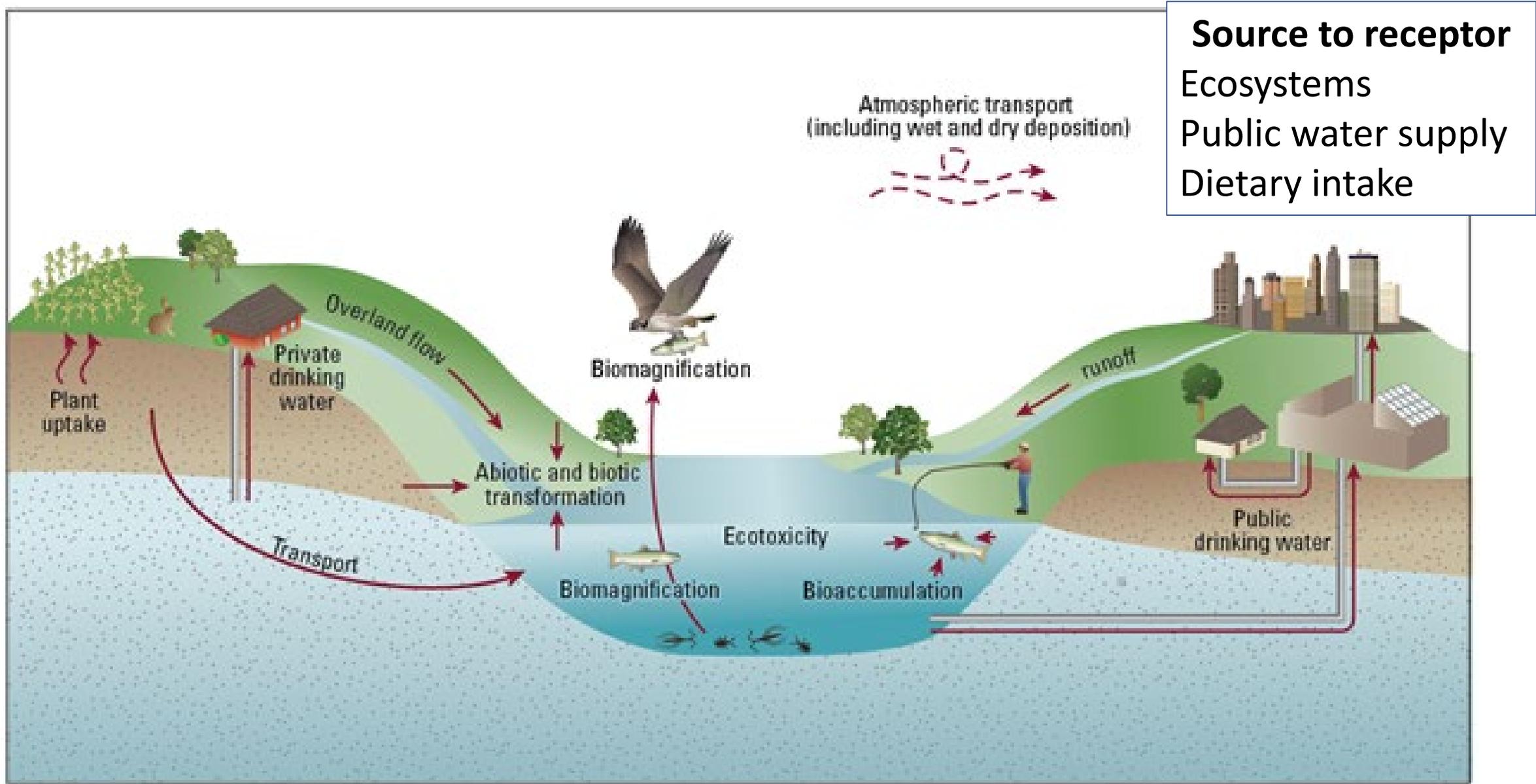
### *Active Ingredients*

Avobenzone 2.7%, Homosalate 9.0%, Octisalate 4.5%, Octocrylene 6.5% } 22.7%

*Inactive Ingredients:* Water, Glyceryl Stearate, PEG-100 Stearate, Cetyl Alcohol, Cetyl Dimethicone, Propylene Glycol, Phenoxyethanol, Caprylyl Glycol, VP/Eicosene Copolymer, Acrylates/C12-22 Alkyl Methacrylate Copolymer, Behenyl Alcohol, Sodium Polyacrylate, Chlorphenesin, Xanthan Gum, Disodium EDTA, Fragrance, Tocopheryl Acetate, Aloe Barbadensis Leaf Juice. } 77.3%

- Inactive ingredients include stabilizers, dispersants, emulsifiers, and fragrances
- Each ingredient is a complex mixtures of chemicals
- Active and inactive ingredients interact and co-occur with modified behavior
- Inactive ingredients not regulated by FDA

# Potential Impacts on the Aquatic Environment and Human Health



# Sources of UV Blockers to the Aquatic Environment



## *Recreational*

- Application
- Wash off
- Fugitive
- Container disposal



## *Wastewater*

- Dilution with shower water
- Modification with detergents
- Removal during treatment
- Dilution after discharge

### UV blockers

$2.1 \text{ g/person/application} \times 3 \text{ applications} \times 0.23 \text{ active} \times 0.25 \text{ washoff factor} = 0.36 \text{ g/capita/day}$

$2.1 \text{ g/person/application} \times 3 \text{ applications} \times 0.23 \text{ active} \times 0.75 \text{ shower factor} = 1.1 \text{ g/capita/day}$

### Pharmaceuticals

Metformin 0.04 g/capita/day

# Analytical Considerations -Robust Standardized Methods

Sampling/Preservation

Isolation/Concentration

Instrumental Analysis

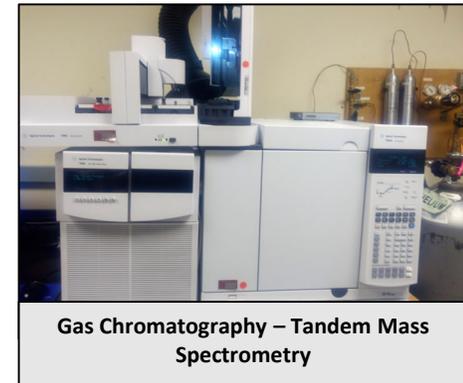
“Instrumental Gold Standards”

## Organic

- Gas Chromatography/Tandem Mass Spectrometry
- Liquid Chromatography/Tandem Mass Spectrometry
- Isotope Dilution Quantitation

## Inorganic

- Inductively Coupled Plasma/Mass Spectrometry
- Standard Reference Materials
  - No current approved USGS methods
  - No current approved USEPA methods
  - No current approved ASTM methods
  - Many study specific ad hoc methods



Gas Chromatography – Tandem Mass Spectrometry

# UV Blocker Aquatic Fate and Transport

## Physicochemical

- Structure
- Solubility
- Degradability
- Transformation products
- Complex mixture interactions

## Environmental

- Redox conditions
- Temperature
- Salinity
- Latitude, altitude, and climate
- Microbial communities

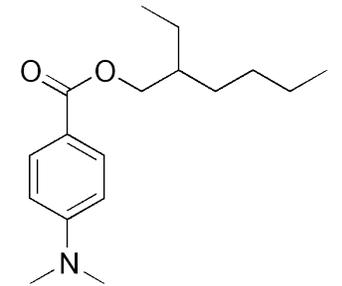
## Hydrological

- Rivers
- Lakes and reservoirs
- Groundwater
- Coastal
- Marine

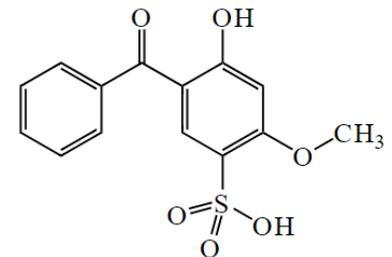
		Water				
	Log Kow	Solubility	HLC	Log Koc	Log BCF	STP removal
Name	unitless	mg/L	atm m3/mole	unitless	L/kg	percent
Aminobenzoic acid	1.4	7970	1.8E-09	1.0	0.5	1.9
Avobenzene	4.5	1.5	3.7E-07	3.3	2.1	56.6
Octocrylene	6.9	0.0038	3.9E-07	5.5	4.2	93.8
Padimate O	5.8	0.20	6.5E-05	3.3	3.5	90.9
Sulisobenzene	0.4	20290	2.7E-16	1.8	0.5	1.9

Parameters Estimated Using EPI Suite™ (USEPA, 2012)

Padimate O



Sulisobenzene



# Environmental Exposure Pathways - Measure and Model

- Fit-for-purpose analytical methods for occurrence measurements
- Monitoring data to determine temporal and spatial variability
- Hydrological model input parameters for sources, loading, transformation, and transport
- Consumer product model input parameters for per capita use, rinse off, wash off, and fugitive application
- Aquatic and human ecotoxicological model input parameters for exposure pathways, toxicity endpoints, and mixture effects



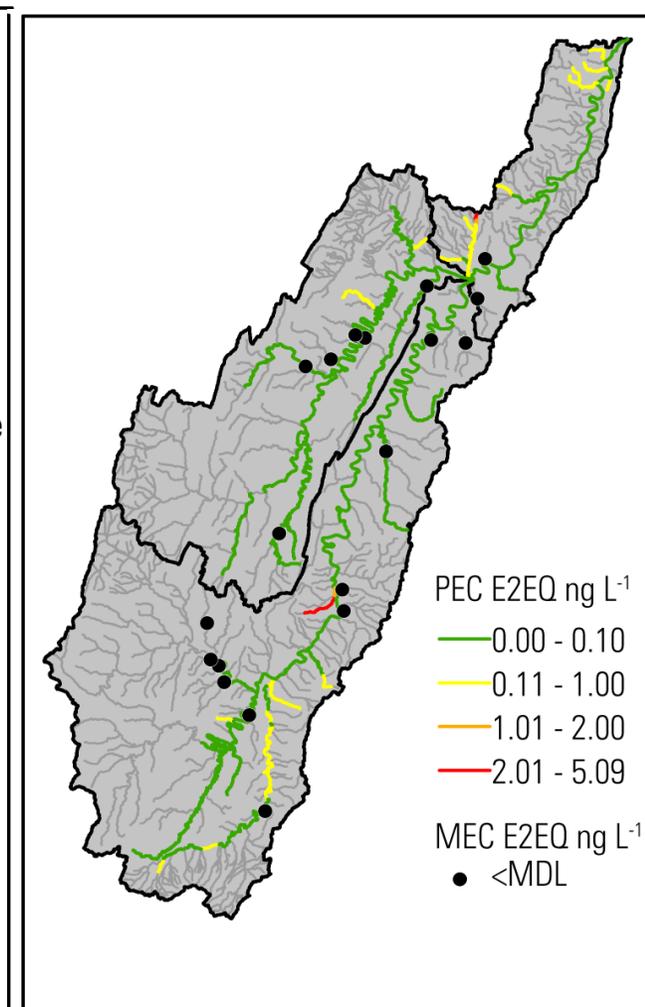
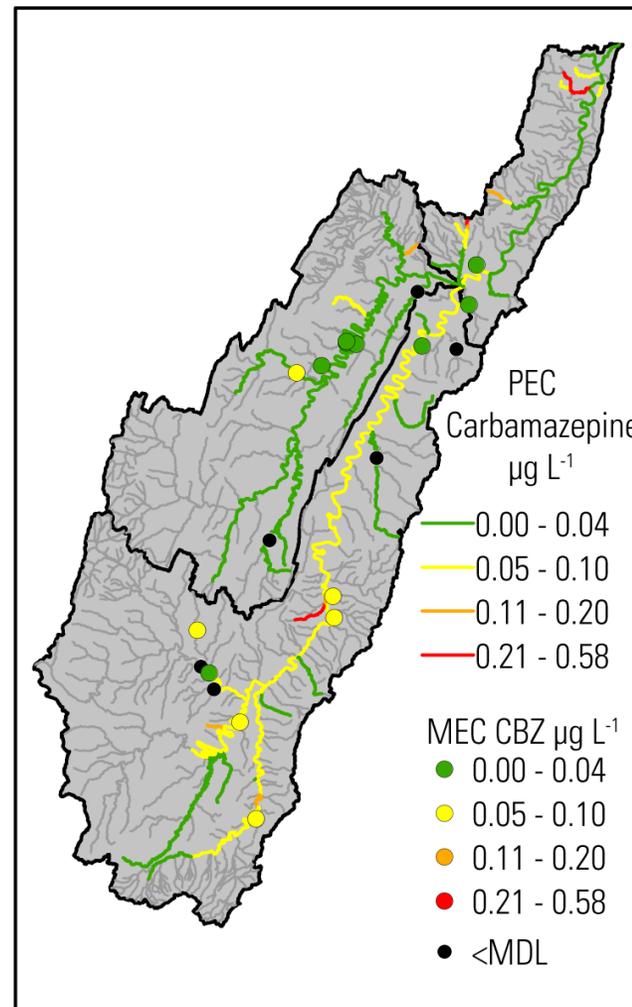
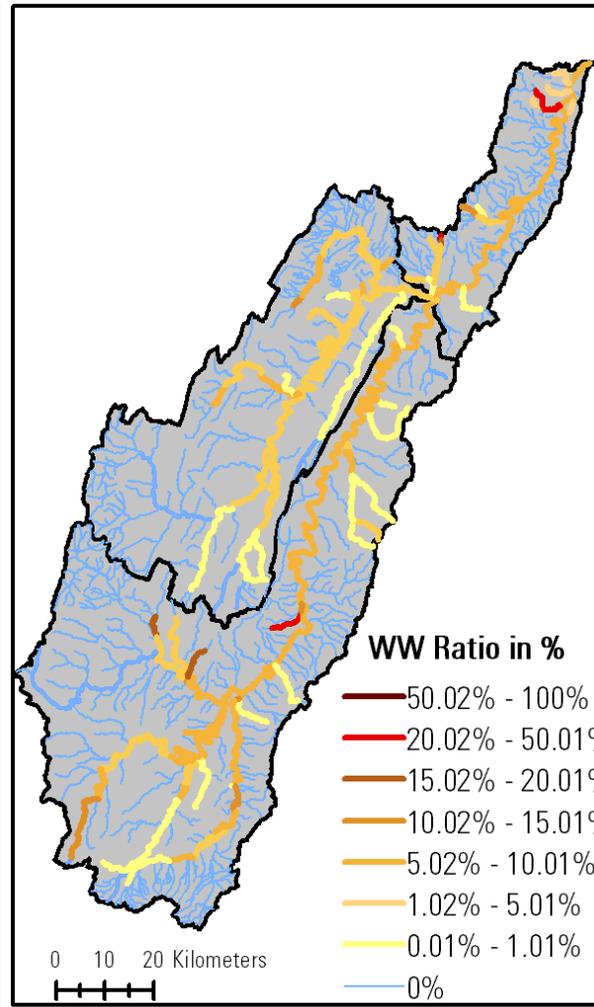
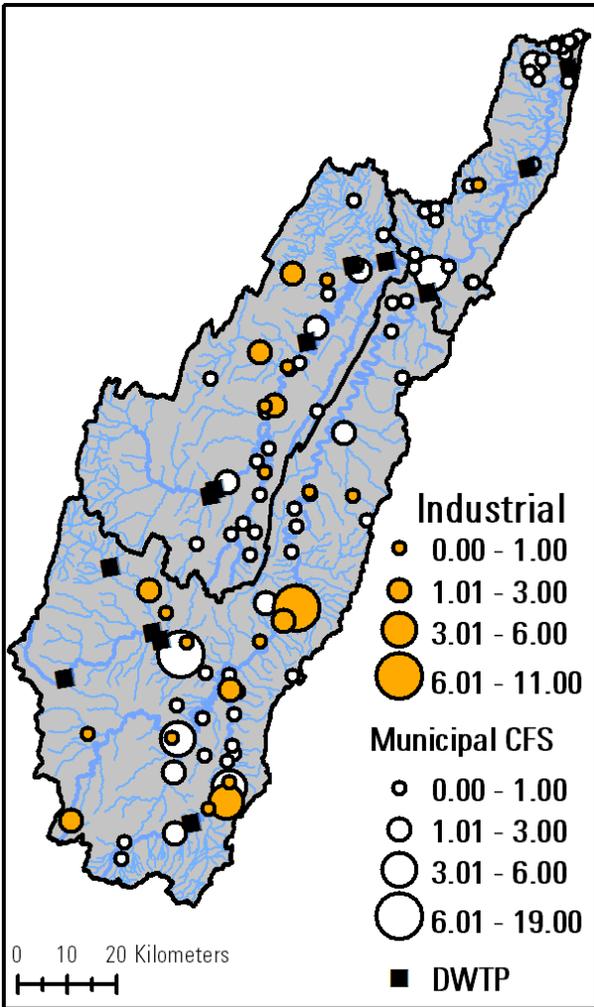
# Wastewater Mapper Tool Predicts Environmental Concentrations

WWTP

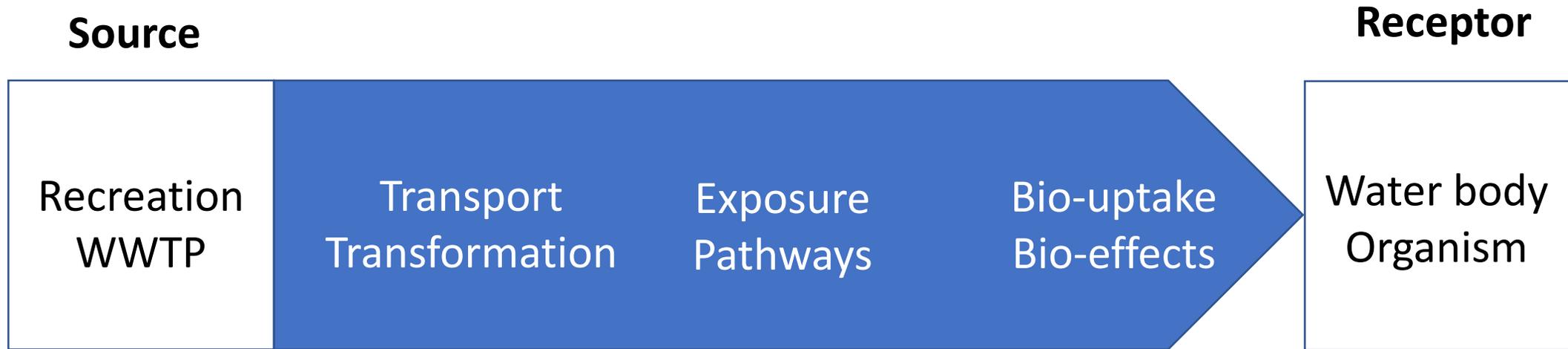
ACCWW

Carbamazepine

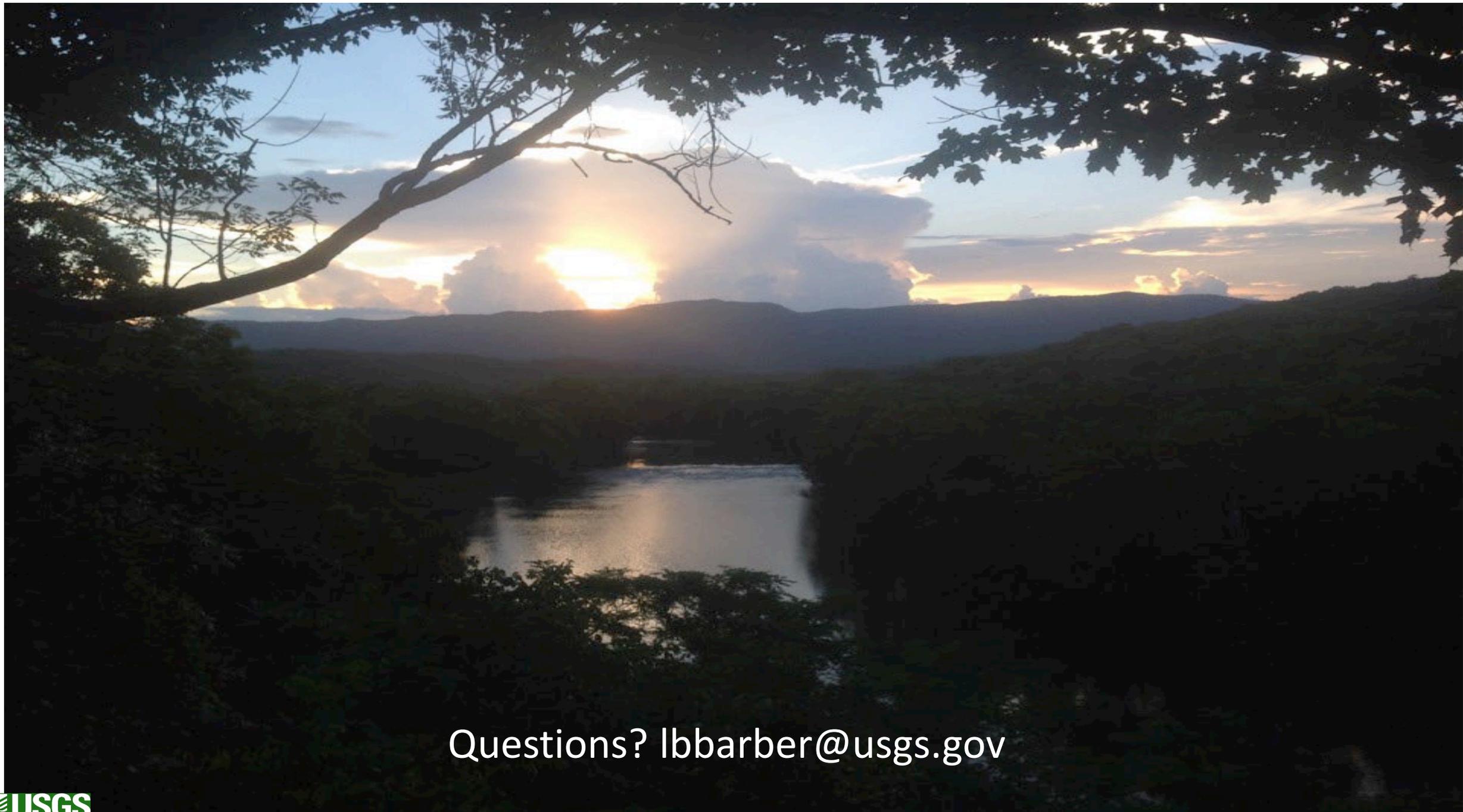
Estradiol Equivalence



# Data Gaps in Understanding UV Blockers in the Aquatic Environment



- National occurrence
- Inland freshwater and coastal marine
- Wastewater and recreation
- Alternative sources
- Drinking water supplies
- Treatment processes
- Fate and transport modeling parameters



Questions? [lbbarber@usgs.gov](mailto:lbbarber@usgs.gov)