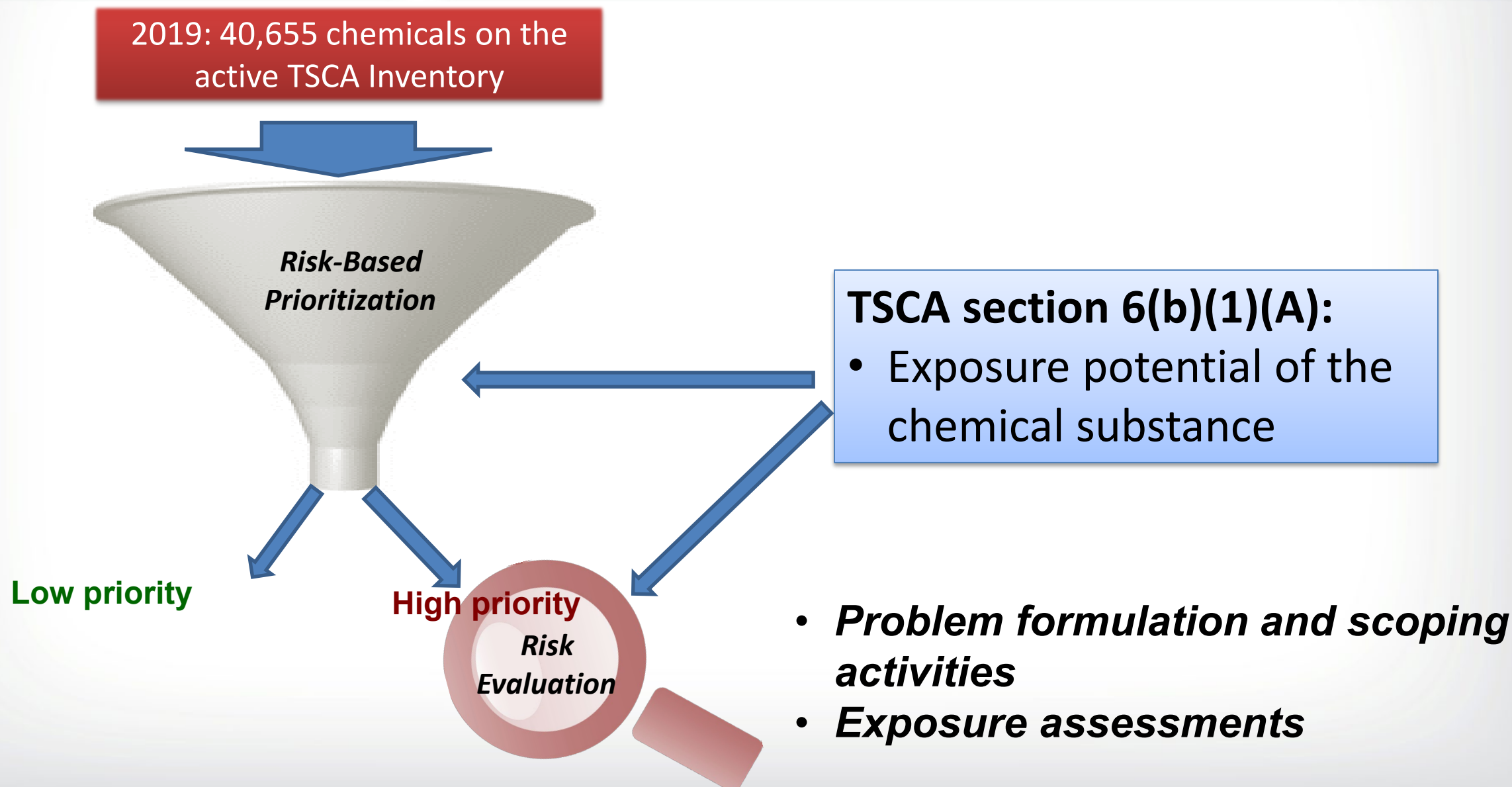




Informatics-Based Approaches for Managing and Curating Exposure Data

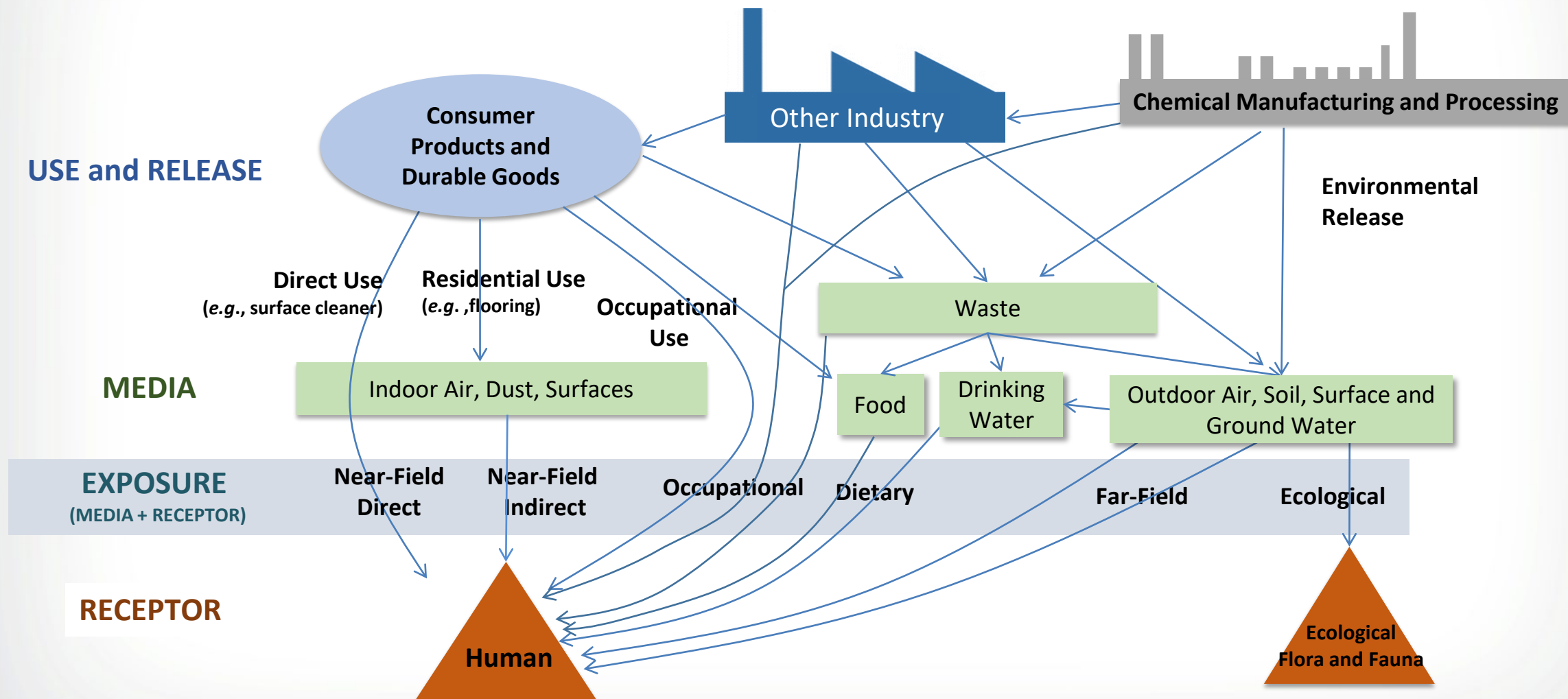
Kristin Isaacs and Kathie Dionisio
Center for Computational Toxicology and Exposure

Computational Toxicology
Communities of Practice Webinar
September 24, 2020

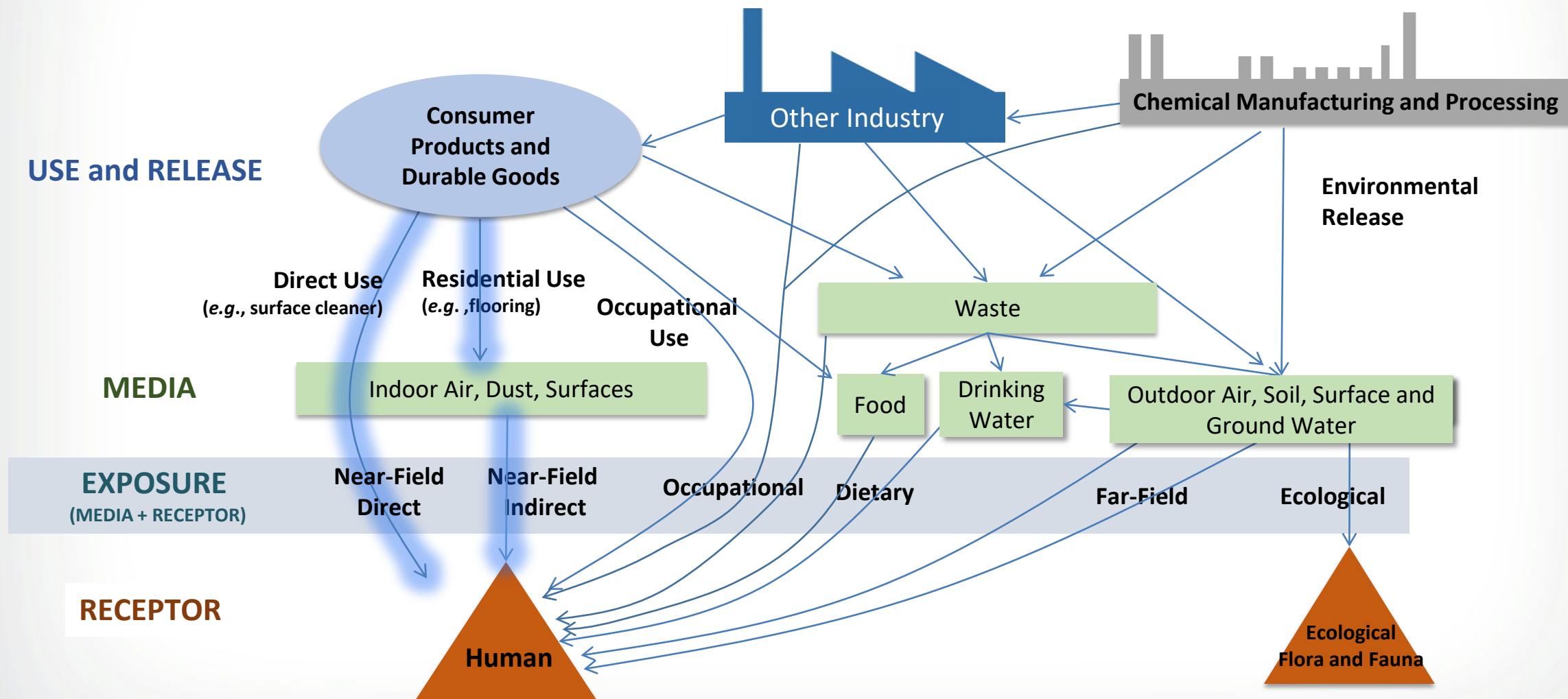


- “Chemical exposure evaluations require ***information to estimate exposure for a variety of high-priority pathways***, including ...consumer products and materials in the indoor environment, as well as occupational, ambient and ecological pathways.”

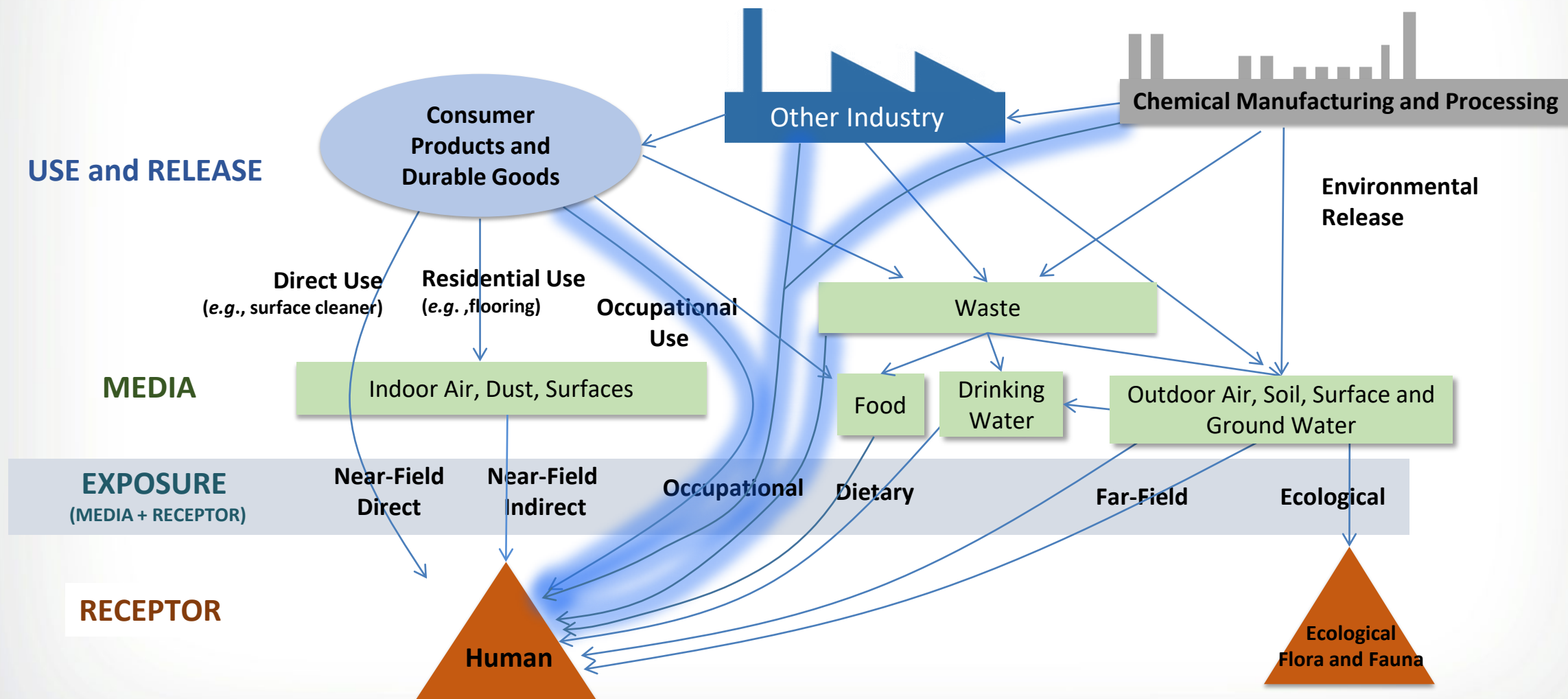
Exposure Pathways



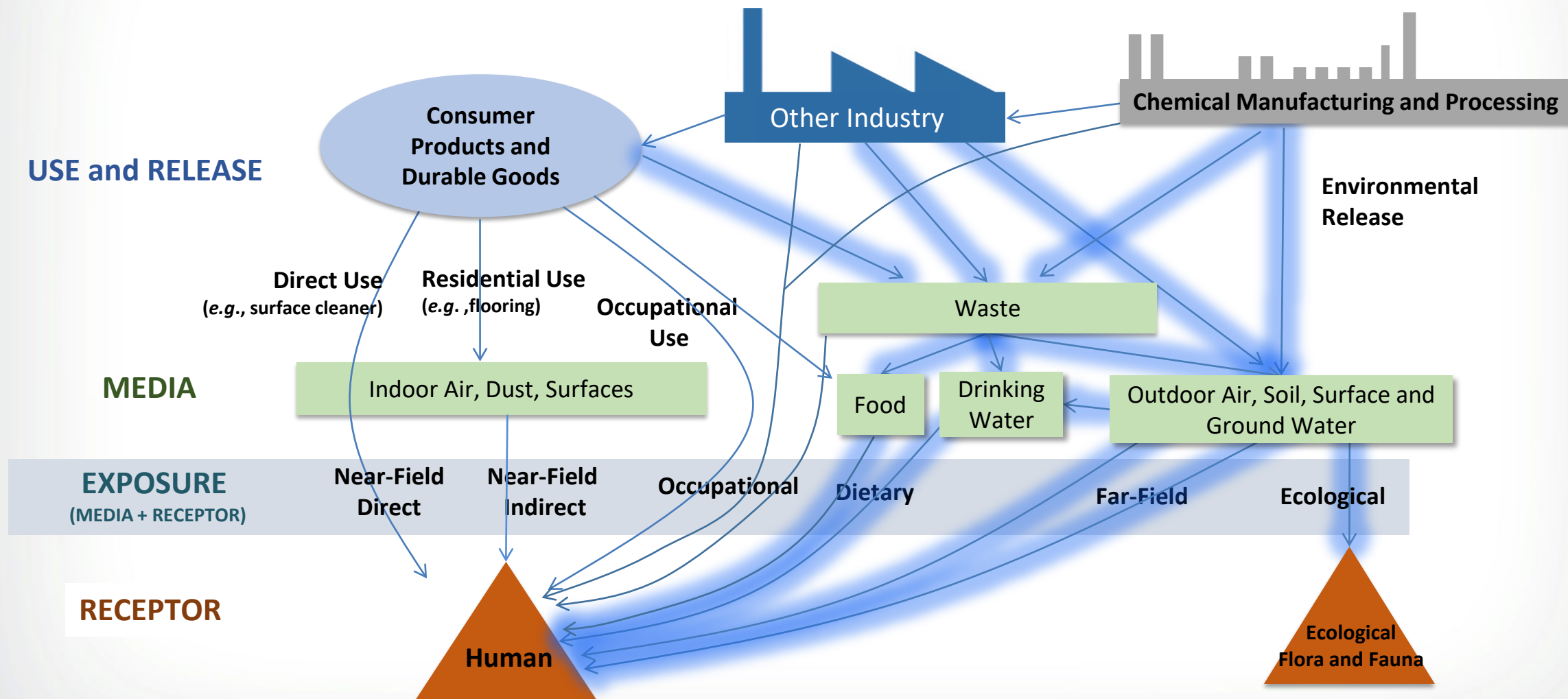
Consumer Pathways



Occupational Pathways



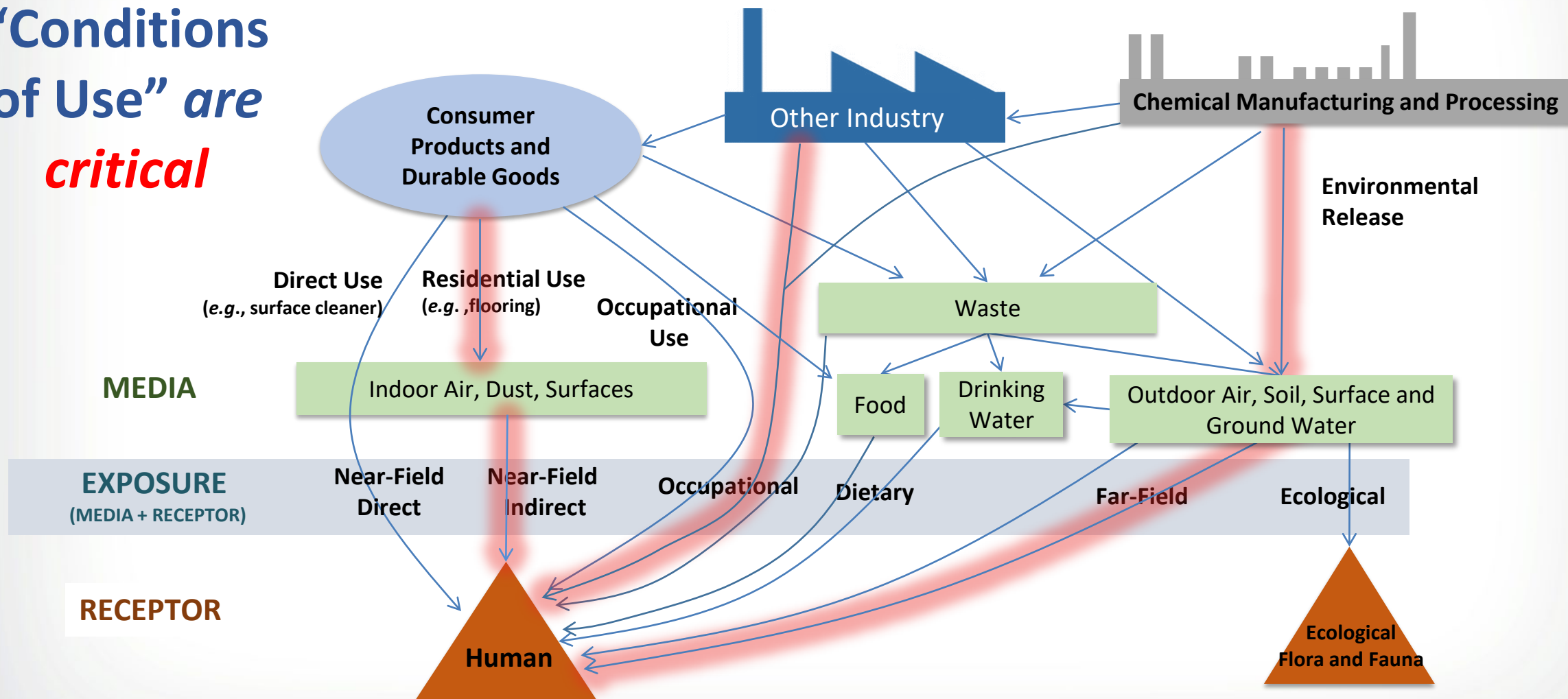
Ambient Pathways





Identification of Relevant Pathways for a Chemical

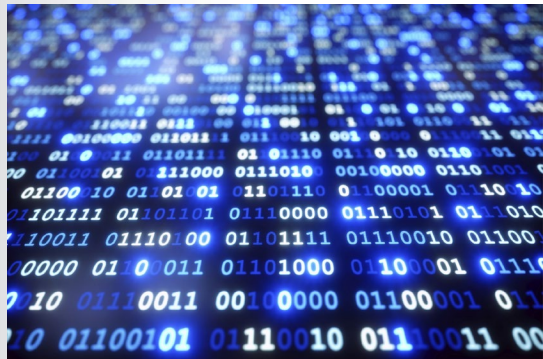
“Conditions of Use” are *critical*





Developing the Required Chemical Use Data to Support TSCA

- “Conditions of use” under TSCA means “the circumstances, as determined by the Administrator, under which a chemical substance is intended, known, or reasonably foreseen to be manufactured, processed, distributed in commerce, used or disposed of”.
- CCTE is collecting, curating, and storing large amounts of publicly available chemical use information
 - **500,000+** documents
 - **3.9 million** chemical records
 - Qualitative and quantitative information
- Developing tools and data infrastructure to directly support risk-based decision making
 - Seamless and timely delivery of data to EPA partners and the public
 - Quality assurance and data provenance





Chemical Use Types and Data Sources

- Specific consumer use
 - Use in particular products or product types



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The Procter & Gamble Company
P & G Household Care
Fabric & Home Care Innovation Center
5299 Spring Grove Avenue
Cincinnati, OH 45217-1087

MATERIAL SAFETY DATA SHEET

MSDS: RQ1305623
RQ1400356

Issue Date: 02/05/2014

SECTION I - PRODUCT IDENTIFICATION

Identity: **Liquid Laundry Detergent***

This MSDS applies to the following Liquid Tide Detergent Brands:

Tide Simply Fresh Refreshing Breeze
Tide Simply Fresh Daybreak Fresh

Emergency Telephone Number: 24hr P&G Operator – 1-800-879-8433

*** This MSDS applies to all uses/handling of these products in a retail package for consumer home use.**

SECTION II - HAZARDS IDENTIFICATION

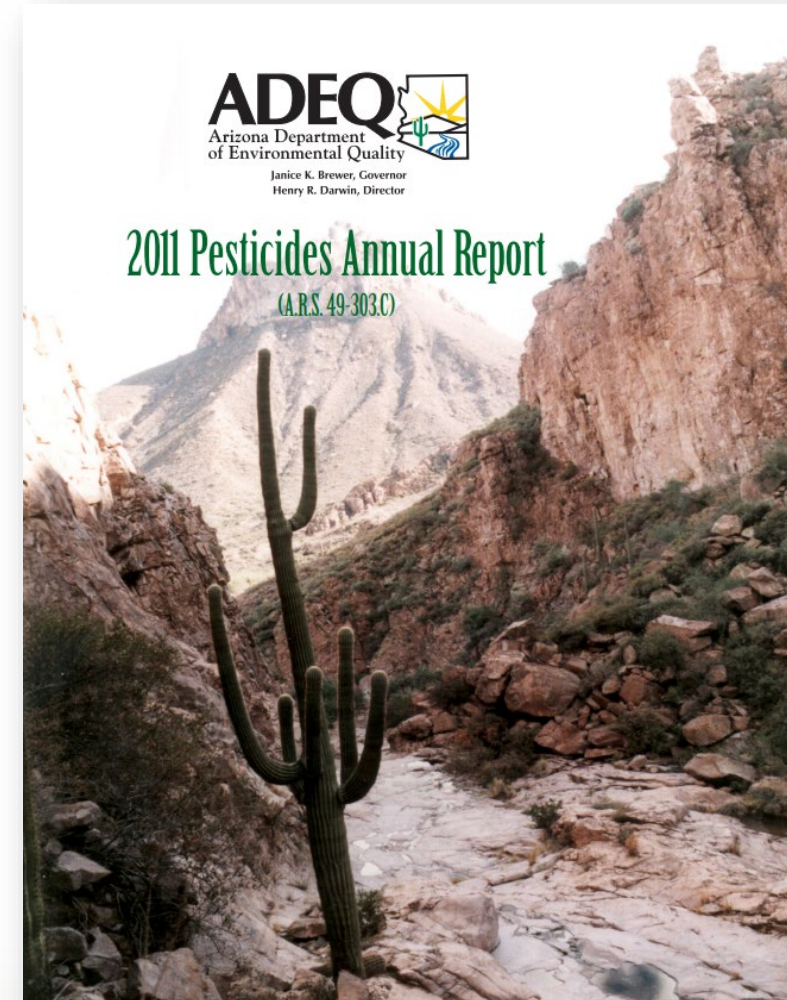
Health Hazards (Acute and Chronic):

Ingestion: May cause transient gastrointestinal irritation.
Eye Contact: May cause mild, transient irritation.
Inhalation: Transient irritation with prolonged exposure to concentrated material.

Signs and Symptoms of Exposure:

Ingestion: May result in nausea, vomiting, and/or diarrhea.
Eye Contact: May cause stinging, tearing, itching, swelling, and/or redness.
Skin: Prolonged contact with concentrated material may be drying or transiently irritating to skin.

- Specific consumer use
 - Use in particular products or product types
- General use
 - Use in particular commercial or industrial sectors





Chemical Use Types and Data Sources

- Specific consumer use
 - Use in particular products or product types
- General use
 - Use in particular commercial or industrial sectors
- Functional use
 - Role the chemical plays in different consumer products or industrial processes

The screenshot displays the Stepan website for the BIO-SOFT® S-120 product. The page is organized into several sections: a top navigation bar with links like 'About Us', 'Products', and 'Markets'; a left sidebar with a 'Products' menu; a main content area with an 'Overview' section describing the product as an anionic surfactant, an 'Application' section listing uses like 'Car/Truck Wash' and 'Industrial Cleaning', a 'Chemical Description' section identifying it as 'LINEAR ALKYL BENZENE (C12.0) SULFONIC ACID', a 'Chemical Groups' section, a 'Markets' section, a 'Properties' table, and a 'Regions of Availability' section. A right sidebar offers 'Product Downloads' such as 'Biodegradability' and 'Ecotoxicity'. A 'REQUEST A SAMPLE' button is prominently displayed at the top right of the main content area.

Property	Value
% Active:	97
Acid Value:	178 min.
Density, g/ml:	1.06
Flash Point, PMCC, °C:	>94
Form @ 25°C:	Liquid
Freeze Point, °C:	-18
Pour Point, °C:	-15
Specific Gravity @ 25°C:	1.06
Viscosity, cps @ 25°C:	960
RVOC, U.S. EPA %:	0



ChemExpoDB

Integrated family of exposure databases, linking data across multiple exposure data streams

- Different types of chemical use data
- Other exposure data (e.g., measured concentrations of chemicals in biological and environmental media)



Factotum

Internal application for the storage, management, and curation of exposure factor data in ChemExpoDB

- Facilitates loading of large quantities of data into ChemExpoDB (raw documents and curated data)
- Allows for tracking of data provenance
- Provides tools for curating data
- Disseminates data to other EPA users (e.g., OPPT)



ChemExpoDB



Factotum



Cleaned,
curated,
harmonized
data set

Web services



CompTox Chemicals Dashboard