



United States
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Development of the Public-Facing ChemExpo Knowledgebase Web Application to Support Delivery of Chemical Use and Consumer Product Data

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Abstract

The US EPA is responsible for evaluating thousands of chemicals for the potential risks to humans and ecosystems, which necessitates information on hazard and exposure potential for each chemical. To support chemical decision-making, EPA's Office of Research and Development (ORD) must identify and characterize relevant exposure pathways - the path of a chemical from source to a receptor. How a chemical is used (e.g. in a consumer, occupational, or industrial context) is critical to determining exposure pathways. The ORD data management and curation application, Factotum, facilitates the rapid collection and distribution of high-quality chemical and exposure related data from public documents to inform chemical exposure and risk assessments. To date, Factotum has been used to collect and curate data from over 560,000 documents, representing 4 million individual chemical records and 35,000 unique chemical substances. A new publicly available data search and visualization tool, called Chemical Exposure Knowledgebase (ChemExpo), is being developed by ORD. ChemExpo will surface data managed and curated by the internal Factotum application. The initial release of ChemExpo will focus on specific chemical substances, chemical composition of consumer products, functional role of chemicals within products and processes, and presence of chemicals on reported specific or general use lists. This new application will display more detailed curated data than currently available on the EPA CompTox Chemicals Dashboard, including additional document metadata; product-level chemical ingredient information; and product category, function category, and chemical summaries. This application will allow for data exploration by chemical, function, and consumer product category to support exposure assessments and other risk-based chemical evaluations. This abstract does not necessarily reflect U.S. EPA policy.

Introduction

- EPA is charged with evaluating risks associated with chemicals in commerce, including consumer and industrial products.
 - As of February 2023, there are **68,968** active chemicals on the EPA's Toxic Substances Control Act (TSCA) Inventory.
- Evaluating chemicals for risk to humans or the environment requires information on hazard and **exposure potential**.
- To support chemical decision-making, EPA's Office of Research and Development (ORD) has developed a robust, well-documented, and accessible database to inform exposure assessments and modeling efforts.

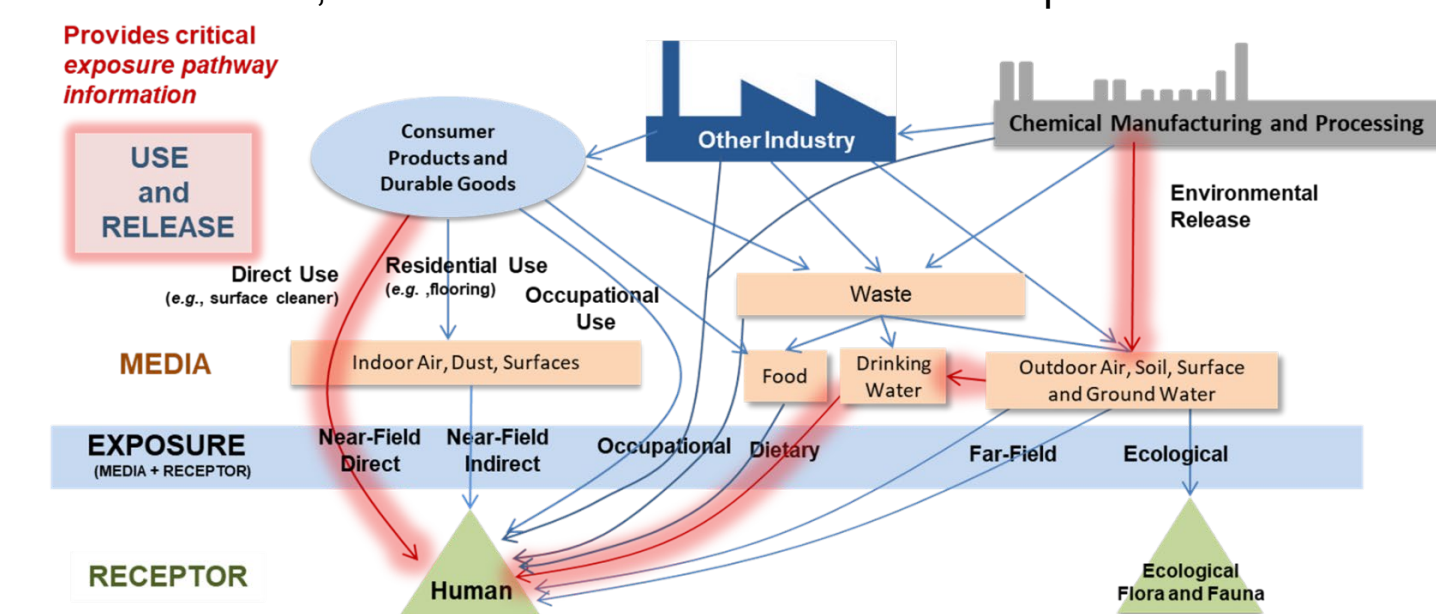


Figure 1. Data on chemical use and release from consumer products and industrial processes provides critical information to characterize human exposure pathways.

Approach

- Factotum** is an existing internal EPA ORD curation and data management application.
- ChemExpo** is a new public-facing web application, built from the streamlined visualization functionality of Factotum.
- Both Factotum and ChemExpo make use of the extensive chemical curation workflows that map chemicals to unique substance identifiers (DTXIDs) via the **DSSTox** database³.
- ORD's **Chemicals and Products database (CPDat)**² Currently, data is surfaced to the public via the **Comptox Chemicals Dashboard (CCD)**⁹, and via a Bulk Release of the CPDat database.

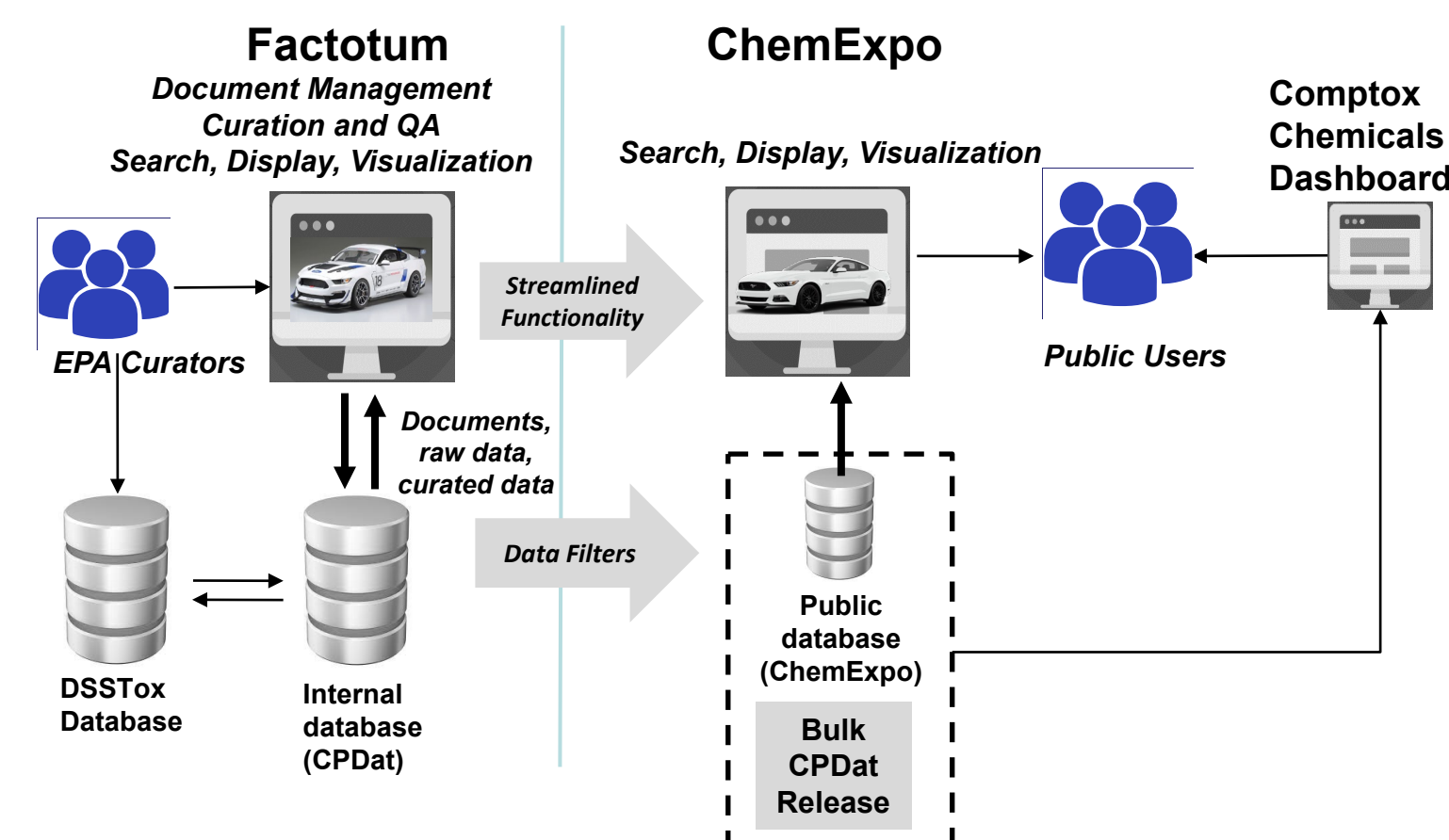
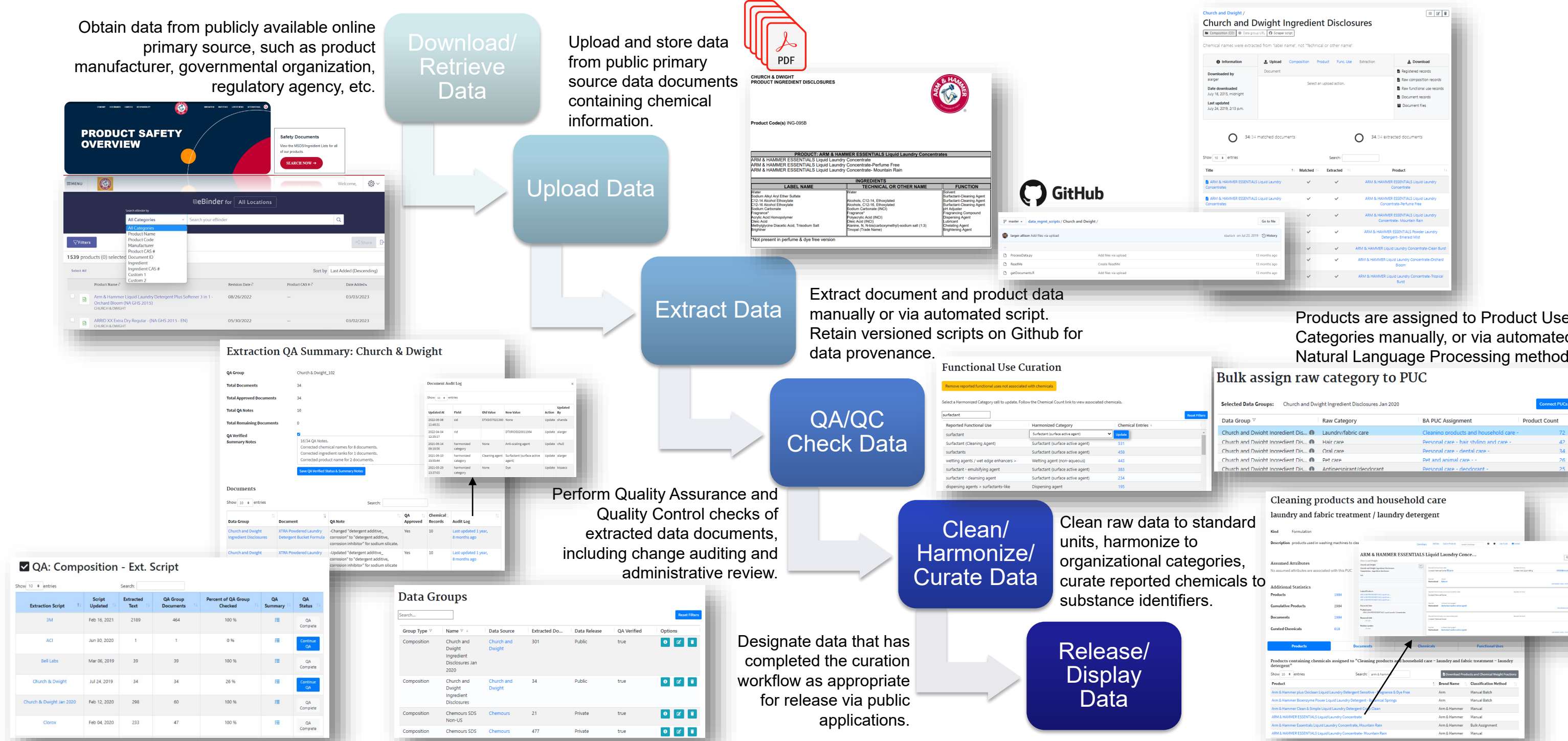


Figure 2. Relationship between Factotum, ChemExpo and Other System Components

Methods

Data Management and Curation via Internal Factotum Application



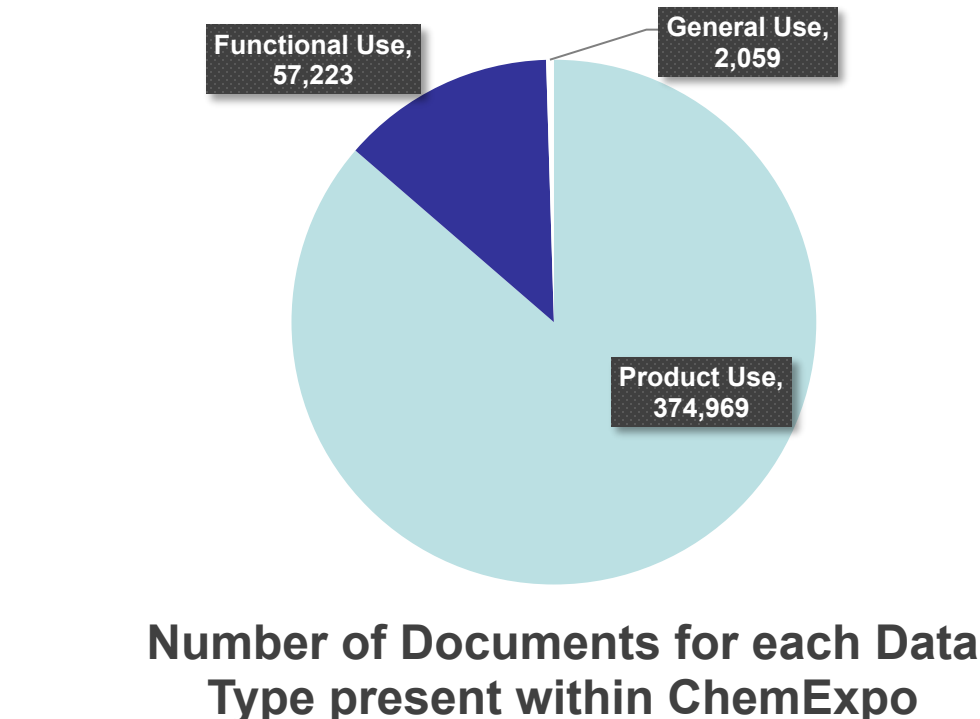
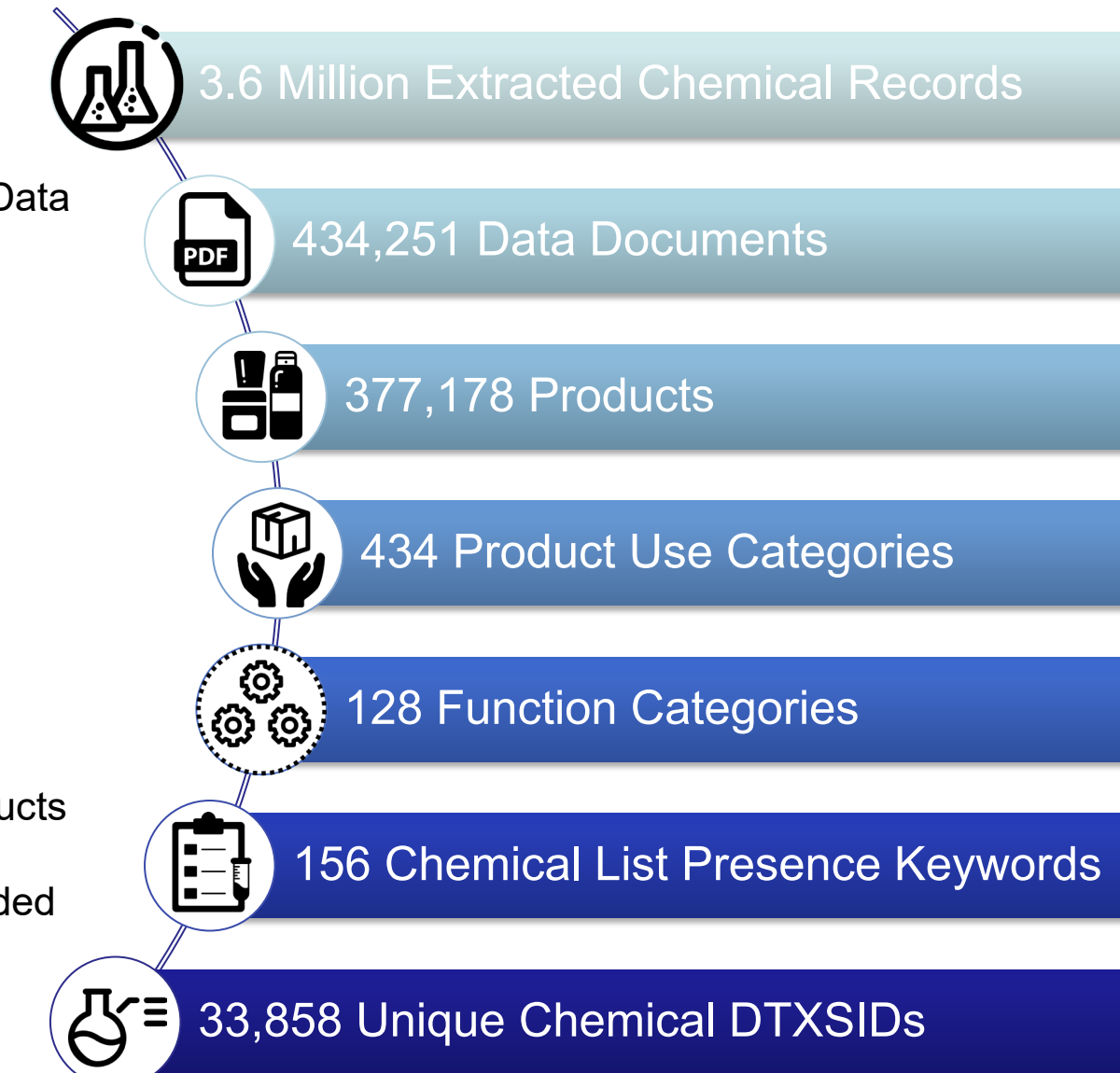
Data Visualization via Public ChemExpo Application



Results

Data available within ChemExpo

- Product use**
 - Use in particular products or product types
 - Documents include standard Manufacturer Safety Data Sheets (MSDS), Ingredient Disclosures
 - Organized by **Product Use Categories (PUCs)**
- General use**
 - Lists of chemicals used in particular commercial or industrial sectors
 - Documents include government reports, published chemical lists
 - Organized by **Chemical List Presence Keywords**
- Functional use**
 - Role the chemical plays in different consumer products or industrial processes
 - Documents include chemical use disclosures provided by manufacturers or regulatory agencies
 - Organized by **Function Categories**⁷



Impact and Future Plans

- The **Factotum/ChemExpo** system will improve the **volume, timeliness, quality, and accessibility of exposure data** available for use and exploration by stakeholders, including the general public.
- Anticipated public release** of the ChemExpo application in **late Spring/Summer 2023** will allow the public access to chemical use data within ORD's Chemicals and Products Database (CPDat)².
- New chemical use data** are being continuously curated via Factotum and will be released on a regular basis.
- Additional data sources and functionality** may be incorporated in future releases based on user feedback.

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