



United States
Environmental Protection
Agency

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

3795/P284

Sakshi Handa¹, Kenta Baron-Furuyama¹, Katherine Phillips¹, Jonathan Wall¹, Beth Horton², Christian Lutz², Allison Larger³, Kristin Isaacs¹, Colleen Elonen¹

¹Center for Computational Toxicology and Exposure, Office of Research and Development, U.S. Environmental Protection Agency, RTP, NC;

²Oak Ridge Associated Universities, Oak Ridge Institute for Science and Education, Oak Ridge, TN; ³General Dynamics Information Technology, Inc (GDIT)

Sakshi Handa | handa.sakshi@epa.gov | 919-541-0636

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.

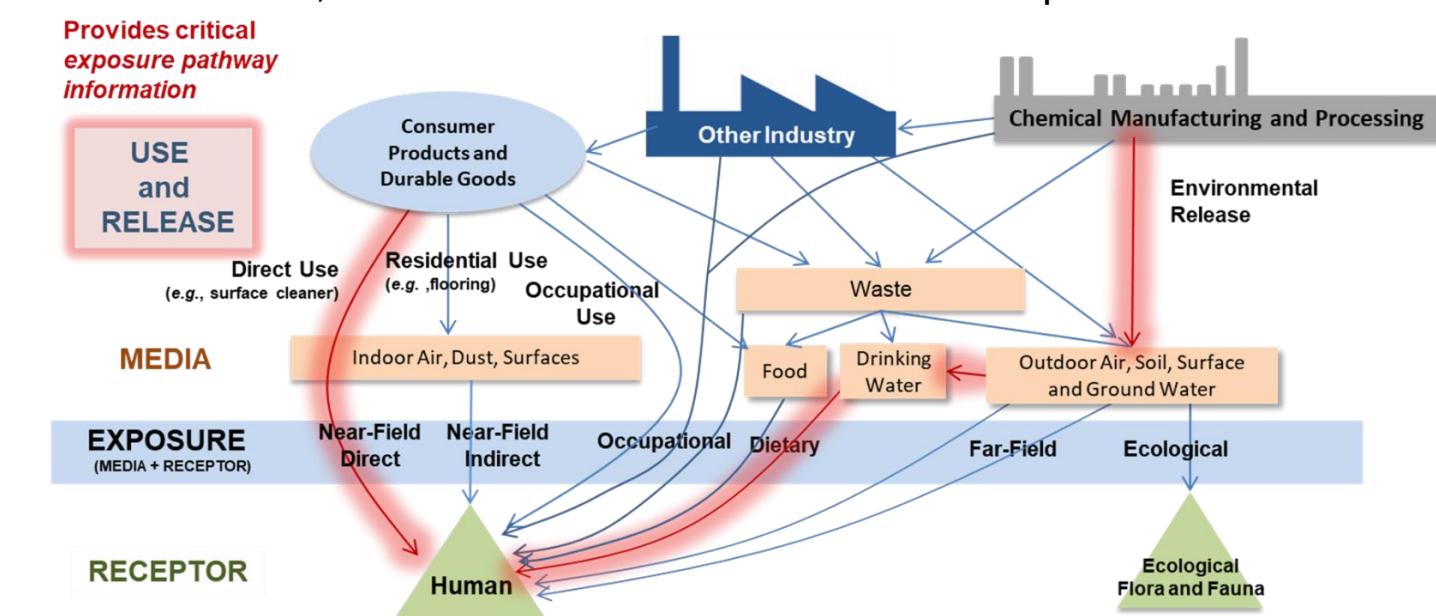


Figure 1. Data on chemical use and release from consumer products and industrial processes provides critical information to characterize human exposure pathways.

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 (DTXSIDs) 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.

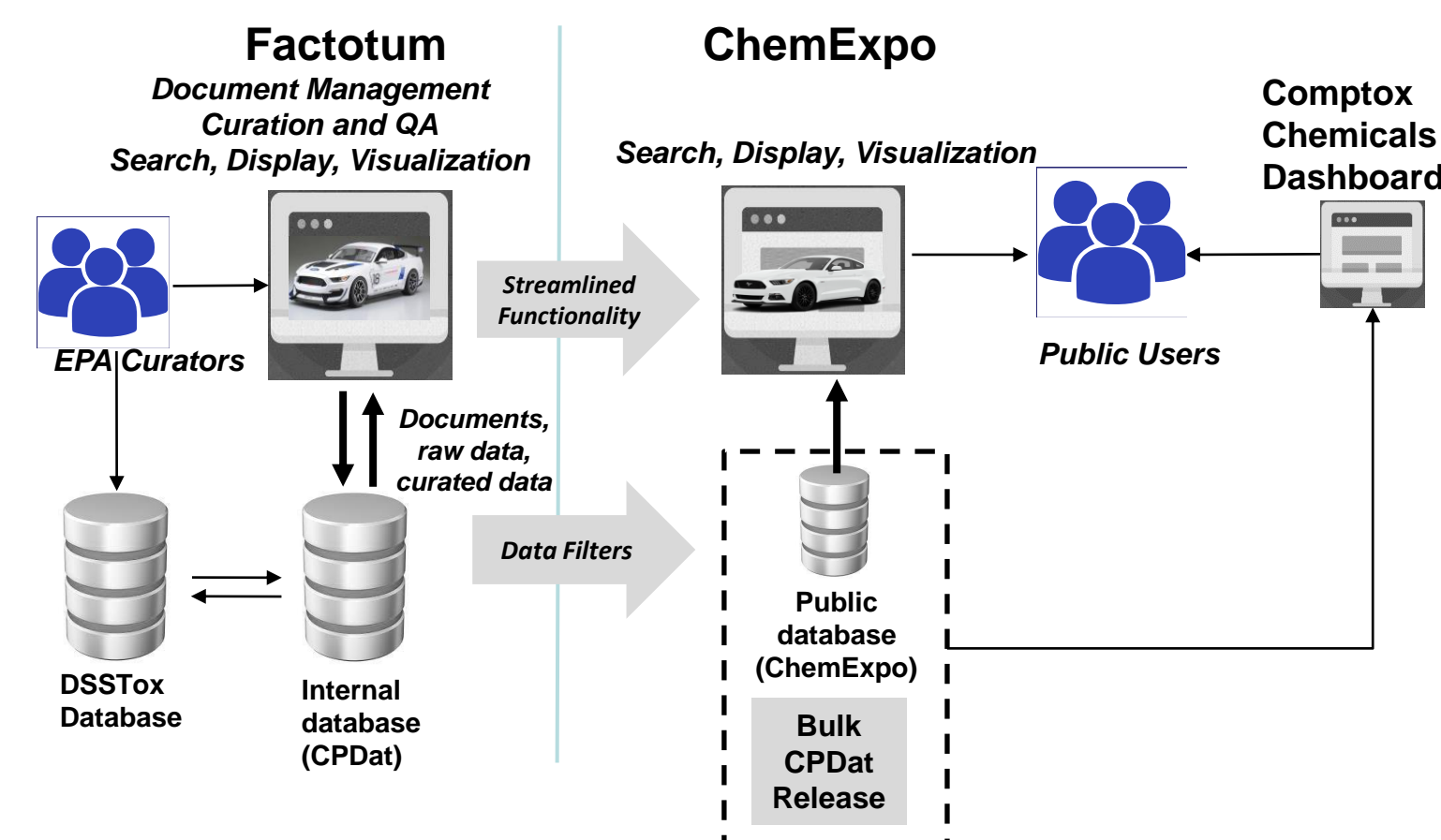
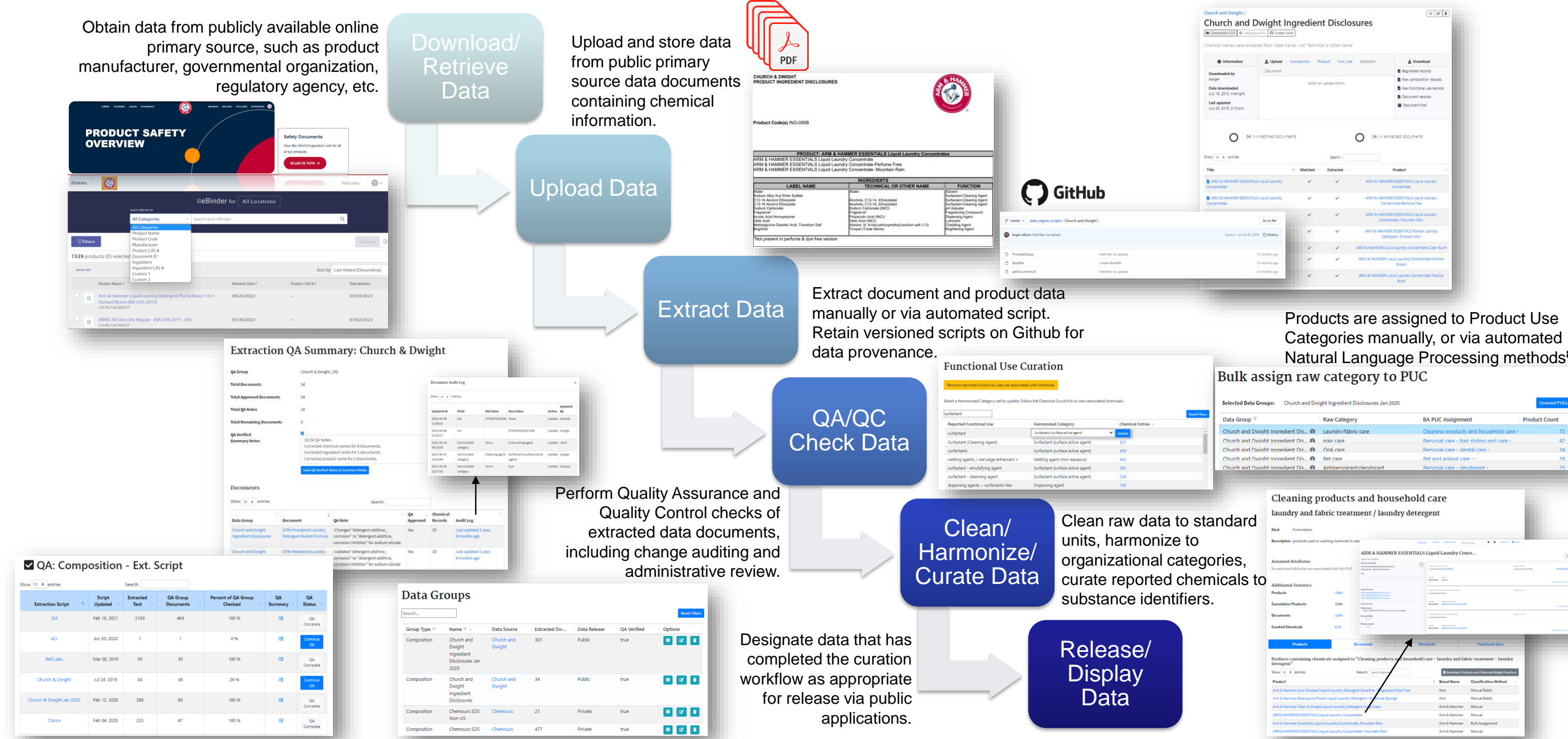


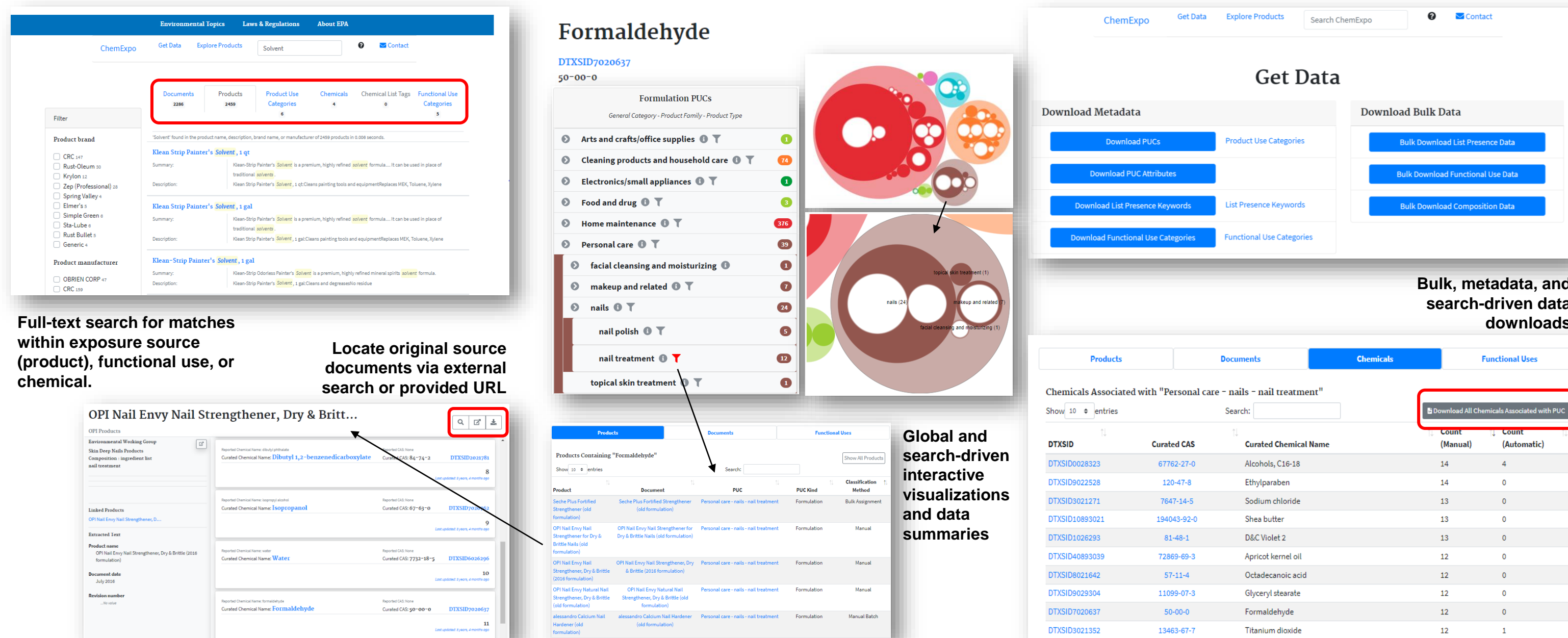
Figure 2. Relationship between Factotum, ChemExpo and Other System Components

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

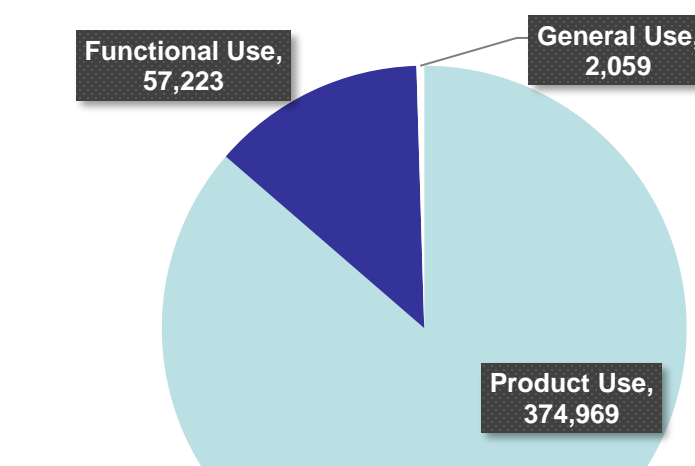


Figure 3. Number of Documents for each Data Type present within ChemExpo

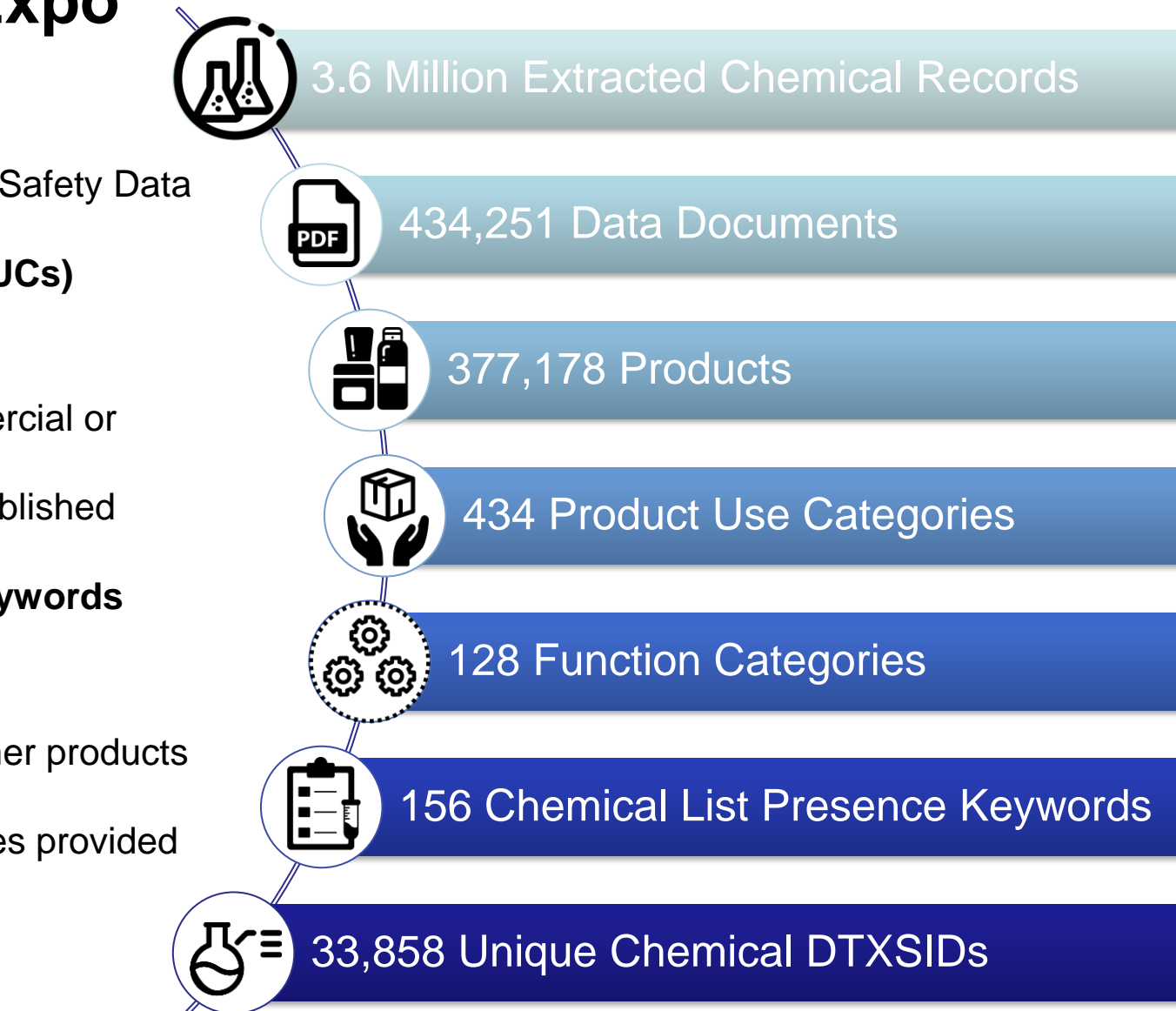
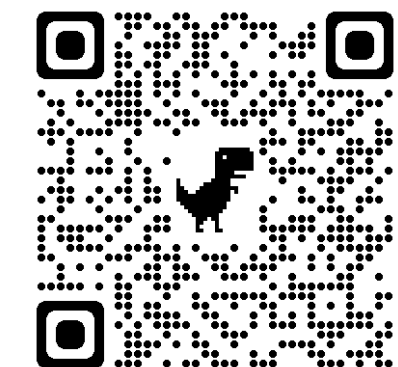


Figure 4. Summary of Distribution of Products within High-Level Product Use Categories (PUCs)

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.



The public ChemExpo application will be available through EPA's Comptox Portal - comptox.epa.gov

References

- Dionisio, Kathie L., Alicia M. Frame, Michael-Rock Goldsmith, John F. Wambaugh, Alan Liddell, Tommy Cathey, Doris Smith, et al. 2015. "Exploring Consumer Exposure Pathways and Patterns of Use for Chemicals in the Environment." *Toxicology Reports* 2: 228-37. <https://doi.org/10.1016/j.toxrep.2014.12.009>
- Dionisio KL, Phillips K, Price PS, et al. The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products. *Sci Data*. 2018;5:180125. Published 2018 Jul 10. doi:10.1038/sdata.2018.125.
- Gruke, Christopher M., Anthony J. Williams, Inthirany Thilanderajirakul, and Ann M. Richard. 2019. "EPA's DSSTox Database: History of Development of a Curated Chemistry Resource Supporting Computational Toxicology Research." *Computational Toxicology* 12 (November): 100966. <https://doi.org/10.1016/j.comtox.2019.100966>
- Isaacs KK, Dionisio K, Phillips K, Bevington C, Egeghy P, Price PS. Establishing a system of consumer product use categories to support rapid modeling of human exposure. *J Expo Sci Environ Epidemiol*. 2020;30(1):171-183. doi:10.1038/s41370-019-0107-5
- Koval, Lauren E., Kathie L. Dionisio, Katie P. Friedman, Kristin K. Isaacs, and Julia E. Rager. 2022. "Environmental Mixtures and Breast Cancer: Identifying Co-Exposure Patterns Between Understudied Vs Breast Cancer-Associated Chemicals Using Chemical Inventory Informatics." *Journal of Exposure Science and Environmental Epidemiology* 32 (6): 794-807. <https://doi.org/10.1038/s41370-022-00451-8>
- Phillips, Katherine A., John F. Wambaugh, Christopher M. Gruke, Kathie L. Dionisio, and Kristin K. Isaacs. 2017. "High-Throughput Screening of Chemicals as Functional Substitutes Using Structure-Based Classification Models." *Green Chemistry* 19 (4): 1063-74. <https://doi.org/10.1039/c6gc02744a>
- OECD 2017. "Internationally Harmonised Functional, Product and Article Use Categories." [https://one.oecd.org/document/ENV/JM/MONO\(2017\)14/en/pdf](https://one.oecd.org/document/ENV/JM/MONO(2017)14/en/pdf)
- Wall, Jonathan T., Scott Burns, Katherine Phillips, Kathie Dionisio, and Kristin Isaacs. (in production). "docuCAT: Automated assignment of documents to structured hierarchical categories in support of chemical assessments."
- Williams AJ, Gruke CM, Edwards J, et al. The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. *J Cheminform*. 2017;9(1):81. Published 2017 Nov 28. doi:10.1186/s13321-017-0247-6

U.S. Environmental Protection Agency
Office of Research and Development

This poster does not necessarily reflect EPA policy. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.