SUPPLEMENTAL METHODS

Methods implemented in the Chemicals and Products Database (CPDat) Chemical List Presence dataset

Within CPDat (Dionisio et al. 2018) v3 exists the Chemical List Presence dataset. This dataset is an update to the US EPA’s Chemical and Product Categories database (CPCat) (Dionisio et al. 2015). All data included in CPCat were reviewed and expanded upon to cultivate a more comprehensive dataset, and as part of an exercise to verify data provenance, all data points were linked to a stored copy of their original data source. In the CPCat dataset, each chemical record was assigned to one or more CPCat terms describing the general use of the chemical. As part of the overarching data update, CPCat terms were inventoried and modernized into a structured, streamlined set of keywords used in the Chemical List Presence dataset within CPDat v3. A keyword is defined as a term that imparts information on how a chemical is used, based on information available in the primary source. One or more keywords can be assigned to a single chemical record to accurately convey the relevant use information, thus accounting for varying levels of detail provided by different data sources. The collection of keywords assigned to an individual chemical record constitutes the “keyword cassette”, which should be interpreted holistically to best comprehend the scope of the chemical’s use. Additionally, larger categories, called “kinds”, were introduced to group related keywords. Keyword kinds aid in the curation process and allow for the quick aggregation of related data. A large motivation for the development of these updated keywords was alignment with current chemical functional use (Development 2017) and consumer product categories (Isaacs et al. 2020).

The scalable nature of this framework allows for the introduction of new keywords and keyword kinds as the dataset grows. In CPDat version 3, the Chemical List Presence dataset includes 136 keywords grouped into 11 keyword kinds. Keywords were manually assigned to each chemical record in the Chemical List Presence dataset after evaluating the contents of the primary source to determine the use of the chemical being described. A level of caution was exercised to not make assumptions or propagate unsubstantiated claims regarding the chemical’s use, focusing the assignment of keywords strictly on information presented in the primary data source. Additionally, care was taken to avoid the assignment of conflicting keywords and to limit the room for subjective user interpretation of a cassette. Resulting keyword cassettes provide a concise overview of an individual chemical’s use, according to the primary source.

A listing of keyword kinds included in the CPDat version 3 release can be found in Table SM1. Keywords, along with their definition and assigned keyword kind, can be found in Table SM2. As an illustrative example of the keyword assignment process, consider a report from the California Department of Pesticide Regulation that chronicles the use trends of pesticides on California’s Proposition 65 list that are known to be reprotoxic. Individual chemicals in this report received a cassette {Pesticides}, as this is what could be confidently inferred about the chemicals’ use according to the original document. Another primary source from the Danish Environmental Protection Agency details hundreds of chemicals associated with children’s personal care products such as shampoo, bodywash, soap, and lotion. These chemicals were assigned keywords resulting in the cassette {children; Europe; Personal Care}. This cassette should be interpreted as there is a relation between the chemical and a personal care product labeled for use by children in Europe. It is important to note that this cassette does not imply a detectable presence of the chemical, as the results of this report were largely based on the declaration of contents for many of the listed products.
It was common for keywords belonging to certain kinds to be used as part of the same cassette, for example, keywords belong to the PUC and Modifier kinds. Combining a keyword belonging to the Modifier kind (“detected”) and a keyword belonging to the PUC kind (“Personal Care – dental care – toothpaste”) creates the keyword cassette (“detected”; “Personal Care – dental care - toothpaste”). A chemical record would be assigned this cassette if the chemical was tested for and found in toothpaste. Modifiers were also commonly used alongside keywords belonging to the Media kind and the Foods & Agriculture kind, to describe a chemical’s presence in specific media or food related substances. The keyword cassette {nondetect; Pesticides; surface_water}, for instance, should be interpreted as a chemical identified as a pesticide, was tested for, but not found, in surface water.
TABLES

Table SM1. Keyword Kinds with definitions included in CPDat version 3. PUC kinds (PUC-article, PUC-formulation, and PUC-industrial) were built upon the previously defined PUC system, a hierarchical system for categorizing consumer products to aid in exposure assessments (Isaacs et al. 2020). PUC kind keywords always refer to a product, and the assimilation of the PUC system into this dataset allows for the integration of Chemical List Presence data with other data in CPDat.

| Keyword Kind | Definition |
|--------------|------------|
| Foods & Agriculture | related to food and agriculture |
| General use | related to general chemical use |
| Location | related to location/origin of the document/list |
| Manufacturing | related to the manufacturing process |
| Media | associated with a specific environmental media, e.g., as in a measurement study |
| Modifiers | keyword modifies other keywords assigned to the same list/chemical combination |
| PUC – article | keyword is a product use category (PUC) of kind “article” |
| PUC – formulation | keyword is a product use category (PUC) of kind “formulation” |
| PUC – industrial | keyword is product use category (PUC) of kind industrial/occupational |
| Specialty list | keyword refers to a recognized, specialty list of chemicals, e.g., a regulatory list |
| Subpopulation | keyword denotes specific population associated or affected by the document/list |
| Keyword                        | Definition                                                                 | Keyword Kind       |
|-------------------------------|-----------------------------------------------------------------------------|--------------------|
| active_ingredient             | active ingredients in a product                                             |                    |
| Pesticides                    | Relating to pesticides or pesticide usage. Includes specific types of      |                    |
|                               | pesticides, e.g. insecticides, herbicides, fungicides, and fumigants; also|                    |
|                               | includes general biocides                                                   | PUC - formulation  |
| agricultural                  | general term pertaining to agricultural practices, including the           | Foods & Agriculture|
|                               | raising and farming of animals and growing of crops                        |                    |
| applied                       | modifier, e.g. for a pesticide applied to a particular crop (as            |                    |
|                               | compared to a pesticide being detected in that crop or food product)      |                    |
| detected                      | chemicals measured or identified in environmental media or products        |                    |
| ground_water                  | of, found in, or related to ground water                                    | Media              |
| Europe                        | Sources specific to a European country or subset of countries              | Location           |
| plastic_additive              | additives used in plastics                                                 | Manufacturing      |
| drinking_water                | water intended for drinking, or related to drinking water; includes        | Media              |
|                               | bottled water, finished water from drinking water treatment plants, and    |                    |
|                               | untreated water that has been denoted as a drinking source                 |                    |
| manufacturing                 | NA                                                                           | Manufacturing      |
| fruits_and_vegetables         | includes fresh, canned and frozen forms, as well as juices and             | Foods & Agriculture|
|                               | sauces (e.g. applesauce), excludes forms intended for consumption by young |                    |
|                               | children (i.e. baby foods); includes green beans and peas                  |                    |
| cotton                        | of or related to the growing of cotton, or processed cotton used as        | Foods & Agriculture|
|                               | a textile for consumer goods                                               |                    |
| pharmaceutical                | includes, medicinal and illicit drugs, biologics, and the salts, esters,   | General use        |
|                               | and hydrates of pharmaceuticals, includes precursors to                    |                    |
|                               | pharmaceuticals, additives, and pharmaceuticals for                        |                    |
|                               | animal/veterinary use                                                      |                    |
| Australia                     | Sources specific to Australia                                              | Location           |
| Personal care                 | General personal care products which can not be assigned to a              | PUC - formulation  |
|                               | more refined category                                                      |                    |
| Canada                        | Sources specific to Canada                                                 | Location           |
| Substances in PCP - Canada    | Substances in cosmetics and personal care products regulated under the    | Specialty list     |
| (4/2014)                      | Canadian Food and Drugs Act (F&DA) that were in commerce between January  |                    |
|                               | 1, 1987 and September 13, 2001; list updated 4/24/2014                    |                    |
| consumer_product              | Indicated as related to, or in, consumer products, but with no more       | General use        |
|                               | specific information designating product category                          |                    |
| Substances in Products -     | Substances in products regulated under the Canadian Food and Drugs Act    | Specialty list     |
| Canada (4/2014)               | (F&DA) that were in Commerce between January 1, 1987 and September 13,    |                    |
|                               | 2001 (list updated 4/24/2014)                                             |                    |
| inert_ingredient              | NA                                                                           | Modifiers          |
| non_food_use                  | chemicals specifically designated as not for food use (e.g., pesticides   |                    |
|                               | approved for non-food use                                                  |                    |
| children                      | pertaining to, or intended for use specifically by children                | Subpopulation      |
| Arts and crafts/Office supplies - | products used to create textured or fiber covered surfaces,             | PUC - formulation  |
| - flocking                    | including artificial snow                                                  |                    |
| Category                                           | Description                                                                 | Modifier                                                                 |
|----------------------------------------------------|-----------------------------------------------------------------------------|--------------------------------------------------------------------------|
| Arts and crafts/Office supplies - general arts and crafts supplies | arts and crafts supplies which can not be assigned to a more refined category | PUC - formulation                                                        |
| Cleaning products and household care - air freshener | home air fresheners, including candles with a fragrance                    | PUC - formulation                                                        |
| Vehicle - car interior - auto air freshener        | products for masking odors or adding fragrance to car cabin air              | PUC - formulation                                                        |
| Cleaning products and household care - laundry and fabric treatment - fabric deodorizer | fabric deodorizers                                                          | PUC - formulation                                                        |
| nondetect                                          | Chemicals that were tested for but not found in media or products. May include concentrations below the limit of detection, and instances where a measurement was not reported due to issues with measuring equipment, QA concerns, or other reasons. | Modifiers                                                                |
| Cons electronics mech appliances and machinery     | Including small and large consumer electronics appliances (e.g. refrigerator, washing machine, vacuum cleaner, computer, phone, smoke detector, electric tools, lamps); includes small electronics with direct personal contact such as massagers; excludes electronics specifically intended for use by children; excludes electronics with direct food contact (e.g. electric blender) | PUC - article                                                           |
| air emissions                                      | release of a chemical from a source to an environmental medium; includes off-gassing | General use                                                              |
| Cleaning products and household care - shoes       | Products related to the care of footwear which do not fit into a more refined category | PUC - formulation                                                        |
| Personal care - body oil                          | lipophilic products applied to skin (excluding baby oils)                   | PUC - formulation                                                        |
| Toys and children's products                      | Toys and articles intended for use by children (not including formulations) (e.g. stuffed toys, blankets, games, baby bottles and pacifiers, dolls) | PUC - article                                                            |
| artificial_sweat                                   | artificial sweat - media specific to the chemical presence                  | Media                                                                   |
| Arts and crafts/Office supplies - home office - pens and markers | writing utensils containing liquid or gel ink                                  | PUC - formulation                                                        |
| Arts and crafts/Office supplies - general arts and crafts supplies - arts and crafts adhesive | glue sticks, glitter glues, fabric glues, craft glue, spray mounts, stencil sprays, and other adhesives used for primarily craft purposes | PUC - formulation                                                        |
| Arts and crafts/Office supplies - general arts and crafts supplies - arts and crafts paint | paints (including acrylic and enamel), colorants (materials that color solid objects), and pigments primarily used for craft purposes | PUC - formulation                                                        |
| Arts and crafts/Office supplies                    | unspecified arts and crafts or office supplies which can not be classified into a more refined category | PUC - formulation                                                        |
| general_foods                                      | unspecified foods or beverages for human consumption; these may be crops (e.g. raw fruits or vegetables) or processed goods | Foods & Agriculture                                                      |
| Medical/dental                                     | Medical and dental supplies and equipment, e.g. medical equipment used in a hospital or doctor's office setting, at home (e.g. wheelchairs, colostomy bag). Includes clothing and personal protective equipment used in medical settings (e.g. scrubs, face masks, gowns, gloves) | PUC - industrial                                                        |
| radioactive                                        | compounds identified as being radioactive                                 | General use                                                              |
| surface_water                                     | of, in, or related to surface water                                        | Media                                                                   |
| soil                                               | of, found in, or related to sediment or soil                              | Media                                                                   |
| Arts and crafts/Office supplies - fabric treatment and dye | Fabric treatments or dyes which can not be assigned to a more refined category | PUC - formulation                                                        |
| artificial_saliva                                  | artificial saliva - media specific to the chemical presence                | Media                                                                   |
| Personal care - body hygiene - hand soap | liquid hand soaps | PUC - formulation |
| CEDI | The U.S. FDA Cumulative Estimated Daily Intake database of publicly available cumulative estimated daily intakes (CEDIs) for a large number of food contact substances | Specialty list |
| Indirect additives food contact (10/2018) | U.S. FDA list of Indirect Additives used in Food Contact Substances; presence of a substance in this list indicates that only certain intended uses and use conditions are authorized by FDA regulations (version of list updated 10/4/2018) | Specialty list |
| wastewater | of, in, or related to wastewater, includes sludge and biosolids | Media |
| Furniture and Furnishings | Items used to furnish a home or workplace, e.g. tables, chairs, sofa, outdoor patio furniture, sofa cover, hammock, mattress, area rug | PUC - article |
| Other indirect contact consumer goods | Misc. consumer goods likely to have indirect contact with the user (e.g. home decor (paintings, decorations), lampshades) | PUC - article |
| Construction and building materials | Materials used for construction (e.g. flooring, tile, sinks, bathtubs, mirrors, wall materials/drywall, wall-to-wall carpets, insulation, playground surfaces); includes semi-permanent fixtures such as faucets and light fixtures | PUC - article |
| residue | chemical residues, typically from drugs or pesticides | Modifiers |
| animal_feed | Includes hay, alfalfa hay, and pastures/rangeland | Foods & Agriculture |
| baby_food | Jarred and canned foods intended for consumption by infants and toddlers (includes formula) | Foods & Agriculture |
| general_crops | Misc. crops, including sunflowers | Foods & Agriculture |
| Road vehicles | Road vehicles for passengers and goods (e.g. cars, trucks, vans) | PUC - article |
| Flavornet | substances on the Flavornet list of compounds found in the human odor sphere | Specialty list |
| Personal care - nails - nail polish | clear or colored nail enamels, polishes, basecoats, topcoats, and other acrylic coatings | PUC - formulation |
| Personal care - nails | products for nail or cuticle treatment or decoration | PUC - formulation |
| Other direct contact consumer goods | Misc. consumer goods likely to have direct contact with the user (e.g. sports equipment, hand-held non-electric tools, jewelry, clothing, jackets, bags/luggage/purses, and other apparel, blankets and sheets, newspapers, adult diapers, feminine hygiene products, pencils and writing implements | PUC - article |
| Cleaning products and household care - laundry and fabric treatment | Cleaning or care products for laundry and fabric treatment which do not fit into a more refined category | PUC - formulation |
| Cleaning products and household care | Cleaning and household care products that can not be placed in a more refined category | PUC - formulation |
| animal_products | Meat, poultry, fish and eggs (includes honey) | Foods & Agriculture |
| prohibited | noted chemical is prohibited from specified use | Modifiers |
| grain | excludes soybean grain (included with legumes); excludes corn grain (included with fruits and vegetables) | Foods & Agriculture |
| legumes | Legumes, excludes green beans and peas (included with fruits and vegetables); excludes peanuts and peanut butter (included with nuts) | Foods & Agriculture |
| nuts | includes peanuts and nut butters | Foods & Agriculture |
| organic | for food or crops that are specified as being grown or produced organically | Foods & Agriculture |
| tobacco | NA | Foods & Agriculture |
| supplements | supplements for human consumption, includes prebiotics, probiotics, and vitamins | Foods & Agriculture |
| Category                                                      | Subcategory                                                                 | Description                                                                                                                                                                                                 | Source                                                                 |
|---------------------------------------------------------------|------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------|
| Arts and crafts/Office supplies                              | children's art and toys - modeling clay                                      | soft modeling compounds                                                                                                                                                                                  | PUC - formulation                                                    |
| Cleaning products and household care                          | shoes - shoe polish or protectant                                             | products applied to footwear to color, polish, clean, or add a protective surface                                                                                                                        | PUC - formulation                                                    |
| Cleaning products and household care                          | carpet and floor - floor polish                                              | products that impart a shine to solid floors                                                                                                                                                             | PUC - formulation                                                    |
| Specialty occupational products                               |                                                                              | Specialty products used in a specific occupational setting, by members of that occupation (e.g. firefighting foam, metal working fluids, products used in portable toilets) | PUC - industrial                                                    |
| Raw materials                                                 |                                                                              | Pure chemicals or ingredients                                                                                                                                                                           | PUC - industrial                                                    |
| OEHHA Proposition 65 (3/2019)                                |                                                                              | California Office of Environmental Health Hazard Assessment Proposition 65; version of list updated 3/18/2019                                                                                                                                 | Specialty list                                                       |
| water                                                         |                                                                              | found in water of a nondescript or unspecified type (e.g. not ground water, surface water, etc)                                                                                                                                 | Media                                                                |
| Vehicle - car interior                                       |                                                                              | formulation products used on the interior of cars, which do not fit into a more refined category                                                                                                                                 | PUC - formulation                                                    |
| Cleaning products and household care                          | oven - oven cleaner                                                          | products used to clean grills, ovens, or range cooktops                                                                                                                                                  | PUC - formulation                                                    |
| Arts and crafts/Office supplies                              | body paint - tattoo ink                                                      | inks used for permanent tattoos                                                                                                                                                                          | PUC - formulation                                                    |
| Personal care - specialized bath products - bath salts        |                                                                              | solid or powdered products added to bathwater including bath salts, soaks, and fizzes                                                                                                                     | PUC - formulation                                                    |
| Personal care - general moisturizing - hand/body lotion      |                                                                              | products specifically marketed for application to hands or body to moisturize or improve skin characteristics (excluding baby lotion)                                                                        | PUC - formulation                                                    |
| Personal care - body hygiene - body wash                      |                                                                              | body cleaners, washes, shower gels                                                                                                                                                                         | PUC - formulation                                                    |
| Personal care - hair styling and care - shampoo              |                                                                              | shampoos, including dual shampoo/conditioner products                                                                                                                                                     | PUC - formulation                                                    |
| Personal care - specialized bath products - bubble bath      |                                                                              | products added to bath water to create bubbles, may provide cleaning, fragrance, or improve skin characteristics (including bubble bath marketed to babies or children) | PUC - formulation                                                    |
| Personal care - dental care - toothpaste                      |                                                                              | toothpastes and dentrifices                                                                                                                                                                               | PUC - formulation                                                    |
| Personal care - fragrance                                    |                                                                              | fragrances, colognes, and perfumes                                                                                                                                                                         | PUC - formulation                                                    |
| Personal care - make-up and related                          |                                                                              | make-up or cosmetic products which do not fit into a more refined category                                                                                                                               | PUC - formulation                                                    |
| Arts and crafts/Office supplies                              | body paint                                                                   | products placed on the skin for decorative purposes (body paints, markers, glitters, play cosmetics, Halloween cosmetics, and henna)                                                                        | PUC - formulation                                                    |
| Personal care - hair coloring                                |                                                                              | general hair coloring products which can not be classified into a more refined category                                                                                                                    | PUC - formulation                                                    |
| Personal care - make-up and related - eye liner               |                                                                              | eye liners or brow coloring products                                                                                                                                                                       | PUC - formulation                                                    |
| Cleaning products and household care                          | laundry and fabric treatment - laundry stain remover                          | stain removers or laundry pre-treatment products                                                                                                                                                          | PUC - formulation                                                    |
| Category                                                                 | Description                                                                                                                                                                                                 | Location       |
|-------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|
| Cleaning products and household care - carpet and floor - carpet cleaner | Carpet cleaning products that may be used directly (or require dilution), includes solutions that may be used by hand or in mechanical carpet cleaners                                                                 | PUC - formulation |
| Home maintenance - caulk/sealant                                        | Liquid or gels designed to seal cracks or fill cracks and depressions on hard surfaces                                                                                                                      | PUC - formulation |
| Personal care - hair styling and care - shampoo-dandruff                | Shampoos, including dual shampoo/conditioner products for treatment of dandruff                                                                                                                          | PUC - formulation |
| Home maintenance - adhesives and adhesive removers - multipurpose adhesive | General purpose repair adhesives including all purpose glues, super glue, and epoxies; not including wood glues                                                                                           | PUC - formulation |
| Cleaning products and household care - general household cleaning - surface cleaner | Products used to clean hard surfaces in the home, including kitchen specific hard surface cleaners                                                                                                       | PUC - formulation |
| Cleaning products and household care - dishwasher and dishes           | Cleaning products used in the dishwasher or on dishes, which do not fit into a more refined category                                                                                                   | PUC - formulation |
| Cleaning products and household care - general household cleaning       | Cleaning products for general household cleaning, which do not fit into a more refined category                                                                                                         | PUC - formulation |
| Cleaning products and household care - laundry and fabric treatment - fabric softener | Products used to improve tactile properties of fabrics that are added to the rinse water of clothes washers (excluding dryer sheets)                                                                 | PUC - formulation |
| Vehicle - car surface treatment - body cleaner                          | Cleaners, shampoos, and washes for auto body exterior (not including wax products or combo wash/wax products)                                                                                             | PUC - formulation |
| Personal care - sexual wellness                                        | Sexual wellness products, including personal lubricants                                                                                                                                                | PUC - formulation |
| Personal care - deodorant                                              | Deodorants and antiperspirants                                                                                                                                                                           | PUC - formulation |
| Personal care - liniment                                               | Products for treatment of muscle or joint pain                                                                                                                                                           | PUC - formulation |
| Personal care - body adhesive                                          | Adhesive products for attaching clothing or accessories to skin                                                                                                                                          | PUC - formulation |
| Personal care - hair styling and care - hair conditioner               | Rinse-out everyday hair conditioners (excluding combo shampoo/conditioner products)                                                                                                                      | PUC - formulation |
| Personal care - make-up and related - toner                            | Face and skin toners and astringents excluding eye related products                                                                                                                                     | PUC - formulation |
| Home maintenance - adhesives and adhesive removers - wood adhesive     | Adhesives specifically designated for gluing wooden surfaces together                                                                                                                                     | PUC - formulation |
| fossil_fuels                                                           | Coal, petroleum, natural gas, and heavy oils                                                                                                                                                            | General use    |
| dairy                                                                   | Milk and foods produced from or containing milk                                                                                                                                                         | Foods & Agriculture |
| Personal care - hair coloring - hair color - permanent                 | Hair colors and dyes characterized as permanent, excludes dyes intended for use by professionals                                                                                                          | PUC - formulation |
| Personal care - hair coloring - hair color - professional              | Hair colors and dyes characterized as for professional use                                                                                                                                                 | PUC - formulation |
| Personal care - sunscreen                                              | Products applied to the skin to block harmful effects of sunlight                                                                                                                                        | PUC - formulation |
| Southeast Asia                                                         | Sources specific to ASEAN countries, governing body for various Southeast Asian countries                                                                                                                | Location       |
| MN Chemical Screening                                                  | Applied to all data sources used in MN DoH chemical screening proof of concept                                                                                                                             | Specialty list |
| New Zealand                                                            | Sources specific to New Zealand                                                                                                                                                                          | Location       |
| Arts and crafts/Office supplies - children's art and toys - crayons    | Wax crayons for coloring or illustration                                                                                                                                                               | PUC - formulation |
| Arts and crafts/Office supplies - children's art and toys              | General children's art supplies and toys which can not be classified into a more refined category                                                                                                        | PUC - formulation |
| Israel | Sources specific to Israel | Location |
|-------|--------------------------|----------|
| restricted | noted chemical is restricted from specified use | Modifiers |
| IFRA Transparency | substances on the International Fragrance Association's ordered register of all fragrance ingredients used in consumer goods by the fragrance industry's customers worldwide | Specialty list |
| WA Children's Safe Product Act (4/2020) | present on the WA State Department of Ecology - Chemicals of High Concern to Children Reporting List (version of list pulled 4/24/2020) | Specialty list |
| fracking | chemicals related to or used during the fracking process | General use |
| Vehicle - car surface treatment - body wax | auto body waxes and coatings, excluding combo wash/wax products | PUC - formulation |
| Cleaning products and household care - dishwasher and dishes - automatic dishwashing additive | products used in automatic dishwashers other than detergents (rinse aids, spot removers, and dishwasher cleaners/scale or rust removers) | PUC - formulation |
| Food contact items | articles intended for food contact, including food-contact packaging (e.g. glasses, plates, pots/pans, food storage containers, cloth napkins and placemats, cutlery, paper plates, and plastic utensils, take-out containers, plastic wrap and foil; includes small electronics with direct food contact (e.g. blender) | PUC - article |
| Landscape/Yard - cleaner | products used to clean hard surfaces outside of the home including decks, driveways, and external walls; includes products used as part of a mechanical cleaning system (e.g. solutions for pressure sprayers) | PUC - formulation |
| Vehicle - car surface treatment | treatments for the surfaces/body of vehicles that can not be otherwise categorized | PUC - formulation |
| Personal care - dental care | Personal dental care products that can not be assigned to a more refined category | PUC - formulation |
| Home maintenance - plumbing | miscellaneous plumbing repair products (putties, tapes, cements) | PUC - formulation |
| Cleaning products and household care - carpet and floor | Household carpet and floor cleaning products that can not be assigned to a more refined category | PUC - formulation |
| Substances Added to Food (formerly EAFUS) (2/2019) | U.S. FDA Substances Added to Food inventory (formerly known as 'Everything Added to Foods in the United States (EAFUS)' (version of list updated 2/8/2019) | Specialty list |
| SCIL (9/2019) | present on the Safer Chemicals Ingredients List (SCIL) (https://www.epa.gov/saferchoice/safer-ingredients); version of list updated 9/14/2019 | Specialty list |
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Isaacs KK, Dionisio K, Phillips K, Bevington C, Egeghy P, Price PS. 2020. Establishing a system of consumer product use categories to support rapid modeling of human exposure. J Expo Sci Environ Epidemiol 30:171-183.
SUPPLEMENTAL FIGURES

Figure S1A. Total sum of squares and silhouette profile for determining the optimal number of chemical clusters ($k$) where $1 \leq k \leq 100$. 
Figure S1B. Total sum of squares and silhouette profile for determining the optimal number of exposure source category clusters (k) where $1 \leq k \leq 31$. 
Figure S2. Distribution of enriched structural features across all UCs evaluated within CPDat (N=6,306 total). Here, ‘enriched structural features’ were identified as ToxPrint chemotypes that were significantly more commonly present in BCs in comparison to NBCs. Note the y-axis starts at 1.
Figure S3. Distribution of physicochemical correlations between U Cs and BCs. Correlations were calculated on a per-cluster basis and combined for visualization.
**Reporting Checklist**

This checklist is used to ensure the quality, transparency, and reproducibility of published results. We require authors attest that these components have been considered and addressed.

| Exposure Assessment Guiding Principle                                                                 | Yes/No/Not Applicable |
|--------------------------------------------------------------------------------------------------------|------------------------|
| Has the method to estimate exposure been described clearly?                                             | Yes                    |
| Has the exposure assessment method been validated/evaluated as a proxy for exposure and is its validity or agreement with other methods described? | Yes                    |
| Is the time period over which the exposure assessment method is considered to be a proxy for exposure appropriate for the research question? | N/A                    |
| If exposure is modeled or measured, were all critical potential routes and sources of exposure considered? | Yes                    |
| If exposure is modeled, how does it vary over space and time and are necessary historical data incorporated? | N/A                    |
| If biomarkers are used as indicators of exposure, could the biomarker measurement have been affected by the outcome (i.e., reverse causality)? | N/A                    |
| Are the strengths and weaknesses of the exposure approach detailed and discussed?                      | Yes                    |