

SUPPLEMENTAL MATERIAL

Exploring Consumer Exposure Pathways and Patterns of Use for Chemicals in the Environment

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Creation of ACToR UseDB

In parallel to constructing CPCat, the authors created the ACToR UseDB using an automated approach to mine the full ACToR database and assign chemicals to a small number of broad chemical use categories (Supplemental Table 1). A total of 514 separate listings (many of them federal, state, and international regulatory listings) for chemicals falling into specific use classes (e.g., U.S. EPA Antimicrobials Re-registration, The International Fragrance Association's List of Fragrance Ingredients) were used to extract a set of distinct ACToR data sets (the full names of all listings used to compile the UseDB are available at www.actor.epa.gov/cpcat). Each ACToR data set was manually assigned to one of 15 broad chemical use categories (e.g., chemicals in the ACToR data set derived from the U.S. EPA Antimicrobials Re-registration list were assigned to the "Antimicrobials" category; Figure 1a).

All chemicals in the full ACToR database (551,763 as of March 31, 2014) were checked against the ACToR data set extracted for the UseDB, and assigned to one or more of the 15 broad UseDB categories (Supplemental Table 1), based on the category associated with the ACToR data set(s) where that chemical appeared. To reduce incorrect category assignments, a small number of manual adjustments were made to the assigned UseDB categories for each chemical. Because potential pesticide residues on raw products carried over into processed foods are considered food additives by the U.S. Food and Drug Administration (FDA), the majority of chemicals assigned to the pesticide category were also marked for food use. To eliminate this overlap, any chemical that was known to be a pesticide was subsequently excluded from the food use category. In this way it is up to the user to identify if pesticide residues are detected in food; however, ambiguity is eliminated that the chemical is deliberately used as a food additive. Expert opinion was also solicited to identify any chemicals that were miscategorized (e.g., one data source classified

progesterone as a fertilizer, it was removed). Lastly, in creating the UseDB, only detected chemicals from the DCPS source within ACToR Data Sets and Lists were included (chemicals analyzed for but not detected were not included).

Because the UseDB aggregates chemical data from a variety of sources, chemicals often had more than one ACToR data set assignment. To provide a weight of evidence for the chemical assignments to the 15 broad UseDB categories, the number of ACToR data sets per chemical which mapped to each UseDB category (i.e., the number of ‘hits’) after making the above adjustments were output. More ‘hits’ per UseDB category indicated stronger support for that category assignment for that chemical. Any chemicals with fewer than three hits for a given UseDB category were manually checked to determine whether or not that use category was appropriately assigned.

CPCat cassettes associated with ethylparaben (Example 1; full list)

agricultural	personal_care bath
agricultural animal	personal_care cosmetics
agricultural crop	personal_care cosmetics baby_use
arts_crafts	personal_care cosmetics bath baby_use
arts_crafts drawing	personal_care cosmetics body
arts_crafts paint	personal_care cosmetics body powder
automotive_care	personal_care cosmetics cream colorant
child_use	detected
cleaning_washing	personal_care cosmetics eye
cleaning_washing flooring	personal_care cosmetics face
cleaning_washing machines dishwashing	personal_care cosmetics fragrance
cleaning_washing stain_remover detected	personal_care cosmetics hair
construction	personal_care cosmetics hair detected
consumer_use_ACToRUseDB	personal_care cosmetics hair_removal
detergent	personal_care cosmetics hair_removal cream
drug	personal_care cosmetics hand cream
drug dietary_supplement	personal_care cosmetics lips
drug inactive_ingredient	personal_care cosmetics lotion
drug veterinary	personal_care cosmetics lotion detected
electronics batteries	personal_care cosmetics nails
electronics batteries consumer_use	personal_care cosmetics perfume
facility salon detected	personal_care cosmetics preservatives
fluid_property_modulator	personal_care cosmetics shampoo detected
food_additive	personal_care cosmetics shampoo hair
food_additive flavor	personal_care cosmetics soap detected
food_additive preservatives	personal_care sanitizer hand
food_additive_ACToRUseDB	personal_care sexual_wellness gel detected
food_contact	personal_care shower gel
fragrance consumer_use	personal_care soap
hunting	personal_care soap hand
industrial cleaning_washing	personal_care sunscreen
industrial_manufacturing_ACToRUseDB	personal_care sunscreen detected
inert_ACToRUseDB	personal_care wash
manufacturing chemical	personal_care wash body
manufacturing cleaning_washing polish	personal_care wash face
manufacturing detergent	personal_care wash hand
manufacturing drug	personal_care_ACToRUseDB
manufacturing export	pesticide
manufacturing metals	pesticide biocide active_ingredient
manufacturing personal_care	pesticide inert_ingredient
manufacturing personal_care cosmetics	pesticide preservatives
perfume	photographic
manufacturing soap	preservatives
paint	raw_material personal_care cosmetics
paraben	sports_equipment
personal_care	surface_treatment

tools personal_care hair
toys
toys arts_crafts
toys arts_crafts drawing
toys baby_use
toys child_use
toys lawn_garden

Consumer-related cassettes selected for use in Example 3 (full list)

adhesive consumer_use	child_use
adhesive powder consumer_use	child_use phthalates detected
adhesive water_based consumer_use	cleaning_washing bathroom consumer_use
air_fresheners consumer_use detected	cleaning_washing carpet consumer_use
air_fresheners fragrance consumer_use	cleaning_washing consumer_use
air_treatment consumer_use	cleaning_washing dishwashing
apparel	cleaning_washing enclosed consumer_use
apparel arts_crafts	cleaning_washing flooring consumer_use
apparel baby_use	cleaning_washing fragrance consumer_use
apparel baby_use diaper	cleaning_washing glass consumer_use
apparel bags	cleaning_washing kitchen consumer_use
apparel clothing handwear phthalates detected	cleaning_washing laundry consumer_use
apparel footwear baby_use	cleaning_washing laundry fragrance
apparel footwear phthalates detected	consumer_use
apparel handwear	cleaning_washing machines dishwashing
apparel jewelry detected	cleaning_washing pet
apparel pet	cleaning_washing sports_equipment
apparel_care	cleaning_washing toilets
apparel_care footwear	cleaning_washing tools consumer_use
appliance air_treatment consumer_use	colorant consumer_use detected
appliance consumer_use	consumer_use
appliance food_contact consumer_use	consumer_use_ACToRUseDB
appliance refrigeration consumer_use	decor baby_use
appliance vacuum consumer_use	decor bathroom
arts_crafts	decor candle
arts_crafts child_use detected	decor lawn_garden
arts_crafts clay detected	decor lighting
arts_crafts drawing	decor lighting lawn_garden
arts_crafts paint	decor walls consumer_use
arts_crafts paper	drinking_water
arts_crafts textile	drinking_water disinfectant
automotive_care consumer_use	drinking_water food_contact plastics
automotive_component batteries	drinking_water_contaminant
consumer_use	drinking_water_contaminant drug detected
automotive_component consumer_use	drinking_water_contaminant pesticide detected
automotive_component interior consumer_use	electronics baby_use
automotive_component tires consumer_use	electronics batteries consumer_use
baby_use detected	electronics sports_equipment
batteries consumer_use	electronics toys child_use
bedding baby_use detected	explosives consumer_use
beverage juice	extermination consumer_use
beverage powder	fertilizer consumer_use
building_material ceramic tile consumer_use	flame_retardant
building_material flooring consumer_use	food
building_material insulation consumer_use	food baby_use
building_material paving consumer_use	food cereal

food cooking_oils
food dairy
food fats
food_additive
food_additive colorant
food_additive flavor
food_additive meat
food_additive preservatives
food_additive sweetener
food_contact
food_contact consumer_use
food_contact plastics
food_residue
food_residue dairy pesticide detected
food_residue fish
fragrance consumer_use
fuel automotive
fuel consumer_use
fungicide consumer_use
furniture bedding
furniture lawn_garden
furniture pet
heating consumer_use
heating fire consumer_use
heating fire lawn_garden
hunting
impregnation consumer_use detected
lawn_garden consumer_use
leather consumer_use
lubricant automotive_care consumer_use
lubricant consumer_use
personal_care
personal_care baby_use
personal_care bath
personal_care cosmetics
personal_care cosmetics after_shave
personal_care cosmetics baby_use
personal_care cosmetics bath
personal_care cosmetics bath baby_use
personal_care cosmetics body
personal_care cosmetics body powder
personal_care cosmetics child_use detected
personal_care cosmetics colorant
personal_care cosmetics conditioner hair
personal_care cosmetics cream detected
personal_care cosmetics cream colorant
detected
personal_care cosmetics deodorant

personal_care cosmetics exfoliator
personal_care cosmetics eye
personal_care cosmetics face
personal_care cosmetics foot
personal_care cosmetics fragrance
personal_care cosmetics hair
personal_care cosmetics hair_dye
personal_care cosmetics hair_dye colorant
personal_care cosmetics hair_removal
personal_care cosmetics hair_removal cream
personal_care cosmetics hand cream
personal_care cosmetics lips
personal_care cosmetics lotion
personal_care cosmetics nails
personal_care cosmetics perfume
personal_care cosmetics powder hair
personal_care cosmetics preservatives
personal_care cosmetics prohibited_ASEAN
personal_care cosmetics restricted_ASEAN
personal_care cosmetics restricted_Europe
personal_care cosmetics restricted_UK
personal_care cosmetics shampoo detected
personal_care cosmetics shampoo hair
personal_care cosmetics skin
personal_care cosmetics skin colorant detected
personal_care cosmetics soap
personal_care dental
personal_care dental floss
personal_care ears detected
personal_care eye
personal_care feminine_care
personal_care feminine_care sanitary_napkins
detected
personal_care feminine_care tampons detected
personal_care first_aid
personal_care foot
personal_care health
personal_care incontinence
personal_care lawn_garden shower
personal_care lawn_garden toilets
personal_care mouthwash
personal_care paper detected
personal_care sanitizer hand
personal_care sexual_wellness
personal_care sexual_wellness gel detected
personal_care sexual_wellness liquid detected
personal_care sexual_wellness toys detected
personal_care shower gel

personal_care skin
personal_care soap
personal_care soap hand
personal_care sunscreen
personal_care thermometer
personal_care tools
personal_care tools hair_removal
personal_care toothpaste
personal_care wash
personal_care wash body
personal_care wash face
personal_care wash hand
personal_care wash scrub
personal_care_ACToRUseDB
pesticide consumer_use
pet
polish apparel_care footwear
solvent consumer_use
sports_equipment
sports_equipment child_use
stoves consumer_use
surface_treatment consumer_use
tea_coffee
textile colorant consumer_use detected
textile consumer_use detected

toilets baby_use
tools apparel consumer_use
tools consumer_use
tools food_contact consumer_use
tools lawn_garden
tools paint consumer_use
tools personal_care
tools personal_care dental toothbrush
tools personal_care hair
tools plumbing consumer_use
toys
toys arts_crafts
toys arts_crafts drawing
toys baby_use
toys child_use
toys decor
toys fragrance child_use detected
toys lawn_garden
toys lawn_garden child_use
toys mouthing baby_use
toys pet
water_treatment consumer_use
writing
writing correction_material
writing ink

Supplemental Table 1: Chemical use categories from ACToR UseDB

Antimicrobials	Substances or mixtures used to destroy or limit the growth of microorganisms, whether bacteria, viruses, or fungi
Chemical/industrial processes	Chemicals used in industry, including those used for chemical processing/manufacturing (e.g., common reagents, solvents)
Chemical warfare	Chemicals used in agents of chemical warfare
Colorants/dyes	Chemicals used in textile or decoration dyes
Consumer use	Chemicals used in consumer products
Fertilizer	Substances added to soil or land to increase fertility
Flame retardant	Chemicals added to polymeric materials, both natural and synthetic, to limit possible combustion
Food use/food additive	Substances intentionally added to food, or food contact materials, including substances regulated by the U.S. FDA which are generally recognized as safe (GRAS), or added to food directly (e.g., an ingredient), indirectly (e.g. food packaging materials), or as a colorant
Fragrances	An ingredient to enhance odor of a consumer product, including personal care products and household care products
Herbicide	Chemicals used to manipulate or control undesirable vegetation
Inert ingredients in pesticides	Inert ingredients in pesticides may not be chemically inert, but are not the active ingredient intended to prevent, destroy, repel, or reduce pests (e.g., a chemical solvent contained in a pesticide product)
Personal care products	Substances used in cosmetics and other items for personal care (e.g., make-up, shampoo, soap, moisturizers, deodorant, perfume)
Pesticides	Ingredients in products designed to prevent, destroy, repel, or reduce pests (e.g., insect repellants, weed killers, fungicides); may include both inert and active ingredients, if inert ingredients were not categorized as such by the source
Petrochemicals	Chemical products derived from petroleum
Pharmaceutical	Human prescription drug products and biological products