USDA IngID Thesaurus: an application dataset for systematic reporting of ingredients used in commercially packaged foods

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A. Background

Commercially processed foods are important contributors to food security (especially in terms of availability of food) and nutrient intake of the US population (Eicher-Miller et al., 2012; Weaver et al., 2014). They provide ≥~50% of energy and several nutrients, including those identified by the Dietary Guidelines for Americans to limit (added sugars, saturated fat, sodium) and to encourage (calcium, folate, iron, total dietary fiber) (Weaver et al., 2014). Dietary intake analysis among youth (aged 2-19 years) indicates increasing trends of consumption of highly processed foods (Wang et al., 2021), with intakes higher among selected minority populations and those with lower levels of education and lower socio-economic status (Baraldi et al., 2018). Intakes of highly processed foods have been linked to negative health outcomes such as excessive weight and other non-communicable diseases (Juul et al., 2018; Lawrence M, 2020). Several reasons for these outcomes have been proposed, including reduced nutritional quality, changes in physical structure of the food due to processing as compared to original whole unrefined foods, and ingredients such as added sweeteners, artificial flavorings, and other food additives (Juul et al., 2021). Public health agencies such as the American Heart Association suggest limiting the intake of highly processed foods as part of their dietary guidance (Lichtenstein et al., 2021).

As per the Code of Federal Regulations (21CFR§101.4), most commercially packaged foods should have ingredients listed on the label using their common or usual name and generally in descending order by weight (ingredients in amounts of 2% or less of the total weight of the product need not be listed in descending order by weight) (Food Labeling, Section 101.4) (US Food and Drug Administration, 2017). Furthermore, composite ingredients such as margarine, that contain two or more sub-ingredients must be listed in descending order by weight inside a parenthesis. Most food composition databases are focused on nutrients and mostly include generic food descriptions (i.e., limited brand name information). They use generic ingredients for nutrient determinations and typically have no specific information on ingredients such as specific sweeteners, added flavorings, and other food additives. Hence, in general, there is a lack of information about ingredients used in packaged foods in the scientific literature.

There has been some progress in the availability of food composition databases for commercially packaged foods in recent years. The USDA Global Branded Food Products Database (GBFPD) (U.S. Department of Agriculture, 2018), as part of USDA's FoodData Central (Fukagawa et al, 2022) makes publicly available label nutrient and ingredient information for over a quarter million packaged foods. The ingredient lists in GBFPD are obtained from label scans and manufacturer supplied data, are presented as free. In 2021, a prototype of IngID, a framework for parsing and systematically reporting ingredients used in commercially packaged foods was

developed using ingredient statements of \sim 6,800 top-selling baked products (Ahuja et al., 2021). The prototype was then used to characterize ingredients in baked products – cookies, crackers, fresh bread and rolls, and pies and doughnuts, with a focus on the intricacies and challenges of using ingredient statements (Ahuja et al., 2022).

B. IngID Thesaurus

Need for IngID Thesaurus

As part of the baked product IngID prototype, blocks of free text containing ingredient lists were obtained from GBFPD and parsed into separate individual ingredients (Ahuja et al., 2021). A review of the ingredient terms revealed that they are complex, inconsistent, contain spelling errors, and may have multiple synonyms for the same ingredient. For example, the ingredient, 'high fructose corn syrup' can be listed in several ways such as 'glucose-fructose syrup', 'high levulose corn syrup', 'glucose-fructose syrup (corn)', 'high fructose corn syrup' and so forth. In a study on added sugars, Scapin et al., (2018) identified 179 terms for added sugar. Similarly, we identified over 1,350 terms for wheat flour. Multiple names for the same ingredient and inconsistencies can impede consumers and researchers from understanding the ingredient lists and their use. The need for a thesaurus for use in data analysis of ingredient lists was highlighted by Cooper (2020) and Ahuja et al., (2021, 2022) in their studies on estimation of ingredient occurrences and co-occurrence networks. Tseng et al., (2022) reported differences in results when ingredient variations and errors are not taken into consideration. Similarly, we found differences in results for the top 5 sweeteners used in beverages, with and without the use of the thesaurus, underscoring the need for pre-processing and data clean-up in studies of commercial ingredients listed on label statements (Ahuja, unpublished data, May 2023). In the past few years, resources such as the National Agricultural Library Thesaurus (NALT) file (https://agclass.nal.usda.gov/), FooDB ('a resource on food constituents, chemistry, and biology', (https://foodb.ca/) and FoodOn (a food ontology system) (Dooley et al., 2018) have been made available in the public domain. However, none of these existing resources include entries of ingredients as listed on packaged foods. For example, FoodDB has an entry for goji, but not goji extract, goji juice concentrate, goji juice powder, or dried goji berries, i.e., the various forms of goji ingredients listed on the labels or its synonyms/spelling errors or variants, such as gojiberry, goji, or goji berry. Recognizing this need, we began work on a thesaurus for the baked products project, which was further expanded and is now being released publicly for the first time as the IngID Thesaurus.

Key features of IngID Thesaurus

• The first publicly available version, IngID Thesaurus Version 1 (2023) contains ~26,000 parsed ingredient terms, that have been assigned ~3,000 PDs, categorized in a taxonomic hierarchy of 16 broad groups (**Appendix 1**).

- These ingredient terms were parsed from ingredient lists of foods sold the most in the U.S. and of different types, ensuring breadth of coverage of the ingredient terms used in ingredient lists in the thesaurus.
- Type of ingredients include 1) single additives/isolated ingredients or agricultural-commodity-type ingredients such as citric acid and coconut oil, respectively, and 2) selected composite ingredients (that contain sub-ingredients), such as baking powder and enriched flours. **Appendix 2** lists some of the composite ingredients included in the current IngID Thesaurus. Composite ingredients such as enriched flours, different types of fats (e.g., margarine, shortening), sweeteners (e.g., powdered sugar), and high sodium ingredients (e.g., hot pepper sauce) were included as they may be of interest to consumers and researchers. The list can be expanded as per research interest.
- The IngID Thesaurus file includes the parsed ingredient term, assigned PD and broad group for each of the parsed ingredients.

Approach

Figure 1 provides an overview of the steps in the development of IngID Thesaurus. To summarize, we identified top-selling categories that contributed ≥ 1% of the total volume sold in the U.S. using point-of-sales data from Information Resources Incorporated (IRI). Thirty-one food categories (excluding alcoholic drinks) of the 173 IRI food categories met this criterion. Details of the data and its use to select top categories have been published earlier (Muth et al., 2016; Ahuja et al., 2021). We selected 16 of the 31 categories for Version 1 of the thesaurus, based on the variety and diversity of the type of ingredients used in their products. The selected categories include - baked products, such as cookies, crackers, fresh bread and rolls, and pies and doughnuts, beverages such as ready-to-drink tea and coffee, juices and juice drinks, candies, dairy products such as yogurt and cheese, frozen and refrigerated entrees, and soups, among others. New, parsed ingredients from additional categories can be included in the next versions of the thesaurus. We obtained ingredient lists (blocks of free text) from GBFPD for foods representing these 16 selected categories and parsed them into individual ingredients. The parsed ingredients were reviewed and parsed ingredients that were equivalent, similar, spelling or usage variants, spelling errors or synonyms were assigned the same Preferred Descriptor (PD). This allows for systematic reporting of these ingredients. Furthermore, the PDs were grouped broadly into a broad taxonomy scheme. The following example illustrates the steps: UPC code, 810253011520, Assorted European chocolate cookies, from food category 'Cookies', listed 'glucose-fructose syrup' as one of its ingredients. We assigned 'High fructose corn syrup' as a PD for 'glucose-fructose syrup', 'high levulose corn syrup', 'glucose-fructose syrup (corn)' (and 49 other spelling and usage variants) and then grouped it broadly as 'Additives and Isolated ingredients (includes sweeteners)' in the IngID Thesaurus.

To assign PDs, we used several existing resources when appropriate. Key resources include the FDA Food Substances Added to Foods inventory (US Food and Drug Administration, 2019a) and PubChem (https://pubchem.ncbi.nlm.nih.gov/) for additives and isolated ingredients; NALT and FooDB for mainly agricultural commodity-type ingredients. About a quarter of the PDs are based on these resources, which facilitates the sharing of data as well as integration with other systems. Many of the PDs were manually assigned by a staff food chemist or nutritionist, as

these resources did not include ingredients as listed on the labels such as spelling errors or were not consistent with our preferred terminology. For example, FDA Food Substances Added to Foods inventory includes 'Agar', however, the PD (variable name - 'Substance; in the FDA file), is 'AGAR (GELIDIUM SPP.)', which is not consistent with our approach of not including the scientific name in the PD, hence, not used. We used several trade association and non-profit organization websites (e.g., https://oldwayspt.org/programs/whole-grains-council), as well as national and international agencies such as Food and Agricultural Organization's Codex Standards, and Wikipedia to guide the process. All assigned PDs were reviewed by another nutritionist, followed by several checks such as to ensure consistency in terminology, spelling, singular or plural, etc., and to identify inadvertent errors.

We used the following general rules to guide us in manually assigning PDs; some of these were detailed earlier (Ahuja et al., 2021), and are commonly used with other ontology systems, such as FoodOn (https://foodon.org/design/curation-rules/).

- The first part of the description should identify the food product, for example, 'barley flour' rather than 'barley, flour', followed by additional descriptors such as 'malted', 'enriched' etc.
- Additional descriptors of a food may include physical characteristics (e.g., light meat), information on fortification (e.g., enriched), product form (e.g., puree or dried), preparation terms (e.g., cooked in oil or roasted), among others.
- The order of processing is represented in the description (e.g., 'pasta, enriched, cooked' rather than 'pasta, cooked, enriched', as the enrichment process is followed by cooking, and not vice versa).
- Singular terms are generally used for PDs, except when referring to a group of ingredients.
- For plant ingredients, we generally limited the taxonomic differentiation of PDs to the species level. Although we were able to define some PDs at the variety level, we did not describe PDs at the level of individual plant cultivars. For example, banana pepper and Anaheim pepper, 2 different cultivars of Capsicum annuum were both assigned the PD, 'hot pepper'.
- The level of specificity in the description of PDs was guided by 1) information present on ingredient lists, for example, the source of protein and starch are generally listed on labels, such as 'fish protein' or "corn starch', but not for enzymes. Therefore, we have ~70 PDs for different types of protein but only 1 PD Enzyme, 2) extent of use of the food. For the most frequently used commodity-type foods such as oil or wheat flour, we attempted more differentiation based on food type, food source, enrichment, processing, combinations, etc. For example, wheat flour has ~70 PDs whereas buckwheat flour has 2 PDs.

Appendix 3 illustrates some of the more specific rules with examples.

C. Conclusion

Here, we present the first version of a novel application dataset - IngID Thesaurus, which includes ~26,000 ingredient terms that have been assigned ~3,000 PDs, categorized under 16 broad groups. IngID includes varied ingredient terms from several food groups. It for the first time makes publicly available a tool that can potentially help reduce pre-processing and data clean-up time for the study of ingredients as listed on labels of commercially packaged foods. It will enable characterization of what is in the food we eat using standardized vocabulary and can potentially help improve our understanding of commercial ingredients, characterizing foods in dimensions other than the traditional nutrient profiles, and development of food ontology, computer programs, and artificial intelligence tools. However, more work needs to be done, especially in including more ingredient terms from additional food categories and expanding the level of detail available for each ingredient such as scientific names (as appropriate), etc.

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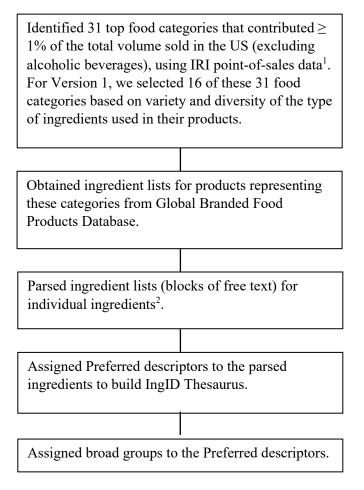
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Figure 1: Schema of the workflow for the development of IngID Thesaurus



¹ IRI: (Information Resources Incorporated) (Information Resources Inc. (IRI), 2016)

² Details of parsing methodology have been published (Ahuja et al., 2021 doi:10.1016/j.jfca.2021.103920)

Appendix 1: Broad groups of ingredients represented in IngID Thesaurus Version 1 (2023), and associated counts

Broad groups of ingredients	Count of unique Preferred descriptors (PDs) ¹ represented	Count of uniquely parsed ingredients assigned PDs ¹
Additives and Isolated ingredients (includes sweeteners)	878	10170
Algae	14	50
Beverages	20	160
Dairy and Dairy Products	214	2560
Eggs and Egg Products	14	116
Eubacteria ²	0	0
Fats and Oils	527	2654
Fruits and Fruit Products	362	1495
Fungi	18	138
Grains and Grain Products	237	2993
Legumes and Legume Products	81	371
Meats and Meat Products	100	603
Nut and Seed Products	78	1042
Seafood and Seafood Products	54	152
Spices, Herbs and Flavorings	215	1752
Vegetables and Vegetable Products	224	1419
Total	3036	25675

¹ The listed counts represent the number of unique PDs or parsed ingredients, not the frequency of their occurrence. These ingredients were parsed from selected top-selling food categories - baked products, such as cookies, crackers, fresh bread and rolls, and pies and doughnuts, beverages such as ready-to-drink tea and coffee, juices and juice drinks, candies, dairy products such as yogurt and cheese, frozen and refrigerated entrees, and soups, among others.

² The group has not been populated yet.

Appendix 2: Examples of composite¹ ingredients included in the thesaurus

Broad groups of ingredients	Examples
Additives and Isolated ingredients (includes sweeteners)	Baking Powder, powdered sugar
Dairy and Dairy Products	butter, buttermilk, fortified fluid milk, cheese, yogurt
Eggs and Egg Products	egg white (with added sulfite agent)
Fats and Oils	vegetable oil, margarine, shortening
Fruits and Fruit Products	Cranberry, sweetened, orange juice from concentrate,
Grains and Grain Products	enriched wheat flour, pasta
Legumes and Legume Products	tofu, cooked chickpeas with salt added
Meats and Meat Products	bacon, pepperoni, ham
Nut and Seed Products	cashew nut, oil roasted, semisweet chocolate
Spices, Herbs and Flavorings	broth, soy sauce, vinegar
Vegetables and Vegetable Products	tomato paste with salt, tomatoes in juice

¹ an ingredient with two or more sub-ingredients listed inside parentheses.

Appendix 3: Examples of parsed ingredients, assigned Preferred Descriptors and thesaurus rules used in the development of IngID Thesaurus

Aspect	Parsed ingredients	Assigned Preferred Descriptor (PD)	Rule for assigning PDs
General: Adjectives in the ingredient description – includes organic, source, proportions, etc.	organic palm oil; organic sustainable palm oil; palm oil (5%);	OIL, PALM	Disregard adjectives
General: Spelling Errors	soybeen oil	OIL, SOYBEAN	Disregard spelling errors
General: Function in the ingredient name	dough conditioner (ascorbic acid)	ASCORBIC ACID	Disregard functions in the name
General: Different forms with different moisture contents	freeze dried strawberry powder	STRAWBERRY, DRIED	Differentiate forms with varying moisture contents
	strawberry puree	STRAWBERRY PUREE	
	concentrated strawberry juice; strawberry concentrate	STRAWBERRY JUICE CONCENTRATE	
General: Non-specific ingredients	pepper	PEPPER	Non-specific PD, with some exceptions for highly popular ingredients
	flour	WHEAT FLOUR	
General: Cooking	almonds (dry roasted)	ALMOND, ROASTED	Differentiate cooking methods (based on NALT³) - baked, broiled, fried, grilled, parboiled, roasted (include toasted). Use cooked for other methods. Disregard cooking methods for flour, puree, and concentrates. Exceptions to the rule - use 'roasted in oil' for fried or oil-roasted nuts, seeds, and cereal grains, and 'cooked in oil' for pasta/noodles
	cashews (roasted in peanut oil)	CASHEW NUT, ROASTED IN OIL	
	pasta (semolina, water, eggs, sunflower oil)	PASTA, COOKED IN OIL	

Aspect	Parsed ingredients	Assigned Preferred Descriptor (PD)	Rule for assigning PDs	
Additives ¹ : Color	annatto for coloring; annatto extract coloring	ANNATTO EXTRACT (FOR COLOR)	Differentiate by source of color. When both extract and color are	
	red #40	FD&C RED NO. 40	listed, use a general PD as in the example of annatto.	
	blue 2 lake red 3	FD&C LAKES/DYES	For combination of certified color additives	
	color (paprika and annatto); colors (from fruits and vegetables)	ARTIFICIAL COLOR	For combination of colors exempt from certification	
Additives: Enzymes	wheat enzyme; protease enzymes; rennet	ENZYMES	Disregard source; limited information given on ingredient lists	
Additives: Fiber, protein, starch, lecithin	oat fiber	OAT FIBER	Differentiate based on	
	soy lecithin	SOY LECITHIN	source of protein, fiber, starch, etc.	
Cereal grains (not flours), Seeds: General	hulled millet; cracked millet	MILLET	Disregard different terms such as hulled,	
	whole flax seed	LINSEED	cracked, whole, whole grain	
Cereal grains, seeds: General	oat flakes; rolled oats	ROLLED OATS	Differentiate between forms; the terminology varies by grain	
Fats: General	coconut oil	OIL, COCONUT	Differentiate based on source. Use SR ² formatting	
Fats: Composite fats – margarine, shortening and vegetable oils	margarine (palm oil, water, salt, mono- and diglycerides, soy lecithin, sodium benzoate, artificial flavor, beta carotene for color and vitamin a palmitate)	MARGARINE, PALM OIL, SALTED	Differentiate by source and type of oils, salt and voluntary fortification; not by additives used.	
	margarine (palm oil, water, soybean oil, salt, contains 2% or less of, mono- and diglycerides, calcium disodium edta (preservative), artificial	MARGARINE, COMPOSITE, PALM OIL, SOYBEAN OIL, SALTED	Use the term 'composite' for margarines with multiple oils; the term 'vegetable' for vegetable oils; and the terms 'animal' or	

Aspect	Parsed ingredients	Assigned Preferred Descriptor (PD)	Rule for assigning PDs
	flavor, annatto (color), vitamin a palmitate)		'vegetable' for type of shortening, as per SR. Oils used are sorted alphabetically
Flours: General	barley flour	BARLEY FLOUR	Differentiate by source
Flours: General	unbromated wheat flour	WHEAT FLOUR	Disregard properties which indicate no processing - unbleached; unbromated
Flours: Enriched Flours	enriched wheat flour (flour, malted barley flour, reduced iron, niacin, thiamin mononitrate (vitamin b1), riboflavin (vitamin b2), folic acid)	WHEAT FLOUR, WITH ADDED MALTED BARLEY FLOUR, ENRICHED (NOT AS PER FDA STANDARDS)	Disregard different forms of fortificants; list fortificants only when the fortificants (such as added ascorbic acid) are different than the standards; when the order is different, add phrase - (Not as per FDA Standards)
Fruits and Vegetables: several different cultivars or varieties	green jalapenos; fresh poblano peppers; hatch chili peppers	HOT PEPPER	Disregard different cultivars
	yellow squash	SUMMER SQUASH	Differentiate for common varieties only
	zucchini squash	ZUCCHINI	
Pasta, noodles	pasta (durum wheat semolina); lasagna pasta (water, semolina wheat flour, egg whites)	PASTA	Disregard different shapes; differentiate the type of grain if not wheat
Salt	udon noodles (water, wheat flour, salt)	NOODLES, SALTED	Include 'salted' in PD

¹ Additives and isolated ingredients (including sweeteners)

² SR: USDA National Nutrient Database for Standard Reference (SR) file (https://fdc.nal.usda.gov/fdc-app.html#/)

³ NALT: National Agricultural Library Thesaurus (NALT) file (https://agclass.nal.usda.gov/)