FoodComEx, a new chemical library for rare food-derived compounds

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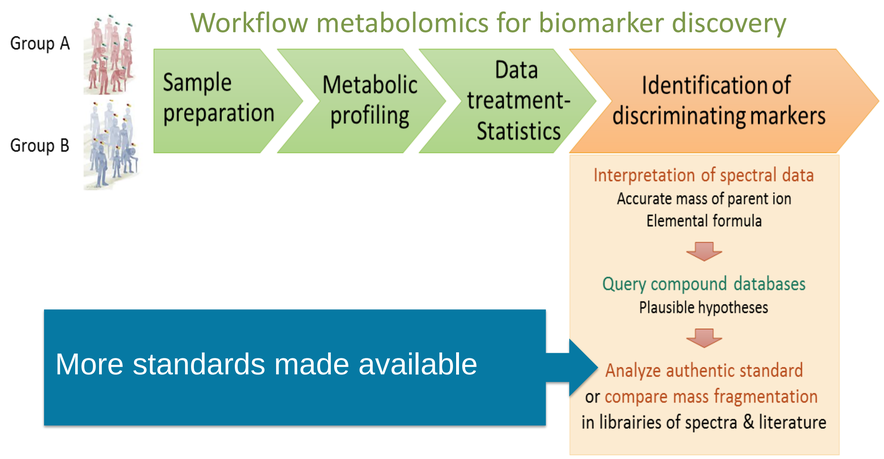
Context

FoodBAll (Food Biomarkers Alliance) is a large collaborative project (22 partners from 11 countries) funded by the JPI HDHL, which includes a systematic exploration and validation of nutritional biomarkers using metabolomics (www.foodmetabolome.org). As the lack of commercial standards is a major limitation in metabolomics and biomarker research, the FoodBAll consortium will develop a new online chemical library to facilitate the sharing of not easily accessible standards for diet-derived metabolites.



Why do we need such a chemical library?

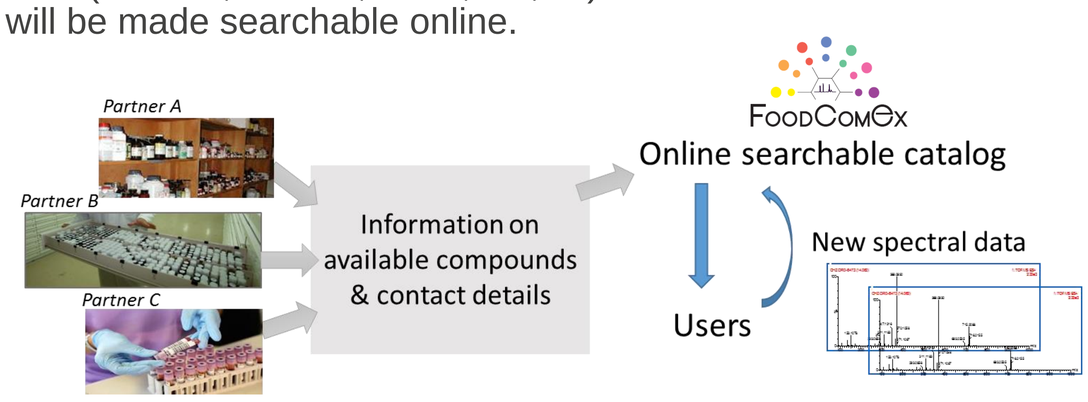
The diversity and complexity of naturally occurring compounds seems to be virtually infinite. For instance, the Dictionary of Natural Products now contains >270,000 compounds. In addition to natural compounds, the human diet contains chemicals resulting from complex reactions occurring during food processing, as well as food additives and food contaminants. Furthermore, ingested compounds are metabolized by the host's enzymes or the gut microbiota. Most of these food-derived metabolites are still unknown.

In recent years, the performance of analytical instruments has improved tremendously, enabling a far more comprehensive exploration of the complex metabolite profiles found in biological matrices such as plant-derived foods or human biofluids. However, a large majority of the detected compounds remain unidentified. In most cases an analytical standard of sufficient purity is needed to confirm a given metabolite's identity with certainty, but the commercial availability of food compounds standards is quite limited.

Major efforts have been made by academic laboratories all over the world to isolate or synthesize many natural products or metabolites on a small scale. FoodComEx aims to improve the availability of these rare standards to facilitate identifications in metabolomics studies as well as for other purposes, for example the study of the biological effects of relevant physiological metabolites of food bioactives in cell models.

How it works

Version 1.0 will be an online catalog of pure compounds and reference materials (food extracts, biofluids from animals fed pure compounds, incubation media from *in vitro* systems to produce metabolites, etc.) made available by FoodBAll partners and external collaborators. The catalog will contain the list of available compounds with associated data including elemental formula, monoisotopic mass, solubility, origin, purity, available quantity, storage conditions, stability, links to existing databases, type of spectral data available and contact details of the laboratory offering to share the standard. The catalog will be queryable by compound name and chemical structure. In the final version, which should be available at the end of 2016, spectral data (GC-MS, LC-MS, NMR, UV, IR) collected in standardized formats will be made searchable online.



Anyone interested in one compound in the catalog will directly contact the provider. A bilateral negotiation will define the terms of collaboration. Contributors and users will have to respect a charter of good practices. An important rule is that the acquirer will have to share the spectral analyses he has acquired on his own analytical platform. This will continuously enrich the content of the chemical library.

FoodComEx coverage

The emphasis lies primarily on food-derived compounds and their human metabolites. However, every compound which may, in any way, be linked to food, diet and nutrition and which is not or rarely commercially available will be welcome. In addition, it will be possible to provide relevant, but not yet fully characterized compounds in order to give others the opportunity to complete structural elucidation.

The Food Compound Exchange will also include a virtual bulletin board where users can post their most-wanted compounds in order to motivate others to isolate or synthesize them.

In addition to pure compounds, the library will contain biological reference materials such as food extracts, animal samples, cell culture media etc. that are thought to contain compounds of interest.

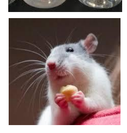
Origin of standards and reference materials

- Chemical synthesis

- Extraction-Purification from foods

- In vitro incubations

  Microsomes, supersomes, isolated enzymes, gut microbiota



- Rodent experiments: *animals fed diet supplemented with pure compounds or food extracts*

Join FoodComEx!

FoodComEx will give researchers all over the world a unique opportunity to acquire standards of diet-related compounds which are not easily available. But of course, participation is the lifeblood of FoodComEx! Therefore, we cordially invite our colleagues from the metabolomics community to join this exciting project and to share their standards, biological materials and spectral data.

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