

### Summary

The Food Compound Exchange (FoodComEx) will give researchers a unique opportunity to acquire standards of food-derived compounds and their metabolites, which might not be commercially available. This initiative will strengthen international collaboration in the fields of food chemistry, nutritional metabolomics and nutrition and health and will certainly facilitate the identification of biomarkers of food intake and the study of health effects of food compounds. But of course, participation is the lifeblood of the Food Compound Exchange! We cordially invite our colleagues from nutrition related disciplines to join this exciting project and share their standards.

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## FoodComEx

### The Food Compound Exchange

A platform for exchange of food compounds  
and derived metabolites

Supported by:



Initiated by:



### Why do we need a public 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 and is growing at a rate of 10,000 compounds a year. In addition to natural compounds, the human diet contains chemicals resulting from complex reactions occurring during food processing, as well as food additives and contaminants. When absorbed by humans, food-derived compounds can be metabolized by intestinal and hepatic enzymes as well as the gut microbiota. However, most of these food 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. While advanced nuclear magnetic resonance and mass spectrometric techniques have extended our abilities to characterize or identify previously unknown compounds, in most cases an analytical standard of sufficient purity is still needed to confirm a given metabolite's identity with certainty.

The major problem is that numerous naturally occurring substances and human metabolites are still commercially unavailable because, from the chemical supplier's perspective, a synthesis would be unprofitable. In contrast, major efforts have been made by academic laboratories all over the world to isolate or synthesize natural products or metabolites on a small scale.

We are proposing the establishment of an online platform to facilitate the exchange of food compounds and their metabolites – the Food Compound Exchange. We believe this kind of public exchange would be of great value for biomarker research and studies on food health effects.

### The FOODBALL project

Biomarker research is still a developing scientific discipline. While several potential dietary and health biomarkers have been recently identified using metabolomics approaches, very few of them have been validated so far. The Food Biomarkers Alliance (FOODBALL), a multinational joint venture comprising 22 partners from Europe and Canada aims to fill this gap by a three-step approach:

1. Discovery of new dietary biomarkers using untargeted metabolic profiling techniques;

2. Systematic validation of existing and newly discovered biomarkers to obtain a good coverage of the food intake in different population groups within Europe
3. Exploring biological effects using biomarkers of intake.

Being the integral part of the first step, reliable identification of biomarkers is of utmost importance for the entire project. The expertise and the resources of the members of the multidisciplinary FOODBALL consortium are being used to establish an online exchange for analytical standards of rare food-derived compounds. However, in order to build up a comprehensive chemical library that may serve a wider range of scientific objectives, the contributions of many colleagues from various disciplines are required.

### Intention and scope

FoodComEx aims to improve the availability of standards by bringing together scientists that can provide compounds and those who need them. The compounds in the library are available to any group that is interested on using them as standards for metabolomics, quantitative analyses or in biological assays. The users will be able to further characterize the compounds, by adding spectral data and other information.

The chemical library is primarily open to any compound present in food, whether it is a natural substance, an additive or contaminant, and their metabolites. However, the scope of the library is not strictly limited and every compound which may, in any way, be linked to food, diet and nutrition and which is not or rarely commercially available is welcome. In the future, we are planning to include biological reference materials (food extracts, animal samples, cell culture media etc.) that are thought to contain compounds of interest and could be of use in the identification of given metabolites.

### How it works

FoodComEx is available as an online catalog via the web portal [www.foodcomex.org]. While the catalog can be browsed without authentication, only registered users are able to include new compounds. FoodComEx contains a list of available compounds that can be searched by compound name, chemical structure, InChI, and other features. The compound provider is invited to supply detailed information regarding the product, including available quantity, storage conditions, stability, safety information and the spectral data (GC-MS, LC-MS, NMR, UV, IR) available.

The compounds included in the virtual library will be kept at the laboratory that owns them. Anyone interested in a compound from the catalog will have the opportunity to contact the provider directly. The conditions for the delivery of the compound are a matter of bilateral negotiation – both parties can decide to exchange the compound for free, for money or in exchange for goods or services. A charter of good practices is available in the website to guide these exchanges. An important rule is that anyone obtaining a compound through the library will have to share any spectral analyses acquired on his or her analytical platform. The use of FoodComEx is free of any charges. All registered providers have the possibility to include their profile in the website, where they can be searched by specialty, institution and area of interest.

What if a highly desired compound remains unavailable? FoodComEx will also include a virtual board where users can post their most-wanted compounds in order to motivate others to isolate or synthesize them.

