FOBI: An ontology to represent food intake data and associate it with metabolomic data

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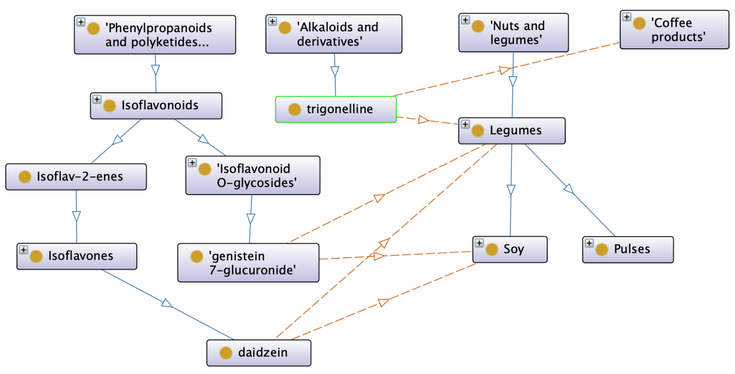
Problem

- Metabolomics is linked to nutrition [1] but, for different reasons, it is difficult to associate these two types of data [1, 2].
  - **heterogeneity found in the information provided by participants** in nutritional studies about what they have eaten.
  - **metabolites are not specific for food** and foods can have more than one metabolite.
- To manage this we have built an ontology, describing foods (and metabolites) in a hierarchichal way that enables a common description of food intake.
- The ontology contains *formal naming*, *definition of the categories*, *properties*, and *relations* between the concepts of two types of data, food and related metabolites.



Methods

- FOBI (Food-Biomarker Ontology) is part of the **OBOFoundry** project: `http://purl.obolibrary.org/obo/fobi.owl`
- FOBI integrates **FoodOn** and **ChEBI** and provides many other food-specific metabolites.
- Project's Github repository: `https://github.com/pcastellanoescuder/FoodBiomarkerOntology`

Applications

- Annotation of foods and their related food biomarkers using a consistent standardized nomenclature.
- Help in hypothesis generation and experimental design.
- Different types of enrichment analysis*.

References

[1] Scalbert A. *et al. The food metabolome: a window over dietary exposure*, The American Journal of Clinical Nutrition. 2014.

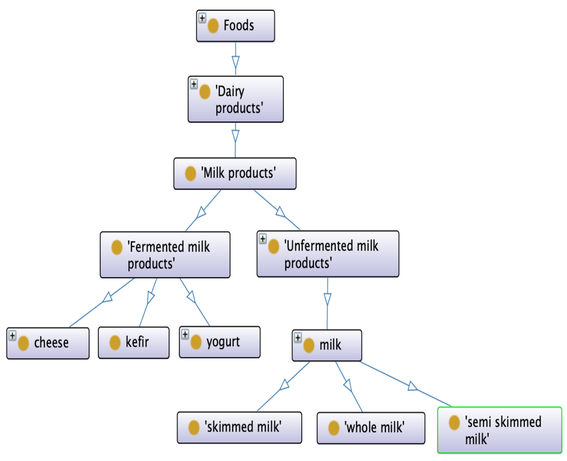
[2] Jones DP, Park Y, Ziegler TR. *Nutritional metabolomics: progress in addressing complexity in diet and health*, Annual Review of Nutrition. 2012.

[3] Feunang, Y. *et al. ClassyFire: automated chemical classification with a comprehensive, computable taxonomy.* Journal of cheminformatics. 2016.

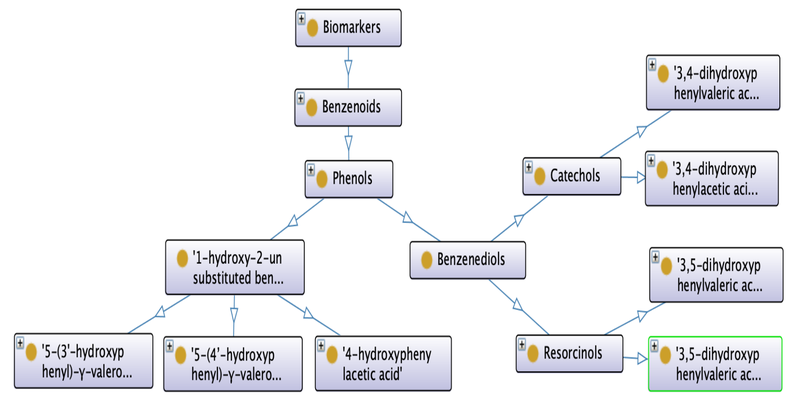
[4] Castellano-Escuder, P. *et al. FOBI: An ontology to represent food intake data and associate it with metabolomic data. Submitted.*

Results

- FOBI [4] is made of two sub-ontologies with more than 1000 entities and 4100 relationships.
- The first ontology describes foods: from simple such as apple to more complex foods such as pizza.
- The second ontology describes metabolites, grouped in their different chemical classes using the *ClassyFire* structure [3].
- The nodes or elements of these two sub-ontologies are connected by the properties of each one, so that if a metabolite is in different foods, it will connect with all of them.
- This ontology allows us to visualize data in a bidirectional way, going from metabolomics to nutritional data or vice versa.

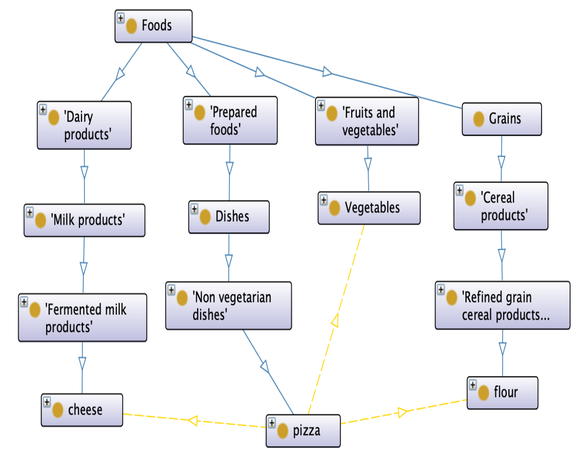


(a) An example of hierachichal structure of foods

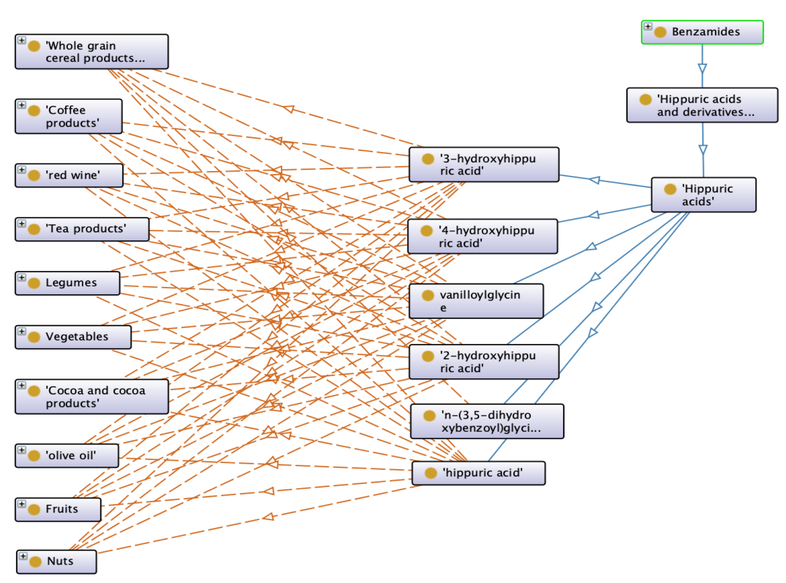


(b) An example of hierachichal structure of metabolites, grouped by *ClassyFire* chemical classes

Figure 1: Examples of FOBI hierarchichal architecture



(a) Prepared foods as *pizza* are related with "simple foods" (as *cheese* or *flour*) by the properties *Contains* and *IsIngredientOf*



(b) Relationships of some *Hippuric acids* with foods that have it related by properties *BiomarkerOf* and *HasBiomarker*

Figure 2: Examples of FOBI properties

Visualization

A Shiny app has been developed to visualize each FOBI entity and its properties.

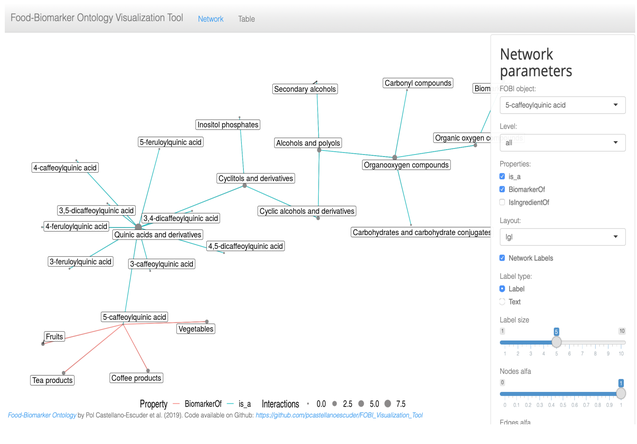


Figure 3: Shiny app to visualize each element of FOBI with their relationships.

Link: `https://polcastellano.shinyapps.io/FOBI_Visualization_Tool/`

Software

- **POMA**: Statistical Analysis Tool for Metabolomics (`polcastellano.shinyapps.io/POMA/`)
- **FOBIEnrichR***: R package for Enrichment Analysis in Nutrimetabolomic Studies. (`github.com/pcastellanoescuder/FOBIEnrichR`)

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