

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

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Problem

- Metabolomics is closely linked to nutrition [1] and is still difficult associate this two types of data [1, 2].
- One reason for this difficulty is the heterogeneity found in the information provided by participants in nutritional studies about what they have eaten.
- Another reason is that the **metabolites are not specific for food and, at the same time, foods can have more than one metabolite**.
- To manage this heterogeneity we have decided to build an ontology, describing foods in a hierarchical way that enables a common description of food intake.
- This ontology contains formal naming, definition of the categories, properties, and relations between the concepts of two types of data, food and related metabolites.

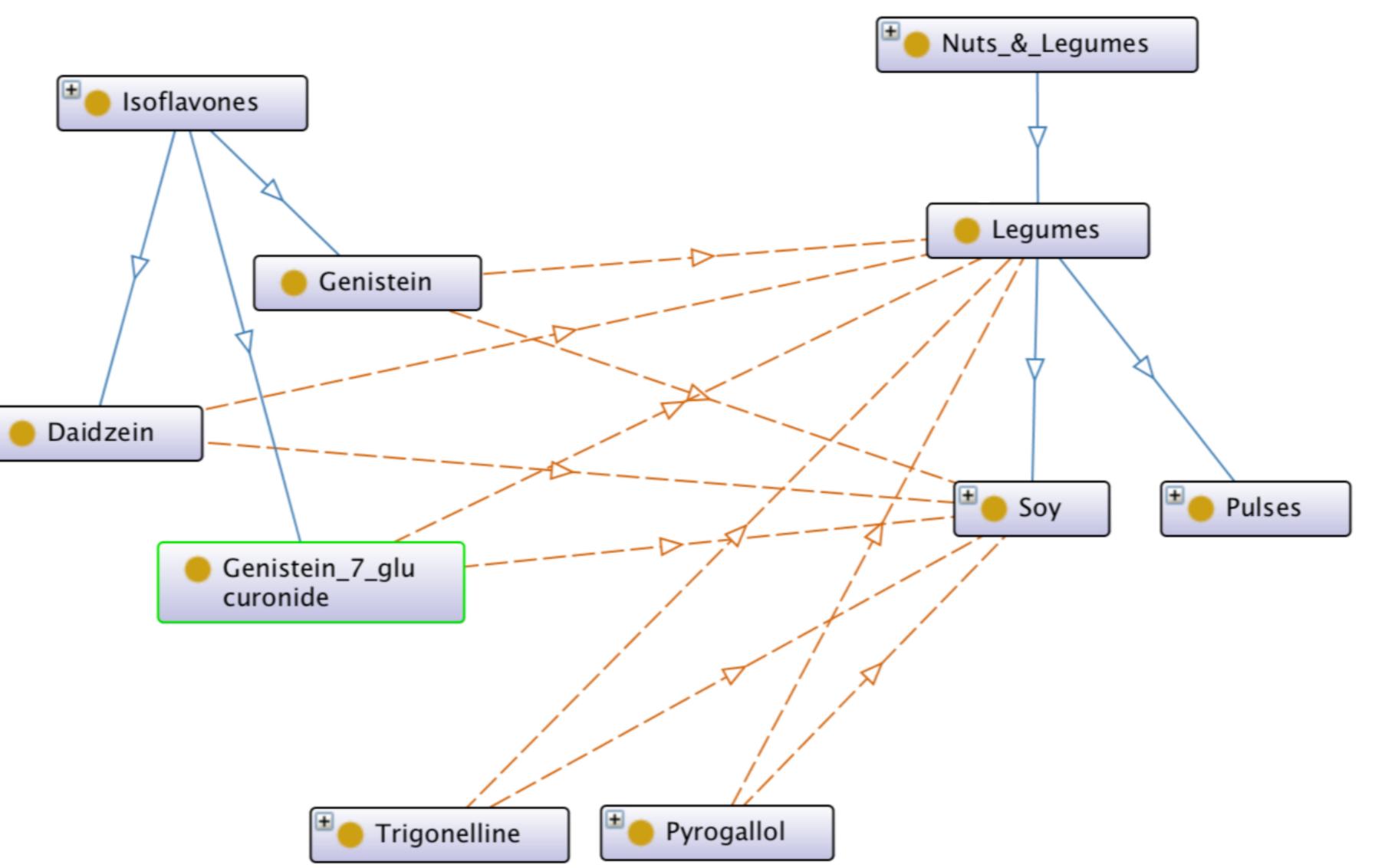


Figure 1: This figure shows that metabolites (on the left) can be in more than one food and each food (on the right) can contain more than one metabolite.

Methods

This ontology has been created using Protégé 5.5.0 version. As is common in ontologies, FBonto (Food-Biomarker Ontology) has been written in OWL language (Web Ontology Language).

Ontology metrics

- Axioms: 2160
- Class Count: 489
- Object Property Count: 4 (*BiomarkerOf*, *hasBiomarker*, *Contains*, *IsIngredientOf*)
- Inverse Object Properties: 2

References

- [1] Scalbert A, Brennan L, Manach C, **Andrés-Lacueva C**, Dragsted LO, Draper J, Rappaport SM, van der Hooft JJ, Wishart DS: *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.

Acknowledgements

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Results

FBOnto is made of two sub-ontologies. The first ontology describes foods: from simple such as fruits and vegetables to more complex foods such as ratatouille. The second ontology describes metabolites, grouped in their different chemical classes. 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.

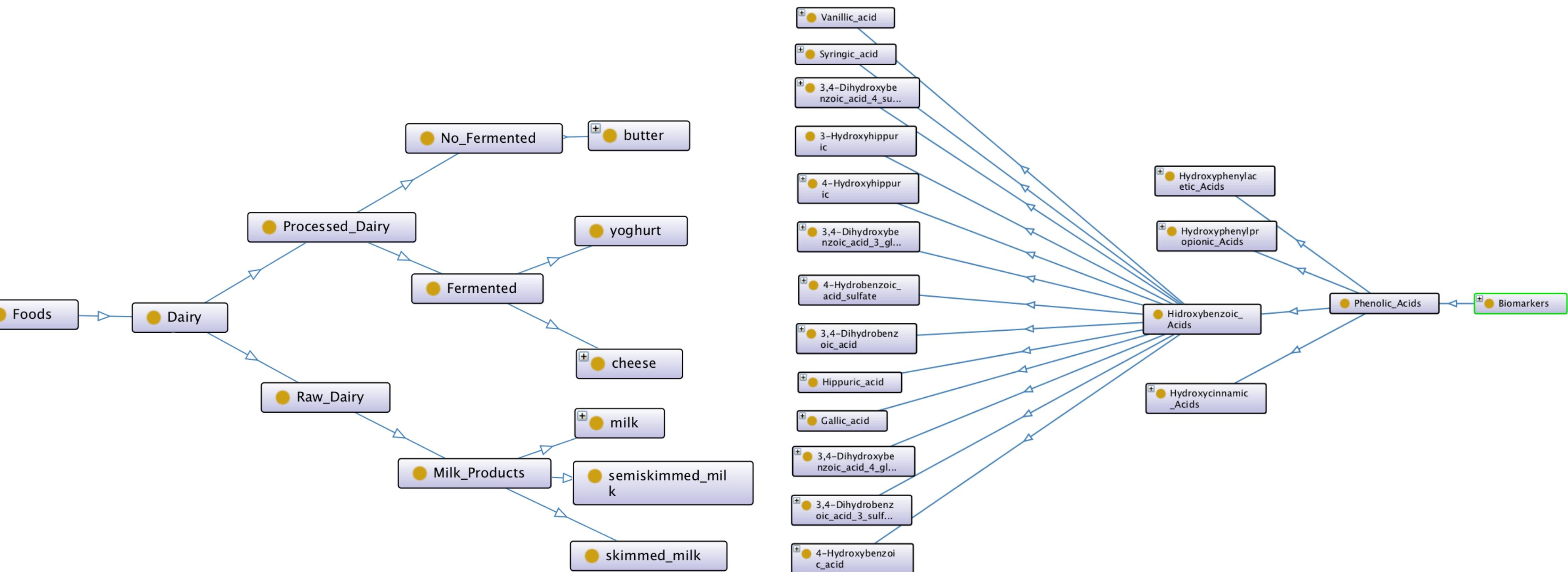


Figure 2: (L) An example of hierarchical structure of foods. (R) An example of hierarchical structure of metabolites, grouped by chemical classes.

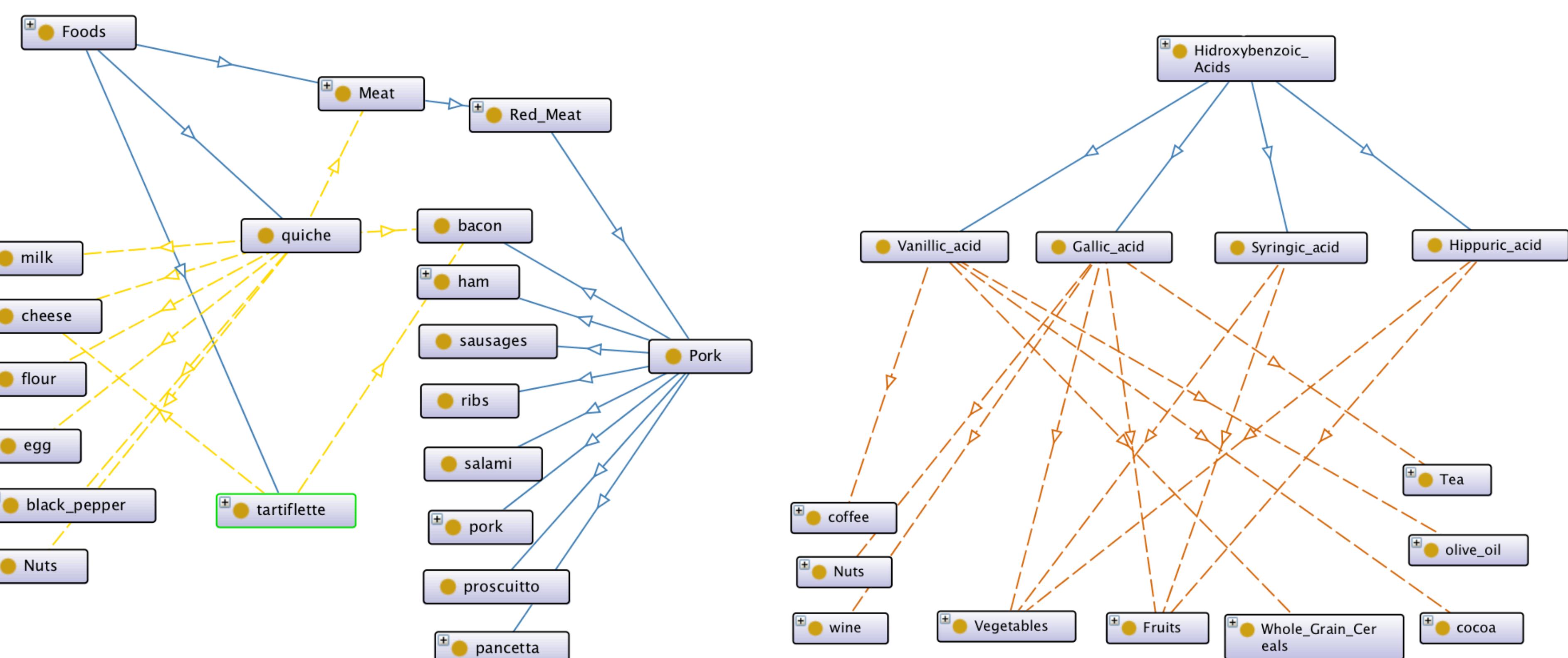


Figure 3: (L) Complex foods as *tartiflette* are related with "simple foods" (as *bacon*) by the properties *Contains* and *IsIngredientOf*. (R) Relationships of some *Hidroxybenzoic Acids* with foods that have it related by properties *BiomarkerOf* and *hasBiomarker*.

Visualization

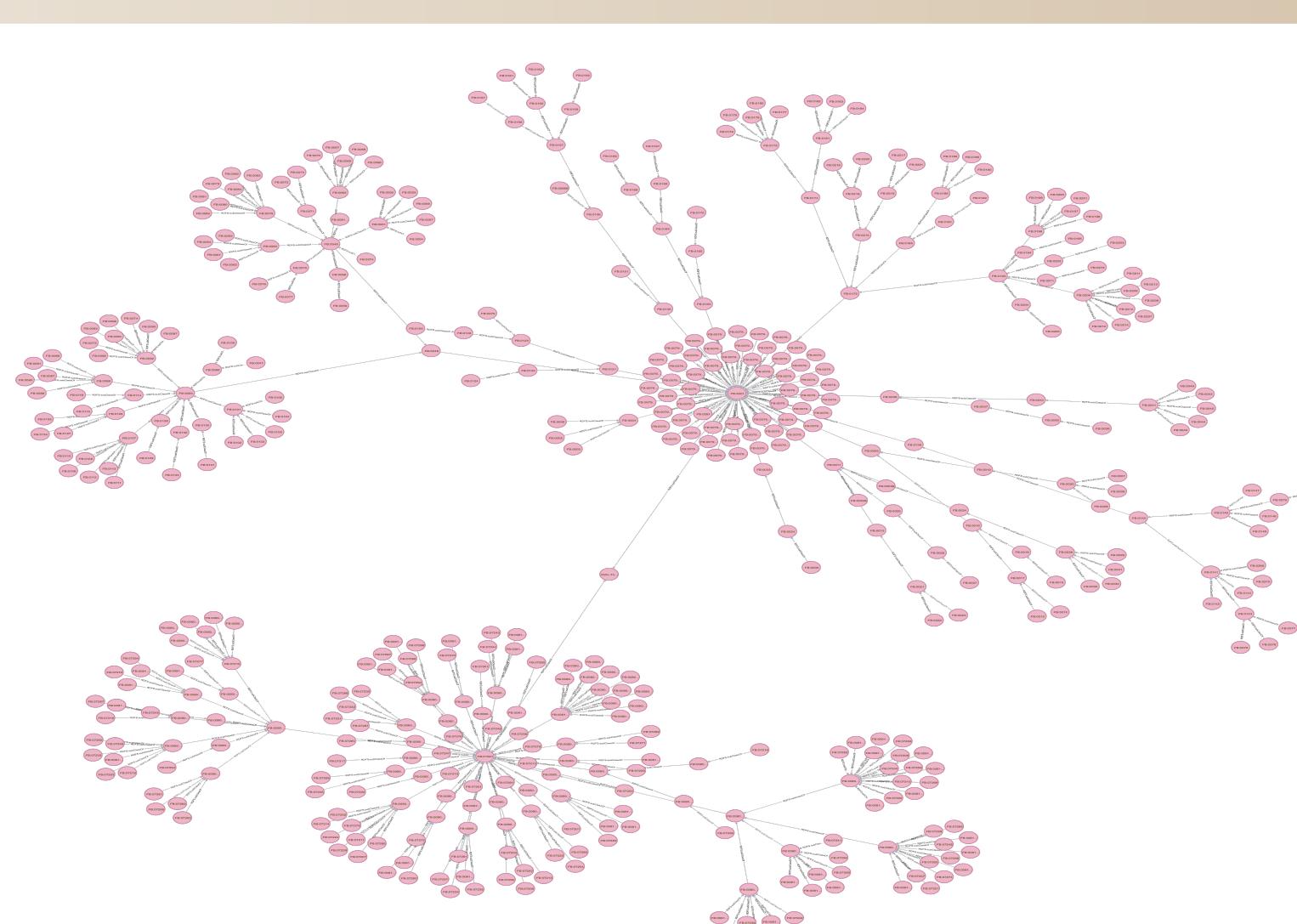


Figure 4: Graph of whole FBonto (without properties). Generated with Neo4j software.

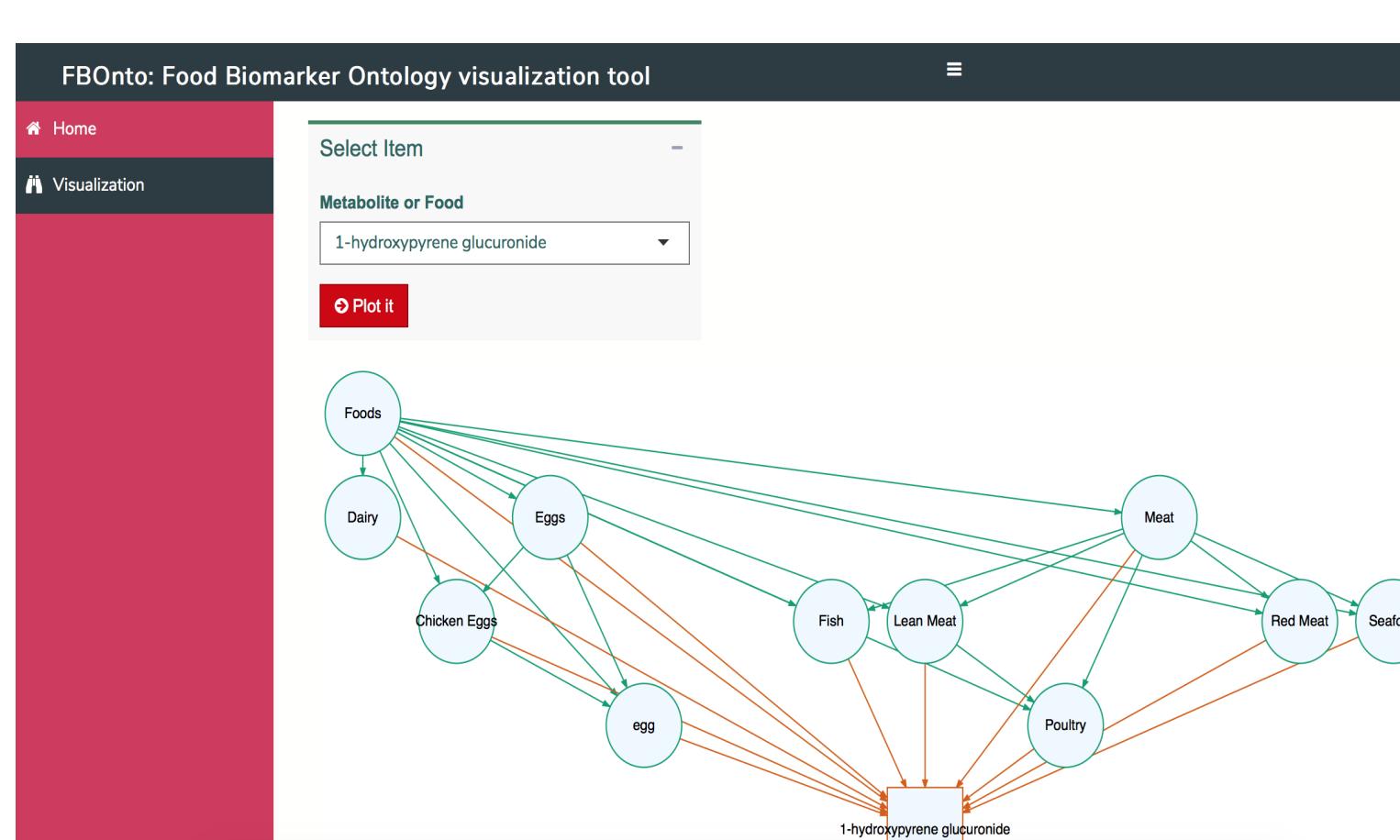


Figure 5: Shiny app to visualize each element of FBonto with their relationships.

Applications

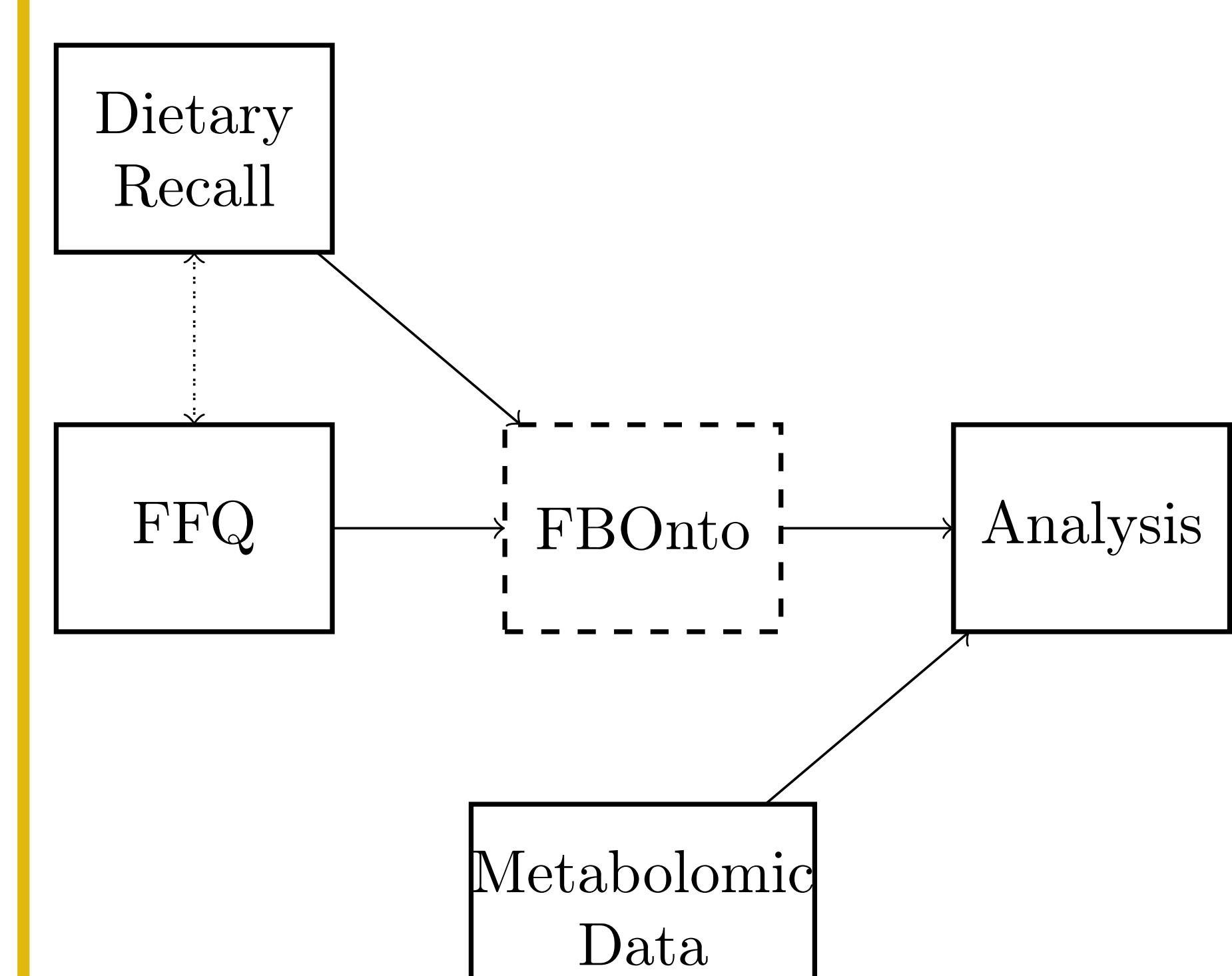


Figure 6: Pipeline analysis using FBonto. 1) Nutritional data come from DR or FFQ. 2) This data is annotated by FBonto and theoretical biomarkers will be obtained. 3) Real metabolite matrix will be integrated with the theoretical matrix obtained from FBonto for the analysis.

