



Centro de Investigación Biomédica en Red

Fragilidad y Envejecimiento Saludable



UNIVERSITAT DE  
BARCELONA

# Food-Biomarker Ontology (FOBI)

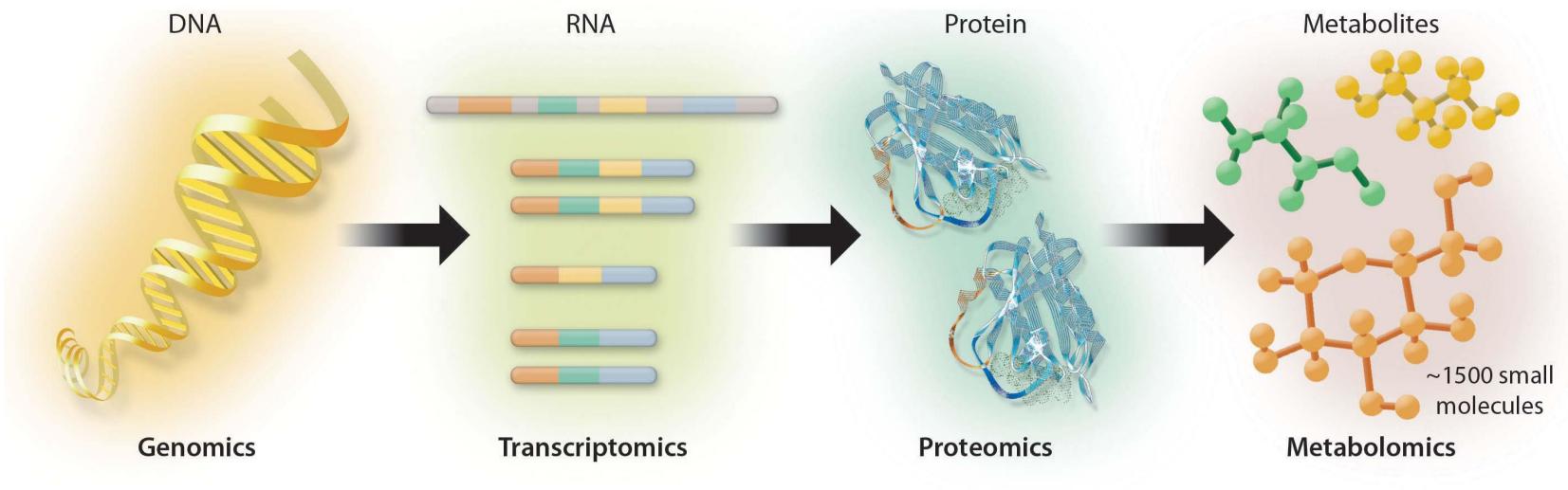
An ontology to represent food intake data and associate it with metabolomic data

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Cristina Andrés Lacueva and Alex Sánchez Pla  
Sep 23, 2020

# Metabolomics

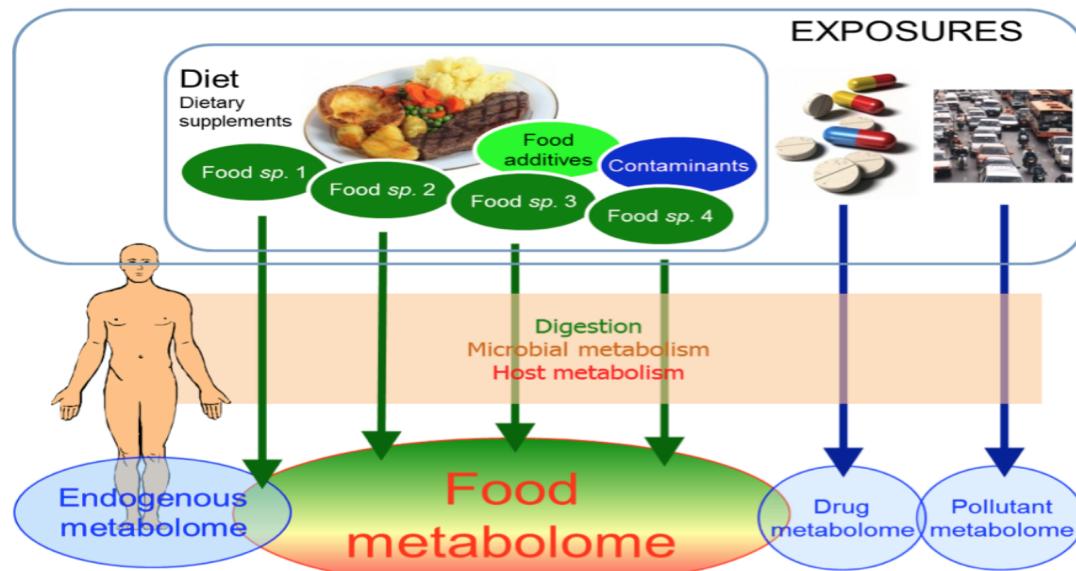
"Metabolomics is the identification and quantification of the small molecule metabolic products (the metabolome) of a biological system. Mass spectrometry and NMR spectroscopy are the techniques most often used for metabolome profiling."\*



\*<https://www.nature.com/subjects/metabolomics>

# The Food Metabolome

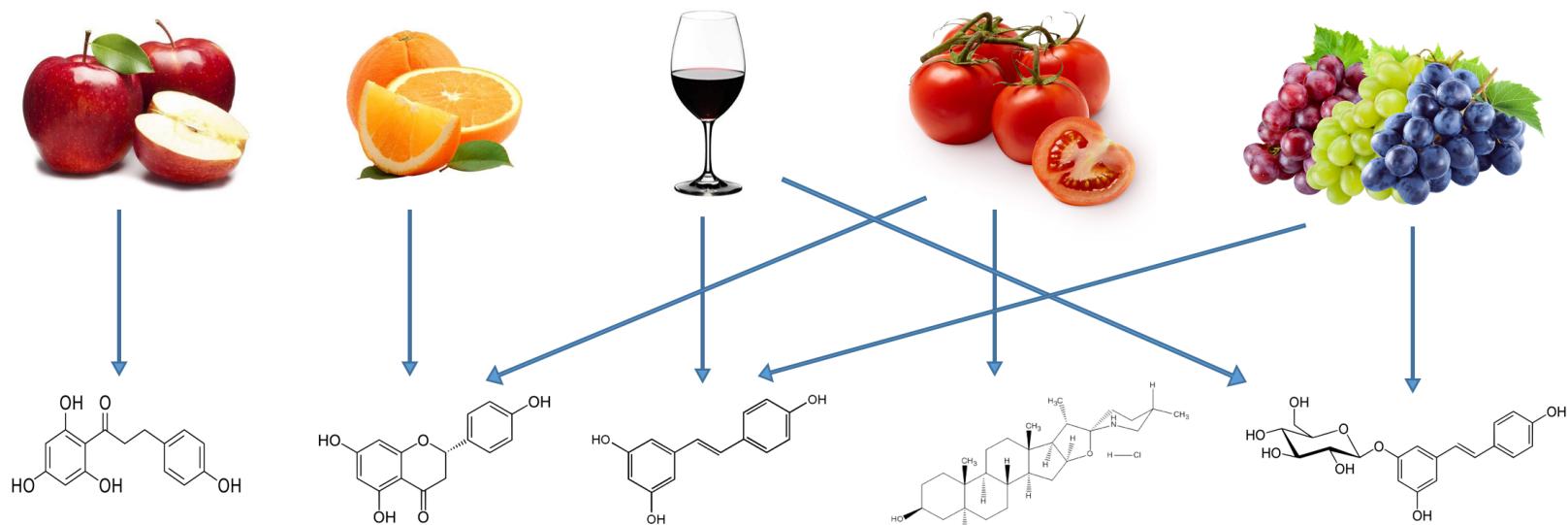
"The food metabolome is the part of the human metabolome directly derived from the digestion and biotransformation of foods and their constituents. With over 25,000 compounds known in various foods, the food metabolome is extremely complex, with a composition varying widely according to the diet." \*



\*<http://foodmetabolome.org/metabolome>

# Our Scenario

- Heterogeneous nutritional data (semantic problem) -> **FoodOn**
- Difficult association of nutritional data with other types of data (semantic and quantitative problem)
- **Unclear relationships between foods and metabolites**



# Aims

- Create an ontology that clearly defines the many complex relationships between **diet derived metabolites** and **foods** in a consistent and homogeneous way
- Reuse previous existing terms to maintain a consistent and standardized nomenclature (OBOFoundry)
  - FoodOn
  - ChEBI
- Propose a consistent starting point for nutrimetabolomic studies
  - Design
  - Validation

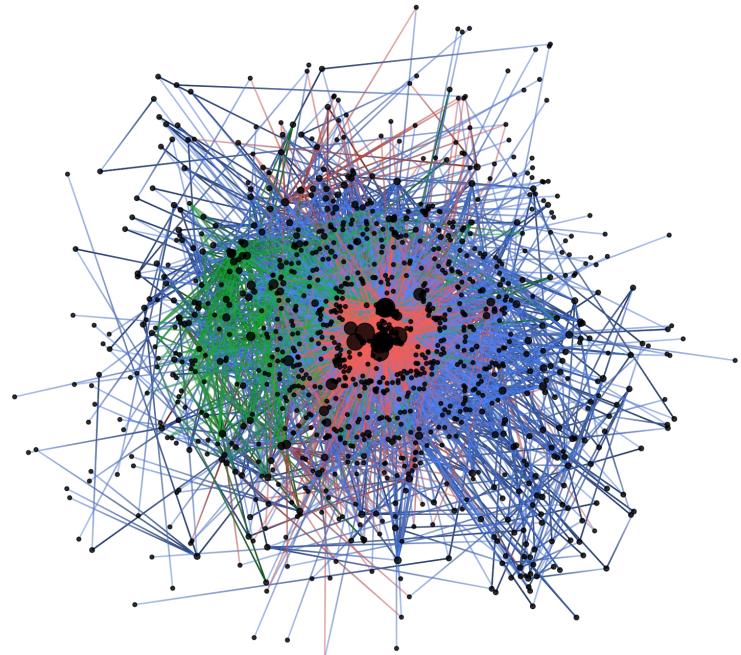


# FOBI (Food-Biomarker Ontology)

🔗 <https://github.com/pcastellanoescuder/FoodBiomarkerOntology>

## Metrics

- 2 sub-ontologies
- 1197 terms
- 4 different properties
- 13 food top-level classes
- 11 biomarker top-level classes
- More than 4700 relationships
- Part of **OBOfoundry project**  
<http://purl.obolibrary.org/obo/fobi.owl>
- FOBI IDs are indexed into the **HMDB**  
(Human Metabolome Database) and  
**FoodDB** (Food Database)



# Sub-Ontologies

## Food sub-ontology

- 13 food top-level classes (according to the related importance with metabolites)
- Most part of the structure adopted from FooDB
- Around 350 terms (306 adopted from FOODON) -> ~ 87%

## Biomarker sub-ontology

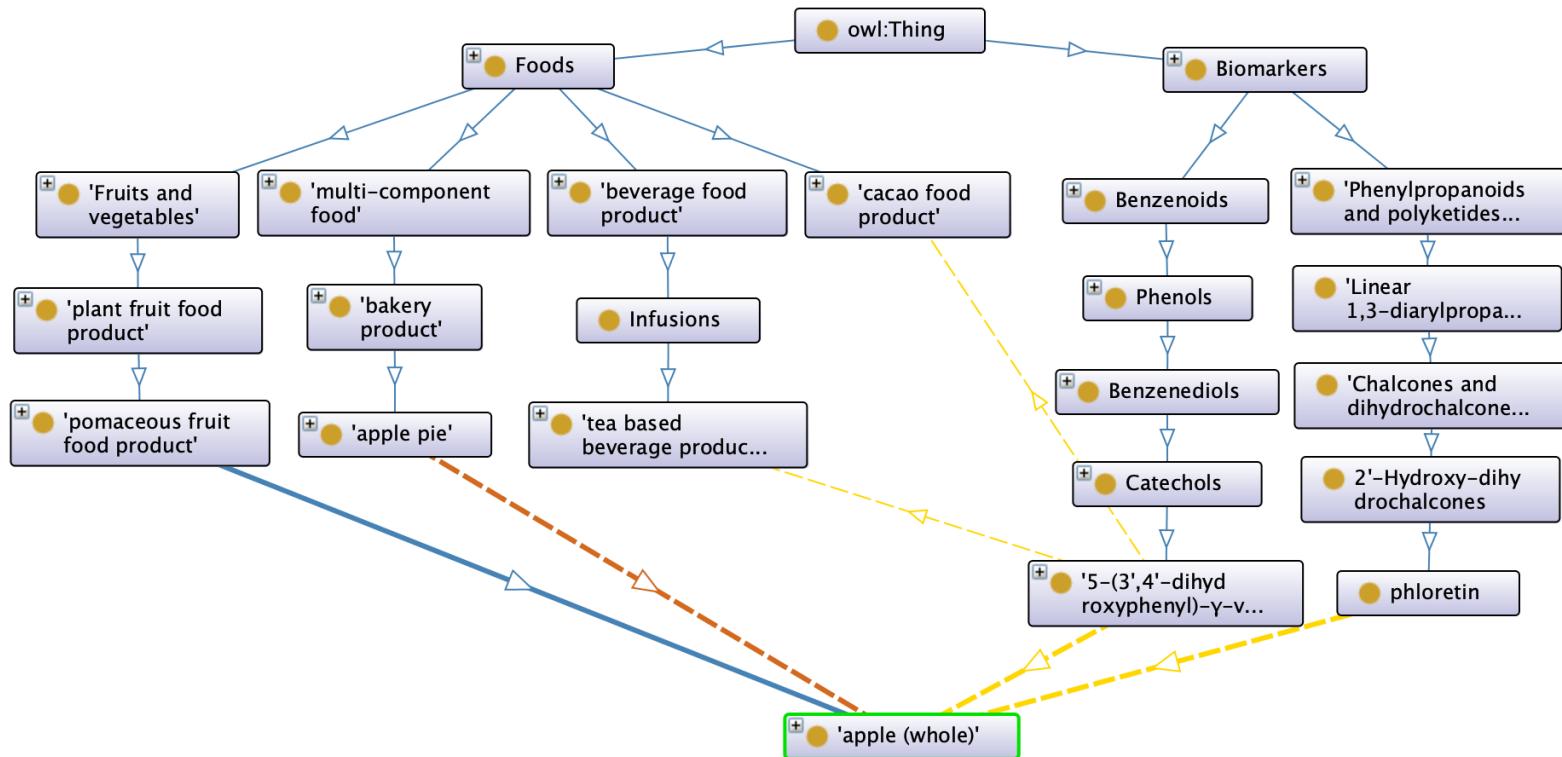
- 11 biomarker top-level classes
- Structure adopted from ChemFOnt (chemical functional ontology)
- Around 850 terms (159 adopted from CHEBI) -> ~ 19%

## Properties

- *BiomarkerOf* and *HasBiomarker* (between Food and Biomarker sub-ontologies)
- *Contains* and *IsIngredientOf* (within Food sub-ontology, to relate raw and multi-component foods)

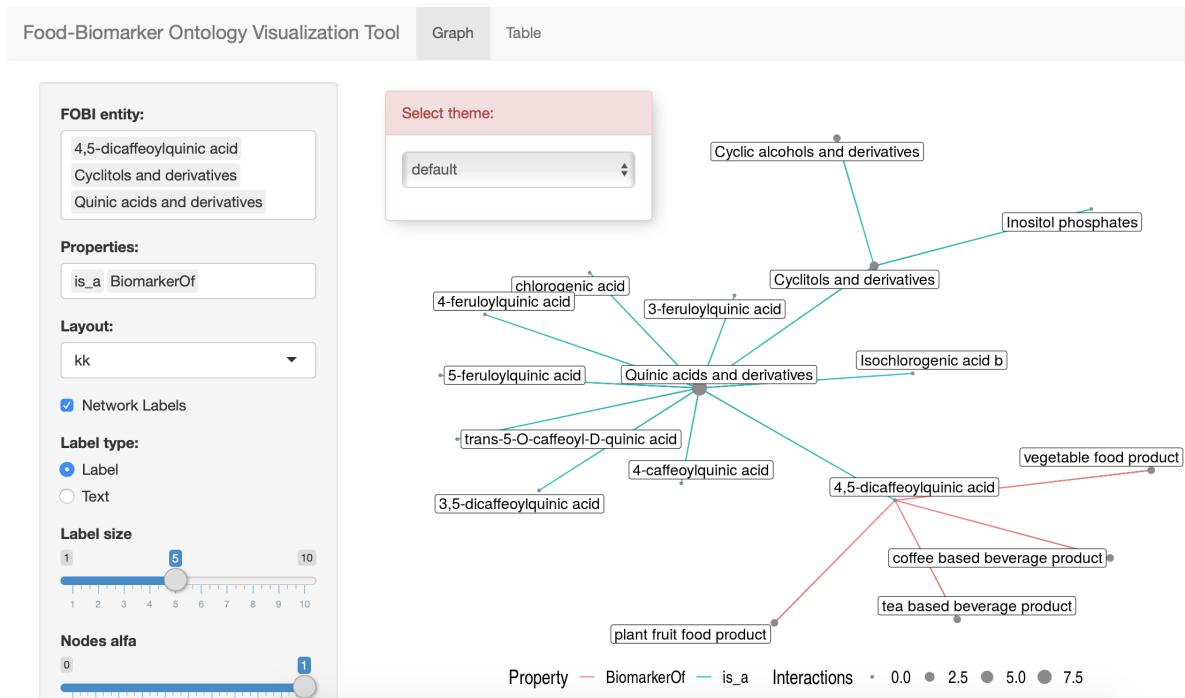
# FOBI Architecture

FOODON:00002473 -> "apple (whole)"



# Applications

- 1) **fobitools** (beta version): R package that provides some FOBI applications like ORA or automatic nutritional text annotation. <https://github.com/pcastellanoescuder/fobitools>
- 2) **FOBI Visualization Tool:** [https://polcastellano.shinyapps.io/FOBI\\_Visualization\\_Tool](https://polcastellano.shinyapps.io/FOBI_Visualization_Tool)



# Acknowledgements



- To the Statistics and Bioinformatics Research Group and Biomarkers and Nutritional & Food Metabolomics Research Group from University of Barcelona
- To **Damion Dooley** for his help on the integration of FoodOn and ChEBI

# Thank you all and absolutely **welcome** **to contribute!**

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