Food-Biomarker Ontology (FOBI)

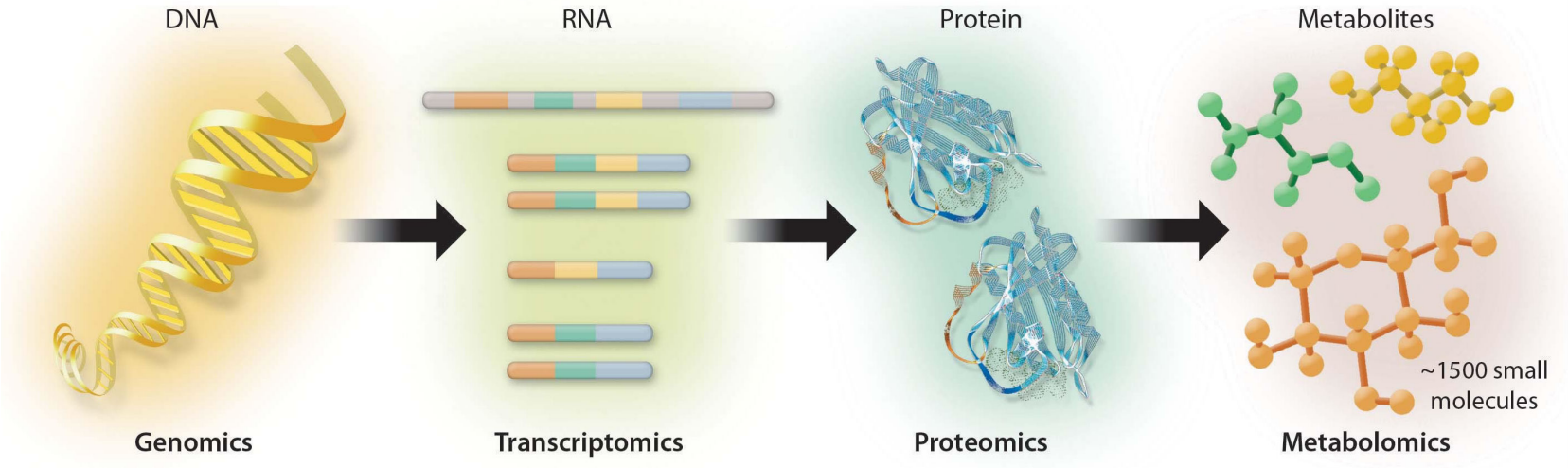
An ontology to represent food intake data and associate it with metabolomic data

Pol Castellano Escuder, Raúl González Domínguez, David S. Wishart, Cristina Andrés Lacueva and Alex Sánchez Pla

Sep 23, 2020

Metabolomics

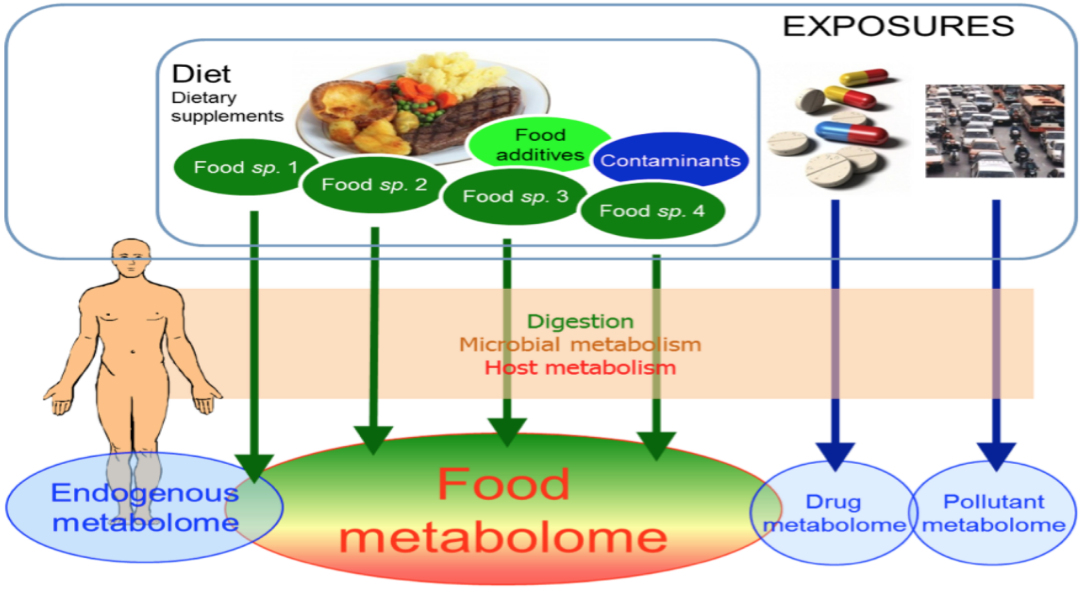
*"Metabolomics is the identification and quantification of the small molecule metabolic products (the metabolome) of a biological system. Mass spectrometry and NMR spectroscopy are the techniques most often used for metabolome profiling."**



*https://www.nature.com/subjects/metabolomics

The Food Metabolome

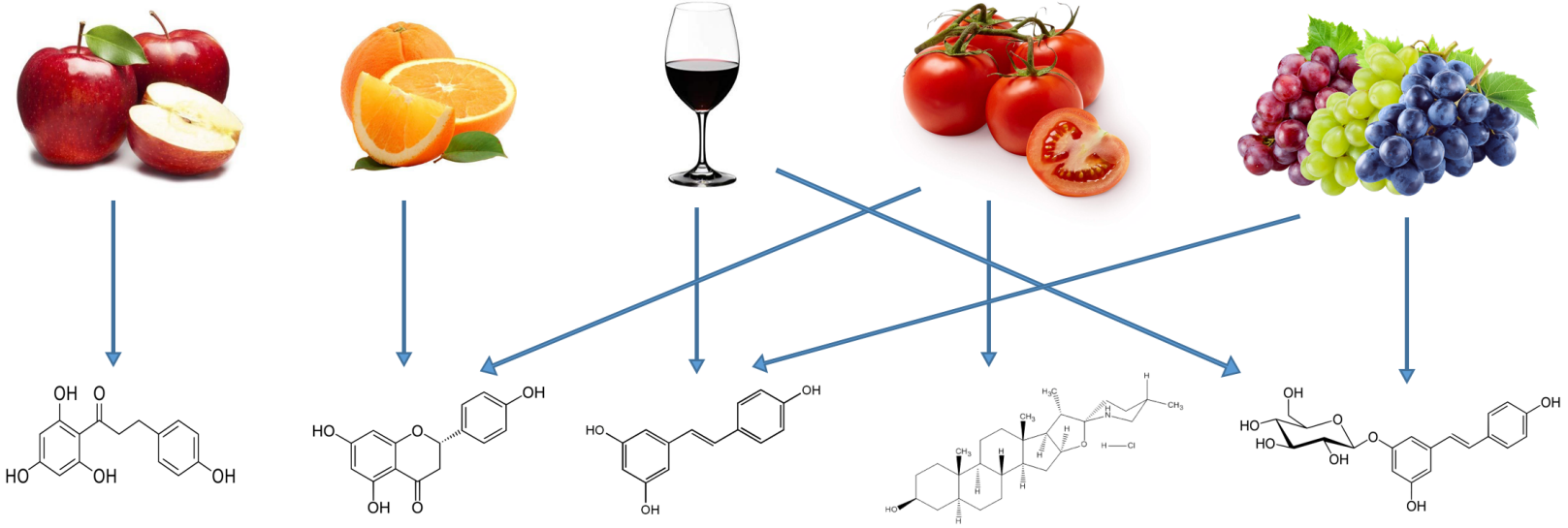
"The food metabolome is the part of the human metabolome directly derived from the digestion and biotransformation of foods and their constituents. With over 25,000 compounds known in various foods, the food metabolome is extremely complex, with a composition varying widely according to the diet." *



*http://foodmetabolome.org/metabolome

Our Scenario

- Heterogeneus 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

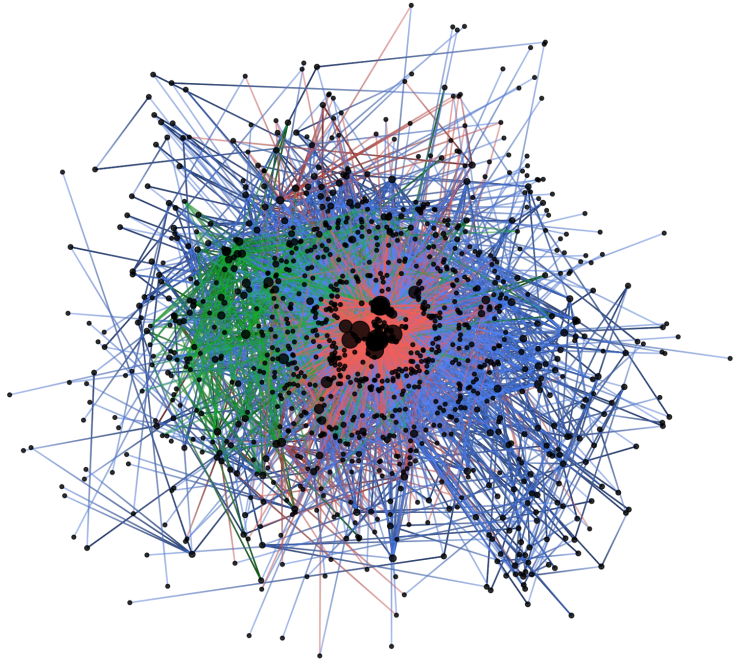
- Propose a consistent starting point for nutrimetabolomic studies
  - Design
  - Validation

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 FooDB (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

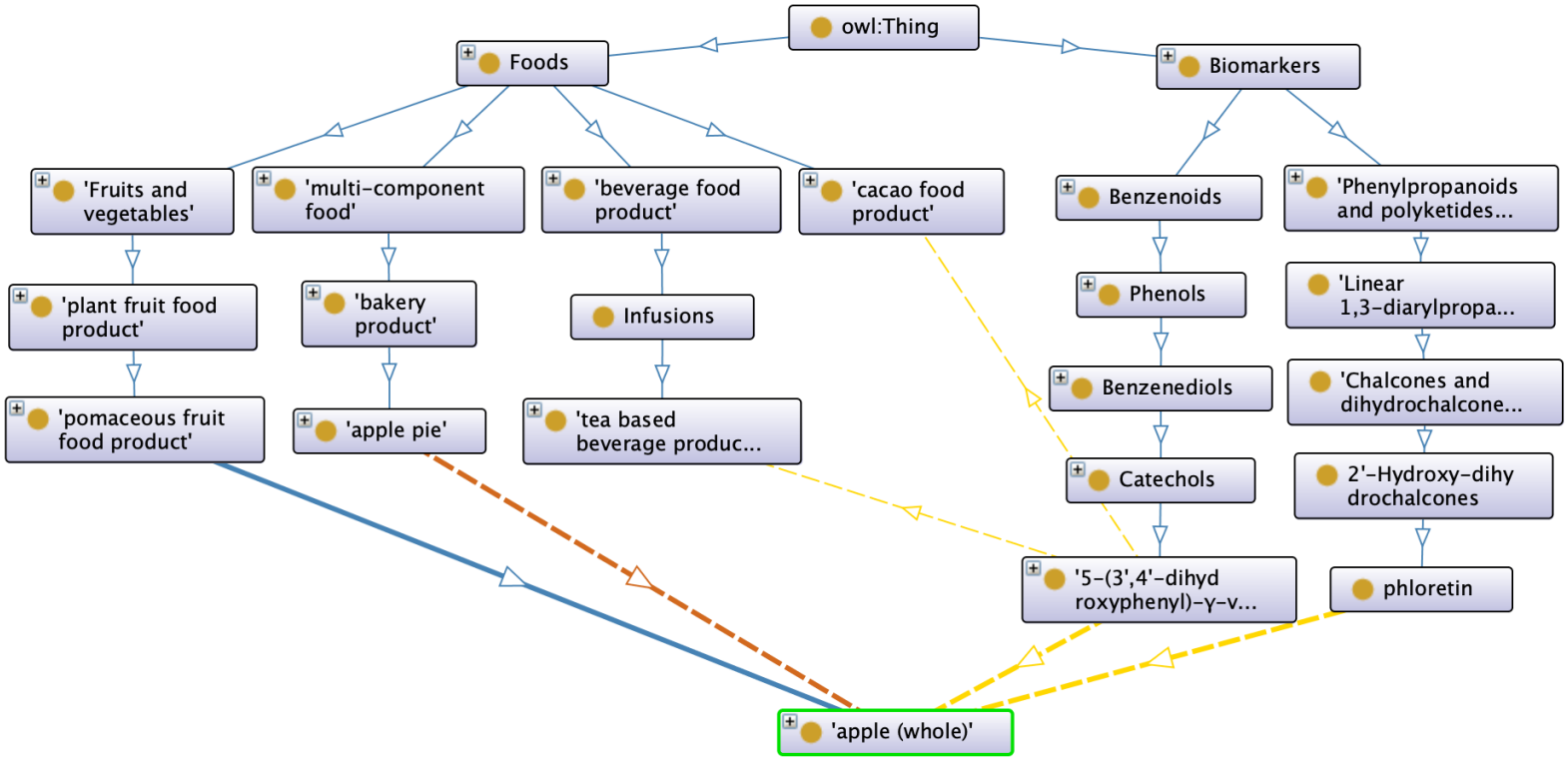
- 11 biomarker top-level classes
- Structure adopted from ChemFOnt (chemical functional ontology)
- Around 850 terms (159 adopted from CHEBI) -> ~ 19%

Properties

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

FOBI Architecture

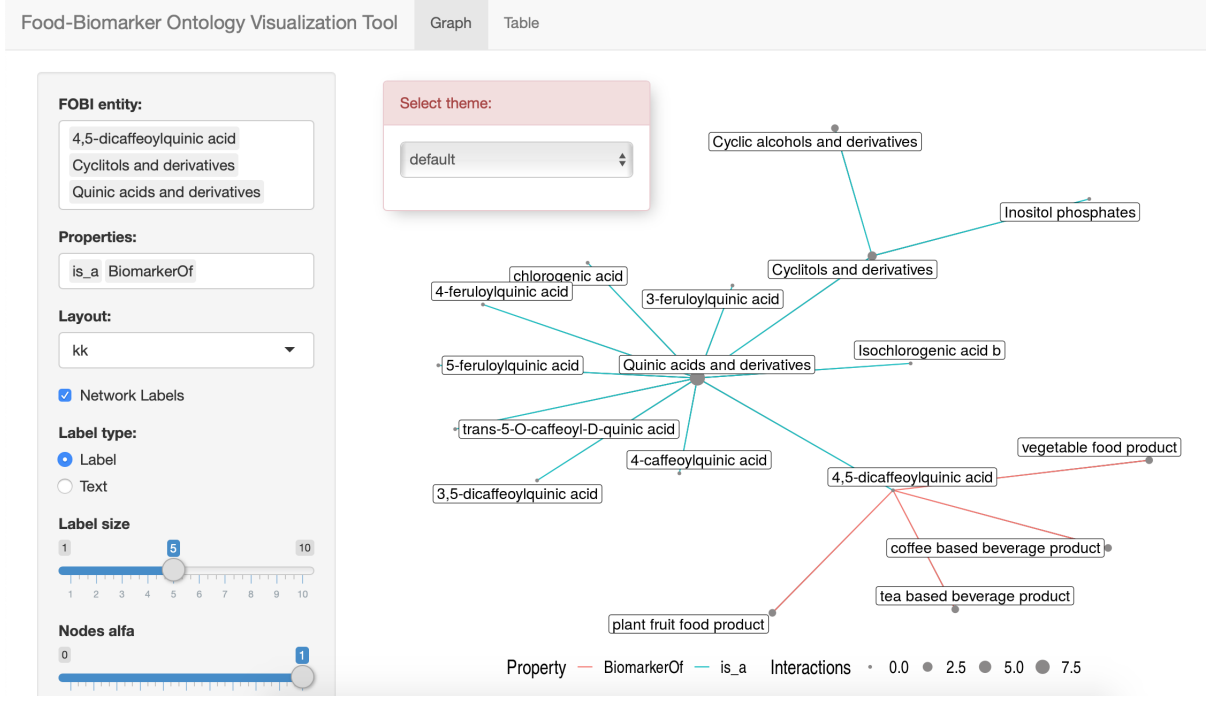
FOODON:00002473 -> "apple (whole)"



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



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!**

polcaes@gmail.com
pcastellanoescuder.github.io/
@polcastellano_
@pcastellanoescuder
University of Barcelona