# FooDrugs

## A go-to application to research potential food-drug interactions

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INNOVATION

EDUCATION

COMMUNICATION

Focus on **Nutrition-Health/Disease** interactions at **molecular** level

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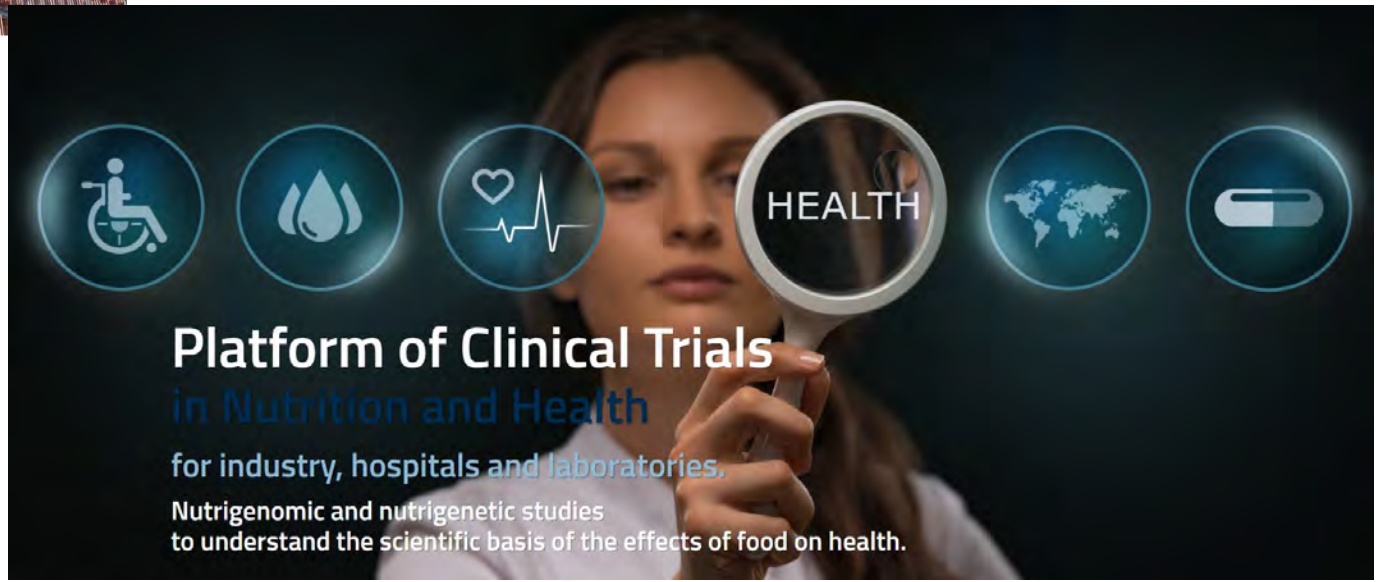


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eit Food

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elixir

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# FooDrugs

## A go-to application to research potential food-drug interactions

https://imdeafoodcompubio.com/index.php/foodrugs/

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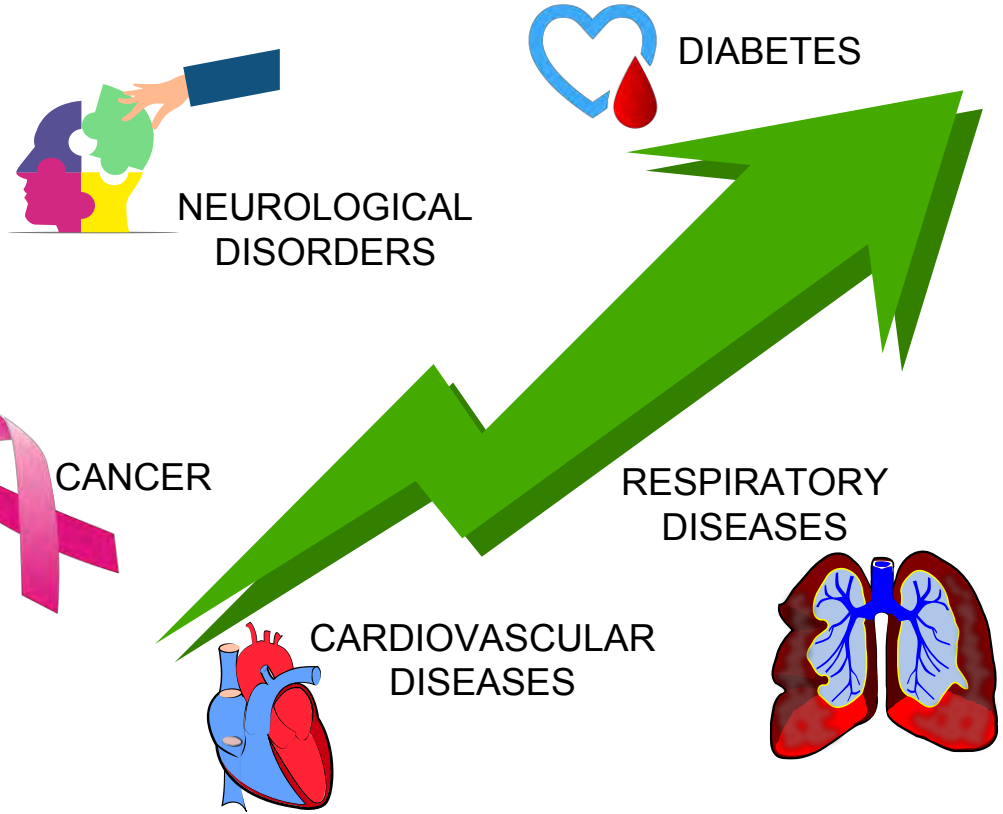
# FooDrugs motivation



Images thank to Pixabay

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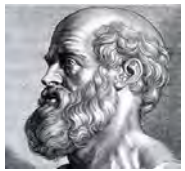
# FooDrugs motivation

Image thanks to Pexels

«The man first wanted to eat to survive, then he wanted to eat well and incorporated gastronomy into his cultural world. He now, in addition, he wants to eat health »
Prof. F. Grande Covian



“Let food be the medicine, and let medicine be the food.” (attributed to Hippocrates)

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Photo: gildemax

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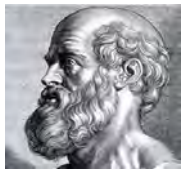

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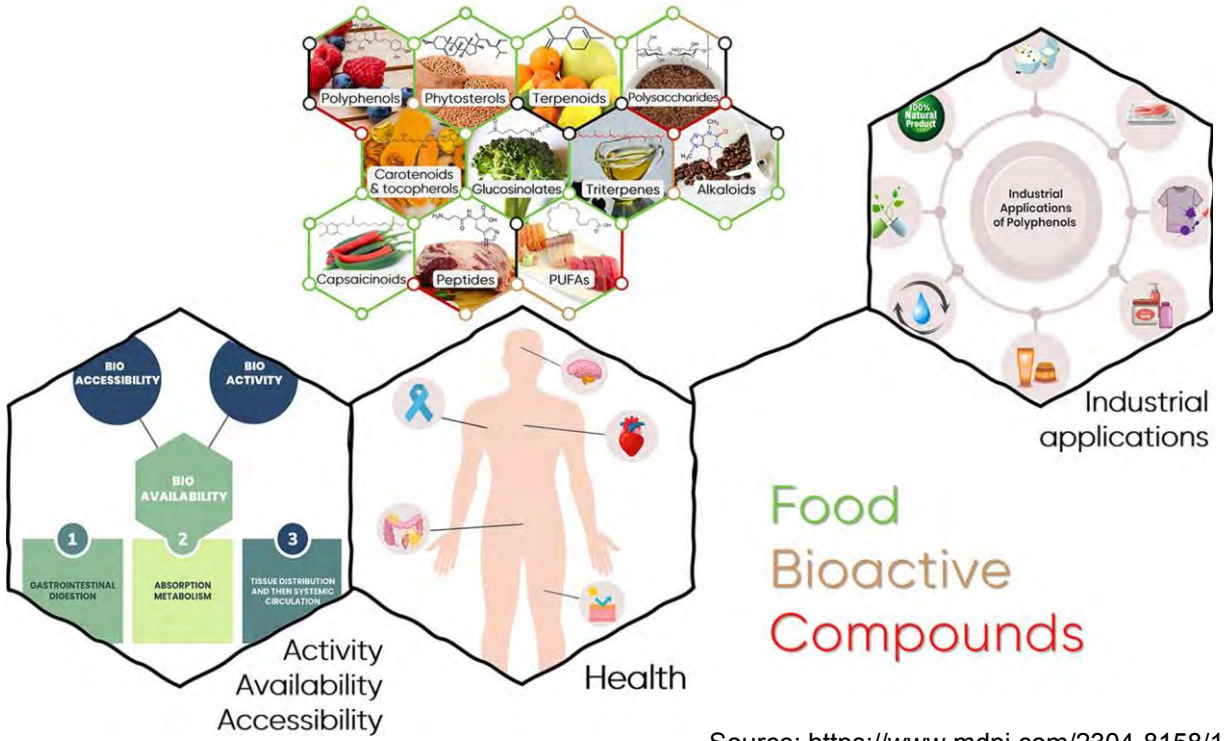
# FooDrugs motivation

Food compounds have different mechanisms of action that have an **effect on health**




Source: https://www.mdpi.com/2304-8158/10/1/37#

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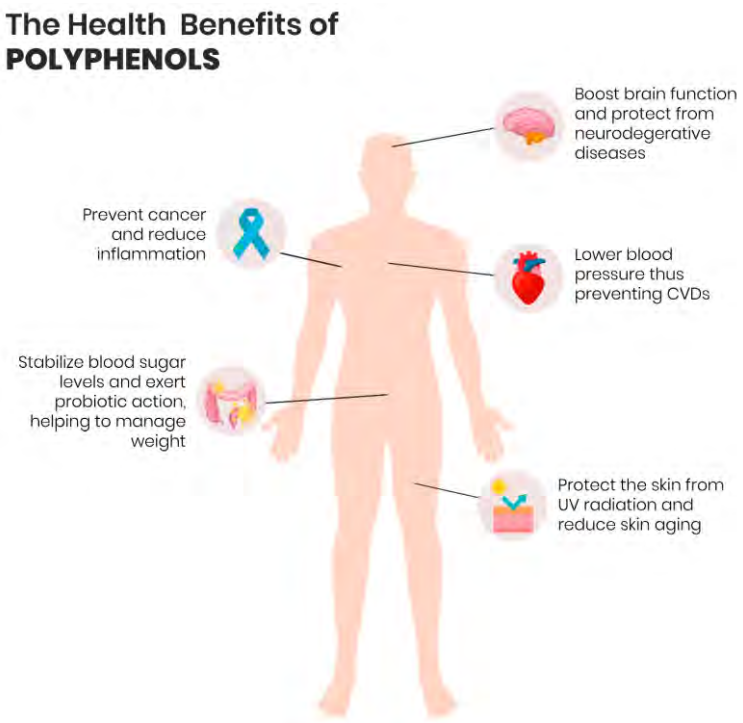


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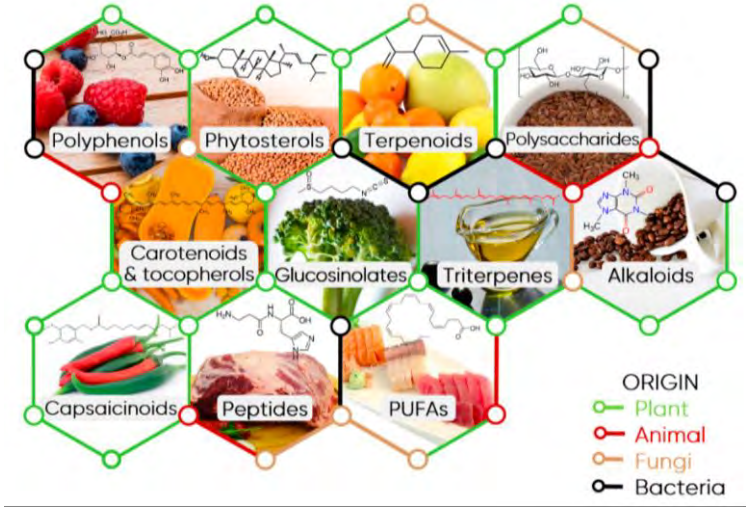


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# FooDrugs motivation

Foods can have **negative** effects on drug efficacy…

EL PAÍS

SUSCRÍBETE INICIAR SESIÓN

EDUCACIÓN MEDIO AMBIENTE IGUALDAD SANIDAD CONSUMO ASUNTOS SOCIALES LAICISMO COMUNICACI

PSEUDOCIENCIAS ›

**“I followed a naturalist diet that interfered with my chemotherapy”**

Desperation in the face of a cancer diagnosis leads many affected to fall into the hands of pseudotherapies

*At the end of the last chemotherapy session for her breast cancer, Isabel Vaquero blurted out, “Now, back home to take my turmeric and the rest of my diet.” The oncologist's face changed, and she said, ‘Did you know that curcumin inhibits the treatment?' “I felt crushed, i followed a naturalist diet that interfered with my chemotherapy."*

https://elpais.com/sociedad/2018/09/28/actualidad/1538152010_345346.html

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# FooDrugs motivation

**Complementary medicine use in cancer patients receiving intravenous antineoplastic treatment**

Uso de medicina complementaria en pacientes oncológicos sometidos a tratamiento quimioterápico intravenoso

Regina Juanbeltz[1,2,3], María Dolores Pérez-Fernández[1], Bianka Tirapu[4], Ruth Vera[3,5], Susana de la Cruz[5], María Teresa Sarobe[1,3]

Farmacia Hospitalaria 2017
| Vol. 41 | N° 5 | 589 - 600 |

- 32.3% of the patients reported **complementary medicine use** during this period recommended by friends or relatives
- 89% were ingesting products by mouth, herbs and natural products being the most commonly used
- The most used supplement was curcumin, among others

British Journal of Clinical Pharmacology

Br J Clin Pharmacol (2018) **84** 679–693 679

REVIEW

**Critical evaluation of causality assessment of herb–drug interactions in patients**

Charles Awortwe[1,2], Memela Makiwane[2], Helmuth Reuter[2], Christo Muller[1], Johan Louw[1] and Bernd Rosenkranz[2]

- 60% cases with adverse drug reactions are due to **herbal supplements**

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# FooDrugs motivation

… or **positively** affect drug efficacy.

frontiers in Oncology

Phenolic diterpenes from Rosemary supercritical extrac inhibit non-small cell lung cancer lipid metabolism and synergise with therapeutic drugs in the clinic

Adrián Bouzas[1,2†], Marta Gómez de Cedrón[1*†], Gonzalo Colmenarejo[3], José Moisés Laparra-Llopis[4], Juan Moreno-Rubio[1,5], Juan José Montoya[2,6], Guillermo Reglero[1,7], Enrique Casado[5], Beatriz Tabares[5], María Sereno[5] and Ana Ramírez de Molina[1*]

nature International weekly journal of science

Letter | Published: 11 July 2018

## Histidine catabolism is a major determinant of methotrexate sensitivity

Naama Kanarek, Heather R. Keys, Jason R. Cantor, Caroline A. Lewis, Sze Ham Chan, Tenzin Kunchok, Monther Abu-Remaileh, Elizaveta Freinkman, Lawrence D. Schweitzer & David M. Sabatini

*Nature* **559**, 632–636(2018) | Cite this article

nature COMMUNICATIONS

## Fatty acids homeostasis during fasting predicts protection from chemotherapy toxicity

Received: 11 January 2021

Accepted: 9 September 2022

Published online: 27 September 2022

Check for updates

Marta Barradas[1,13], Adrián Plaza[1,13], Gonzalo Colmenarejo[2], Iolanda Lázaro[3], Luis Filipe Costa-Machado[1], Roberto Martín-Hernández[2], Victor Micó[4], José Luis López-Aceituno[1], Jesús Herranz[2], Cristina Pantoja[1], Hector Tejero[5], Alberto Diaz-Ruiz[6], Fatima Al-Shahrour[5], Lidia Daimiel[4], Viviana Loria-Kohen[7], Ana Ramirez de Molina[7,8], Alejo Efeyan[9], Manuel Serrano[10], Oscar J. Pozo[11], Aleix Sala-Vila[3,12] & Pablo J. Fernandez-Marcos[1]

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# FooDrugs motivation

**Problem:** No resources about Food-Drug Interactions (FDIs), only about Drug-Drug Interactions (DDIs)

Drugs.com Know more. Be sure. — 4688 drugs with food interactions. Include food, alcohol, high blood pressure and cholesterol interactions

DRUGBANK — 2290 FDI recommendations from 1262 compounds

MEDINDIA — 138 drugs with FDI, 499 FDI recommendations

MedlinePlus Información de salud para usted — 87 herbs and natural products, 945 total FDI recommendations

Some DDI resources contain a few FDIs → **Not homogeneous information**

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# FooDrugs motivation

**Problem:** the knowledge and training of health professionals in known food-drug interactions is unsatisfactory [1]

| Questions | Correct answers, N (%) |
|---|---|
| Amiodarone with grapefruit | 179 (59.7) |
| Atorvastatin with grapefruit | 211 (70.3) |
| Levothyroxine with cauliflower | 125 (41.7) |
| Diazepam with caffeine | 134 (44.7) |
| Coumadin with green vegetables | 239 (79.7) |
| Theophylline with excessive coffee and tea | 196 (65.3) |
| Tetracycline with milk and dairy products | 262 (87.3) |
| MAOI with cheese and fermented food | 204 (68.0) |
| Digoxin with wheat bran | 147 (49.0) |
| Levodopa with protein-rich food | 161 (53.7) |
| Antibiotics with grapefruit juice | 198 (66.0) |
| Spironolactone with potassium rich foods | 160 (53.3) |

**Table 2:** Knowledge assessment for pharmacists about food-drug interactions (n = 300)

Zawiah et al., 2020. *PloS One*, *15*(6), e0234779.

1: Benni et al., n.d.; Couris et al., 2000; El Lassy & Ouda, 2019; Enwerem & Okunji, 2015; Osuala et al., 2021; Zawiah et al., 2020

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# FooDrugs motivation

In summary …

- **Increased consumption** of foods with an active role to prevent non-communicable diseases [1]
- **Increased side effects** with increasing health cost [2]
- **Information disperse** and/or incomplete
- **No dedicated system** for Food-Drug interactions
- **Lack of training** [3]

*1: Choi, and Ko. 2017.*
*2: Topolska, Florkiewicz, and Filipiak-Florkiewicz 2021; Ali, Alam, and Ali 2021; Baker et al. 2022*
*3:*Benni et al., n.d.; Couris et al., 2000; El Lassy & Ouda, 2019; Enwerem & Okunji, 2015; Osuala et al., 2021; Zawiah et al., 2020

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# FooDrugs

**Text Mining component**

**Molecular component**

mySQL Database

**Work package 4**

**Deliverable 4.9**

FooDrugs

**Web service**

Hostinger cloud service

**Work package 5**

**Deliverable 5.8**

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# FooDrugs

FooDrugs database (July, 2023) includes:

*Text Mining component*

| | |
|---|---|
| Number of documents | 439,338 |
| Number of potential FDIs | 1,108,429 |
| Number of food bioactives | 50,960 |
| Number of drugs | 161,809 |

*Molecular component*

| | |
|---|---|
| Number of studies | 150 |
| Number of samples | 3,923 |
| Number of potential positive FDIs | 1,759,322 |
| Number of potential negative FDIs | 1,590,097 |
| Number of food treatment conditions* | 462 |

*Each condition is defined as a food or bioactive per time point, concentration, cell line, primary culture or biopsy, and per study.

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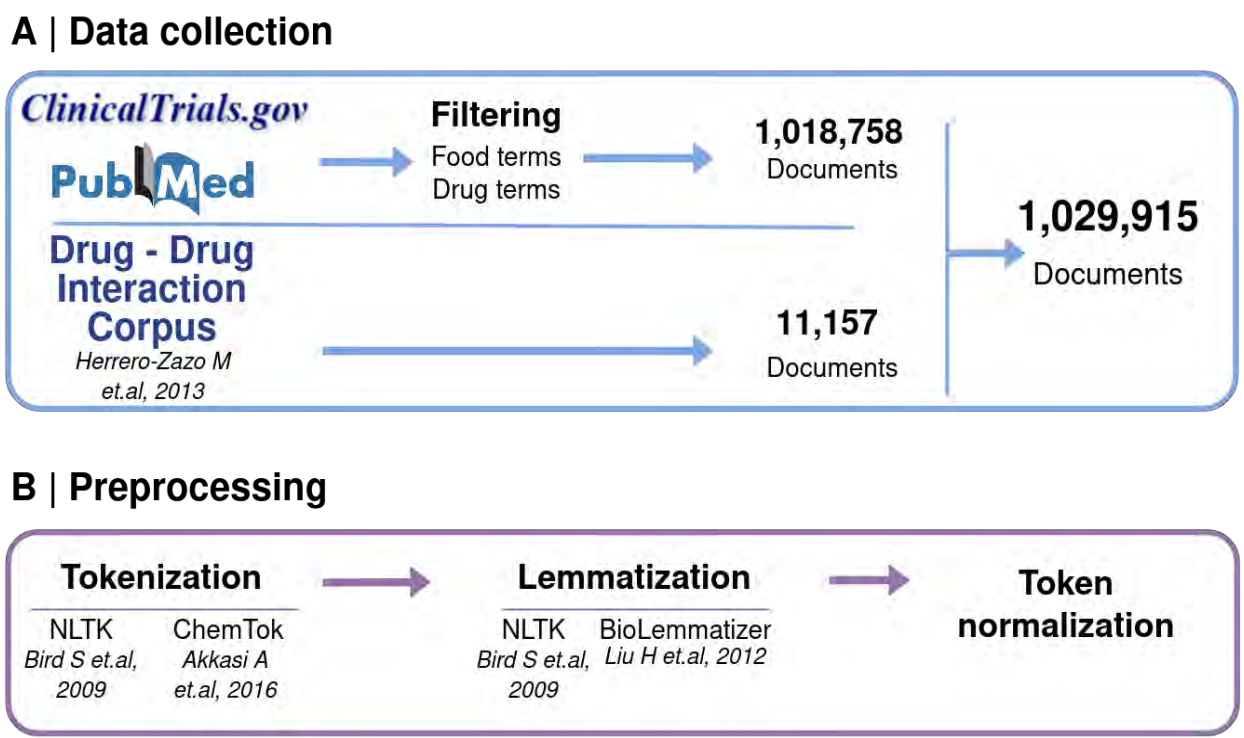
# FooDrugs - Text mining component




**A)** Data collection was performed by collecting documents containing at least one food and drug term in their description, as well as the whole DDI corpus. **B)** Data preprocessing step is applied to the documents for better integration in the pipeline.

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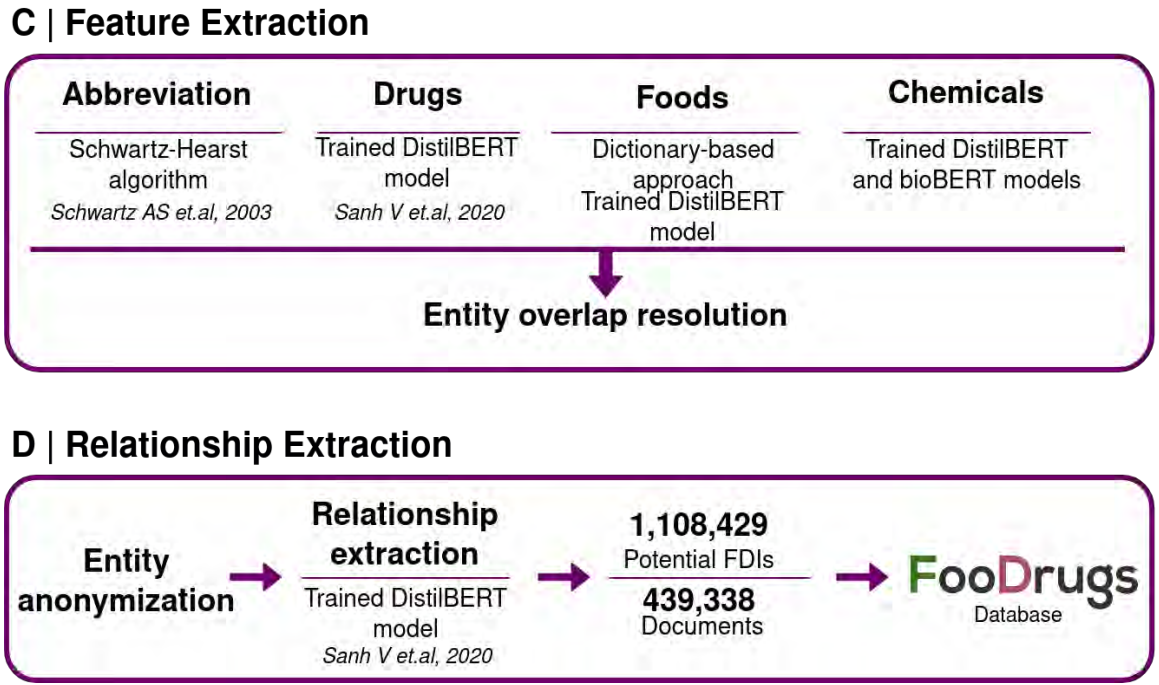


**C)** In the Feature extraction step, different entities are recognised in the text via different methods, and entity overlap resolution is done when necessary. **D)** Finally, for Relationship extraction, entities are anonymized to work with the relationship extraction model used, and the resulting FDIs and documents are stored in the FooDrugs database.

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# Foodrugs: TM selection strategy

Food terms list

Drug terms list

Source

Documents from Source with Foods in description

Documents from Source with Drugs in description

Documents from Source with **both**

Example valid document

**Resveratrol-loaded core-shell nanostructured delivery systems: Cyclodextrin-based metal-organic nanocapsules prepared by ionic gelation**

Chao Qiu [1], David Julian McClements [2], Zhengyu Jin [1], Yang Qin [3], Yao Hu [3], Xueming Xu [1], Jinpeng Wang [4]

Affiliations + expand

PMID: 32087520 DOI: 10.1016/j.foodchem.2020.126328

... Moreover, the encapsulation efficiency of resveratrol within the nanocapsules increased appreciably after coating them with chitosan (from 66.5 to 91.3%). The chitosan coating was also shown to increase the antioxidant activity and photostability of the encapsulated resveratrol…

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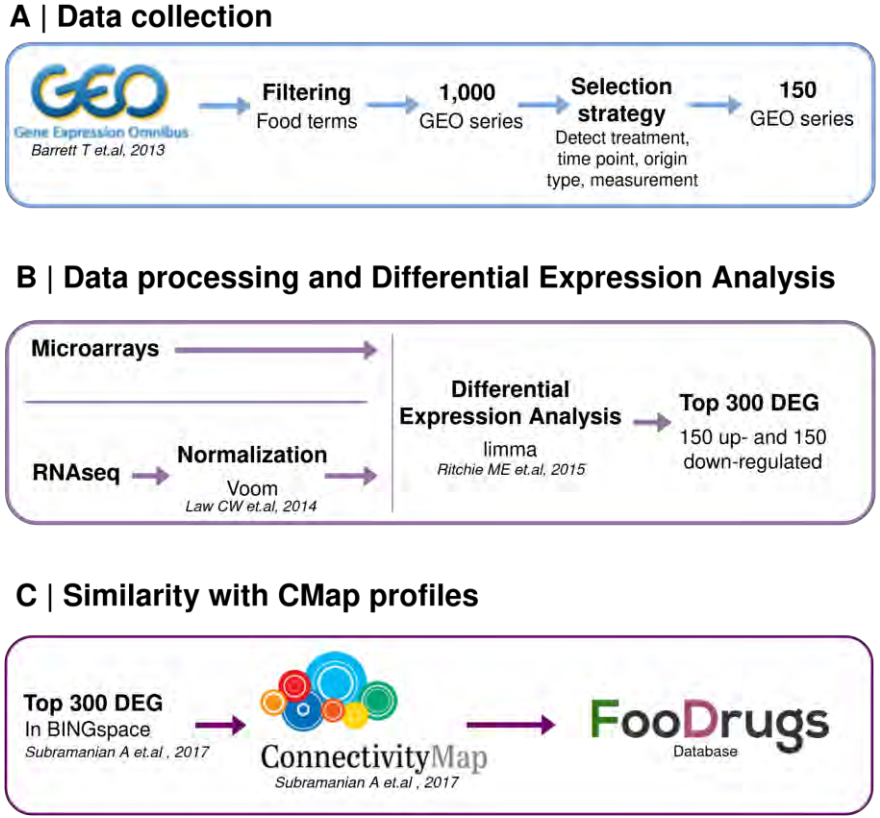


**A)** Data collection consists of the search of food transcriptomic studies with food keywords. **B)** Data processing is performed and differential expression analysis with limma to get 150 up- and down-regulated genes in food condition vs control. **C)** Genes present in BINGspace sent to CMAP to compute similarity scores with drug transcriptomic profiles.

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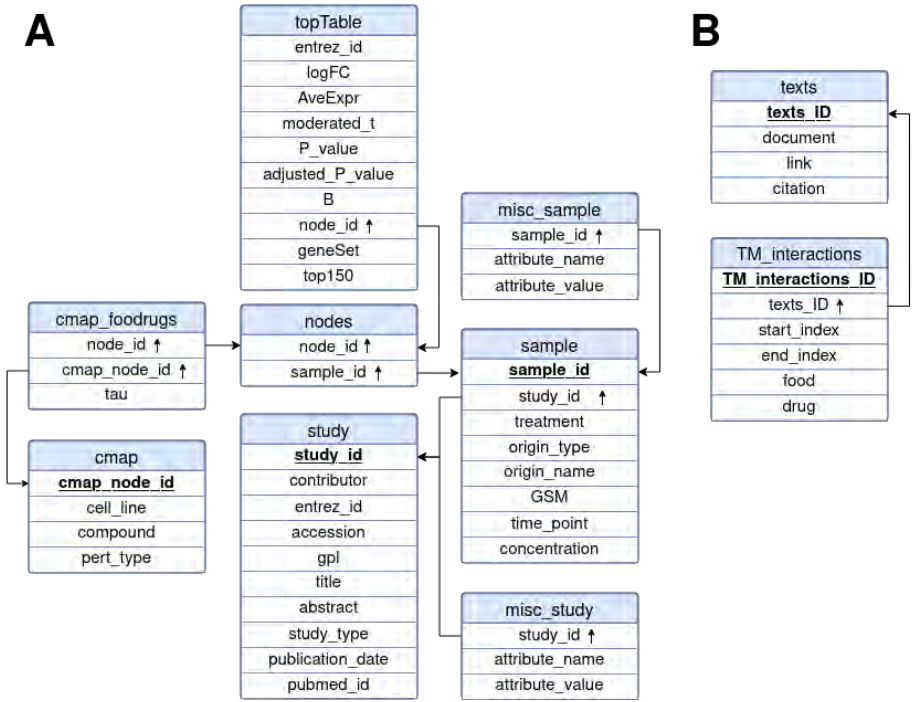
# FooDrugs - Database




Relational model for the FooDrugs database. Primary keys for each table are marked in bold and underlined. Foreign keys are marked by an arrow pointing upwards. The database is formed by two independent components: **A)** a molecular component, built from GEO studies involving food compounds or bioactives; and **B)** a text mining component, built using NLP.

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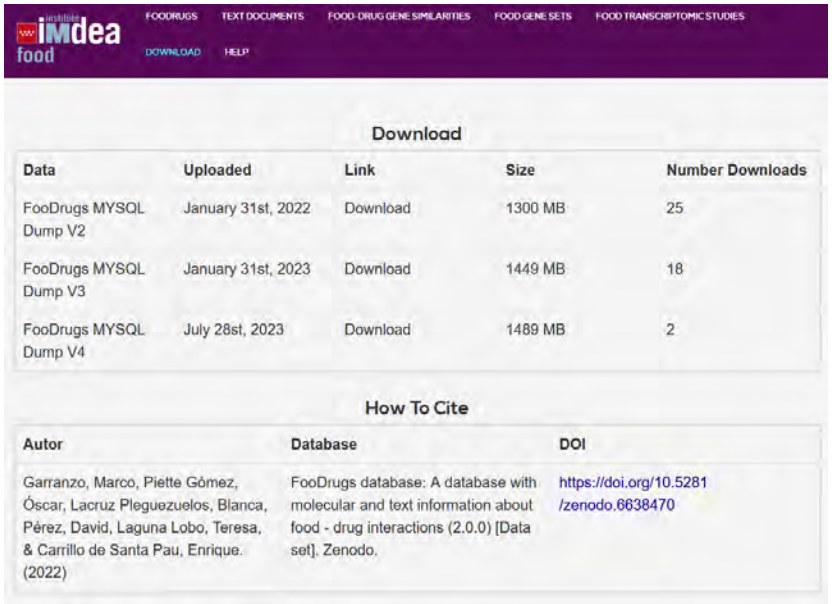


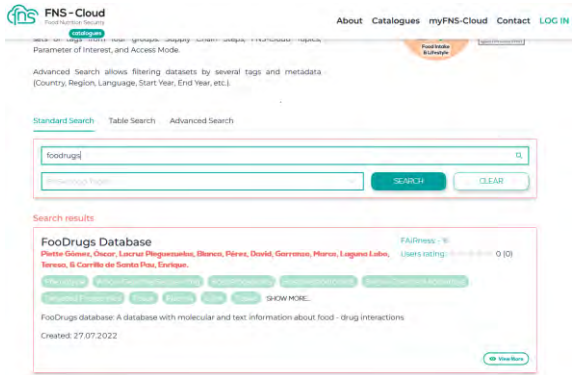


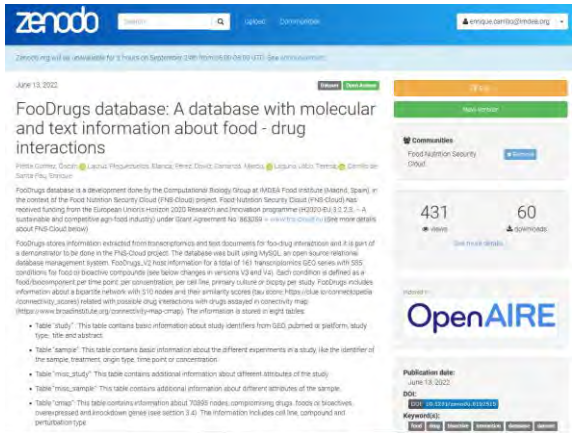


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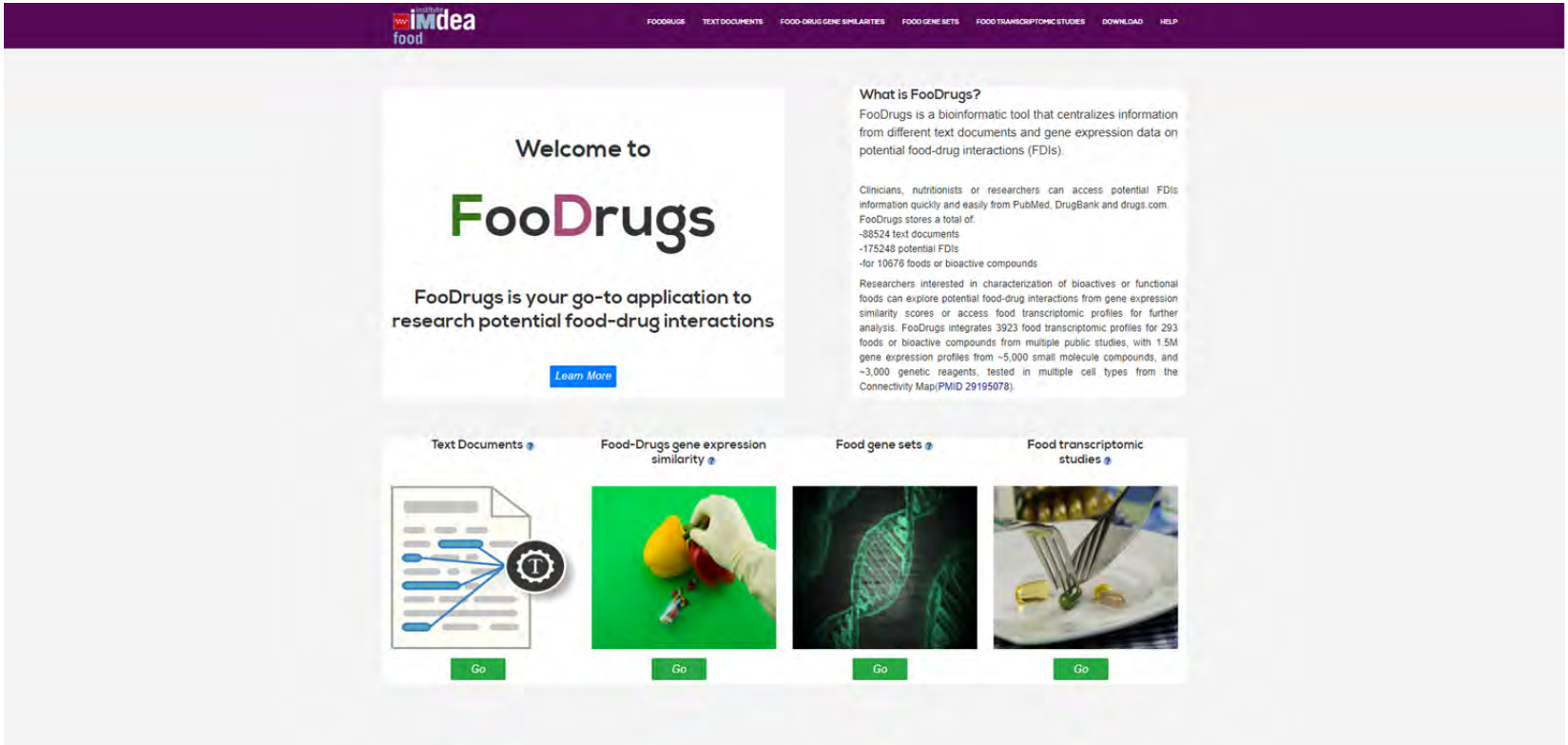
# Webtool

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# Webtool

**Food-Drugs Interactions Database**
10.5281/zenodo.8192515

## FooDrugs
Webtool

| Text Mining | Food-Drug Gene Similarities | Food Gene Set | Food Transcriptomic Studies |
|---|---|---|---|
| Open a query to explore information about potential food-drug interactions in text documents from the FooDrugs database.<br><br>Downloadable Tables.<br><br>Links to go to the article. | Open a query to explore similar gene signatures between foods and drugs or genetic reagents from the FooDrugs database.<br><br>Enrichment Analysis with CMAP,KEGG,Mesh and DrugBank<br><br>Downloadable Tables.<br><br>Links to go to the GEO Study. | Open a query to access information for transcriptomic gene sets in food datasets stored in FooDrugs database.<br><br>Enrichment Analysis with Reactome , WikiPathways and GeneOntology<br><br>Downloadable Tables with Ensembl Information.<br><br>Links to go to the GEO Study. | Open a query to access information for the food datasets stored in FooDrugs database.<br><br>Downloadable Tables.<br><br>Links to go to the GEO Study. |

10.5281/zenodo.7551055

Drugs.com · NIH ClinicalTrials.gov · KEGG · MeSH · WikiPathways · PANTHER · PubMed · ConnectivityMap · GEO Gene Expression Omnibus · reactome · GEO Gene Expression Omnibus · GEO Gene Expression Omnibus · DRUGBANK · GENEONTOLOGY Unifying Biology · Ensembl

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# Usability Testing

The usability testing was divided in 3 Scenarios

- Scenario 1 for Molecular Researchers

  -Extensive network of potential interactions from transcriptomic data.

- Scenario 2 for Clinicians & Nutritionists

  -On food-drug interactions to ensure the correct usage of supplements.

- Scenario 3 for Transcriptomic Researchers

  -Area of identifying and studying the molecular mechanisms of food-bioactive compounds

*Hana Musinovic*

*Siân Astley*

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# Usability Testing

Interviews for FooDrugs usability testing were carried out in a two step process.

- Sassari consortium meeting

  -Food and nutrition researchers and IT specialist. 8 Users

- Guided interviews during October 2022

  -Mix of experts from differents areas and organizations. 11 Users

**Deliverable 5.8**

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# FooDrugs Interviews results surveys

| System Usability Scale | Strongly Disagree | Disagree | Neutral | Agree | Strongly Agree |
|---|---|---|---|---|---|
| I would use FooDrugs frequently | | 3 | 4 | 7 | 4 |
| I found FooDrugs unnecessarily complex | 3 | 9 | 5 | 1 | |
| I thought FooDrugs was easy to use | | 3 | 5 | 6 | 4 |
| I would need support use FooDrugs | 6 | 6 | 3 | 1 | 2 |
| I found the various functions of FooDrugs were well integrated | | 2 | 6 | 8 | 2 |
| There was too much inconsistency in FooDrugs | 3 | 10 | 2 | 2 | 1 |
| Most people would learn to use FooDrugs quickly | | 3 | 2 | 10 | 3 |
| I found FooDrugs cumbersome to use | 5 | 8 | 3 | 2 | |
| I felt confident using FooDrugs | 1 | 4 | 6 | 5 | 2 |
| I would need to learn a lot of things before I could get going with FooDrugs | 3 | 9 | 2 | 4 | |

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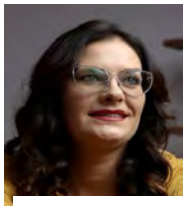
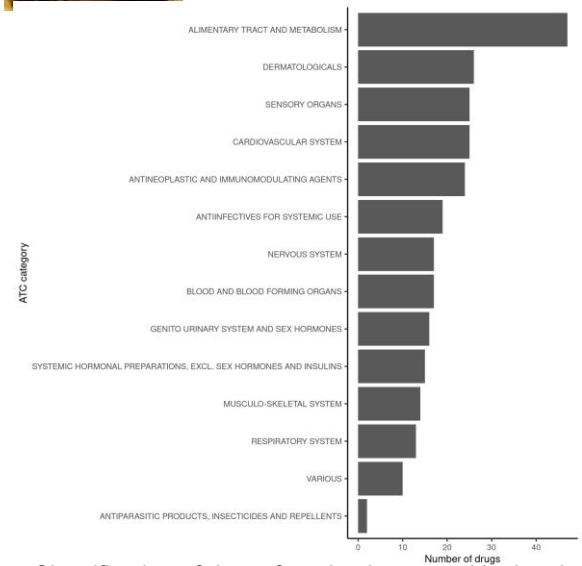
# User case vitamin D

University of Belgrade
INSTITUTE FOR MEDICAL RESEARCH
National Institute of Republic of Serbia
www.imi.bg.ac.rs



*Jelena Milešević*




Classification of drugs found to interact with vitamin D in FooDrugs database, according to ATC classification

**Problem:**

- Vitamin D, a fat-soluble vitamin essential for maintaining bone health, is a recommended food supplement to reduce risk of fractures in elderly people [1]
- However different trials have shown inconsistent results [2]

**Hypothesis:**

Different types of drugs can interrupt absorption of vitamin D in the gut, or consume it, as a derivative of cholesterol, causing vitamin D deficiency.

# FooDrugs

878 texts from different sources, containing 1,146 interactions of vitamin D with 238 drugs


1. Bischoff-Ferrari HA, et al., 2005
2. Gallagher JC. 2016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# E-Learning course

https://www.fns-cloud.eu/foodrugs/#/

FooDrugs

**This course aims to introduce and explain the FooDrugs tool.**

Developed by: IMDEA Food Institute

Authors: David Pérez, Óscar Piette, Marco Garranzo, Blanca Lacruz, Teresa Laguna and Enrique Carrillo.

Sections:

- Introduction to Food-Drug interactions
- FooDrugs webtool tutorial

Prifysgol Cymru
Y Drindod Dewi Sant
University of Wales
Trinity Saint David

***Annette Fillery-Travis***

***Lowri Harris***

***Rachel Davies***

***Alice De Angeli***

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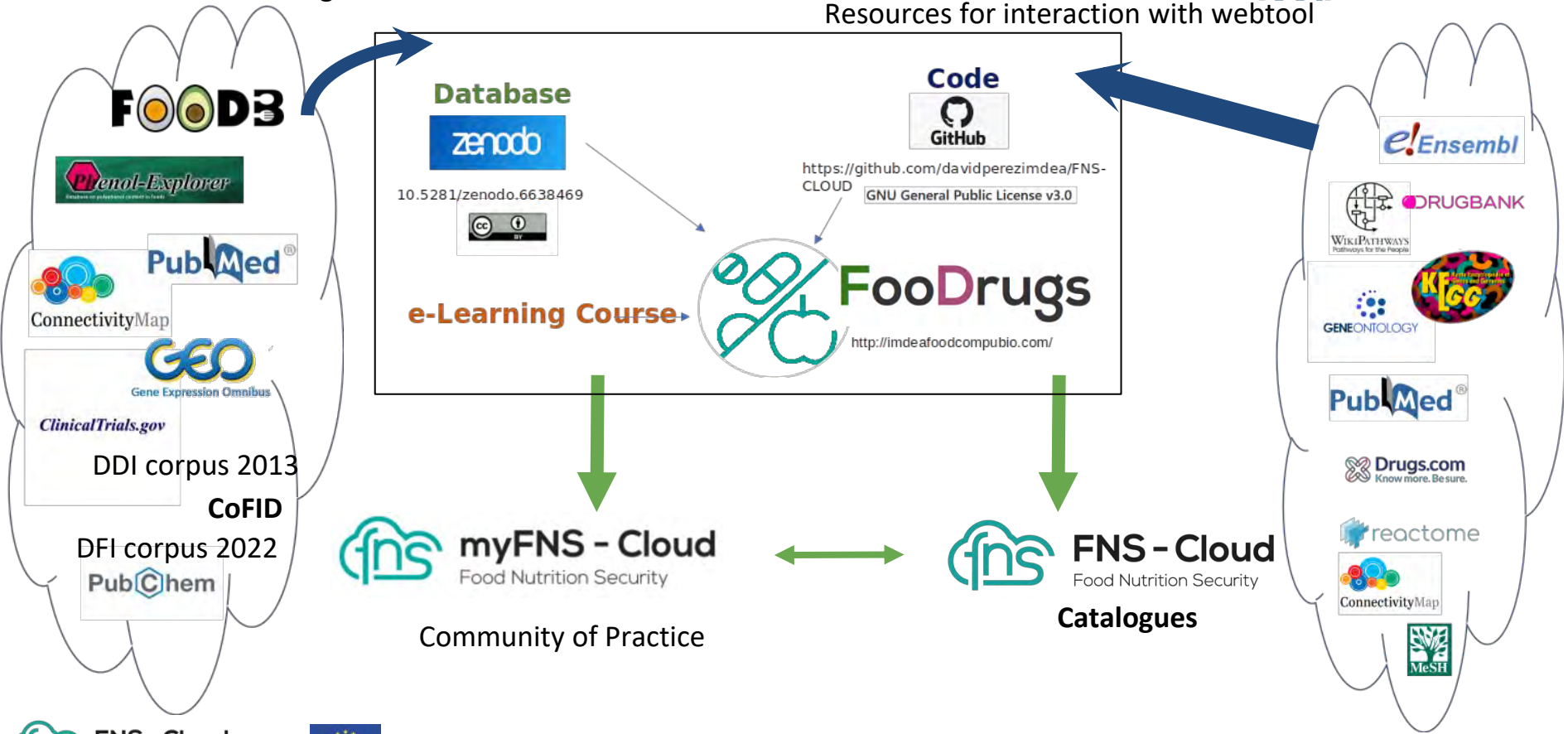
# Resources linked to FooDrugs

Resources for Database generation

Resources for interaction with webtool

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# Resources generated from FooDrugs

- FooDrugs database (*Creative commons license)*
- FooDrugs Web page (*Free Access*)
- Code to generate resource (*GNU*)
- E-Learning course (*Free Access*)
- Included in the FNS-catalog
- Publication under review (Database Journal. CC-BY License)

***Juan Luis Rodrigues (RTDS)***

***Javier de la Cueva***

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# Dissemination

institute IMDEA food

ECCB2022

SeqN 2021

BioinfoCAM

EFFoST

elixir

ITU MBG Student Club

ISMB ECCB 2023 LYON FRANCE July 23-27 ISCB

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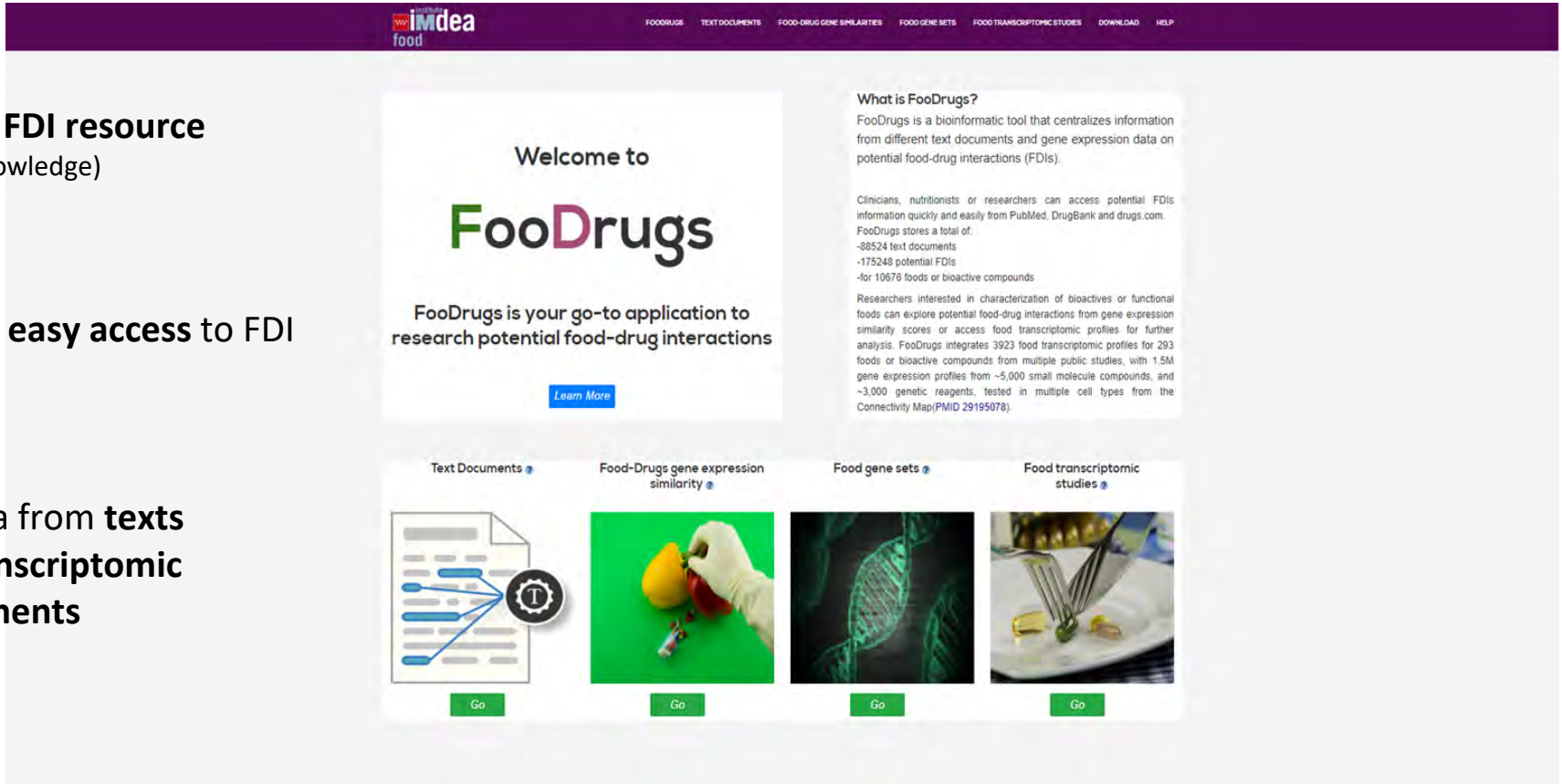
# Final summary

**Largest FDI resource**
(in our knowledge)

Provide **easy access** to FDI

FDI data from **texts** and **transcriptomic experiments**

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# Final summary

- Valuable Resource for Researchers and Clinicians: FooDrugs addresses the pressing need for a centralized repository of FDI information. This resource offers researchers and clinicians a convenient and free platform to access critical data, facilitating their investigation of potential FDIs and enabling personalized dietary recommendations for patients based on their medication regimen.

- I think that these resources collectively present a relevant tool for researchers working in the field

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# Acknowledgements

## Computational biology group

**Former members**

## Acknowledgements

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Food Nutrition Security

*Siân Astley*

*Hana Musinovic*

*Javier de la Cueva*

*Susan Coort*

*Chris Evelo*

*Rachel Davies*

*Alice De Angeli*

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RTDS GROUP

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# Questions?

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# FooDrugs

## A go-to application to research potential food-drug interactions

https://imdeafoodcompubio.com/index.php/foodrugs/

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# User cases with survey monkey

http://imdeafoodcompubio.com/

Clinicians and Nutritians

https://www.surveymonkey.co.uk/r/CJWJ3PS

Molecular researchers

https://www.surveymonkey.co.uk/r/CJHQCXM

Transcriptomic researchers

https://www.surveymonkey.co.uk/r/CQMBNDD

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# FooDrugs

## A go-to application to research potential food-drug interactions

**Enrique Carrillo de Santa Pau**

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