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FoodComEx, a new chemical library useful for the food bioactives community

Claudine Manach, C. Weinert, Jarlei Fiamoncini, Estelle Pujos-Guillot, Maria Ulaszewska, Franck Giacomoni, Fulvio Mattivi, Mireia Urpi Sarda, Cristina Andres-Lacueva, S.E. Kulling, et al.

► To cite this version:

Claudine Manach, C. Weinert, Jarlei Fiamoncini, Estelle Pujos-Guillot, Maria Ulaszewska, et al.. FoodComEx, a new chemical library useful for the food bioactives community. 1. international conference on Food Bioactive and Health 2016, Sep 2016, Norwich, United Kingdom. hal-01595601

HAL Id: hal-01595601

<https://hal.science/hal-01595601>

Submitted on 5 Jun 2020

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FoodComEx, a new chemical library useful for the food bioactives community



Claudine MANACH
Human Nutrition Unit, UMR1019 Clermont-Ferrand

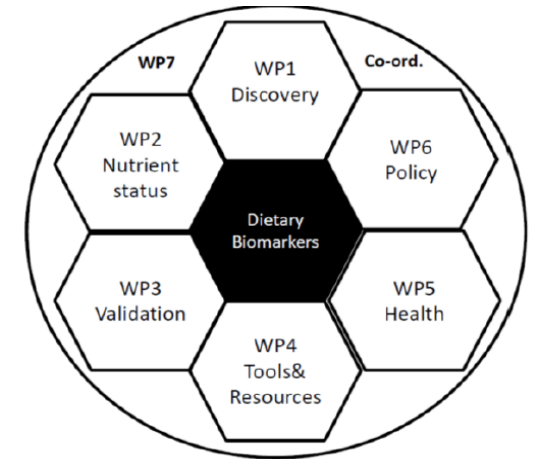
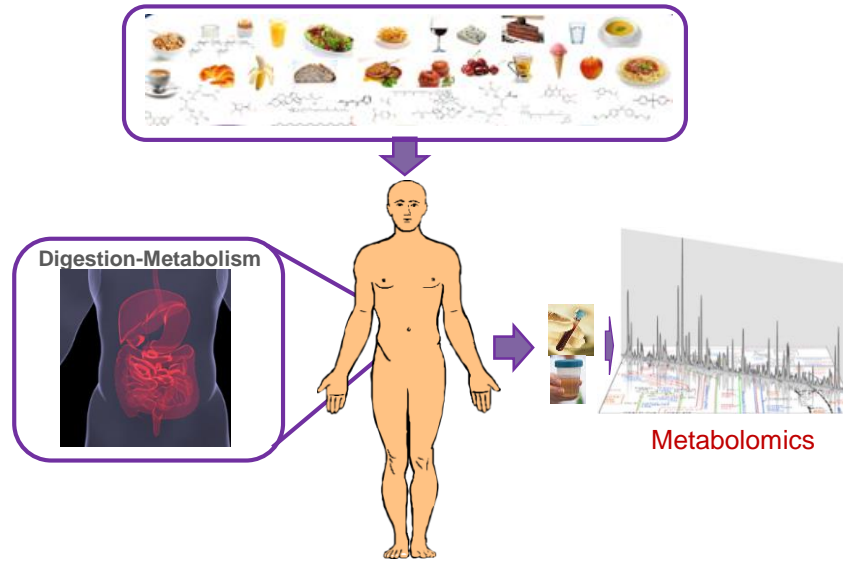
FOOTBALL PROJECT - THE FOOD BIOMARKER ALLIANCE



- Janv 2015-Dec 2017. 4,38M€
- 22 partners, PI: E. Feskens, Wageningen, NL



Aim:
Identification and validation of dietary biomarkers using metabolomics



- Intervention studies in 7 centers to identify new biomarkers of food intake
- Inventory of known dietary biomarkers and new validation scoring system
- New tools and resources for research on the food metabolome and biomarker discovery (WP4)



WHY FOODCOMEX?

Standards for food-derived compounds are needed for:

- Validation of identifications in untargeted metabolomics studies
- Development of quantitative methods of analysis for particular metabolites or biomarkers
- Testing the biological activities of isolated metabolites in *in vitro* models

For many food-derived compounds,
standards are not commercially available

A RESOURCE TO FACILITATE SHARING OF STANDARDS : FOODCOMEX

- Many compounds have been synthesised or isolated in academic laboratories

FoodComEx

Browse About Register Log In Links

Search compounds Search

Library
Virtual Board
Providers
Production/Isolation Methods

<http://foodcomex.org/>

FoodComEx

Welcome to the **Food Compound Exchange**,
a new collaborative exchange platform for rare food-derived compounds!

The lack of commercial standards for food-derived metabolites is a major limitation in nutritional metabolomics. It also hampers the study of the cellular and molecular effects of physiological metabolites of food nutrients and non-nutrients *in vitro* models.

FoodComEx is a new chemical library initiated in the **FoodBALL** (Food Biomarkers Alliance) project to facilitate the sharing of not easily accessible standards for food compounds and their human metabolites.

FoodComEx is a virtual library, with compounds stored in the laboratory

> Browse Library
> How It Works
> Virtual Board

Only a few example compounds available online

We believe that FoodComEx will strengthen international collaboration in the field of metabolomics and beyond, but its success depends on your participation! You are invited to share your standards and browse our library if you are searching for a specific compound. Start now!

Please [contact us](#) for more information!

[Download the Flyer](#)

NuGO week is coming up!
nugo.org/nugoweek-2016/

David Arndt
@DavidEArndt
It's time for some **FOODBALL!**
foodmetabolome.org

A RESOURCE TO FACILITATE SHARING OF STANDARDS : FOODCOMEX

Labo A



Labo B



Labo C



Information on available
compounds
& contact details



Online catalog



- Chemical synthesis



- Extraction-Purification from foods



- Biofluids from animals fed pure compounds or food extracts



- In vitro incubations
*Microsomes, isolated enzymes,
microbiota*

A RESOURCE TO FACILITATE SHARING OF STANDARDS : FOODCOMEX



Foodcomex Compounds

1-Methyl-pyrogallol-3-O-sulphate (FCE031318)

[Back to Compounds](#)

Batch Actions ▾

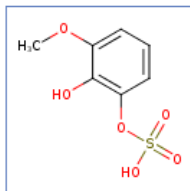
Record Information

Version	1.0
Creation date	2016-01-06 21:21:34 UTC
Update date	2016-01-13 19:45:20 UTC
FoodComEx ID	FCE031318

Chemical Information

FoodDB Name	1-Methyl-pyrogallol-3-O-sulphate
Description	Not Available
CAS Number	Not Available

Structure



[MOL](#) [SDF](#) [PDB](#) [SMILES](#) [InChI](#)

FDB02994

FDB031313

4-hydroxybenzoic acid
4-O-sulphate

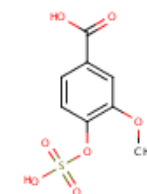
Chemical synthesis

Powder

Name
Chemical structure
Description
Synonyms
Taxonomy
Mode of production
Purity
Available quantity
Storage conditions-Stability
Physico-chemical properties
Spectral data available
Contact details

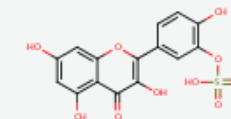
Address Contact Email Structure

BET,
tugal
rventura@itqb.unl.pt,
csantos@itqb.unl.pt



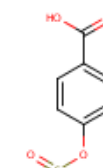
csb@usal.es

n en
Unidad



de
Spain

BET,
tugal
rventura@itqb.unl.pt,
csantos@itqb.unl.pt

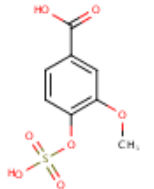
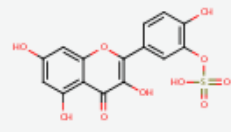
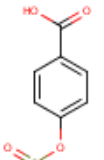


A RESOURCE TO FACILITATE SHARING OF STANDARDS : FOODCOMEX



Foodcomex Compounds

Batch Actions ▾

<input type="checkbox"/>	FoodComEx Id	Compound Name	Origin	Storage Form	Maximum Quantity	Storage Condition	Contact Name	Contact Address	Contact Email	Structure
<input type="checkbox"/>	FDB029964	Vanillic acid 4-sulfate	Chemical synthesis	Powder	Production upon request		Rita Ventura, Claudia Santos	ITQB-UNL/IBET, Oeiras, Portugal	rventura@itqb.unl.pt, csantos@itqb.unl.pt	
<input type="checkbox"/>	FDB029941	Quercetin 3'-sulfate	Chemical synthesis	Freeze-dried	Milligram amounts when produced. Production upon request	Room temperature in a dryer	Celestino Santos Buelga	Grupo de Investigación e Polifenoles, Cromatología, Facultad de Farmacia, Universidad de Salamanca, Spain	csb@usal.es	
<input type="checkbox"/>	FDB031313	4-hydroxybenzoic acid 4-O-sulphate						ITQB-UNL/IBET, Oeiras, Portugal	rventura@itqb.unl.pt, csantos@itqb.unl.pt	

Bilateral negotiation with the provider
(*Charter of good practices online*)

A RESOURCE TO FACILITATE SHARING OF STANDARDS

The screenshot shows the top navigation bar of the FoodComEx website. The logo 'FoodComEx' is on the left. The navigation menu includes 'Browse', 'About', 'Register', 'Log In', and 'Links'. A search bar is on the right with the text 'compounds' and a 'Search' button. A dropdown menu is open under 'Browse', listing 'Library', 'Virtual Board', 'Providers', and 'Production/Isolation Methods'. A green oval highlights the 'Virtual Board' and 'Providers' options, with a green arrow pointing down to a list of features.

<http://foodcomex.org/>

- A virtual board to request unavailable compounds
- A providers directory to foster collaborations
- A repository of shared production methods

accessible standards for food compounds and their human metabolites.

FoodComEx is a virtual library, with compounds stored in the laboratory where they have been isolated or synthesized. Anyone interested in one compound will directly contact the laboratory offering to share the compound. A reference spectral library for food-derived compounds and their metabolites will be made available from the data shared by users.

We believe that FoodComEx will strengthen international collaboration in the field of metabolomics and beyond, but its success depends on your participation! You are invited to share your standards and browse our library if you are searching for a specific compound. Start now!

Please [contact us](#) for more information!

[Download the Flyer](#)

Tweets by @DavidEArndt

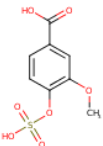
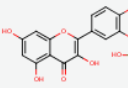
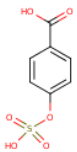
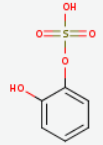
David Arndt
@DavidEArndt
NuGO week is coming up!
nugo.org/nugoweek-2016/
20h

David Arndt
@DavidEArndt
It's time for some FOOTBALL!
foodmetabolome.org
30 Aug

FC ADMIN / **Foodcomex Compounds** New Foodcomex Compound

Contributors can enter and update their data

Batch Actions ▾

☐	FoodComEx Id	Compound Name	Origin	Storage Form	Maximum Quantity	Storage Condition	Contact Name	Contact Address	Contact Email	Structure	
☐	FDB029964	Vanillic acid 4-sulfate	Chemical synthesis	Powder	Production upon request		Rita Ventura, Claudia Santos	ITQB-UNL/IBET, Oeiras, Portugal	rventura@itqb.unl.pt, csantos@itqb.unl.pt		View Edit Delete
☐	FDB029941	Queroetin 3'-sulfate	Chemical synthesis	Freeze-dried	Milligram amounts when produced, Production upon request.	Room temperature in a dryer	Celestino Santos Buelga	Grupo de Investigación en Polifenoles. Unidad de Nutrición y Bromatología, Facultad de Farmacia, Universidad de Salamanca, Spain	csb@usal.es		
☐	FDB031313	4-hydroxybenzoic acid 4-O-sulphate	Chemical synthesis	Powder	Production upon request		Rita Ventura, Cláudia Santos	ITQB-UNL/IBET, Oeiras, Portugal	rventura@itqb.unl.pt, csantos@itqb.unl.pt		
☐	FDB031315	Catechol 1-O-sulphate	Chemical synthesis	Powder	Production upon request		Rita Ventura, Claudia Santos	ITQB-UNL/IBET, Oeiras, Portugal	rventura@itqb.unl.pt, csantos@itqb.unl.pt		

Compound: Vanillic acid 4-sulfate (FDB029964)

Export

Details

Description:

Origin:

Storage form:

Maximum quantity:

Storage condition:

Spectra Data Available Upon Request:

Purity:

Stability:

Delivery time:



- Hopefully FoodComEx will facilitate the sharing of standards that are not commercially available
- Its usefulness will depend on the number of compounds that will be shared

More information on the website

<http://foodcomex.org/>

ACKNOWLEDGEMENTS



Rosa Vazquez Fresno
Tanvir Sayed
David Arndt
Allison Pon
Albert remus Rosana
David Wishart



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Christoph Weinert
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