



HAL
open science

PhytoHub V1.4: A new release for the online database dedicated to food phytochemicals and their human metabolites

Andreia Bento da Silva, Franck Giacomoni, Balthazar Pavot, Yoann Fillatre, Joseph Rothwell, Bergona Bartolomé Sualdea, Catherine Veyrat, Rocio Garcia-Villalba, Cécile Gladine, Rachel Kopec, et al.

► To cite this version:

Andreia Bento da Silva, Franck Giacomoni, Balthazar Pavot, Yoann Fillatre, Joseph Rothwell, et al.. PhytoHub V1.4: A new release for the online database dedicated to food phytochemicals and their human metabolites. The 1. International Conference on Food Bioactives & Health, Sep 2016, Norwich, United Kingdom. 2016. hal-01607427

HAL Id: hal-01607427

<https://hal.science/hal-01607427v1>

Submitted on 3 Jun 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

PhytoHub V1.4: A new release for the online database dedicated to food phytochemicals and their human metabolites

A. Bento da Silva¹, F. Giacomoni², B. Pavo², Y. Fillâtre², J.A. Rothwell², B. Bartolomé Sualdea³, C. Caris-Veyrat⁴, R. Garcia-Villalba⁵, C. Gladine², R. Kopec⁴, P. Hollman⁶, R. Landberg⁷, C. Morand², C. Nunes dos Santos¹, L. Nyström⁸, E. Pujos-Guillo², M. Rosario Bronze¹, F. Tomas-Barberan⁵, M. Urpi-Sarda⁹, W. Wiczowski¹⁰, C. Knox¹¹, C. Manach²

¹ITBQ Oeiras, Lisbon, Portugal; ²Human Nutrition Unit, INRA Clermont-Ferrand-Theix, France, claudine.manach@clermont.inra.fr; ³CIAL, CSIC-UAM, Madrid, Spain; ⁴INRA Avignon, France; ⁵CEBAS-CSIC Murcia, Spain; ⁶RIKILT Wageningen University, The Netherlands; ⁷Swedish University of Agricultural Sciences, Uppsala, Sweden; ⁸Institute of Food, Nutrition and Health, ETH Zurich, Switzerland; ⁹University of Barcelona, Spain; ¹⁰PAN, Olsztyn, Poland; ¹¹OMx, Edmonton, Canada

PhytoHub (www.phytohub.eu) is an online database dedicated to all phytochemicals commonly ingested with the diet. It is the first database to collate information on phytochemical metabolites for metabolomics studies, and should facilitate identification of unknowns in non-targeted LC-MS profiling. More than 980 food phytochemicals have been inventoried so far. PhytoHub V1.4 contains the most consumed flavonoids (n=259), phenolic acids (n=167), stilbenes (n=26), ellagitannins (n=21), coumarins (n=22), miscellaneous polyphenols (n=39), betalains (n=53), glucosinolates and isothiocyanates (n=29), other N-containing compounds (n=73), carotenoids (n=39), phytosterols (n=15), other terpenoids (n=193) thiosulfinates (n=22), phytoprostanes (n=16) as well as 394 known human or animal metabolites of these compounds. Every metabocard provides a downloadable chemical structure as well as identifiers, synonyms and physico-chemical properties. It also includes the dietary sources with references and a link to the FooDB food card (<http://foodb.ca/>). The known metabolites extracted from the literature by experts are given with biofluid location and literature references. Collaborators from the COST Action POSITIVE have been very active to compile knowledge on polyphenol known metabolites. Since the metabolism of many phytochemicals has not been studied yet, *in silico* prediction of metabolism will be added in the future. Mass spectral data come from online libraries of spectra such as RIKEN ReSpect and MassBank, and will be complemented by experimental and literature data. For a queried monoisotopic mass or molecular formula, PhytoHub returns a downloadable list of metabolites or phytochemical precursors, along with their spectral data and possible dietary and metabolic origins. For a queried food, it returns a list of its phytochemicals and their metabolites likely to be present in biofluids after consumption. Custom advanced searches are also possible. PhytoHub will be updated continuously. PhytoHub has become a community database open to new collaborators for curation of data on dietary sources, known metabolites and analytics.

Support: ANR Project ALIA-007-PhenoMeNEp; COST Action FA 1403 POSITIVE; JPI HDHL FoodBALL project