PhytoHUB: a new database dedicated to dietary phytochemicals and their human metabolites for nutritional metabolomics

Franck Giacomoni, Yann Fillatre, J.A Rothwell, Craig Knox, Roman Eisner, Daniel Cesaire, Mercedes Quintana, Blandine Comte, Estelle Pujos-Guillot, Claudine Manach

P12-11

PhytoHUB: A NEW DATABASE DEDICATED TO DIETARY PHYTOCHEMICALS AND THEIR HUMAN METABOLITES FOR NUTRITIONAL METABOLOMICS

Franck Giacomoni[1], Yoann Fillatre[1], J.A. Rothwell[1], Craig Knox[2], Roman Eisner[2], Daniel Cesaire[1], Mercedes Quintana[1], Blandine Comte[1], Estelle Pujos-Guillot[1], Claudine Manach[1]

[1]Human Nutrition Unit, UMR 1019 INRA / University of Auvergne, Clermont-Ferrand, France, [2]In Siliflo Inc, Edmonton, Canada

The “food metabolome” comprises all metabolites present in biological fluids that are directly derived from the digestion of food. A large proportion of the food metabolome consists of phytochemical metabolites, which are products of intestinal and hepatic or microbial metabolism of molecules such as polyphenols, terpenoids and alkaloids. Identification of unknowns in metabolome profiles is a laborious step-by-step process and often a bottleneck in biomarker discovery. One major limitation for the interpretation of the food metabolome profiles is the incompleteness of existing databases with regard to phytochemical metabolites.

As part of the ANR PhenoMeNep project, we have designed an online database called PhytoHUB, dedicated to the study of the phytochemical part of the “food metabolome”. The database will contain all phytochemicals present in edible plants and their known metabolites manually extracted from the literature. Since the metabolism of many phytochemicals has not been studied in humans, a list of predicted metabolites will be generated from expert knowledge of the metabolism of each phytochemical class and and analysis of precursor functional groups on precursor phytochemicals. Mass spectral data will be included from various sources: literature, other databases on plant phytochemicals and experimental data from our collaborative platforms.

Built with MySQL and Perl processing chains, an efficient relational design will underpin a powerful and intuitive web interface. For a queried monoisotopic mass or molecular formula, the database will return a list of possible metabolites, along with their physic-chemical properties, spectral data and possible dietary precursors linked to food sources. For a queried food, it will return a list of metabolites likely to be present in biofluids after consumption.

PhytoHUB will be the first publicly accessible database to collate information on phytochemical metabolites from a metabolomics standpoint, and should facilitate identification of unknowns in non-targeted profiling. A first version of the database is planned for 2013.

ANR Phenomenep ALIA-2010-007 / Conseil Regional Auvergne-FEDER post-doc grant (YF)