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## **PhytoHUB :a new knowledge database on dietary phytochemicals and their human metabolites**

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**Title:** PHYTOHUB: A NEW KNOWLEDGE DATABASE ON DIETARY PHYTOCHEMICALS AND THEIR HUMAN METABOLITES

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**Abstract:** 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 a new database tailored to the study of the phytochemical component of the food metabolome. The database will be an inventory of dietary phytochemicals and their known metabolites described in the literature. It will also include the most likely metabolites predicted *in-silico* for these dietary phytochemicals. 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 elemental formula, the database will return a list of possible metabolites, with their physicochemical 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 its consumption. PhytoHUB will be the first database publicly accessible to collate information on phytochemical metabolites from a metabolomics standpoint, and should improve the identification of discriminant ions in non-targeted profiling.

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