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

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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.

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