DATABASE FOR PHYTOCHEMICALS DETECTION IN MARS

File name: db_PHYTO_240531
Number of compounds: 29,750
Classification: 10 main classes and 70 sub-classes
Number of MS/MS spectra: 10,826
Type of MS/MS spectra: rule-based fragmentation (virtual)

Details: The database contains the structure, formula, exact mass, MS1 of 29,750 phytochemicals and 10,826 MS2 information. The dataset of 29,750 phytochemicals was collected from four databases (KEGG, LipidMaps, HMDB, and PhenolExplorer) and classified into 10 main classes and 70 subclasses.
The MS2 rule-based fragmentation was applied to different subclasses of phytochemicals. In particular, it has been adopted for the classes of flavonoids, alkaloids and Phenolic acids and derivates.

Nomenclature assignation: an identification code (ID) consisting of an alphanumeric string of four and different number is assigned to each phytochemical in the database. In addition, a common name is associated to each compound based on the common nomenclature used on KEGG, LipidMaps, HMDB, and PhenolExplorer databases.

Fragmentation rules: fragmentation rules were coded from experimental fragmentation of phytochemicals collected from literature[1-17] and from *in-house* acquired data.

References

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