M-IOLITE

An integrated software suite for streamlining GC-MS metabolomic data analysis *(http://miolite2.iceht.forth.gr)*

M-IOLITE is a software suite for streamlining GC-MS metabolomic data analysis, developed by the Metabolic Engineering & Systems Biology Laboratory (MESBL), FORTH/ICE-HT, Patras, Greece and supported by ELIXIR-GR structural funds.

It comprises:

a) a standardized GC-MS metabolomic profile repository based on a validated metabolite derivative peak library of >900 peaks;

b) a module for specialized GC-MS metabolomic data validation, normalization and filtering;

c) a module for unknown metabolite peak identification, based on the MESBL peak library, reconstructed metabolic networks of model organisms, meta-analysis of the M-IOLITE data repository and pattern recognition analysis methods.

M-IOLITE is available as an executable file, freely provided to academic users.

Standardized GC-MS metabolic profile repository based on validated metabolite peak library

From the M-IOLITE initial window (Fig. 1), the user can select to upload his/her raw or normalized GC-MS metabolic profile based on a standardized template , along with details about the experimental design, biological system and profiling method used (Fig. 2). During uploading, the user is questioned for first encountered metabolite peak names, given the option to select from expected names (in case of typos) or introduce new unknown peaks tothe MESBL peak library, stored initially as "unreviewed".

The MESBL metabolite peak library comprises (Fig.3):

(a) an in-house peak dataset of >900 peaks (429 reviewed) collected from runs of standard compounds and multiple experiments in various systems, based on the metabolite-centric profile analysis of 6 different analysts, and annotated using commercial and publicly available metabolite peak databases , extended by

(b) a revised and appropriately filtered by our group version of the public GOLM peak dataset (http://gmd.mpimp- golm.mpg.de/).

Fig. 1 : M-IOLITE initial window

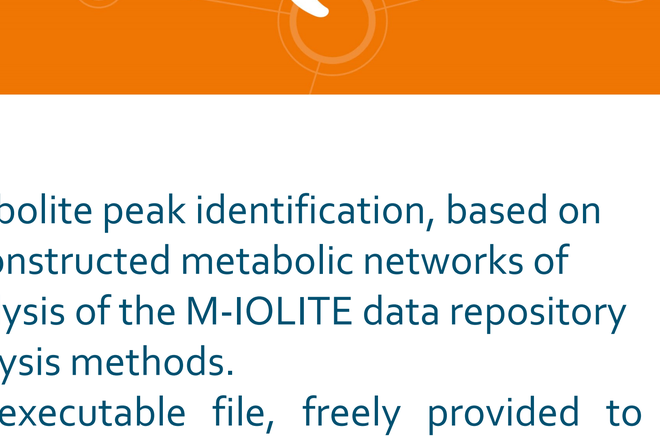

Fig. 2 : The metabolic profile dataset uploading page

Specialized GC-MS metabolomic data validation, normalization & filtering methods

M-IOLITE employs specialized GC-MS metabolic profile dataset validation (QC), normalization & filtering methods (Fig.4), developed by our group (Kanani & Klapa (2007) *Metab. Eng*. 9:39-51; Kanani et. al. (2008). *J Chromatogr. B* 871: 191-201; Papadimitropoulos et. al. (2018) *Methods Mol. Biol.* 1738: 133-147). It is noted that the employed QC method is the only available that does not require the availability of QC samples and can be applied *a posteriori* given the availability of at least three technical replicates for some samples. The user can subsequently upload the normalized dataset to the M-IOLITE profile repository.

The position of the known metabolites in a profile dataset within the KEGG-annotated metabolic network of the selected organism can be visualized in KEGG Atlas. Moreover, the user can get directly connected to the TM4/MeV omic data analysis software (http://mev.tm4.org) and use the normalized profile dataset in its stored format for further multivariate statistical analysis.

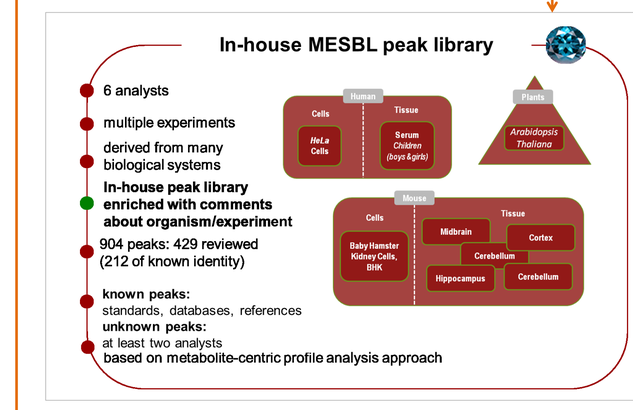

Fig. 3 : The MESBL metabolite peak library.

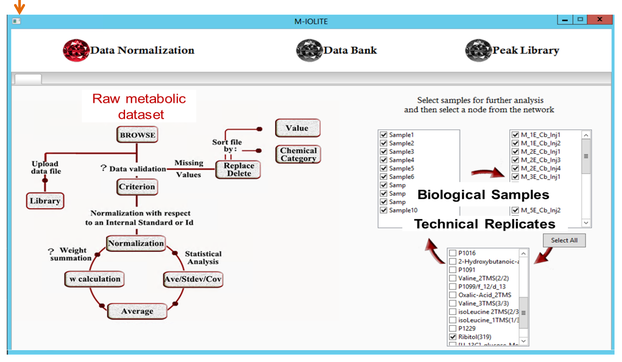

Fig. 4 : The M-IOLITE data normalization module window.

Unknown metabolite identification module based on profile pattern recognition and network analysis

M-IOLITE contains a module for unknown metabolite peak identification, based on the educated integration of information from the extended MESBL metabolite peak library, reconstructed metabolic networks of model organisms, meta-analysis of the M-IOLITE data repository and pattern recognition analysis methods (Fig. 5). Currently, the reconstructed metabolic network in human (https://vmh.uni.lutia) is added, the incorporation of additional model organisms is ongoing. The optimization of this module is part of the ELIXIR metabolomics case-study.

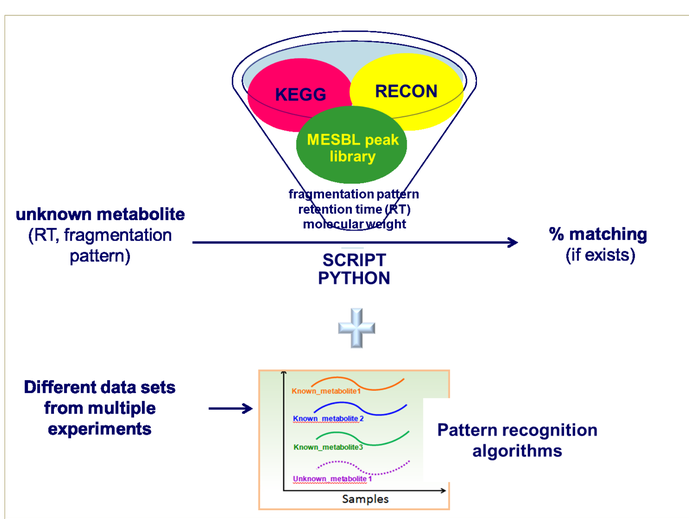

Fig. 5 : The workflow of the unknown metabolite identification module in M-IOLITE.

Contact

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https://bio.tools/M-IOLITE