M-IOLITE: An integrated suite for the streamlining of metabolomic analysis

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ABSTRACT

The mass spectrometry (MS) metabolomics workflow is a multistep procedure involving analytical and computational parts [2]. As the metabolomic analysis application is expanding to various biological systems and contexts, there is a need for standardized data repositories for all types of biological samples. Moreover, MS analysis being producing a vast amount of unidentified compound data, there is a need for unknown peak identification methods. The computational steps of the MS metabolomic workflow include data normalization, validation and filtering methods, while it is imperative that the acquired metabolic profiles are studied in the context of metabolic network structure and regulation. In the case of Gas Chromatography(GC)-MS metabolomics, the additional metabolite extract derivatization step introduces needs for specialized normalization and data validation methods [1-2]. In this context, there is a need for the development of software suites that can assist the user to safely deposit the metabolomic data in a standardized way and then carry out all the normalization, analysis and network reconstruction processes. The currently publicly available software suites cover either the repository or the data analysis capabilities. Especially, for GC-MS metabolomic data, there is currently no suite incorporating the specialized normalization methods or integrating metabolic network analysis into data interpretation and peak identification.

We are developing a software suite, named M-IOLITE, for streamlining GC-MS metabolomic data analysis, integrating (a) the capabilities of a standardized repository, (b) specialized normalization and filtering methods and (c) metabolic network analysis for data interpretation and unknown peak identification. A beta version of the software comprising the first two capabilities is ready and expected to become available for academic use by the end of the year. We are currently working on connecting the suite with registered reconstructed metabolic networks of model organisms (eg Recon 1-2 for human) to provide the additional capability of an educated interpretation of the metabolomic data and unknown peak identification through pattern recognition analysis with respect to the expected topology of the metabolic networks.

REFERENCES

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