FlashNote

Metabolomics workflows? Sustainability please!

Non-targeted data processing in metabolomics is a time consuming task. It is often unavoidable to find yourself lost in a forest of peaks, wondering what is important – and more critically how you can find it. Eventually, a more effective workflow with tools like statistical treatment, annotation, and data base interrogation can be established – which can be quite a relief. So when a beloved tool of your pipeline gets withdrawn or discontinued, it can be a serious setback. Thankfully, with Bruker's MetaboScape® software, you get the best of both worlds: Open source flexibility and trusted sustainability!

Challenge

The metabolomics research community has developed a rich landscape of tools to tackle a particularly diverse set of challenges within the field, extending from raw data to biological interpretation. Unfortunately, not all of these tools will receive long-term support and often become unavailable or otherwise obsolete. Therefore, it can be a considerable risk to rely on these tools within your workflow. Sustained support of all tools within your data processing workflow is paramount.

Solution

MetaboScape offers a sustainable pipeline, regularly updated and enriched by community feedback from users like you. Our quick development cycle ensures we are always at the cutting edge of the analytical techniques used for data acquisition and analysis.

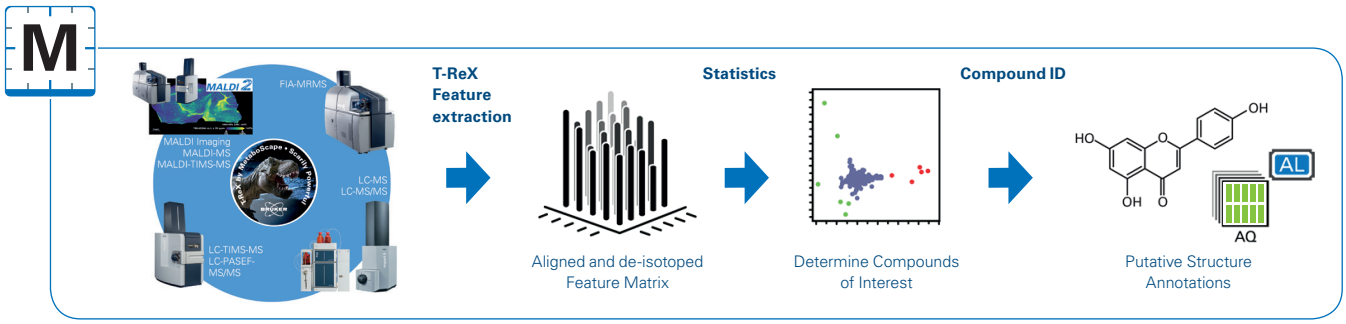
MetaboScape, the sustainable all-in-one package

MetaboScape provides a complete set of tools to help you tackle large datasets containing a huge number of metabolites in large sample cohorts. Identifying biologically relevant metabolites is greatly enhanced by the statistical pipelines, annotation tools, and pathway mapping offered in this unique software. Bruker is committed to maintaining support for these implemented open source tools, while also extending export/import functionalities to external tools developed by the research community – the best of both worlds. Open source flexibility and trusted sustainability!

Dr. Dimitri Heintz, *Institut de biologie moléculaire des plantes, CNRS, Strasbourg, France:*

"One of the things we like very much with MetaboScape is the fact that we have a software not dependent inherently on websites or open source tools. Once we developed a pipeline using an open source program and few weeks after it was not available anymore. For us, this meant time and effort was lost and we had to go back to the starting line! As we are "at the service" of research teams and even industrial collaborators, we have to be sure that a developed processing pipeline will be sustainable."

Authors: Claire Villette[1], Aiko Barsch[2], Dimitri Heintz[1]; [1] Institut de biologie moléculaire des plantes, CNRS, Strasbourg, France; [2] Bruker Daltonik, Bremen.



Claire Villette, Institut de biologie moléculaire des plantes, CNRS, Strasbourg, France:

"The necessary tools for non-targeted data processing are contained in MetaboScape.

The ease-of-use graphical interface allows even novice users to process metabolomics datasets.

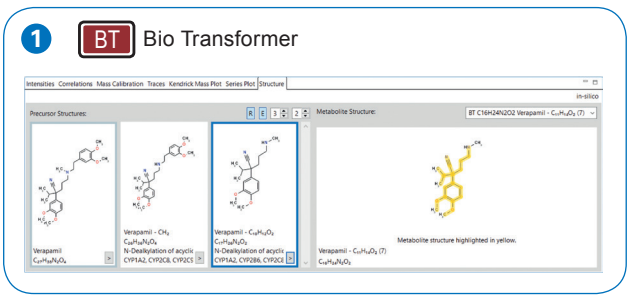
No need for advanced bioinformatics skills, command-lines and source-coding, every tool is available from a click, and processing parameters are still accessible to the user.

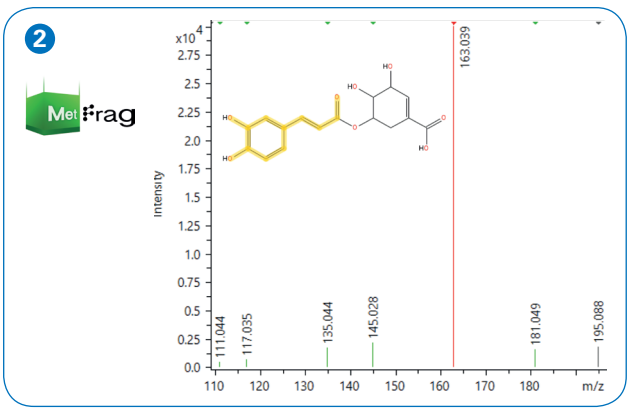
This complete set of tools brings rapidity and efficiency in data processing by also providing support for open source tools such as:

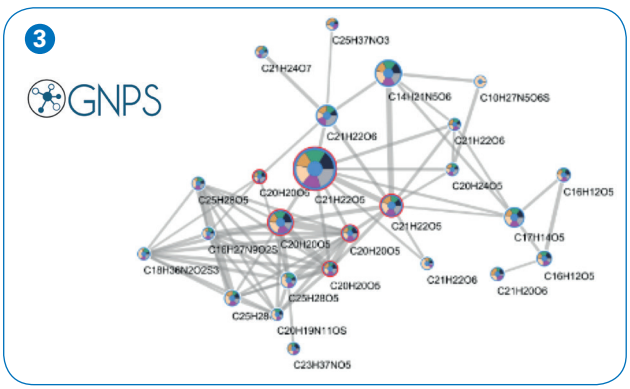
① Support for annotation using BioTransformer [1] to determine possible predicted metabolites biotransformations.

② Implemented MetFrag [2] functionality in MetaboScape helps choosing the most likely metabolite candidate based on *in-silico* fragmentation.

③ Dedicated file exports, e.g. to GNPS [3] for feature based molecular network analysis, helps interpreting the relevant biological information."







Disclaimer: BioTransformer, MetFrag and GNPS are no Bruker products and restrictions to utilize these software tools might apply.

References

[1] Djoumbou FY, et al. (2019). Journal of Cheminformatics, **11**:2 DOI: 10.1186/s13321-018-0324-5

[2] Wolf S, et al. (2010). BMC Bioinformatics, 201011:148. DOI:10.1186/1471-2105-11-148

[3] Nothias LF, et al. (2020). Nature Methods, **17**:905-908. DOI:10.1038/s41592-020-0933-6

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