FlashNote

Look Out! T-ReX 3D will simplify your metabolomics data processing!

In discovery metabolomics research, the ultimate goal is to quickly pinpoint and confidently identify differentially expressed metabolites in large cohorts of complex samples. Automated workflows are required in order to execute all data processing tasks efficiently. Bruker's MetaboScape 3.0 software features T-ReX 3D, a powerful, easy to use algorithm which quickly and reliably conducts all steps of data pre-processing.

Challenge

The initial data processing in discovery metabolomics workflows establishes the basis for all subsequent statistical calculations, as well for all compound identifications. Therefore, it is absolutely necessary that this data pre-processing is reproducible and robust. Problems can arise from incorrectly merged molecular features or missing values in the calculated bucket table. Such a distortion may lead to "false" results as well as incorrect identifications.

Solution

T-ReX 3D is an innovative feature extraction algorithm which is implemented in the recently released MetaboScape 3.0. It uses a sophisticated adduct handling and ensures a robust and region complete feature extraction. All compound-relevant information from large cohorts of complex samples is extracted, automatically. The T-ReX algorithm is optimized for speed, crunching through loads of data in a matter of minutes.

Look out!

T-ReX 3D will simplify your data processing to such a degree that you might even forget how complex your data is!

Dr. Mario E. Gomez Hernandez
Associate Director, Advanced Mass Spectrometry Facility. Florida International University

"MetaboScape is an impressive tool. It is extremely powerful to run through large data sets with replicates in a fraction of the time compared to our previous workflow. In addition, the annotation capabilities provided by SmartFormula and supporting custom made lists with target compounds is extremely useful and a personal favorite. […] With MetaboScape, I have been able to not only identify target compounds in a large set of samples, but also run the statistics applying the PCA and PLS models for different preparative conditions. For this particular set of samples, the PCA model has generated the best results showing the specific variations of target lipids according to specimen type and conditions."

Authors: Ulrike Schweiger-Hufnagel, Aiko Barsch, Sven Meyer / Bruker Daltonik, Bremen

❶ Mass calibration

A good mass calibration is the absolute prerequisite for correct identification of compounds. MetaboScape uses a parameter-free algorithm for convenient and reliable mass recalibration.

❷ Retention time alignment

The non-linear retention time alignment is absolutely parameter-free. It compensates for shifts that can occur when measuring large sample cohorts.

❸ Adduct handling

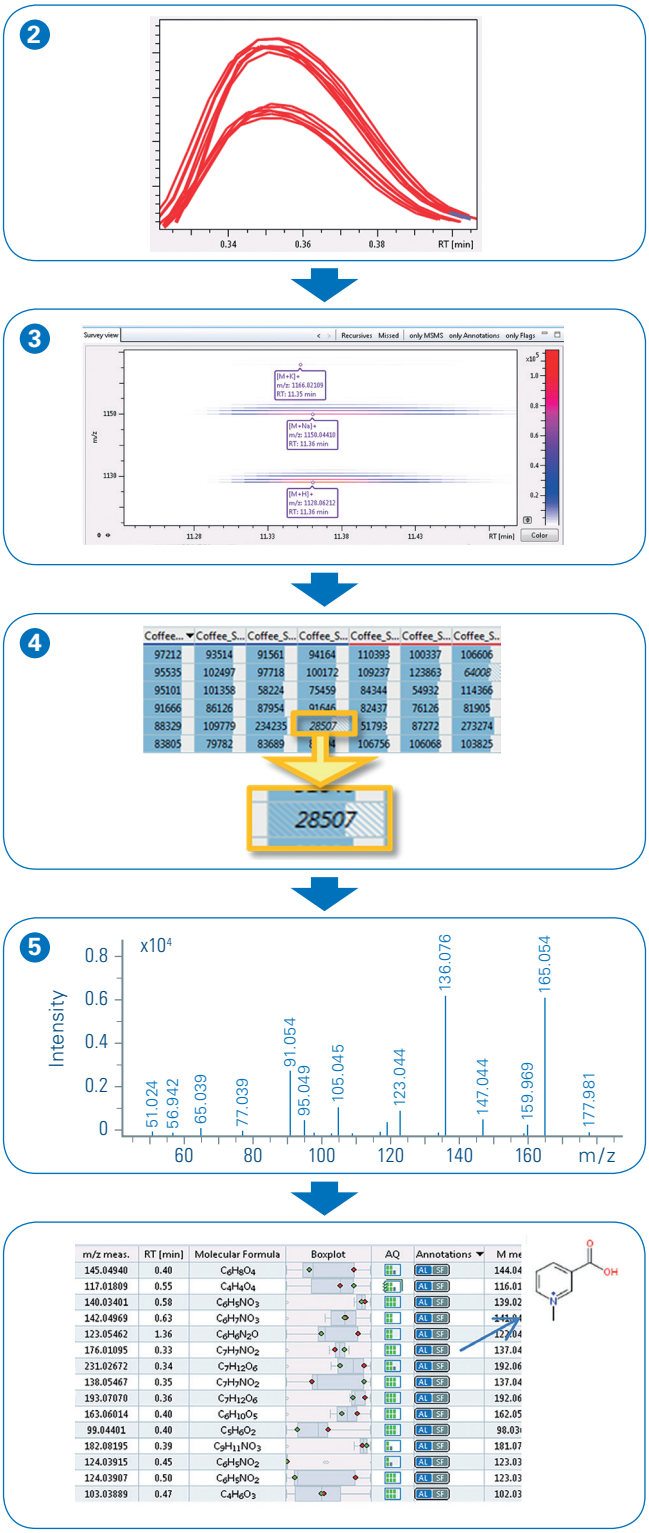
Peaks from adducts, fragments and other charge states are combined into one bucket. This reduces the multiple appearance of the same compound in a bucket table, significantly simplifying subsequent statistical calculations.

❹ Feature Extraction

The region complete feature extraction uses a recursive approach in the event that some features are not detected in all samples, e.g. due to fluctuations in intensity. This improves the robustness of the bucketing process and thus of the statistical results. All cells with shaded backgrounds in the bucket table (right) were determined by region complete bucketing.

❺ MS/MS spectra

MS/MS spectra are automatically connected to the respective buckets. This increases confidence in identification results made via spectral library searches or validated with *in-silico* generated fragment spectra.



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