nature portfolio

https://doi.org/10.1038/s41596-022-00710-w

Supplementary information

Using MetaboAnalyst 5.0 for LC–HRMS spectra processing, multi-omics integration and covariate adjustment of global metabolomics data

In the format provided by the authors and unedited

Supplementary Materials

Using MetaboAnalyst 5.0 for LC-HRMS spectra processing, multi-omics integration and covariate adjustment of global metabolomics data

[1]Zhiqiang Pang, [1]Guangyan Zhou, [2]Jessica Ewald, [3]Le Chang, [1]Orcun Hacariz, [2]Niladri Basu, [1,3*]Jianguo Xia

[1]Institute of Parasitology, McGill University, Montreal, Quebec, Canada

[2]Department of Natural Resources Sciences, McGill University, Montreal, Quebec, Canada

[3]Department of Human Genetics, McGill University, Montreal, Quebec, Canada

*Correspondence:

Tel: 1-514-398-8668

Email: jeff.xia@mcgill.ca

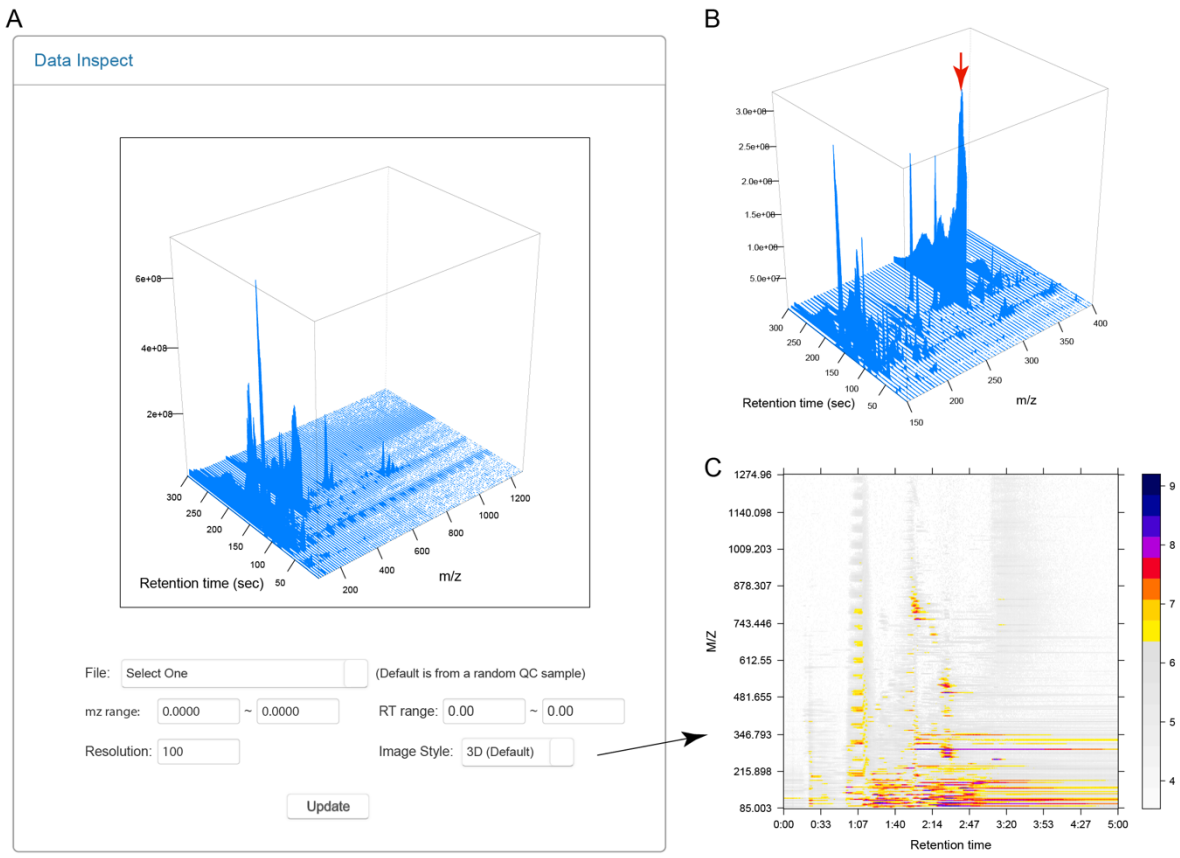

Figure S1 | Global raw spectra inspection. (**A**) A screenshot of 'Spectral Inspection' dialog. User could view the global spectra of sample 'QC_001.mzML' in a 3D view. Different files and view range from RT and m/z dimension can be easily updated. The default resolution is 100, which can be higher to over 1,000 to view every single detail. (**B**) A zoom-in view of m/z range (150~400). There is at least one potential contaminants peak (marked by the red arrow), which is quite intensive and persists over half of the entire chromatogram. Therefore, it is recommended to enable the 'Contaminants Removal' option. (**C**) An example of the data in 2D heatmap view.

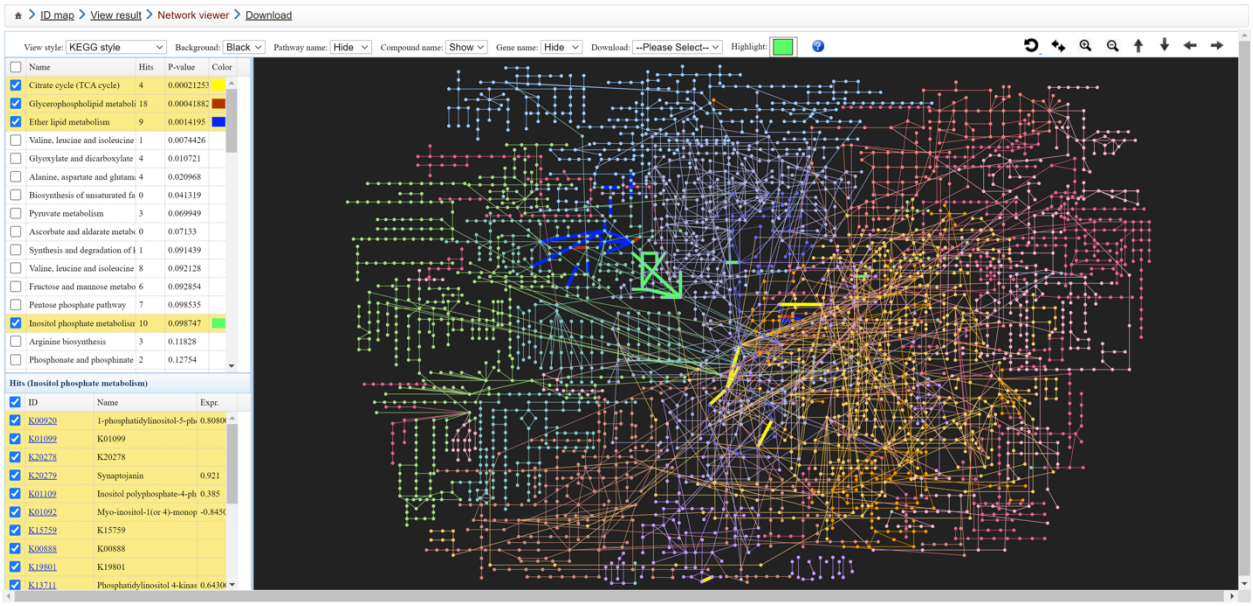

Figure S2 | Network view of the integrated pathways. There are four pathways have been highlighted in the network. The details of the pathways are displayed from the right side.

Table S1. Key parameters for peak picking, alignment and annotation

Steps	Parameters	Explanations and guidance
Peak Picking	Peak Width	Peak width values in second, include minimum value and maximum value.
	ppm	Tolerated mass deviation in one part per million (ppm). Empirically, a value between 2~5 is recommended for orbitrap, but 15~30 is commonly used for Time-of-Flight (TOF).
	mzdiff	Minimum m/z value for peaks with overlapping retention time
	snthresh	Signal-to-noise threshold, default is 10.
	noise	Noise level for filtration, default is 1,000. The higher of the value, the less features will be detected.
	prefilter	Scan filter to discard peaks less than minimum scan number (prefilter) or abundance (value_of_prefilter).
	fwhm	Full-width at half-maximum, default is 30. This parameter is only used for Matched Filter algorithm.
Peak Alignment	Method	Algorithms to perform retention time correction, including LOESS and Obiwarp.
	Bandwidth	Bandwidth of Gaussian smooth kernel. For Q-exactive orbitrap, the recommended value is 2~5, while for TOF, 5~15 is preferred.
	MinFraction	Minimum fraction of samples to be grouped. A value larger than 0.5 is recommended to ensure the quality of features.
	minSamples	Minimum number of samples for grouping as a peak to present. Default is 1.
	maxFeatures	maximum number of peaks to be defined in one m/z slice for peak grouping. Default is 100.
Peak Annotation	Polarity	To specify the ion mode of mass spectrometer when doing the acquisition. 'Positive' and 'Negative' are provided for selection
	Adducts	Potential adducts are highly related with chromatographic conditions. User could manually define the adducts' annotation rule or use the standard option by default.
	Perc_fwhm	Percentage of '*fwhm'*. This parameter defines the boundaries to group features as one group for annotation.
	Mz_abs_iso	Allowed variance of mass for isotopes searching.
	Max_charge	Maximum charge of isotopes
	Max_iso	Maximum number of isotopes.
	Corr_eic_th	Correlation threshold value for EIC correlation.
	Mz_abs_add	Allowed variance of mass for adducts searching.