Electronic Supplementary Material (ESI) for Molecular Omics.

Supplementary Information for "MetaboKit: a comprehensive data extraction tool for untargeted metabolomics"

Pradeep Narayanaswamy[1,*], Guoshou Teo[2,*], Jin Rong Ow[3], Adam Lau[4], Philipp Kaldis[3,5], Stephen Tate[4], Hyungwon Choi[2,3,#]

Affiliations

1. Sciex, R&D, Singapore
2. Department of Medicine, Yong Loo Lin School of Medicine, National University of Singapore, Singapore
3. Institute of Molecular and Cell Biology, A*STAR, Singapore
4. Sciex, Concord, Canada
5. Department of Clinical Sciences, Lund University, Sweden

*These authors contributed equally to this work.

#e-mail: hyung_won_choi@nus.edu.sg

Supplementary Table 1.

List of 86 metabolite standards (out of 91) with annotation from single compound injection analyses. For identification results in MS-DIAL and XCMSonline, we included identifications without MS/MS matching for both parent ions and ISFs.

Supplementary Table 2.

Evaluation of sensitivity of compound identification from DDA analysis of 91 metabolite standard mixture (positive and negative ion modes). The table also includes the original identification reports from all software packages in comparison. XCMSonline did not return any output for the negative mode analysis.

Supplementary Table 3.

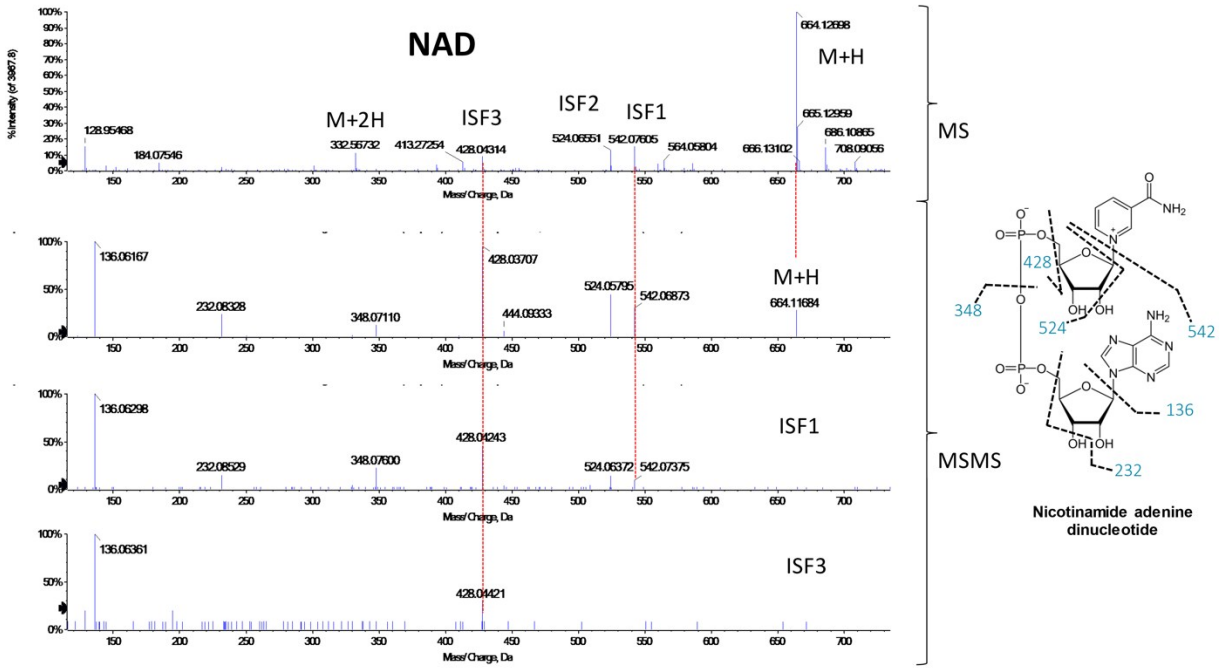
DDA analysis output files for mouse liver samples. Each sample was analyzed four times: two extraction methods (aqueous fraction and organic fraction) in positive and negative ion modes. As such, there are four files for each software package.

Supplementary Table 4.

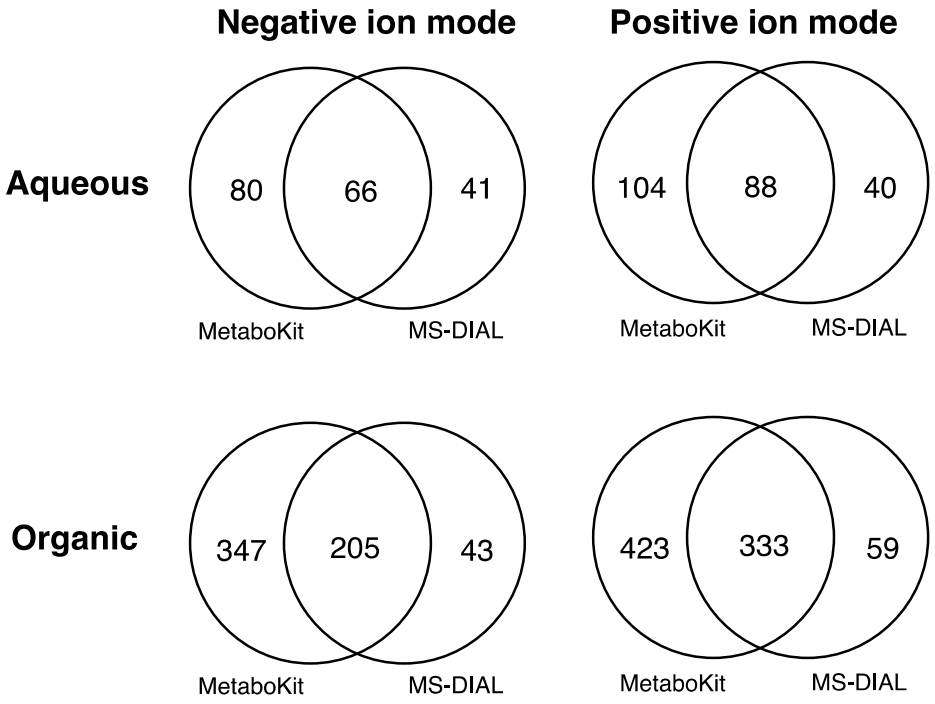
DIA analysis output files for the metabolite standard mix in a series of spike-in concentrations (positive and negative ion modes). The tabs with the suffix "_Quality" contains average abundance values and concentration-specific coefficients of variation. For MS2-level quantification, we applied the mapDIA software to derive a single value for each compound from its multiple product ions.

Supplementary Table 5.

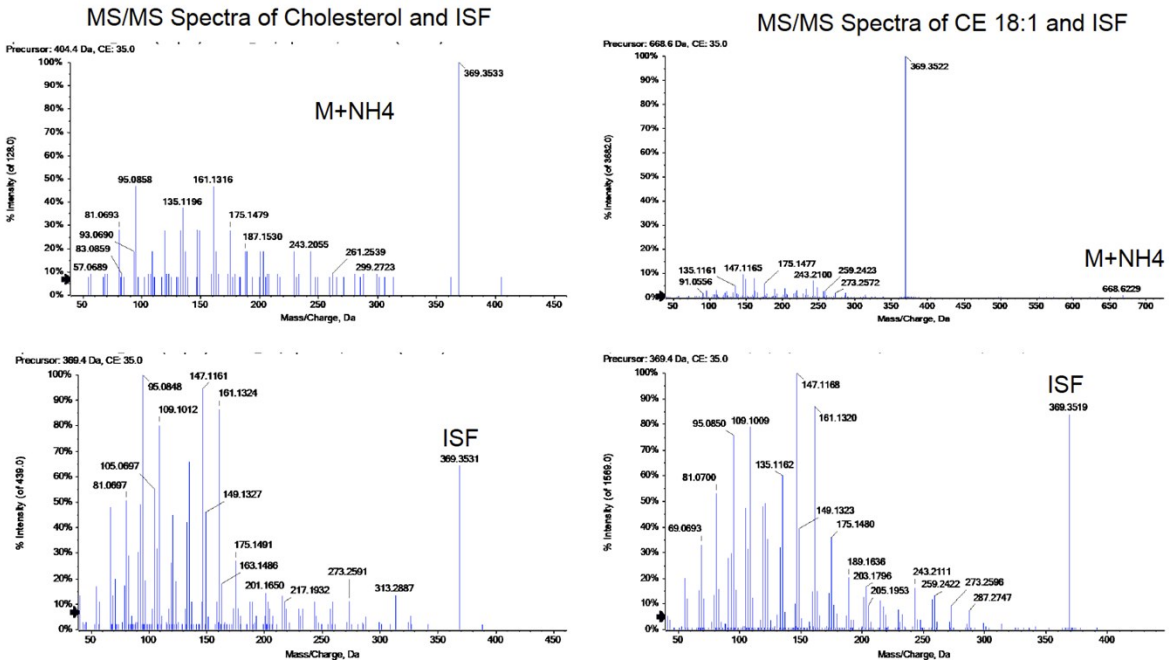
DIA analysis output files for mouse liver samples (aqueous and organic fractions in positive and negative ion modes). For MS2-level quantification, we applied the mapDIA software to derive a single value for each compound from its multiple product ions. The tabs with the suffix "_mapDIA" contains differential metabolite abundance analysis from the mapDIA software.



Supplementary Figure 1 | Comparison MS/MS spectra of NAD and its in-source fragments. The red dotted line marks the m/z of the ISF ions in the full scan where NAD was detected. All product ions of the parent ion [M+H] and two ISFs were aligned along the m/z axis.



Supplementary Figure 2 | Comparison of the metabolite identifications (per peak, with overlap in compound names from different fractions and ionization modes) in the DDA analysis between MetaboKit and MS-DIAL. The intersection of each Venn diagram was strictly limited to the exact same compound names only. Compound identifications without MS/MS evidence from MS-DIAL were excluded in the comparison.



Supplementary Figure 3 | Comparison of cholesterol and its ISF with water loss (left), and CE 18:1 and its ISF (right) in terms of MS/MS fragmentation. Top panel and bottom panels are product ion spectra of the parent compound and the corresponding ISF.