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Comparison of two metabolomics data processing approaches using a standard metabolomics reference material

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In order to capture the most complete profile of an organism's metabolic state, a combination of data acquisition and processing techniques are required. Targeted analysis may be used to accurately measure concentrations of important central metabolites, but in order to create a profile of biologically significant but less well-studied compounds, LC-MS analysis is required. LCMS instruments with accurate mass capability can profile these samples even if the target metabolites are not known in advance.

Such untargeted metabolomics requires the use of highly reproducible chromatography provided by HPLC or UHPLC pumps to provide sufficient data quality for successful statistical analysis. Tandem mass spectrometry is also required in order to identify metabolites of interest. Data processing software and data storage capability beyond what ordinary personal computers can conveniently provide is needed to establish an effective metabolomics workflow.

Many different data processing workflows for metabolomics have been suggested. In the present work, aspects of two complementary data processing workflows incorporating either XCMS Online or a proprietary feature picking and data alignment software in combination with the statistics program SIMCA-P were used. The NIST SRM 1950 Metabolites in Human Plasma certified reference material was used for the analysis in order to provide a common frame of reference with other studies. The results demonstrate that both techniques may be adequately used to process metabolomics data and that the choice of data processing workflow may depend on factors unique to each analysis. Several particular results from each data processing workflow are highlighted in detail.

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