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MASTR-Quant: An Open-Source Web-based Software Tool for the Quantitive Analysis of Mass Spectrometry-based Data

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Software

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Summary

Targeted analysis in mass spectrometry uses a calibration curve to derive the concentration of a substance, by comparison to a set of samples of known concentration. This is canonically done by a form of linear regression.

`MASTR-Quant` is an open-source, web application that allows users to calculate the concentration values of features in mass spectrometry data through visualizing and defining calibration curves based on a range of adjustable parameters. `MASTR-Quant` presents the user with options including and excluding data points to define linear or quadratic calibration ranges. The tool also includes options to assign individual internal standards to specific analytes by applying weighting factors, background subtraction and dilution ratios, normalization of the data based on internal standards and other external measurements, and the option for assessing the quality of data through the calculation of coefficient of variation values of each sample group. The final output is downloadable as an Excel file with multiple sheets containing detailed results of the individual steps involved in the calculation process.

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