

# MSI QUANTIFY: A MICROAPP FOR THE AUTOMATED PROCESSING OF QUANTITATIVE MASS SPECTROMETRY IMAGING DATA

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## INTRODUCTION

Material quantification in mass spectrometry imaging (MSI) is a challenge in the analysis of complex mixtures due to ionization-efficiency variations, matrix effects, and the lack of appropriate standards. Typical quantitative experiments involve spotting a series of known amounts of a compound of interest on tissue. A calibration curve is then constructed from these regions, mapping the signal intensity of the mass of interest to the concentration of the drug. A new micro-app called MSI Quantify is presented which provides tools to assist in the data-processing workflow associated with these experiments, including image visualization, region selection, calibration curve fitting and error estimation.

## HIGHLIGHTS

- Compatible with Waters™ MassLynx™ RAW files or custom .csv text files from processed data containing (x,y) coordinates and m/z intensities
- Load dilution series and dosed tissue data together in a single project
- Use interactive drawing tools to define regions of interest (ROI)
- Generate calibration curves from the dilution data including normalization with applied or internal standards
- Apply the calibration curves to additional regions within dosed tissue data to predict new dose

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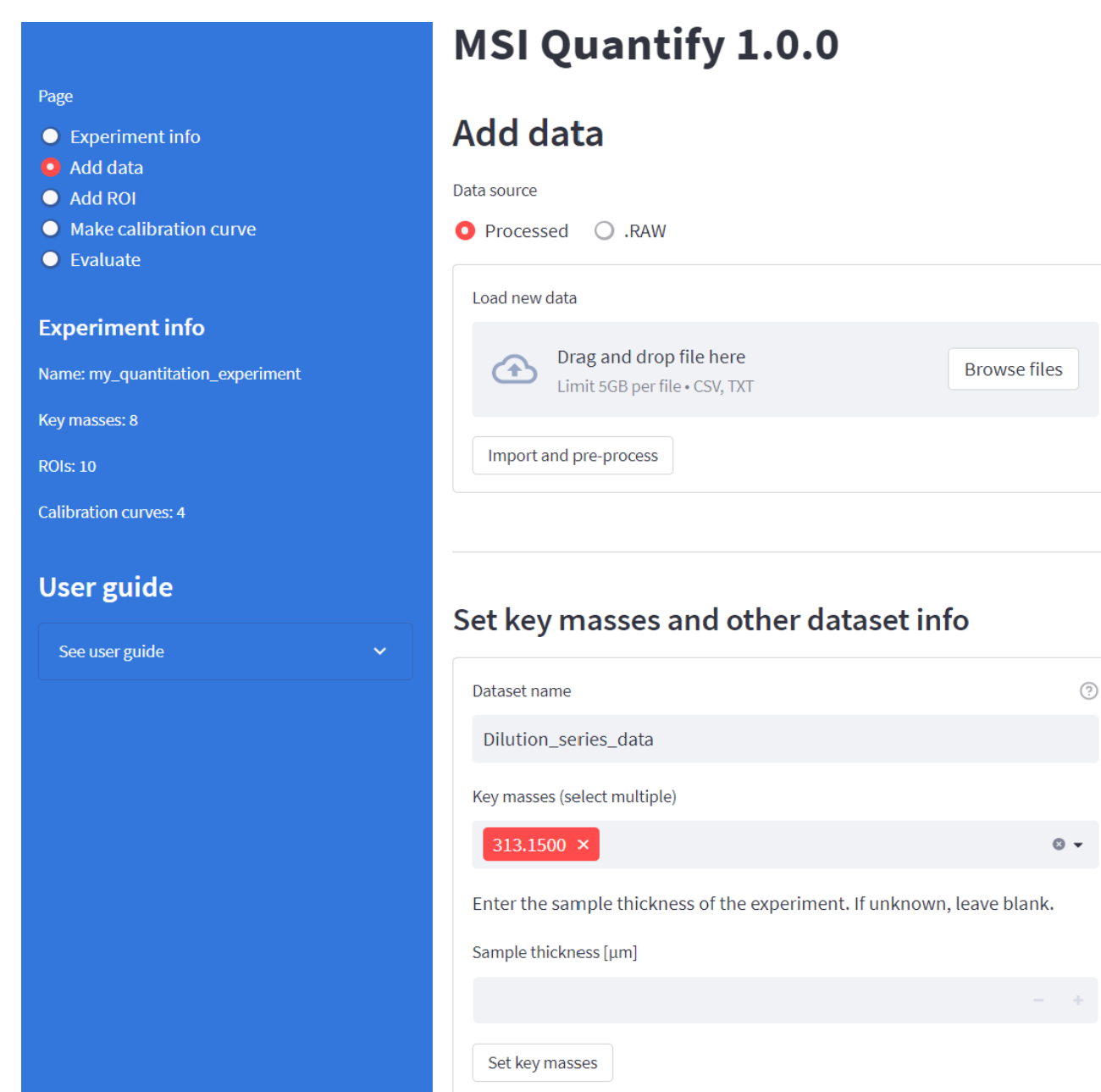


Figure 1. App layout and data import page with form for loading pre-processed text data.

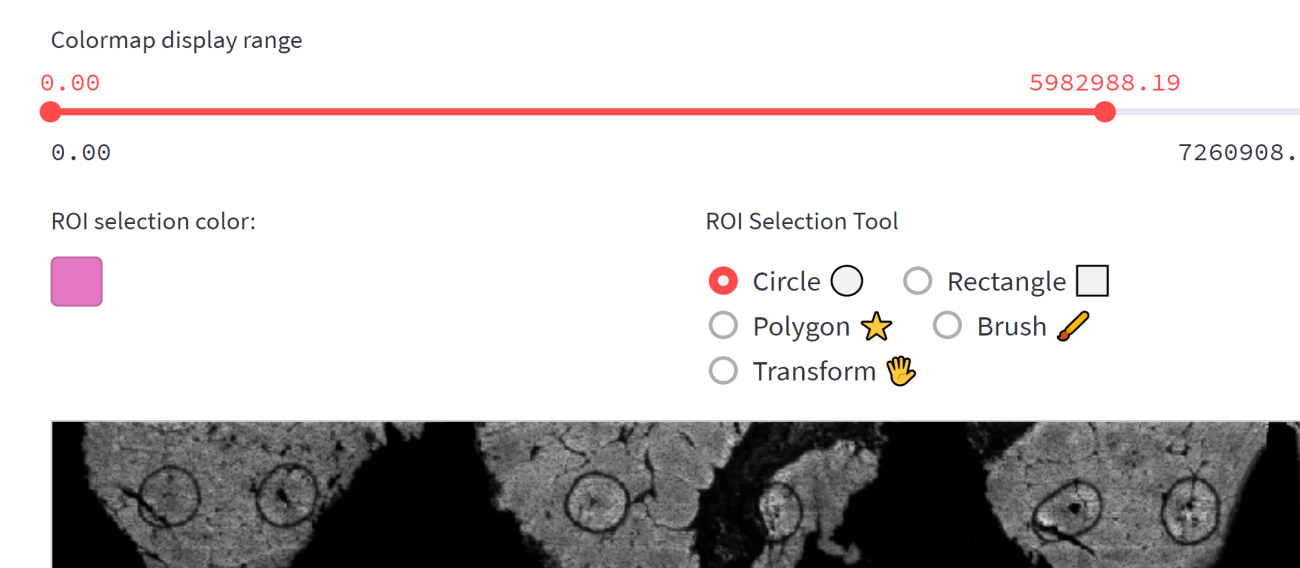


Figure 2. Interactive drawing tools to define regions of interest for dilution series or areas within dosed tissue.

## RESULTS



Figure 3. (Top) Visualization of regions of interest from dilution series. (Middle) Input form for custom labels, dose quantities, and units. (Bottom) Resulting calibration curve with associated confidence interval.

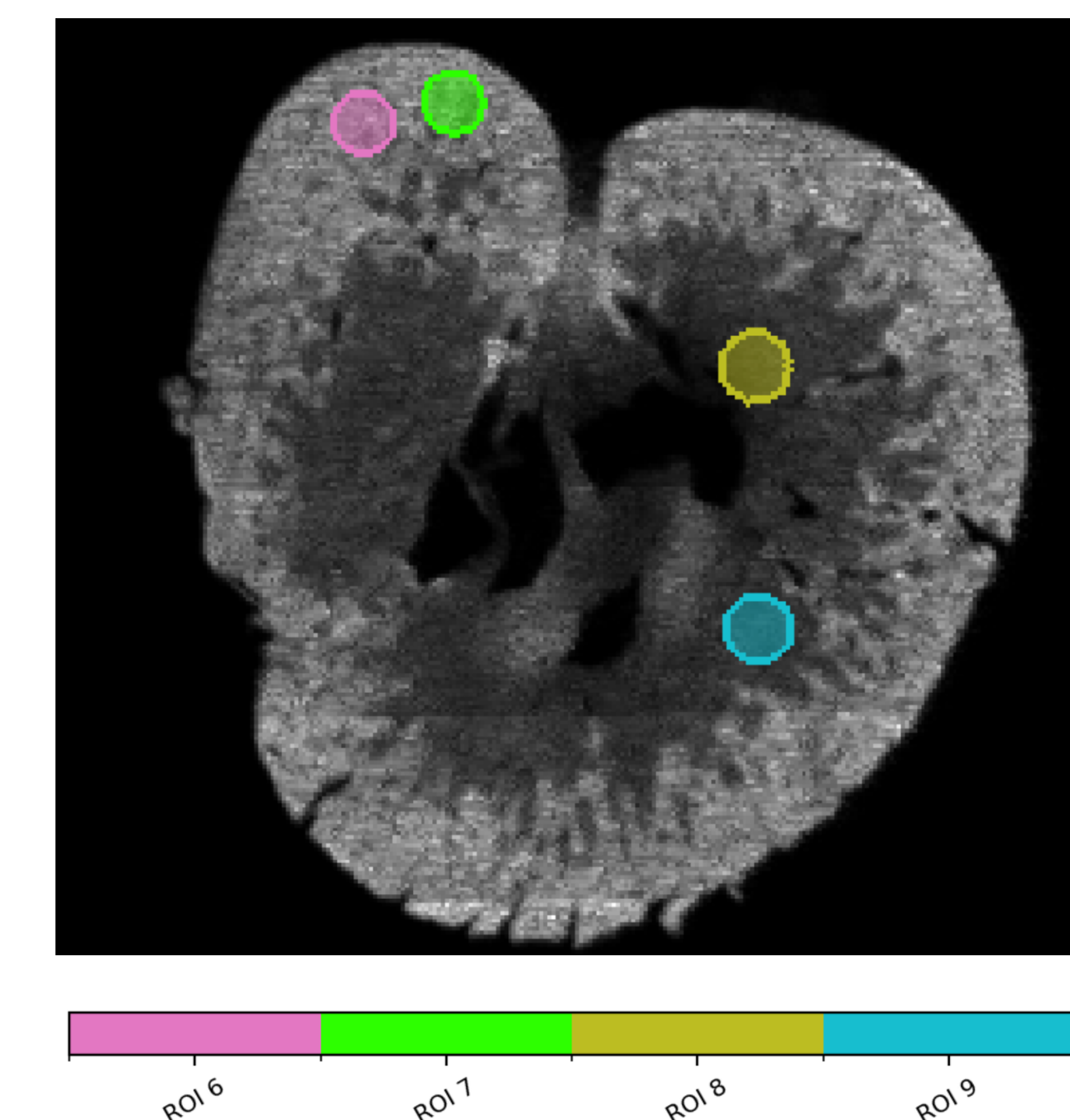


Figure 4. (Top) Visualization of regions of interest defined on a dosed mouse kidney sample. (Bottom) Predicted dose with confidence interval for each region using the calibration curve.

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