

A Complete Wine Analysis Using Multiplets Detection

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Introduction

qNMR is the “gold standard” for compound quantification and has wide application. The quantitative analysis of mixtures poses special challenges.

The routine quantitation of wine components – wine-omics - has tremendous benefit for safety and Quality Assurance.

We can identify relevant components, such as:

- ethanol content → *labelling*
- methanol content → *limited by law*
- benzoic acid, diethylene glycol → *forbidden substances*
- acetic acid at elevated levels → *unwanted smells or tastes*
- shikimic acid, proline → *grape variety discrimination and ripeness*

We show a *visual description* of the practical use and utility of this technology as applied in a validated NMR analysis of wine components.

SMA basics

The core Mnova functionality is used together with an advanced plug-in, SMA (Simple Mixtures Analysis).

GSD quickly deconvolutes all peaks

A compound is represented by a Multiplet area in a spectral region

The user defines a formula that converts the area to concentration

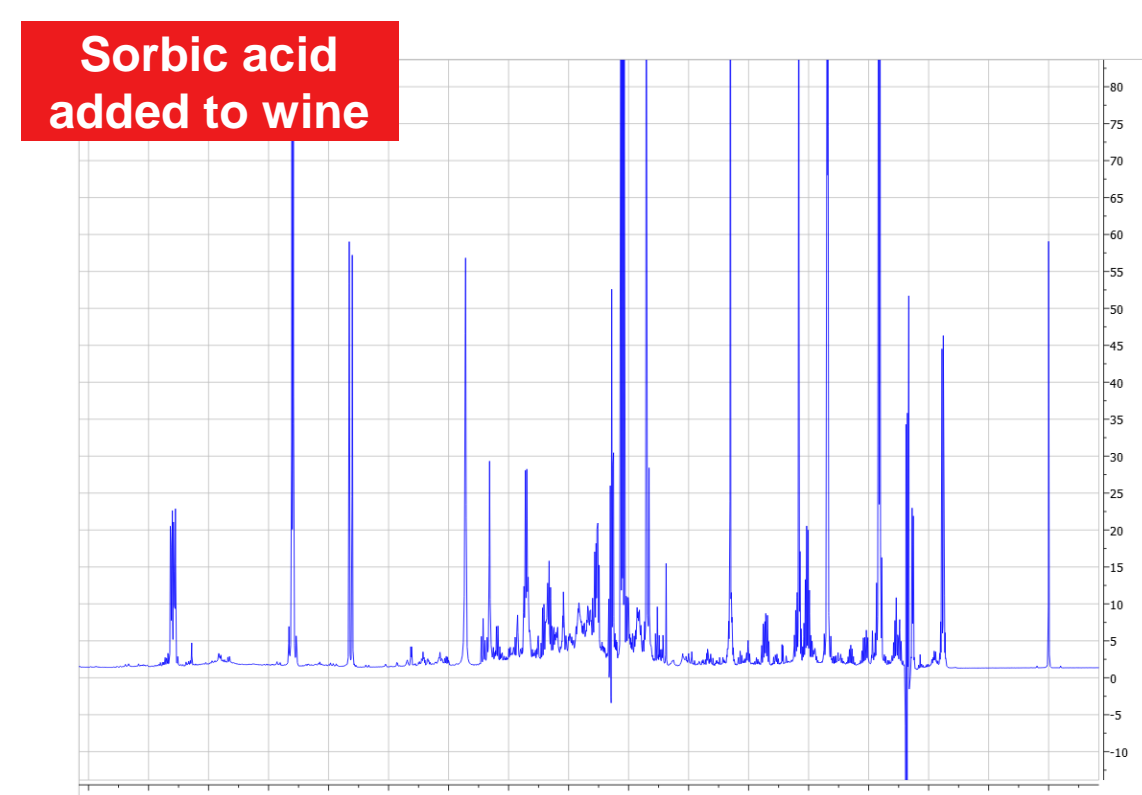
Errors in multiplet detection are flagged, allowing the user to correct them by hand and quickly redo the calculation

For higher throughput the analysis can be performed in batch mode, or as the data are produced by the NMR spectrometer

Poster #21

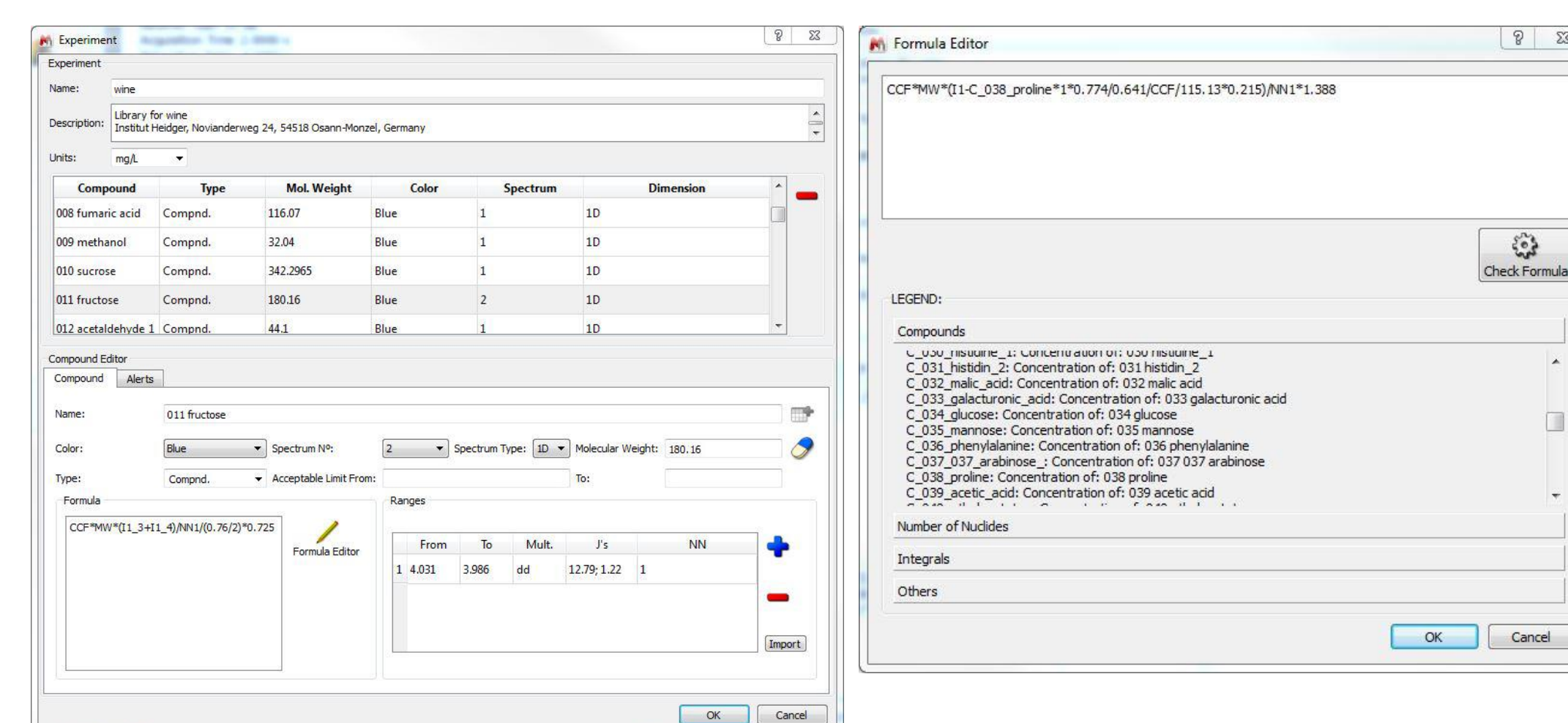
Using Mnova Simple Mixtures Analysis (SMA), more than 50 components of wine can be routinely quantified in an analysis, and ca 50 analyses performed per day by an analyst

Basic setup- validation

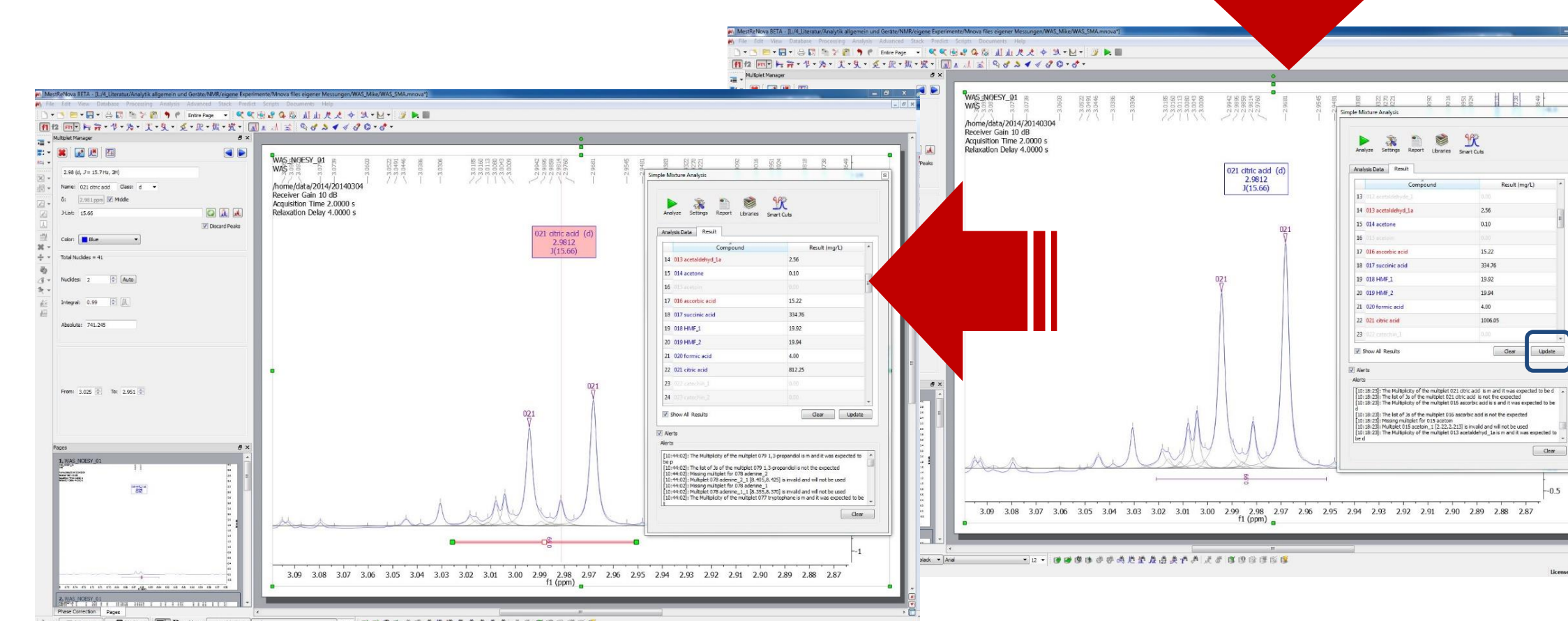
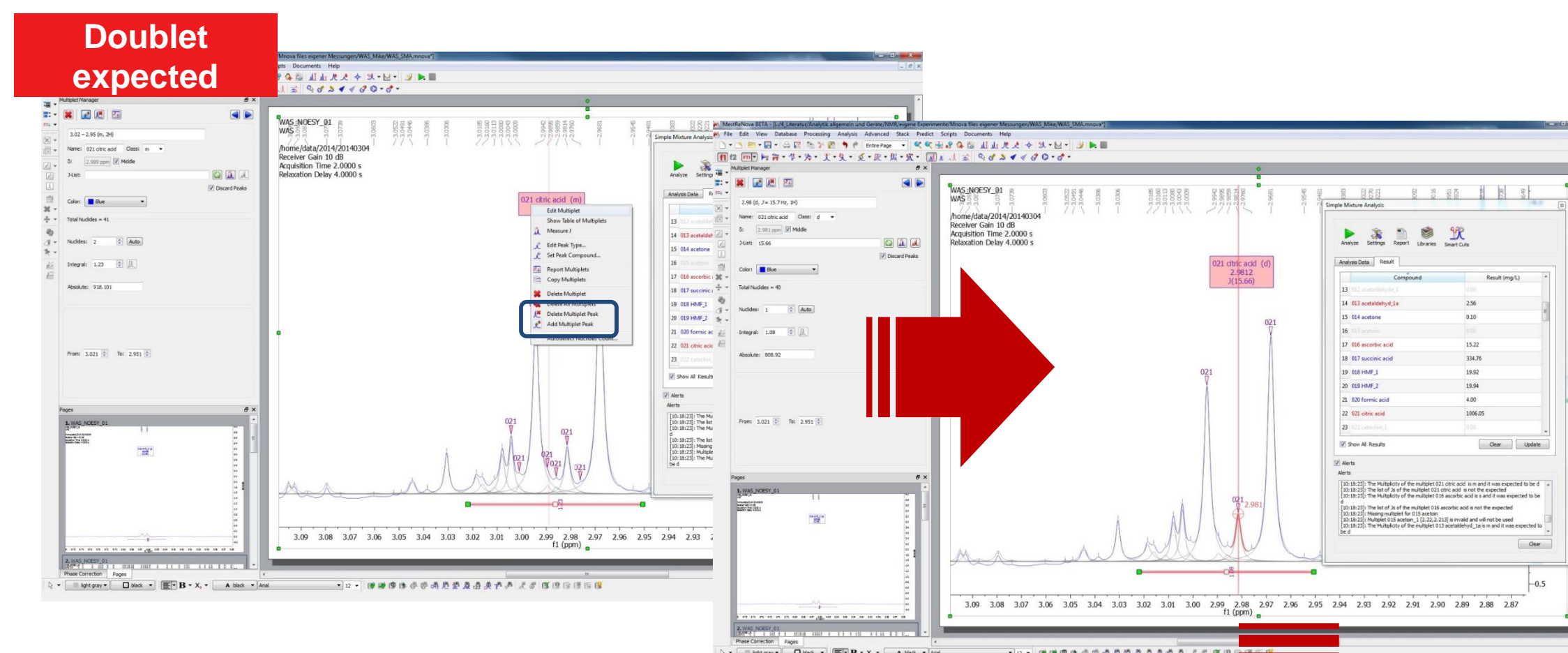
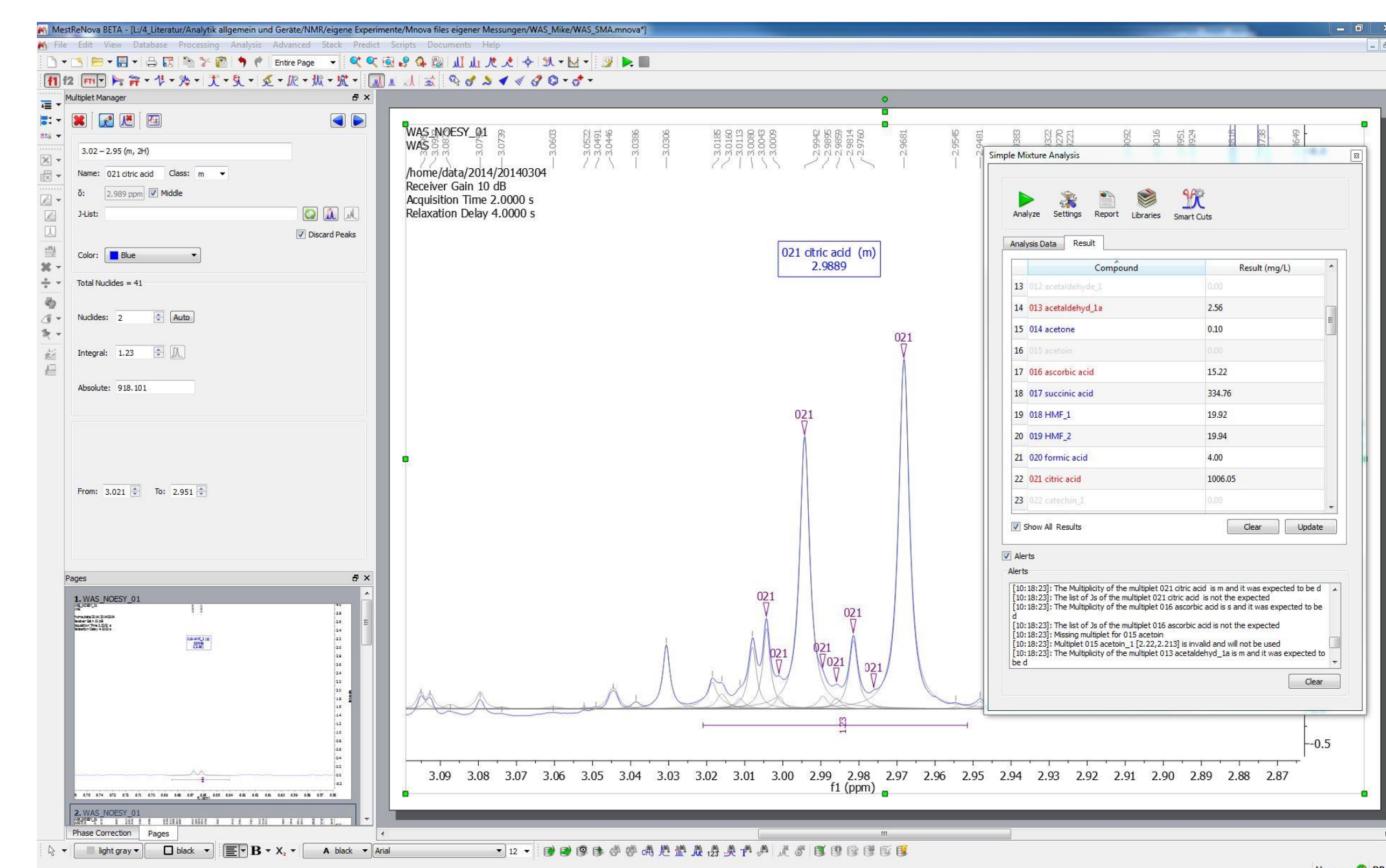


1D ¹H NMR sample spectra with the addition of known components, and at standard pH levels. Clever use of the Formula Editor in Mnova SMA was customized for each component.

The wine experiment - design

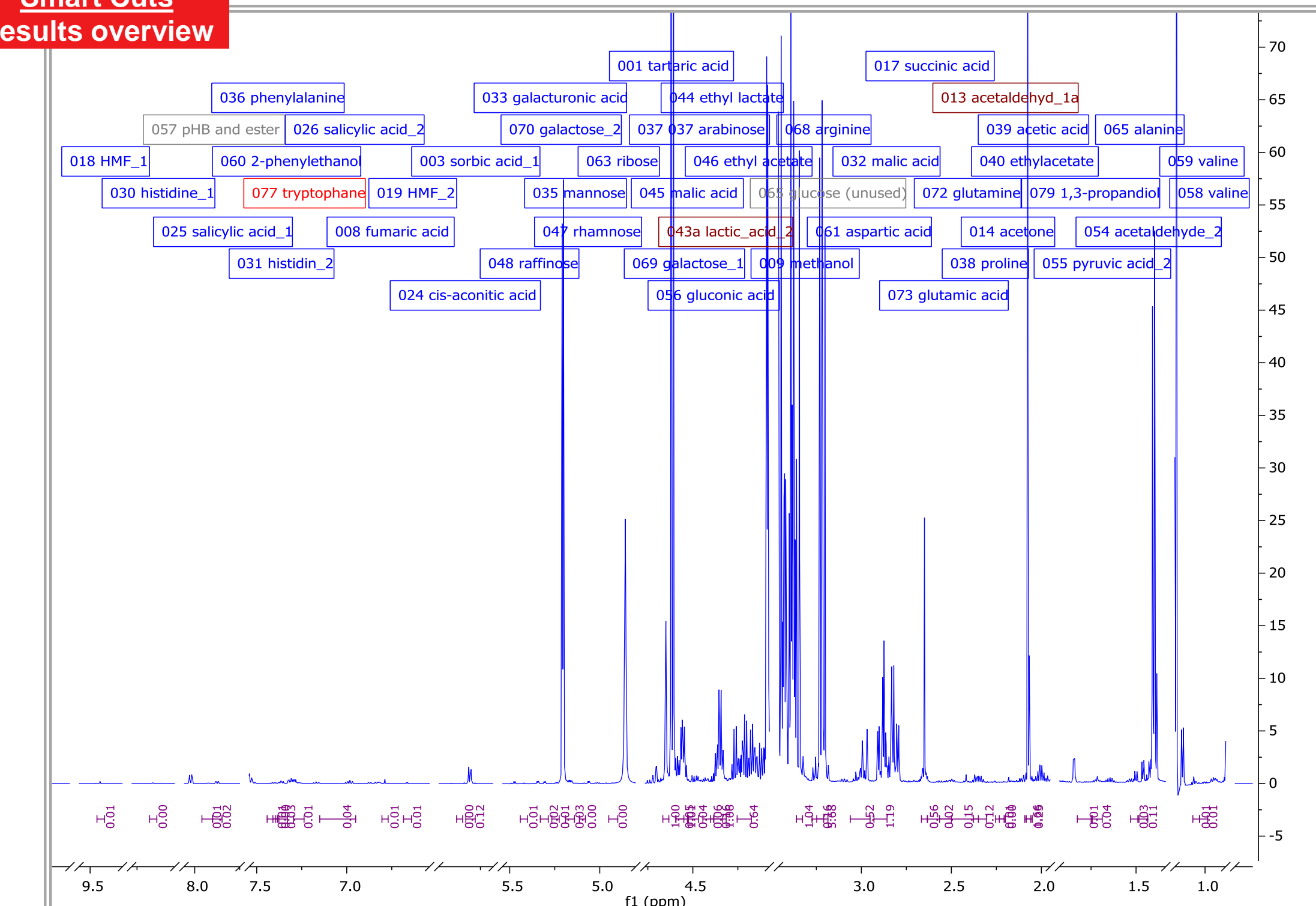


SMA Analysis: See and fix problems

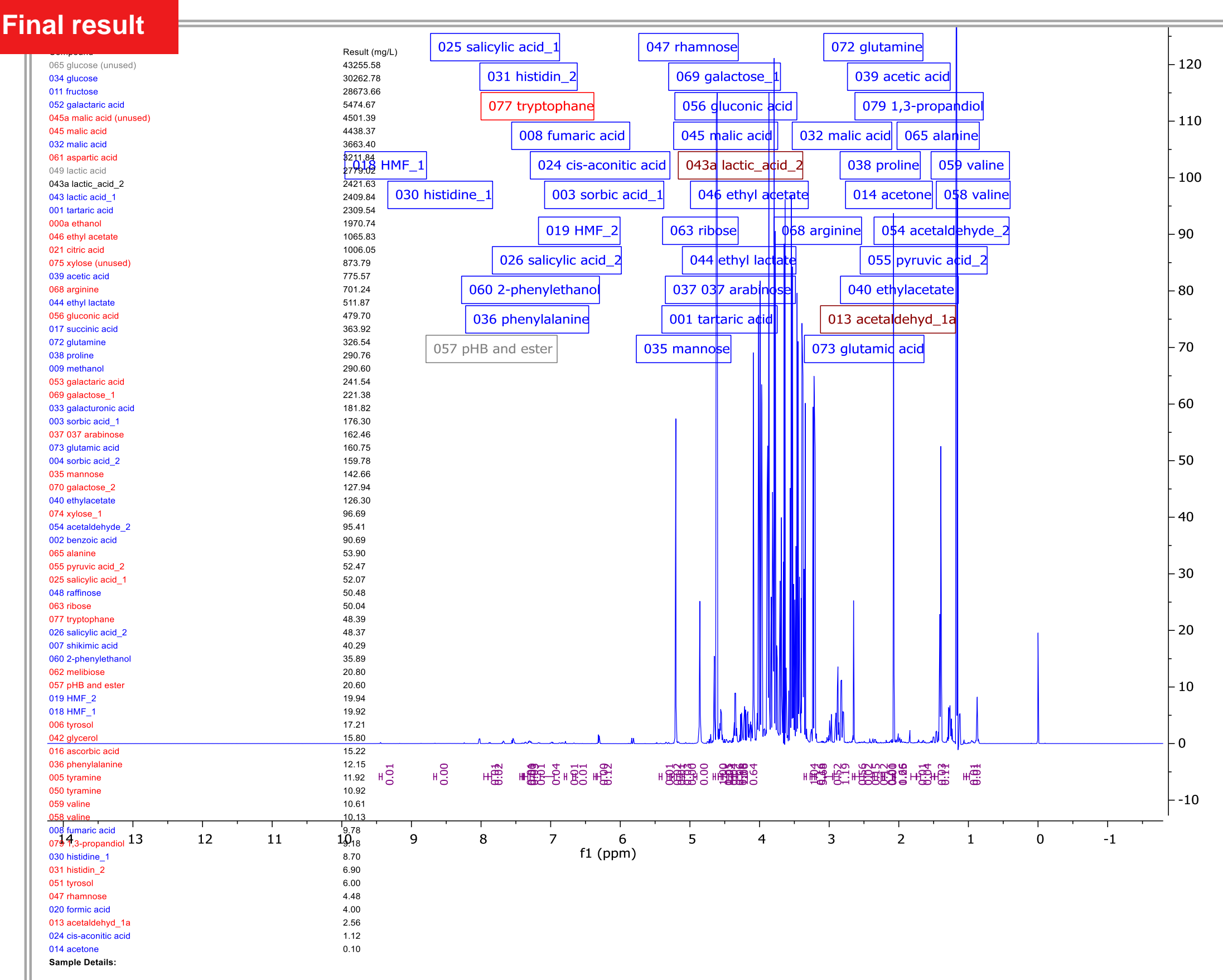


Final results

Smart Cuts Results overview



Final result



Conclusions

A targeted approach to wine component quantitation can lead to an effective and quite high throughput NMR analysis. Method development and optimization of software performance are vital first steps. The routine analysis of NMR is then quick and robust, with a sensible division between fully automated tasks and assisted, visual checks.