

A Complete Wine Analysis Using Multiplets Detection Dr Michael Bernstein¹; Agustín Barba¹; Dr Susanne Klein²; Dr Andrea Dreiseitel²; Daniel Heidger² and Volker Heidger² ¹Mestrelab Research S.L., Spain, www.mestrelab.com²Institut Heidger, Germany, http://www.institut-heidger.de

🛤 Formula Editor

CCF*MW*(I1-C_038

030_nisuaine_ 031_histidin_2 032_malic_acid

033_galacturor 034_glucose: C 035_mannose: 036_phenylalar 037_037_arabi 038_proline: C 039_acetic_acid

021 citric acid (m) 2.9889

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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 imited by law
- \blacktriangleright benzoic acid, diethylene glycol \rightarrow forbidden substances
- acetic acid at elevated levels \rightarrow unwanted smells or tastes
- \blacktriangleright shikimic acid, proline \rightarrow 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

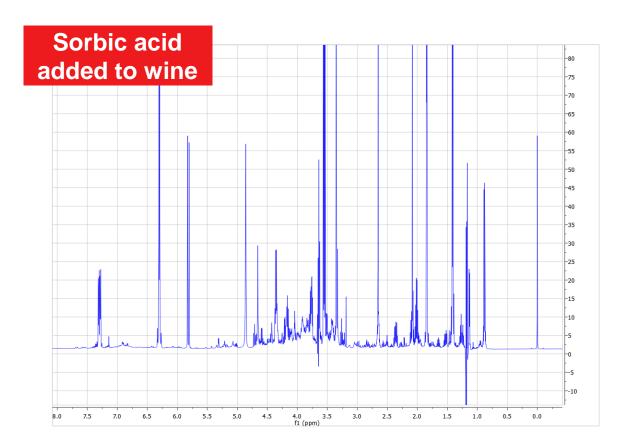
The user defines a formula that converts the area to concentration

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

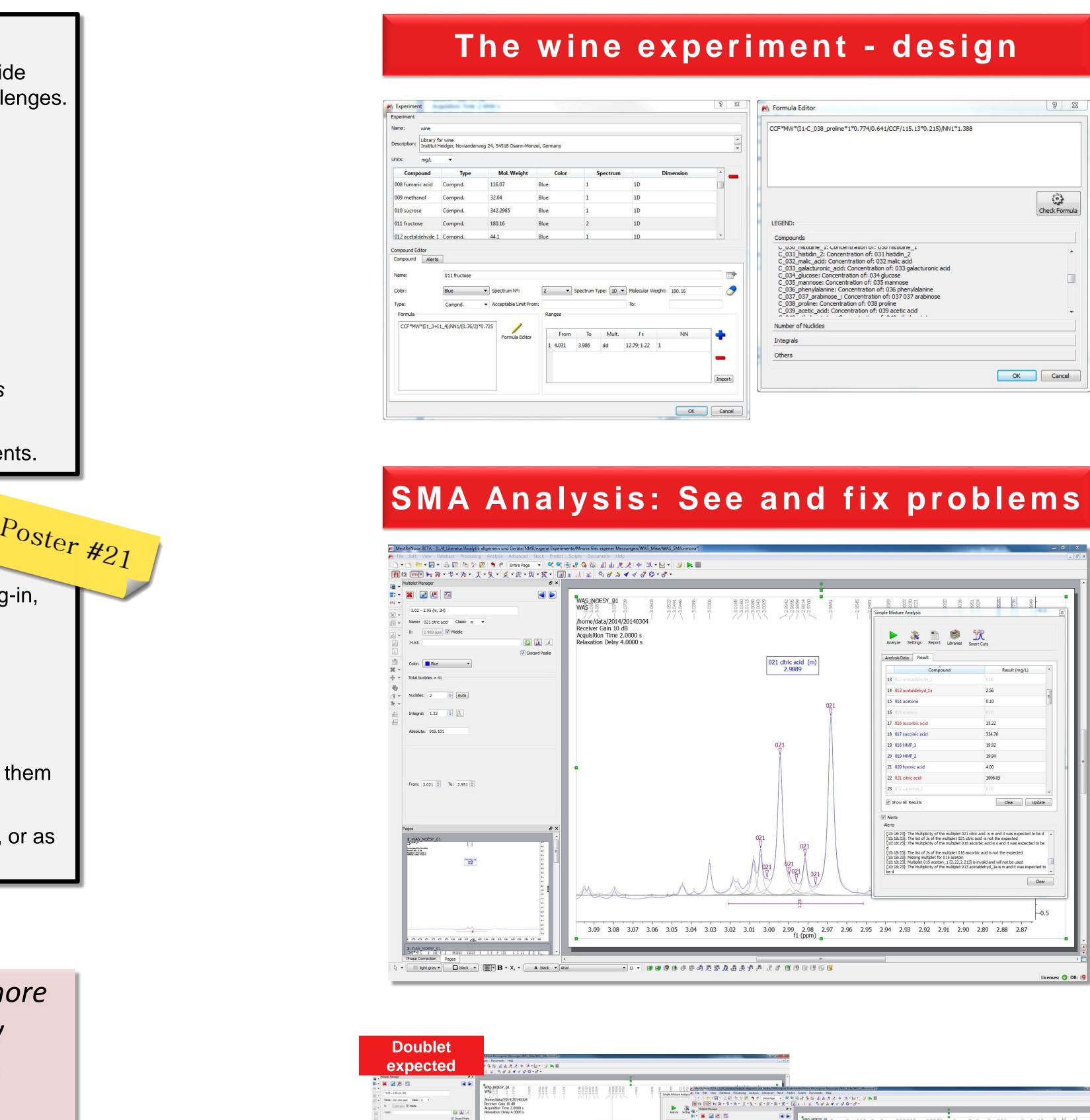
For higher throughput the analysis can be performed in batch mode, or as the data are produced by the NMR spectrometer

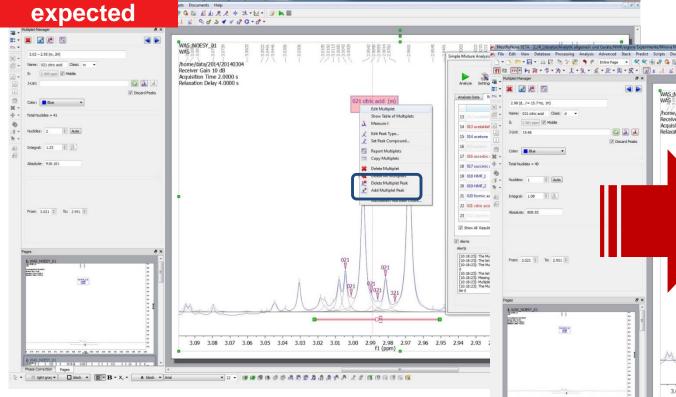
Using Mnova Simple Mixtures Analysis (SMA), more than 50 components of wine can be routinely quantified in an analysis, and ca 50 analyses performed per day by an analyst

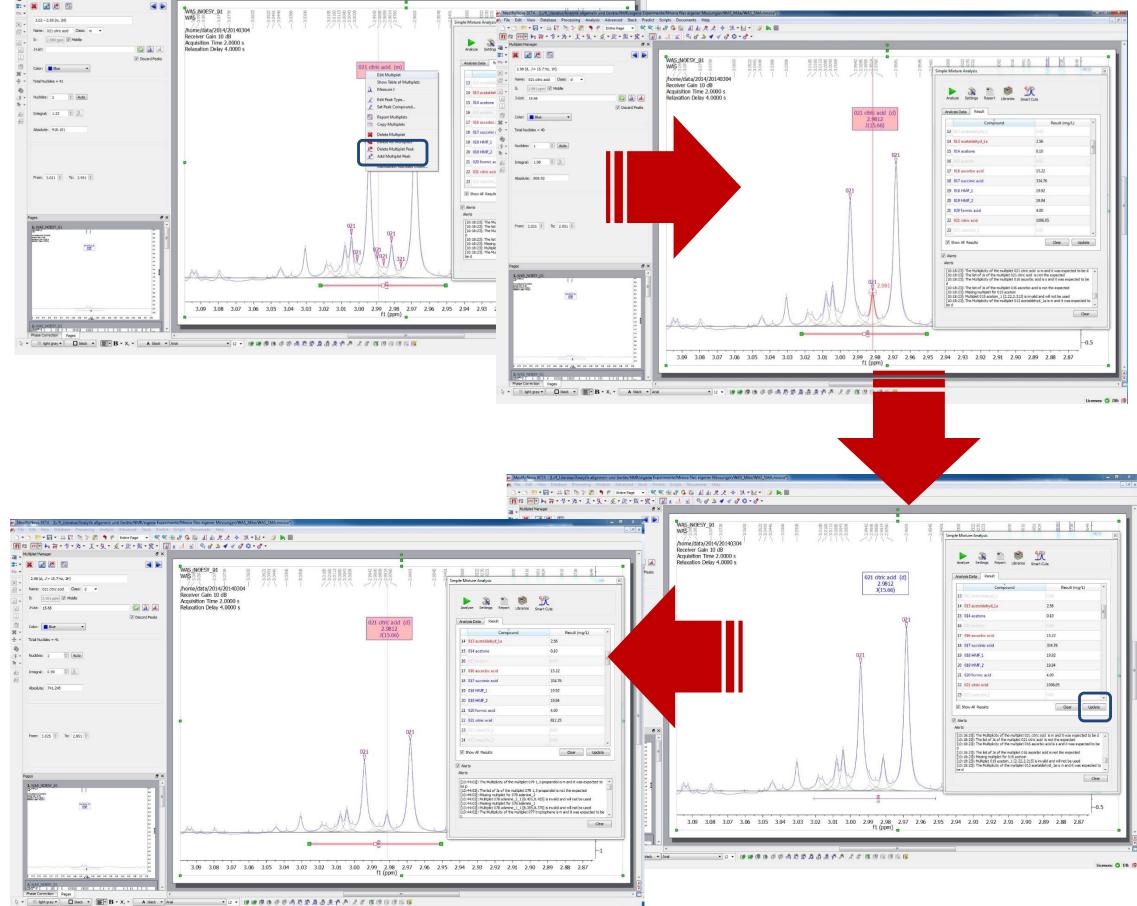
Basic setup-validation



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.



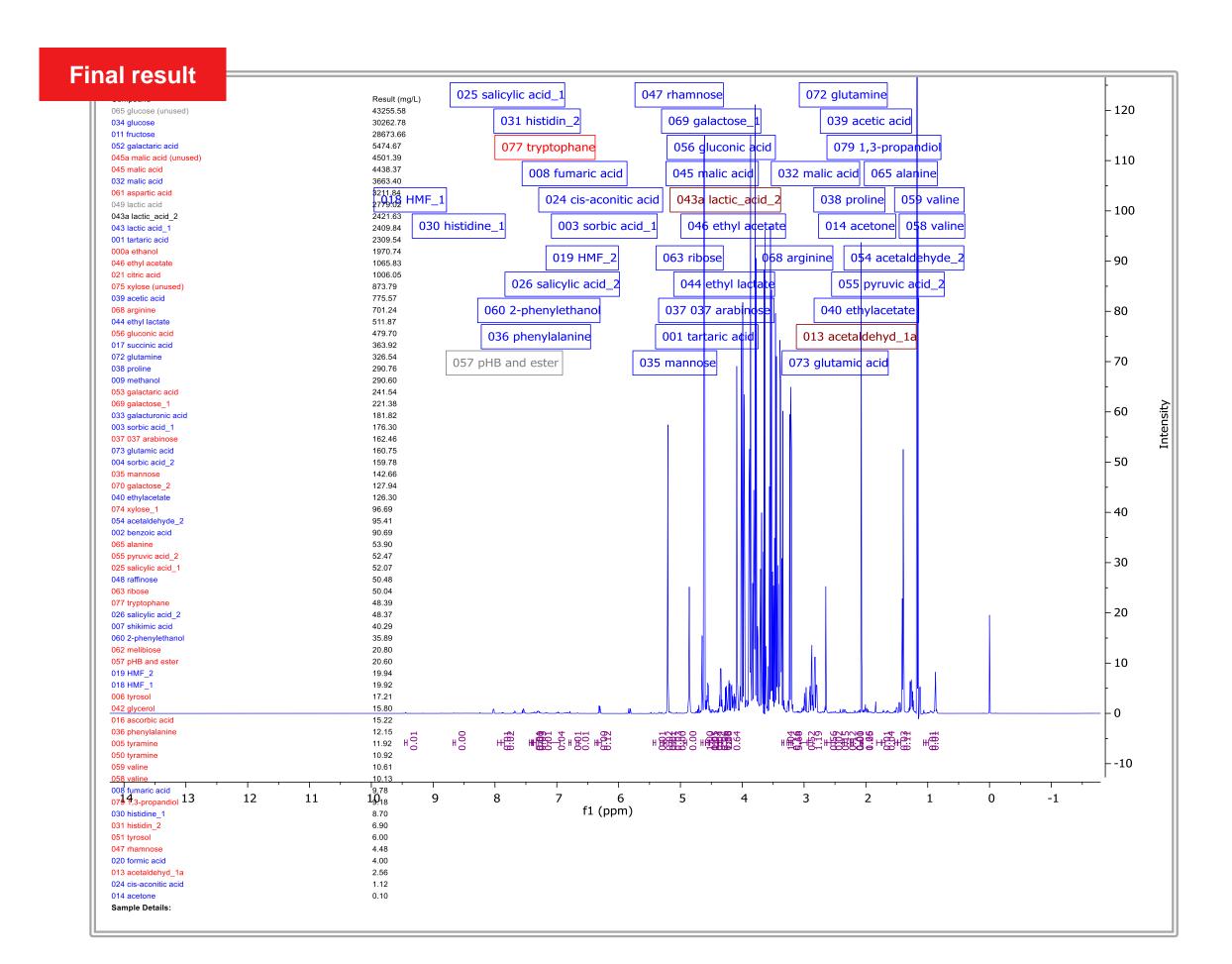




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centration of: 034 glucose ncentration of: 035 mannose :: Concentration of: 036 phenylalanine	
e_: Concentration of: 037 037 arabinose entration of: 038 proline Concentration of: 039 acetic acid	
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21	Analyze Settings Report Libraries Smart Analysis Data Result Compound 13 012 acetaldehyde_1 14 013 acetaldehyde_1 15 014 acetone 16 015 acetoin 17 016 ascorbic acid 18 017 succinic acid 19 018 HMF_1 20 019 HMF_2 21 020 formic acid 22 021 citric acid 23 022 catechin_1	Result (mg/L) Image: Constraint of the second	
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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.





Final results

