

Comparison of GC-MS and NMR metabolite identification in white wines: insights into the chemical basis for wine body

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Novel Aspect: Direct comparison of NMR and MS-based metabolomic profiles in a wine sensory study

Introduction

Gas chromatography-coupled mass spectrometry (GC-MS) and nuclear magnetic resonance spectroscopy (NMR) are the two most frequently used tools in metabolomic studies; both generate high-density, diverse chemical data sets, each with specific advantages and drawbacks. Few studies in the literature report independently-curated metabolite lists and resulting experimental conclusions for the same sample set with the purpose of a direct comparison of the two technologies. This study sought to compare MS- and NMR-based metabolite profiles in the characterization of white wines including varieties Chardonnay, Viognier, Pinot gris, Riesling and Sauvignon Blanc. The ultimate goal of this work was to identify compositional differences in these wines which correlate to wine sensory properties.

Methods

Commercially available wine samples were concentrated under vacuum to remove ethanol and D₂O-exchanged. GC-MS samples were derivatized using a methoximation and silylation protocol. Analysis was performed on a Leco Pegasus GC-TOF-MS. Automatic alignment and identification using a mass spectral/retention index database was performed using BinBase software. NMR samples were pH adjusted and supplemented with chemical shift reference sodium trimethyl-silylpropionic acid. One dimensional ¹H- and two dimensional ¹H-¹³C-NMR spectra were collected on a Bruker 600 MHz spectrometer equipped with cryogenic probe. One dimensional NMR spectra were assigned using Chenomx software. Univariate and multivariate statistical analyses were performed in Statistica DataMiner. Sensory assessments of the wines were performed by a trained panel of judges using descriptive analysis techniques.

Preliminary results

One key attribute of any wine is its body, or viscous mouthfeel properties; despite the importance of body on the style and quality of wine, its precise origin remains unclear. Prior work in the impact of rheological properties on wine body has led to a partial understanding of a few chemical constituents influencing this sensory quality (i.e. glycerol, sugar and ethanol), however, a more comprehensive understanding of the chemical and physical properties related to wine body remains to be determined. Metabolomic profiling in conjunction with sensory assessments allow for the identification of individual constituents responsible for the overall viscosity or body of a wine. The metabolite profiles of seventeen white wines were determined independently using GC-TOF-MS and ¹H-NMR. Over 300 metabolites are reliably detected in all wine samples by GC-TOF mass spectrometry as verified by the BinBase database. Over 100 of these are uniquely identified by retention index-based mass spectral libraries. One dimensional NMR data yields far fewer metabolites (<50) as identified by the commercially available software Chenomx Suite. This list comprises a sub-set of those metabolites detected by GC-TOF-MS. Independent analysis of the GC-TOF-MS and binned NMR data results in similar clustering of the wine samples in PCA space. Additionally, sensory data obtained using descriptive analysis techniques were correlated to the chemical data. Partial least squares (PLS) multivariate models were used to explain the mouthfeel viscosity rating of the seventeen white wines. Most notably, wines scored higher for viscous mouthfeel appear to contain significantly higher levels of lactic and succinic acids, as well as significantly higher levels of 10 of the 18 amino acids identified. The independently calculated MS and NMR models present new insights into the chemical basis for wine mouthfeel properties.