Sneaky stinkies: the challenges associated with analysing volatile sulfur compounds

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Background

- Volatile sulfur compounds (VSCs) often have a negative effect on wine aroma, imparting 'reductive' aromas such as 'rotten egg' and 'sewage'.
- Common examples are hydrogen sulfide (H_2S) and methanethiol (MeSH) .
- There are many challenges with the analysis of these compounds, as they have **low molecular mass**, **high volatility** and **can loosely bind to other compounds.**
- Various methods exist for the quantification of VSCs. Differences in sample preparation, the matrix analysed and the method of sample introduction may influence which 'pool' of VSCs is being quantified.

Research questions

- How do the three methods compare?
- What are any differences showing about the available pool of VSCs in a wine sample?

Experimental design

- Five wines of different varieties were analysed in replicate with each method.
- The results of H_2S and MeSH were compared.

GC-SCD
- Salt samples (2 g salt in 10 mL sample)
- Headspace cool-on-column injection
- Gas chromatography separation and sulfur chemiluminescence detection

GC-MS
- Brine-releasable samples (1 mL sample + 9 mL brine)
- Headspace solid phase microextraction injection (SPME)
- Gas chromatography separation and mass spectrometry detection

LC-MS
- Samples derivatised with N-(2-ferroceneethyl)maleimide (FEM)
- Liquid chromatography separation and mass spectrometry detection

Results

H_2S

- GC-SCD and GC-MS methods, which analyse wine headspace, produced similar results.
  ► Methods are comparable.
- The LC-MS method quantified a higher concentration of H_2S compared to the GC methods.
  ► The LC-MS quantified a larger pool of H_2S present in the liquid.
  ► Suggests that this method could measure latent sources or loosely metal bound H_2S species in certain wines.

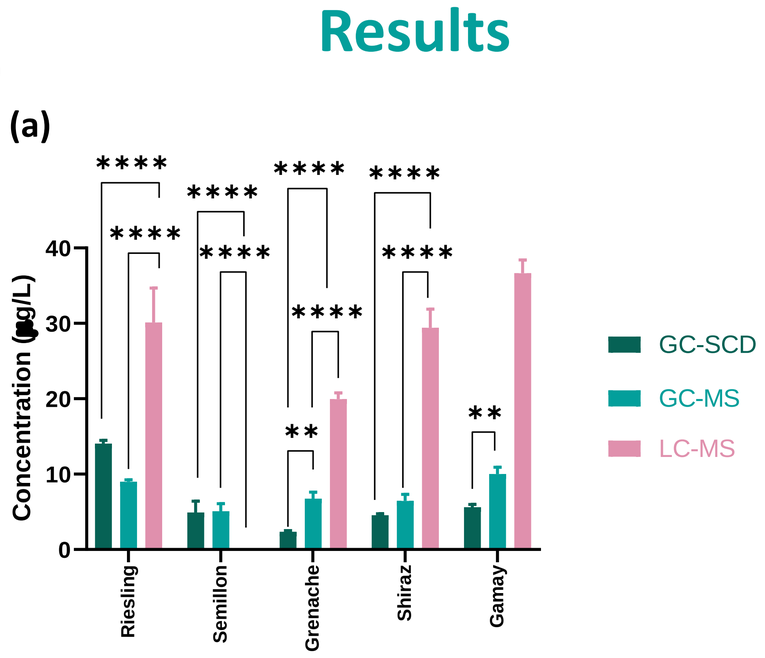

Figure 1. Concentration (µg/L) for H_2S determined by each method (a) and a PCA plot comparing the methods (b)

MeSH

- Results were more comparable when comparing the headspace and liquid phase methods.
- PCA showed that there were no differences between the methods.
  ► Either GC-SCD or GC-MS can be used for headspace analysis
  ► Suggests that there is a smaller difference in equilibrium between the headspace and liquid phase sources of MeSH.

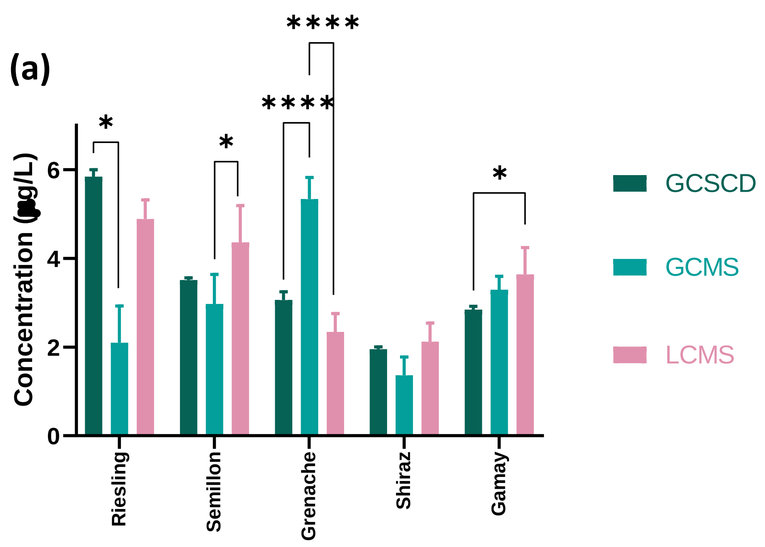

Figure 2. Concentration (µg/L) for MeSH determined by each method (a) and a PCA plot comparing the methods (b)

Take-home messages

- The quantification of H_2S continues to be complex, due to the various forms that can exist in wine.
- There are differences between headspace and liquid phase analysis of H_2S.
- MeSH is easier to quantify, with all methods comparable.

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