# LC-MS METABOLOMICS SHOWS A SMART WAY TO REDUCE SULFITES IN WINE

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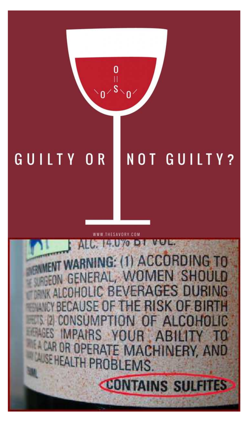
FONDAZIONE EDMUND MACH · MEZZACORONA · NOMACORC THE SYMBOL OF ASSURANCE



## Introduction

The impact of minute amounts of headspace oxygen on the post-bottling development of wine is generally considered to be very important, since oxygen, packaging and storage conditions can either damage or improve the quality of wine, in terms of its characteristics.

## Experimental Design

The sample set included 12 white wines from 6 varieties. 10 samples of each wine were bottled using the standard industrial process, with inert headspace and variable exposure to oxygen (Low $O_2$), along with a further 10 bottles produced using the same line, but without inert gas and with extra headspace (High $O_2$). The wines were analyzed after two months of storage.

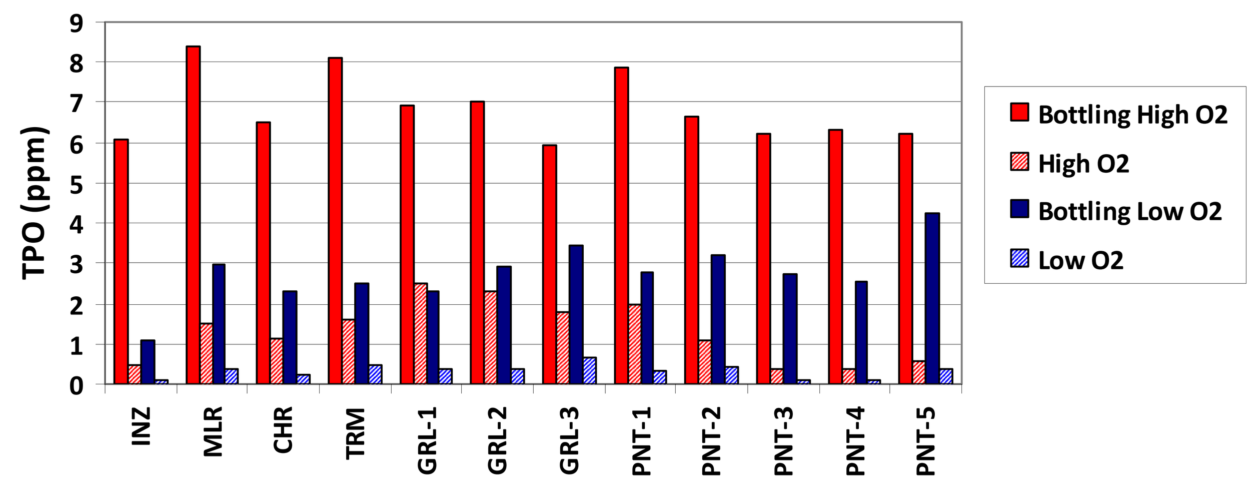
| | | | Bottles bottled | |
|---|---|---|---|---|
| Variety | Code | Wine | Low $O_2$ | High $O_2$ |
| Pinot gris | PNT | x 5 | x 10 | x 10 |
| Grillo | GRL | x 3 | x 10 | x 10 |
| Chardonnay | CHR | x 1 | x 10 | x 10 |
| Muller Thurgau | MLR | x 1 | x 10 | x 10 |
| Traminer | TRM | x 1 | x 10 | x 10 |
| Inzolia | INZ | x 1 | x 10 | x 10 |

Total 240 bottles

## Results I

The mean concentrations of total package oxygen (TPO) in each wine under the two bottling conditions (respectively, High vs Low $O_2$) at the time of bottling and after two months of storage.

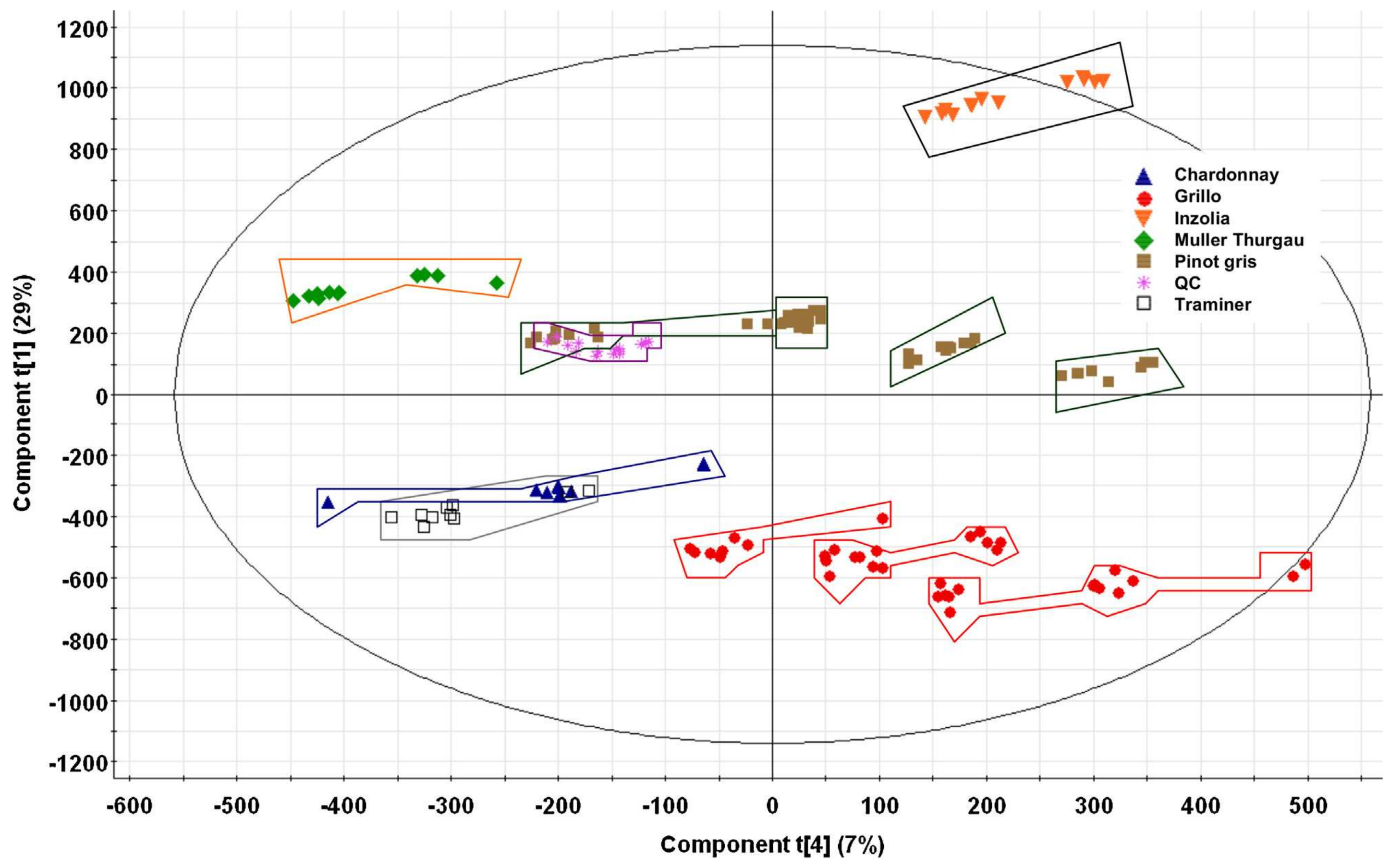
NomaSense™ oxygen analyzer

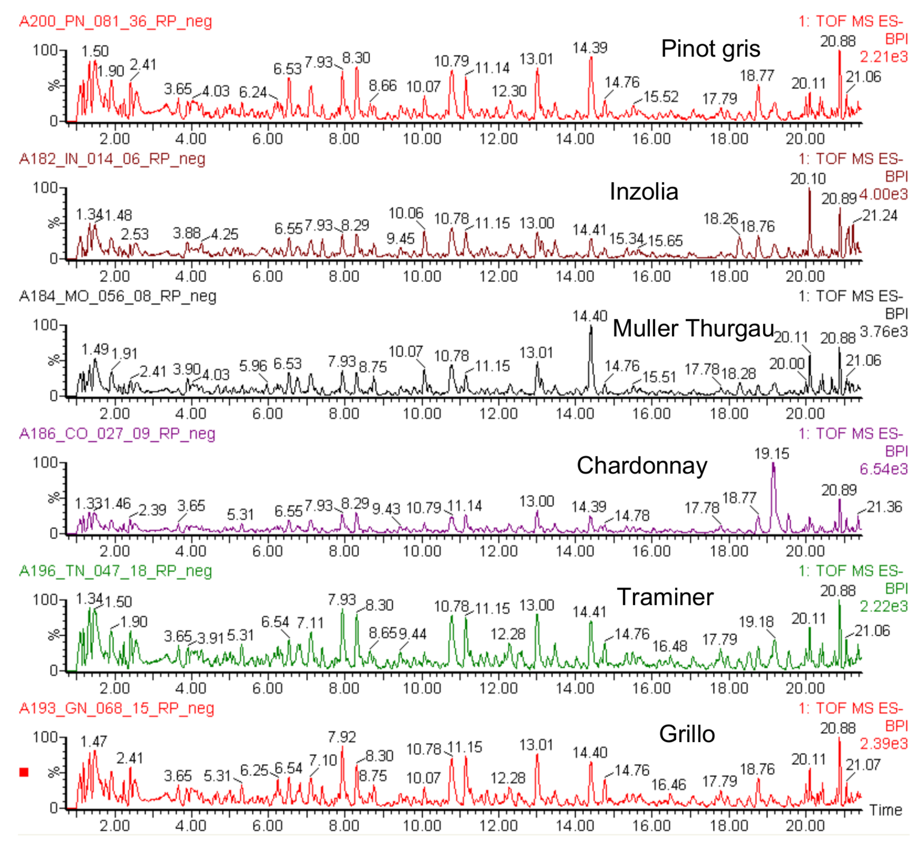



Low $O_2$ High $O_2$

## Results II

UHPLC-QTof MS untargeted analysis pointed out the power of metabolomics to discriminate the various wines; but supervised multivariate statistical analysis were necessary to detect $O_2$ related markers. This was due to the "statistical noise" generated by the cultivar variability.



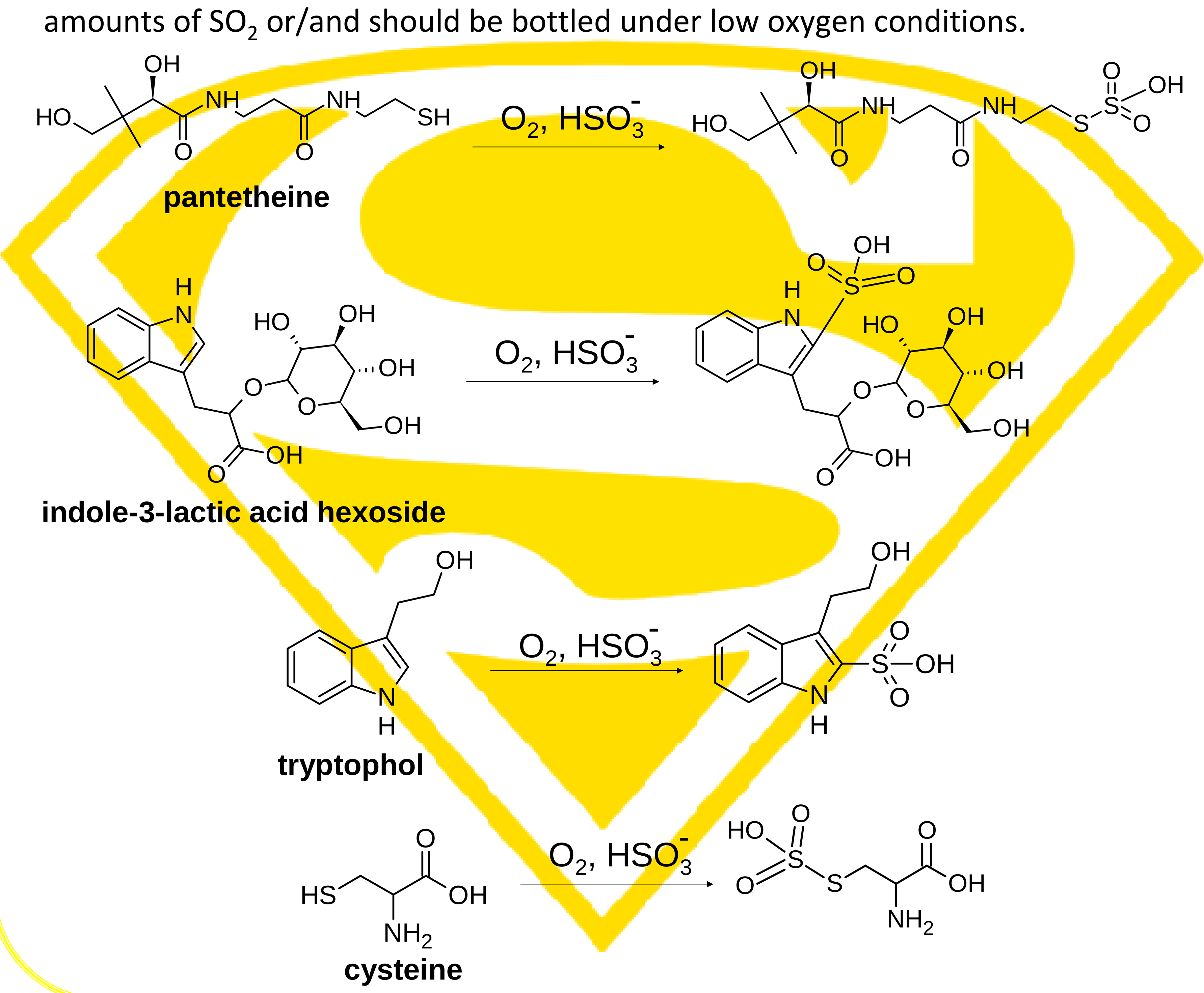



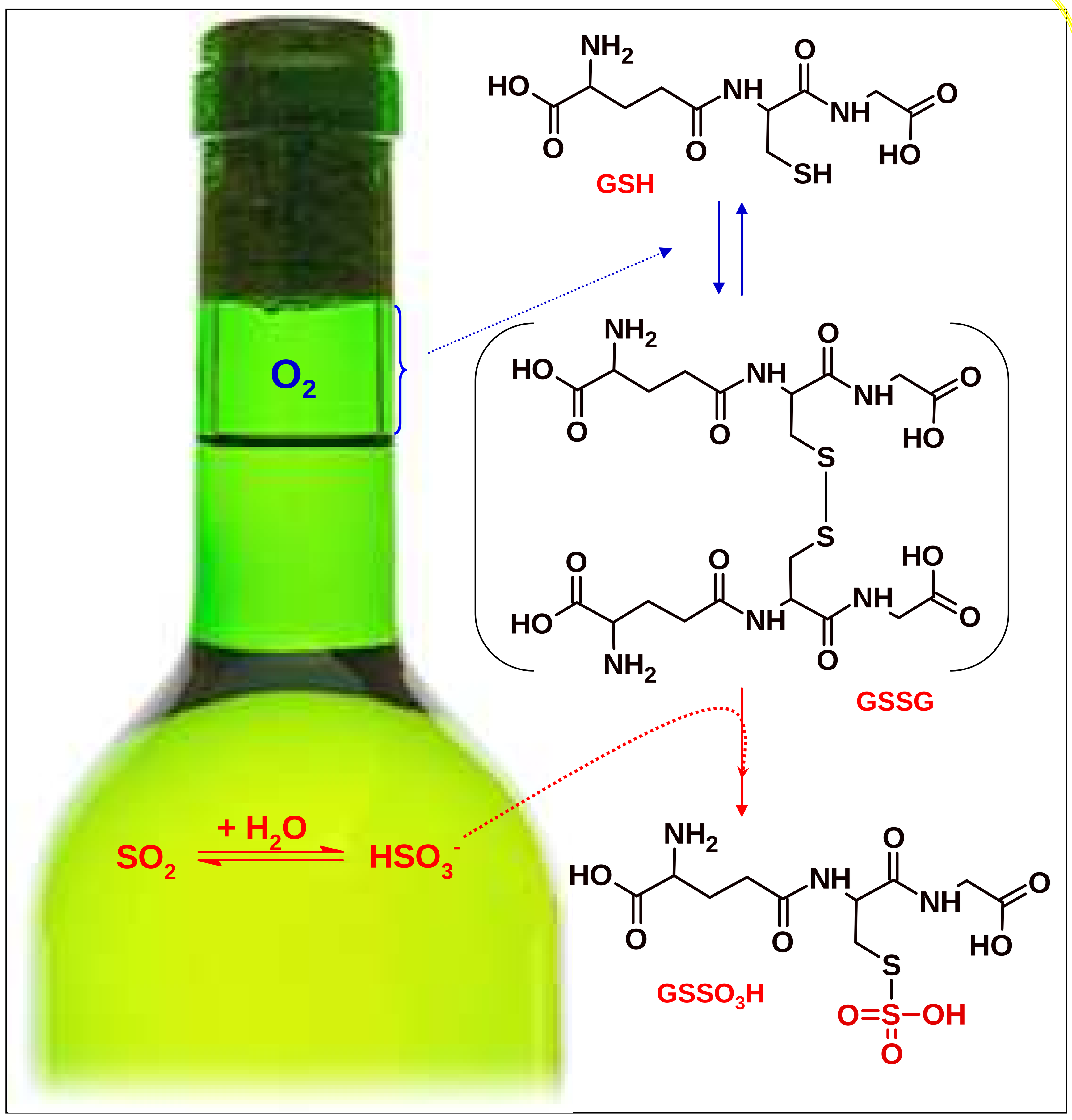

## Results III

New reactions discovered: The main reactions driven by $O_2$ were involving Sulfur. The antioxidant $SO_2$, added to protect wine from unwanted reactions, takes part in various reactions, several of which were unknown in wine to date and would appear to be of practical significance.

Possible additive interaction effects, between $SO_2$ and glutathione, should be revaluated, since these could also turn out to be antagonistic, and their co-addition/co-presence could provide less effective protection.

Wines containing large amounts of indoles might require the addition of larger amounts of $SO_2$ or/and should be bottled under low oxygen conditions.




The co-presence of glutathione (GSH) and $SO_2$ in wine has as a result the formation of *S*-sulfonated glutathione ($GSSO_3H$). The mechanism of the reaction requires first the oxidation of GSH to GSSG (glutathione disulfide), which reacts very fast to produce $GSSO_3H$. This is the cause why GSSG is not detectable in wine.

**For further information read: Arapitsas, P.; Ugliano, M.; Perenzoni, D.; Angeli, A.; Pangrazzi, P.; Mattivi, F. Wine metabolomics reveals new sulfonated products in bottled whitewines, promoted by small amounts of oxygen, Journal of Chromatography A, vol. 1429, pp. 155-165, 2016.**