

# GC-MS/MS METHOD FOR THE DETERMINATION OF OFF-NOTES IN WINE & WINE- RELATED PRODUCTS



## Introduction

Off-notes are components that can develop during the vinification process. Off-notes provide negative smells and tastes to the wine. Some of them are carcinogenic. Therefore it is important to determine the presence of off-notes in wine.

# GC-MS/MS TECHNOLOGY EXPLAINED

GC-MS stands for gas chromatography (GC) in which a mass spectrometer (MS) is used. The GC-MS/MS, also known as triple quadrupole, works with double detection, which greatly increases the precision of the measurements. The volatile components are brought to the injection port of the device with a special needle, provided with a polymer film. This technique is called Solid Phase MicroExtraction (SPME). The high temperature of the injection port cause the substances to be released.



Gas chromatography is still the technique of choice for measuring aromas and off-notes. MS/MS, the double detection, is the application that can determine the specific substances in low concentrations at the parts per trillion level due to the very sensitive measurements.



# GC-MS/MS TECHNOLOGY EXPLAINED

Team leader and chemist Mark Ekkerman explains the technique. “We take 1 millilitre of sample and heat it up to make a large part of the substances volatile. All substances have a certain mass, the GC-MS/MS can detect these different substances with an advanced form of gas chromatography.

Suppose we smell cork, then we are talking about 2,4,6-trichloroanisole (TCA). Cork smell is very volatile. People perceive 2,4,6-TCA at the level of 2 parts per trillion (ppt) in wine. That is the so called ‘threshold value’. Analytically, you must be able to measure below the threshold value to confirm whether the observation is correct. Thanks to the GC-MS/MS we are able to detect around 1 ppt for wines. The system detects 31 ‘off-notes’. The technology originates from the food industry, but it is completely adapted to our needs.”



With our method we are able to detect 31 different off-notes in wine and wine related products. The overview below shows the 31 off-notes, together with the characteristic smell and taste of each off-note.

Off-note	Characteristic Smell / Taste	Off-note	Characteristic Smell / Taste
Hydrogensulfide	Rotten egg	6-Chloro-o-cresol	Hospital
Methanethiol	Onion, cabbage	Geraniol	Floral
Acetaldehyde*	Bruised apples	2,4,6-TCA	Cork
Ethanethiol	Skunk, gas like	Geosmin	Damp soil
Dimethyl sulfide	Cabbage, sulfurous	Guaiacol	Fire, smoke
2-Propanal*	Foul, pungent	2,3,6-TCA	Cork
Ethylacetate	Nail polish	2-Bromophenol	Medicinal
Methanol*	Alcoholic	2,6-Dichlorophenol	Antiseptic
Dimethyl disulfide	Rotten vegetable	4-Ethylphenol	Band aid
Styrene	Plastic	2-Acetylaniline	Sweet, floral
Acetic acid	Acidic	Decanoic acid	Rancid, sweat
2-Methylisoborneol	Peat, mouldy	2,3,4-TCA	Cork
Butyric acid	Sour milk, sweat	2,4,6-TBA	Cork
Isovaleric acid	Cheesy, sweat	Indole	Pig faeces
2-Ethylfenchol	Floral, spicy		

\*The off-notes marked with a \* are carcinogenic





## ORGANOLEPTIC THRESHOLD

The organoleptic threshold was determined by spiking the off-notes to different wines. The tasting panel received 3 glasses. Two of those glasses were filled with a wine and one contained the wine spiked with an off-note. For each off-note series of 4 different concentrations were spiked as a starting point, hereafter the spike concentrations were narrowed down.

The panel started tasting the set with the highest concentration. When they distinguished the spike from the blanks, a set with a lower spike concentration was presented. Every time the panel correctly distinguished the spike, a lower concentration was presented until they could not distinguish the spike from the two blanks.

The threshold is then fixed at the lowest concentration that the taste panel could distinguish from the blanks.



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