

# Fate of tropical odorants in wine:

## Identification and stability of 2-methyl-4-propyl-1,3-oxathiane

Xingchen Wang<sup>1</sup>, Liang Chen<sup>1</sup>, Dimitra Capone<sup>1,2</sup>, David Jeffery<sup>1,2</sup>

<sup>1</sup> Department of Wine and Food Science, The University of Adelaide (UA), PMB 1, Glen Osmond SA 5064, Australia

<sup>2</sup> Australian Research Council Training Centre for Innovative Wine Production, UA, PMB 1, Glen Osmond SA 5064, Australia

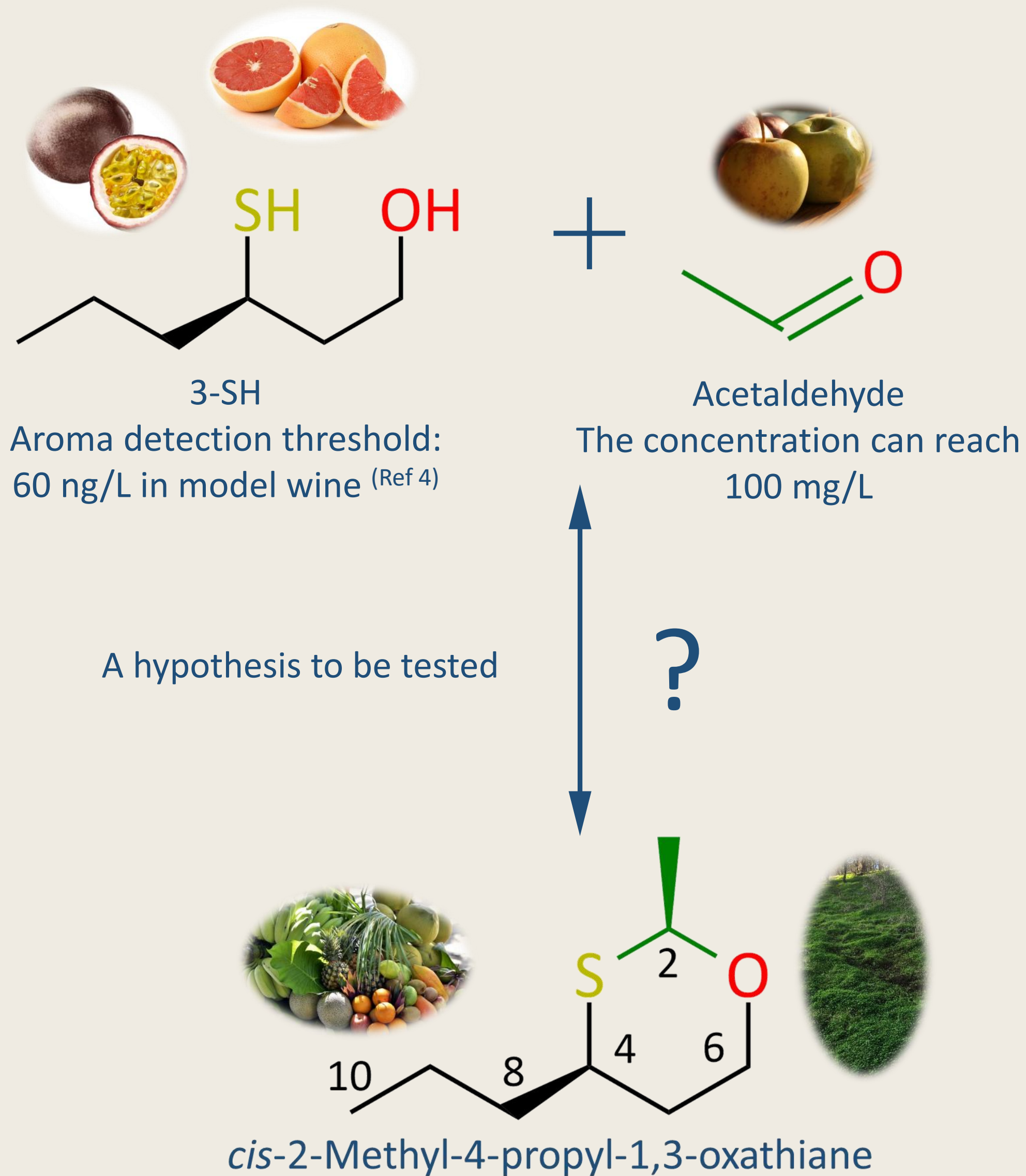
xingchen.wang@adelaide.edu.au



Wine Australia

### BACKGROUND

- 3-Sulfanyl-1-hexanol (3-SH) contributes to "passionfruit" or "grapefruit" aromas in wine (Ref 1) and is one of the most important volatile compounds for wine such as Sauvignon Blanc. Previous research showed 3-SH aroma can be influenced by acetaldehyde. (Ref 2)
- Acetaldehyde and 3-SH also occur in passionfruit, and are presumed to lead to formation of 2-methyl-4-propyl-1,3-oxathiane (**1**), (Ref 3) which is associated with "tropical fruit", "green", and "slight burnt" aromas. On that basis, such a transformation was also assumed to occur in wine.



- The aim of the project is to investigate the presence and stability of **1** to partially explain the fate of 3-SH in wine.

### METHOD



#### Method development & compound identification

- Preliminary method developed leading to the identification of *cis*-**1**
- Further identification by co-injection experiment, mass spectra, and linear retention indices
- Labelled standard synthesis and further optimised method developed using SIDA method



#### Perception threshold & commercial wine analysis

- Threshold determination in Chardonnay wine
- Different grape varieties and country of origin
- Relationship between 3-SH and *cis*-**1** investigated



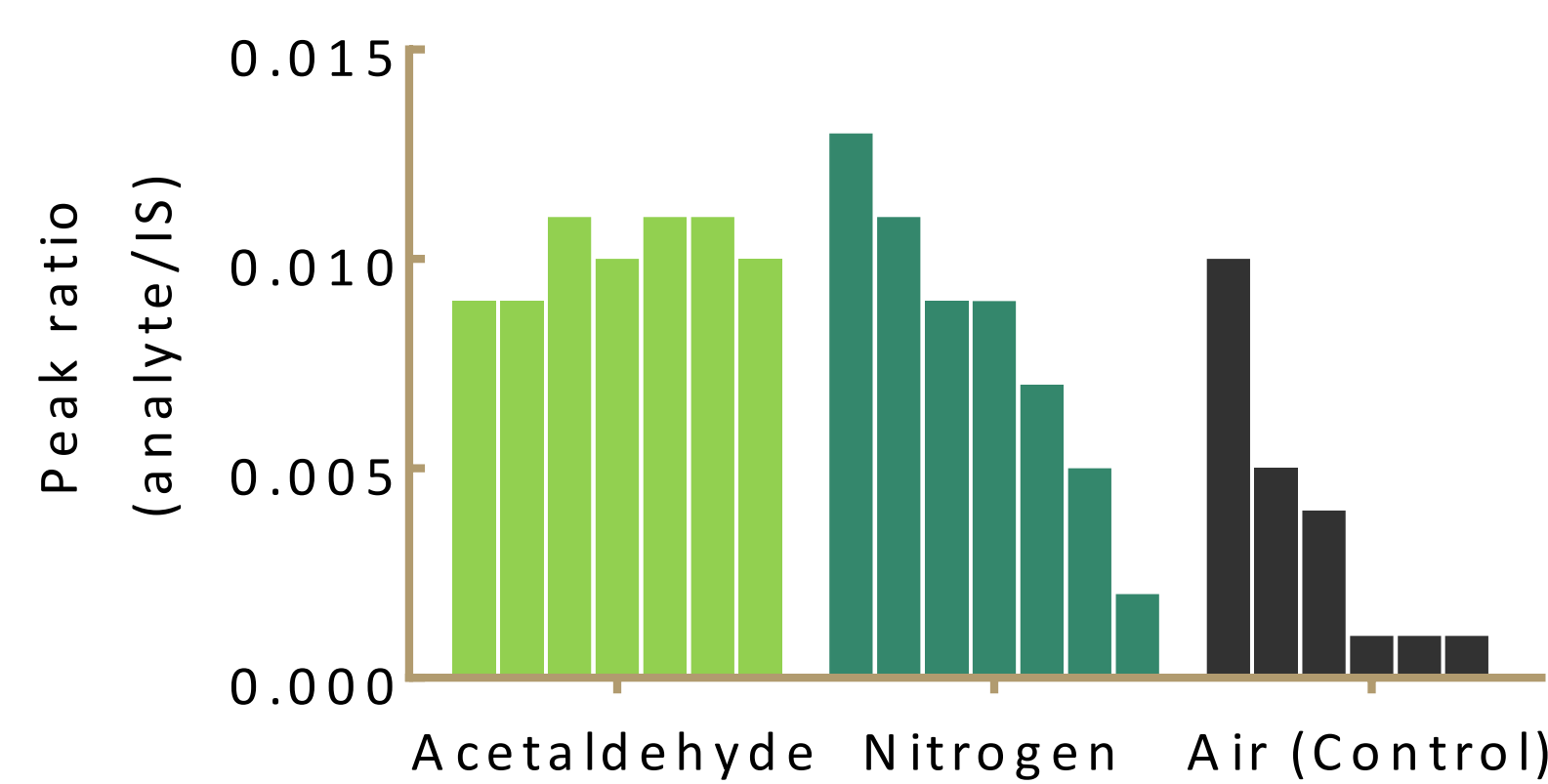
#### Stability during storage, various parameters are investigated

- Temperature impact
- pH impact
- Anoxia, SO<sub>2</sub>, and acetaldehyde impact

### CONCLUSIONS & OUTLOOK

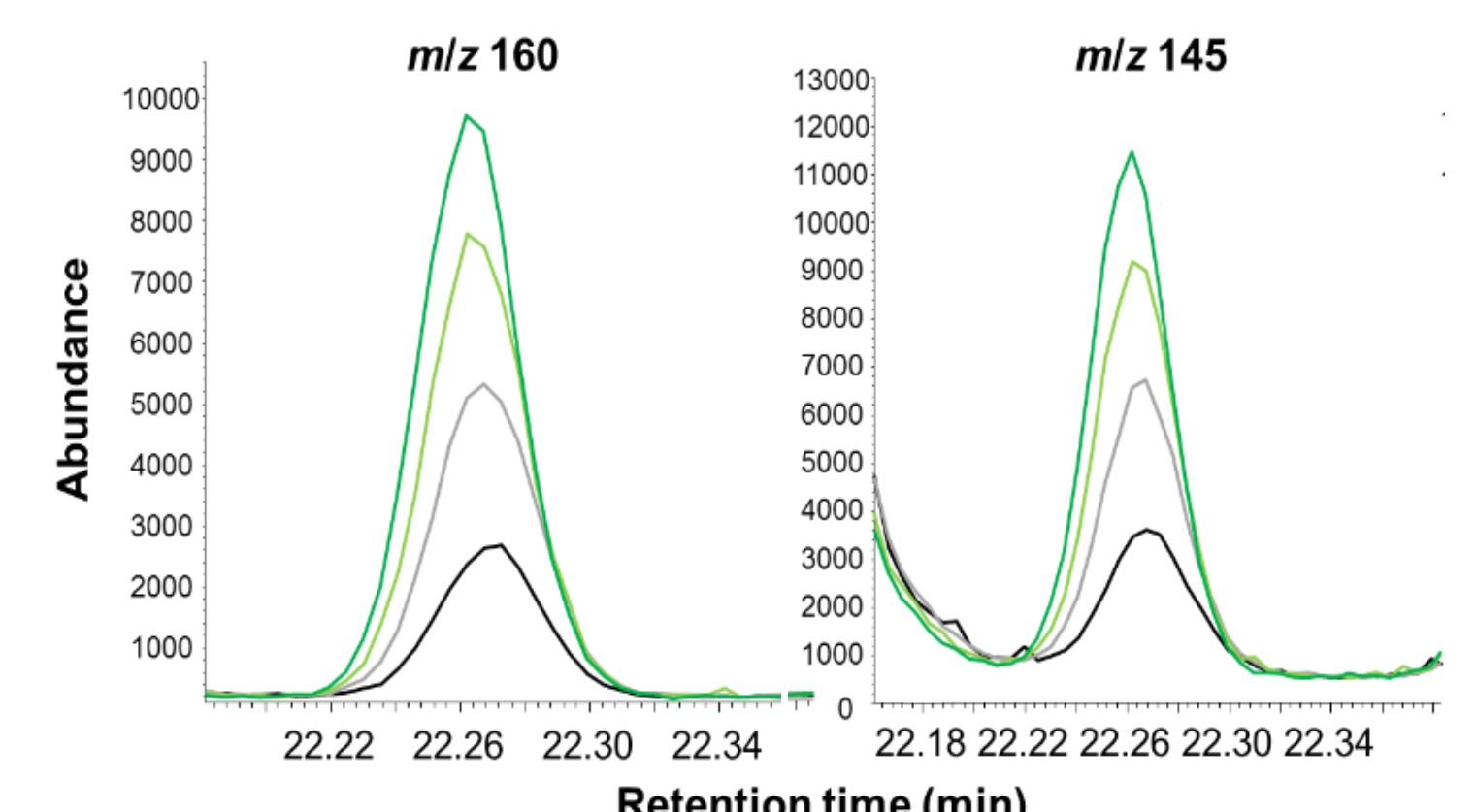
- First identification of *cis*-**1** in wine and a targeted SIDA-HS-SPME-GC-MS method was developed for quantification
- Could explain the partial loss of 3-SH in wine and could potentially be a source of 3-SH in wine
- Relatively stable over a short period of time and ongoing studies are currently being undertaken, including the timing of formation of *cis*-**1**.

### METHOD DEVELOPMENT & COMPOUND IDENTIFICATION (Ref 5)



Acetaldehyde necessary to maintain *cis*-**1** when spiked into model wine

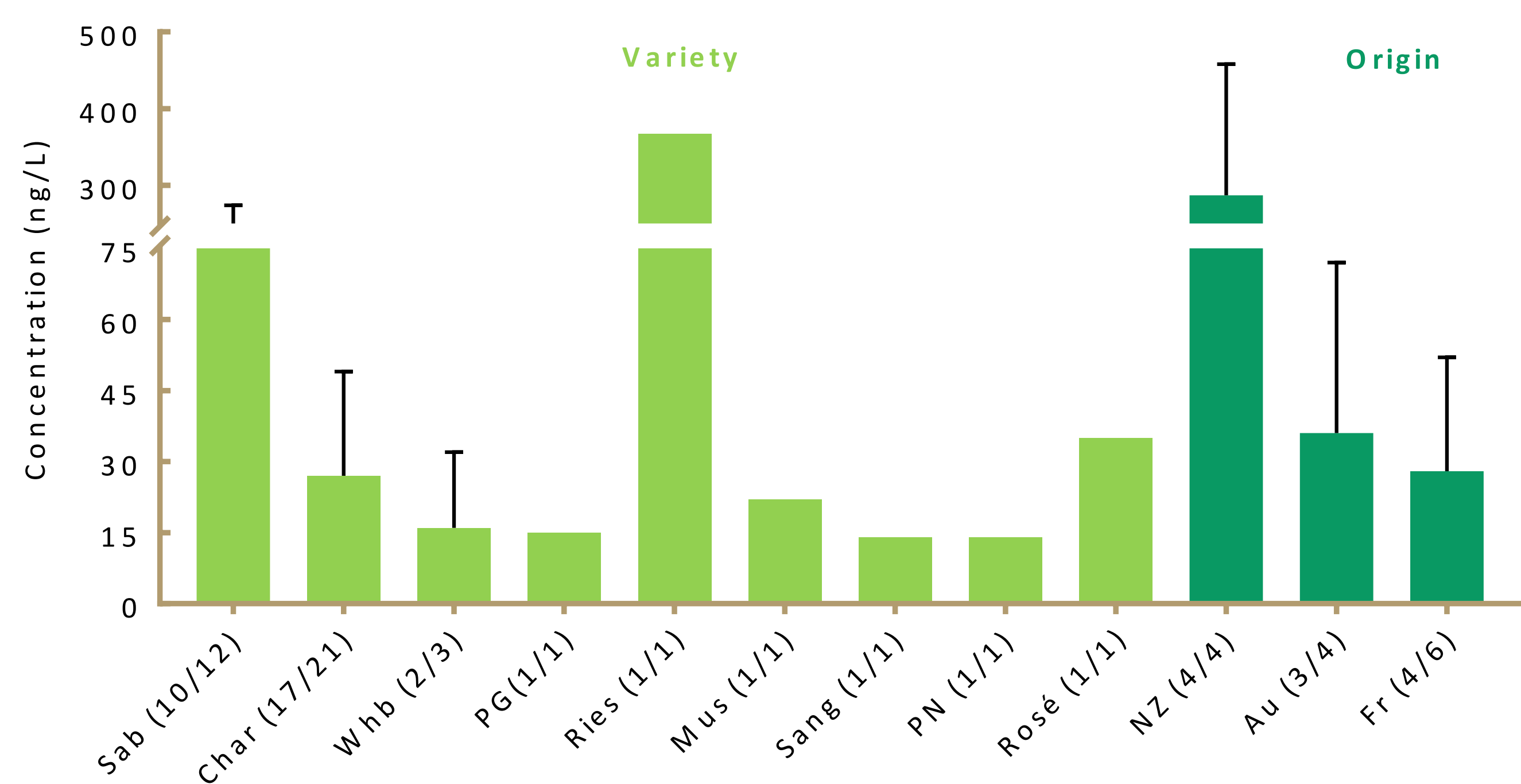
- Acetaldehyde addition preserves **1** from decreasing in model wine
- Deuterated analyte synthesis and peak identity of *cis*-**1** verification performed by co-injection in a Sauvignon Blanc wine
- Mass spectra and linear retention indices on two GC columns were used to confirm the identity of *cis*-**1** in wine
- Stable isotope dilution assay (SIDA) HS-SPME-GC-MS method developed for accurate quantitation of *cis*-**1** in wine.



Overlaid selected ion chromatograms of co-injection experiments

### PERCEPTION THRESHOLD & COMMERCIAL WINE ANALYSIS (Ref 5)

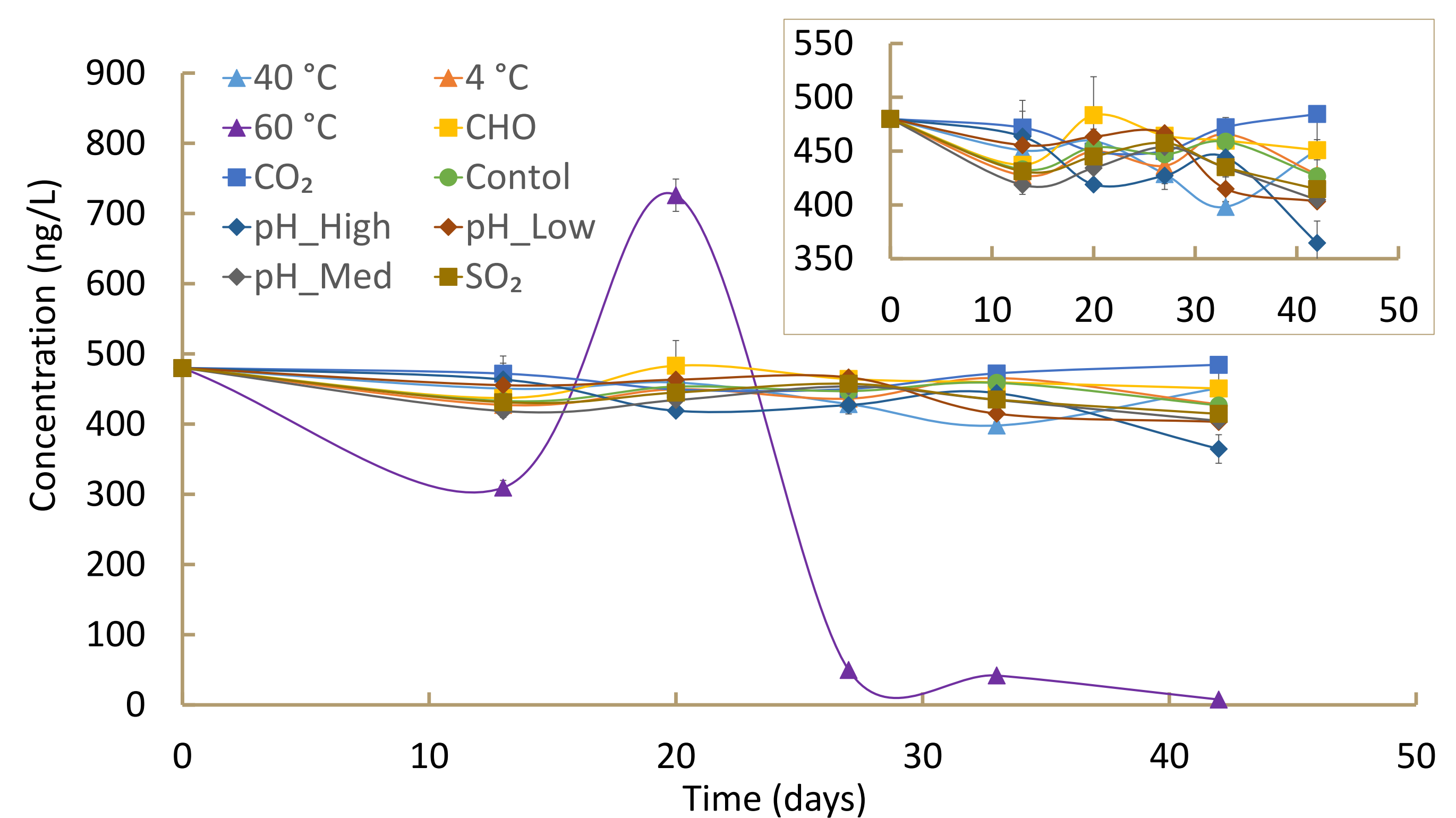
- Aroma detection threshold of **1** (mixture of *cis/trans*=85/15) in a Chardonnay wine was determined to be 7.1 µg/L
- Oxathiane *cis*-**1** present in 35 out of 42 wines varied by grape variety and country of origin, and strongly correlated with 3-SH concentration ( $r=0.72$ )
- Concentrations of *cis*-**1** ranged from undetectable to 460 ng/L (<7.1 µg/L) – varied by country of origin
- Although *cis*-**1** was found below its aroma detection threshold, it could account for the disappearance of an important amount of 3-SH.



\* Sab: Sauvignon Blanc, Char: Chardonnay, Whb: white blend, PG: Pinot Gris, Ries: Riesling, Mus: Muscat, Sang: Sangiovese, PN: Pinot Noir, NZ: New Zealand, Au: Australia, Fr: France.

### STABILITY DURING STORAGE

- The stability of *cis*-**1** was tested under accelerated storage conditions
- Oxathiane *cis*-**1** appears to be stable in most treatments over 42 days.
- A significant decrease of *cis*-**1** was seen in wine stored at 60 °C over 42 days



(Ref 1) Tominaga, T.; Niclasi, Y.; Frerot, E.; Dubourdieu, D. *J. Agric. Food Chem.* **2006**, *54* (19), 7251-7255.  
 (Ref 2) Coetzee, C.; Brand, J.; Jacobson, D.; Du Toit, W.J. *Aust. J. Grape Wine Res.* **2016**, *22*, 197-204.  
 (Ref 3) Winter, M.; Furrer, A.; Willhalm, B.; Thommen, W. *Helv. Chim. Acta.* **1976**, *59*, 1613-1620.  
 (Ref 4) Tominaga, T.; Furrer, A.; Henry, R.; Dubourdieu, D. *Flavour Fragr. J.* **1998**, *13*(3), 159-162.  
 (Ref 5) Chen, L.; Capone, D.L.; Jeffery, D.W. *J. Agric. Food Chem.* **2018**, *66*, 10808-10815.

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