



## Supporting Information

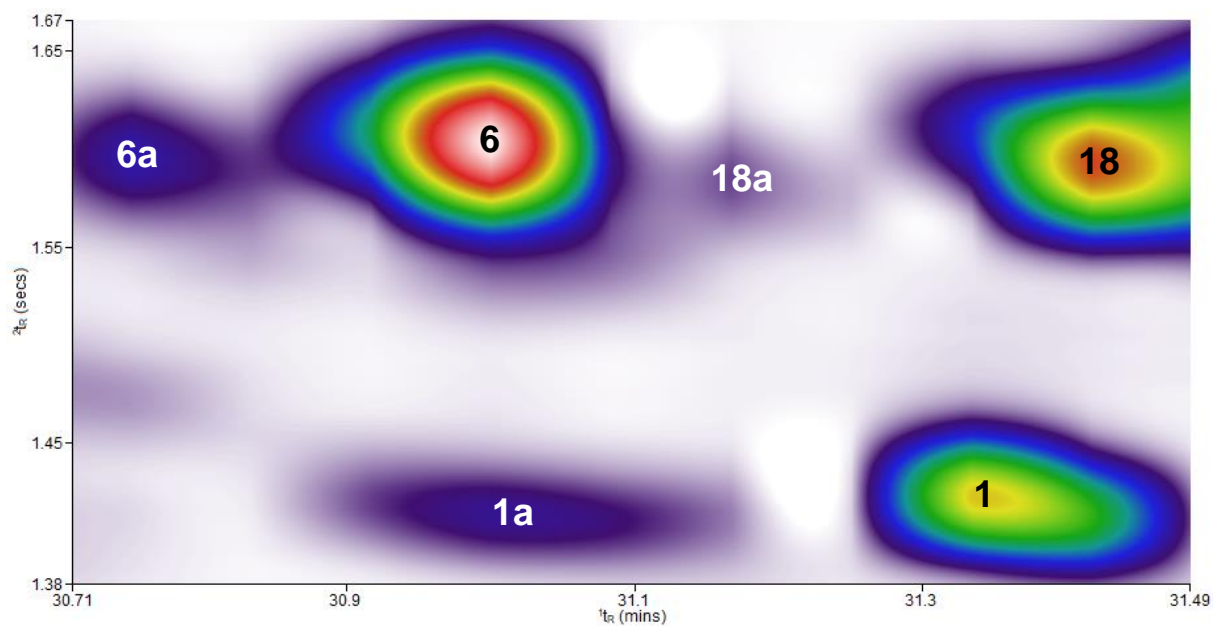
for

### **Analysis of sesquiterpene hydrocarbons in grape berry exocarp (*Vitis vinifera* L.) using in vivo-labeling and comprehensive two-dimensional gas chromatography–mass spectrometry (GC×GC–MS)**

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### **Enlarged 2D chromatogram showing the separation of $\beta$ -elemene, $\alpha$ -guaiene and $\beta$ -ylangene**



**Figure S3:** Enlarged, two-dimensional contour plot after successful administration of  $d_3$ -MVL to isolated exocarp of grapes of the red wine variety Lemberger. The regions labeled with the numbers **6**, **18** and **1** correspond to the genuine sesquiterpenes  $\beta$ -ylangene,  $\alpha$ -guaiene and  $\beta$ -elemene. **6a** ( $d_8$ ), **18a** ( $d_9$ ) and **1a** ( $d_9$ ) are the isotopologues with the highest, possible incorporation of deuterium when  $d_3$ -MVL is used as precursor (the maximum possible number of deuterium atoms incorporated is given in brackets).