



## Supporting Information

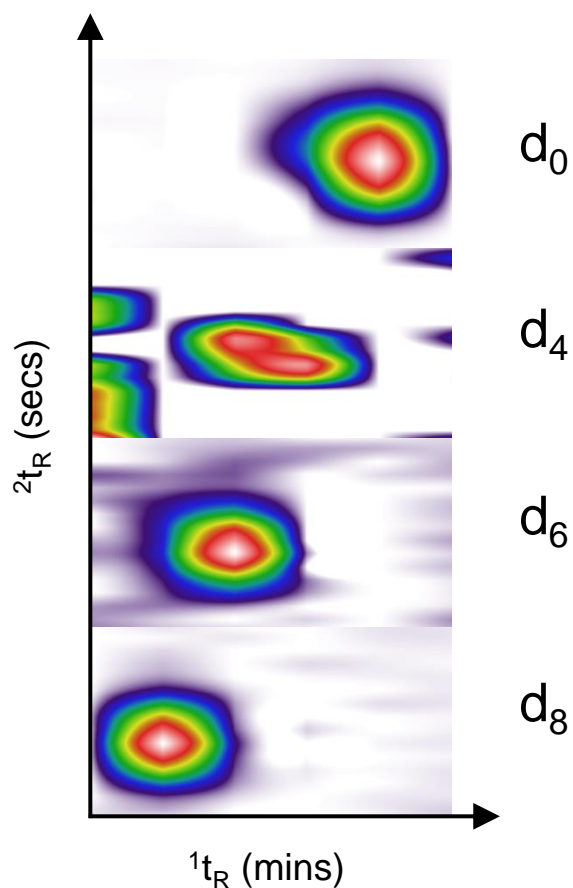
for

### **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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*Beilstein J. Org. Chem.* **2019**, *15*, 1945–1961. [doi:10.3762/bjoc.15.190](https://doi.org/10.3762/bjoc.15.190)

**Extracted ion chromatograms (EIC) of genuine ( $d_0$ ), partially labeled ( $d_4$ ,  $d_6$ ) and fully deuterium-labeled ( $d_8$ )  $\alpha$ -cubebene after administration of [6,6,6- $^2\text{H}_3$ ]-( $\pm$ )-mevalonolactone ( $d_3$ -MVL) to isolated exocarp of grape berries (Lemberger cultivar)**



**Figure S2:** Enlarged sections of a GCxGC chromatogram showing the detected peaks (blobs) of genuine ( $d_0$ ), partially labeled ( $d_4$ ,  $d_6$ ) and fully deuterium-labeled ( $d_8$ )  $\alpha$ -cubebene after feeding experiments using  $d_3$ -MVL. The individual contour plots were obtained by selecting the corresponding mass-to-charge ratios:  $m/z = 204$  ( $d_0$ ),  $m/z = 208$  ( $d_4$ ),  $m/z = 210$  ( $d_6$ ) and  $m/z = 212$  ( $d_8$ ). The gas chromatographic separation of the shown isotopologues is due to the inverse isotope effect, whereby compounds with higher deuterium incorporation elute earlier.