



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)

Philipp P. Könen and Matthias Wüst

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

3D view of signals from genuine and deuterated α -cubebene, α -ylangene and δ -elemene after feeding experiments using d_3 -MVL

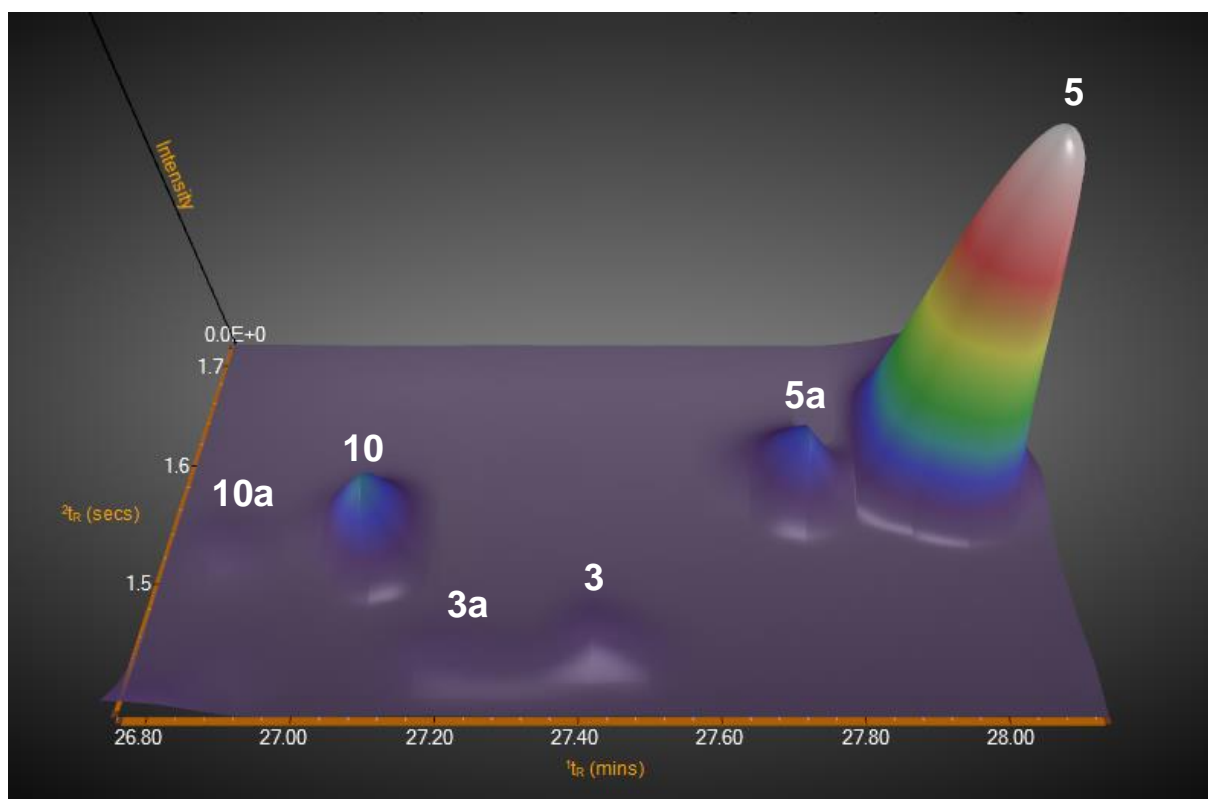


Figure S1: Section of a surface chart (TIC) of a HS-SPME–GC×GC–TOF–MS measurement of genuine sesquiterpene hydrocarbons and their deuterated isotopologues after feeding grape berry exocarp of the grape variety Lemberger with d_3 -MVL. The data is displayed in 3D format, so that the signal intensities are represented in the form of conical signals. Shown are the signals of the two tricyclic sesquiterpene hydrocarbons α -cubebene (d_0 , **10**; d_8 , **10a**) and α -ylangene (d_0 , **5**; d_8 , **5a**) as well as the monocyclic compound δ -elemene (d_0 , **3**; d_8 , **3a**).