

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

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Putative formation pathway of d_8 -(E)- β -caryophyllene and d_9 - α -humulene starting from d_9 -farnesyl pyrophosphate

$$(6,6,6^{-2}H_3]-(\pm)-\text{mevalonolactone}$$

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$$(5,6,6^{-2}H_3)-(\pm)-\text{mevalonolacto$$

Scheme S1: Possible formation of the sesquiterpene hydrocarbons d_8 -(E)- β -caryophyllene and d_9 - α -humulene in grapes from d_9 -farnesyl pyrophosphate (d_9 -FPP). The assumed structural formulas of d_8 -(E)- β -caryophyllene and d_9 - α -humulene are based on feeding experiments of isolated exocarp of the grape variety Lemberger using d_3 -MVL.