

1. Supplementary figures

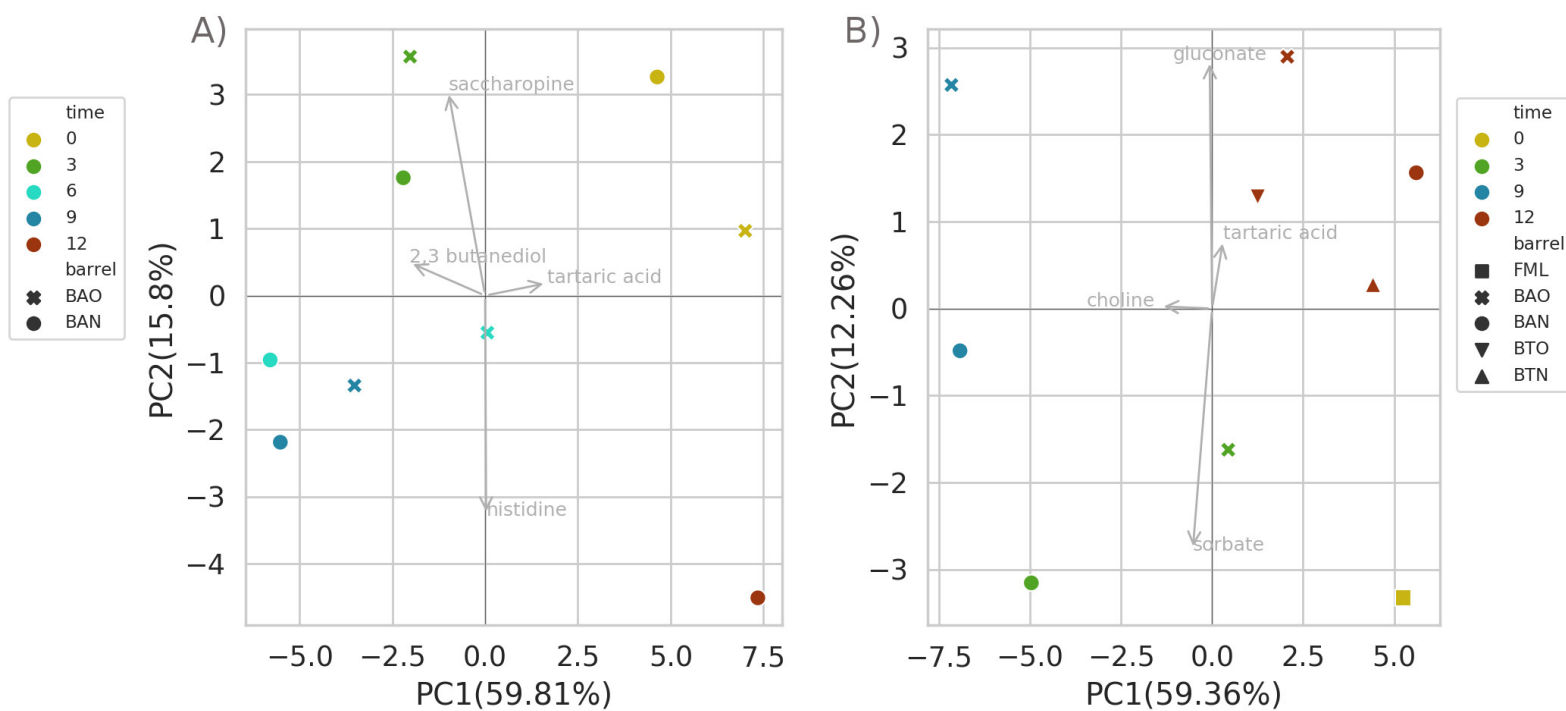


Figure S1: PCoA for cellars FB (A) and ICVV (B) based on the NMR metabolites. Metabolites with highest loadings or practical significance are shown. Acronyms BAN and BAO refer to new and old barrel respectively, FML to final malolactic fermentation stage and BTN and BTO to bottle-aged wine from new and old barrel respectively.

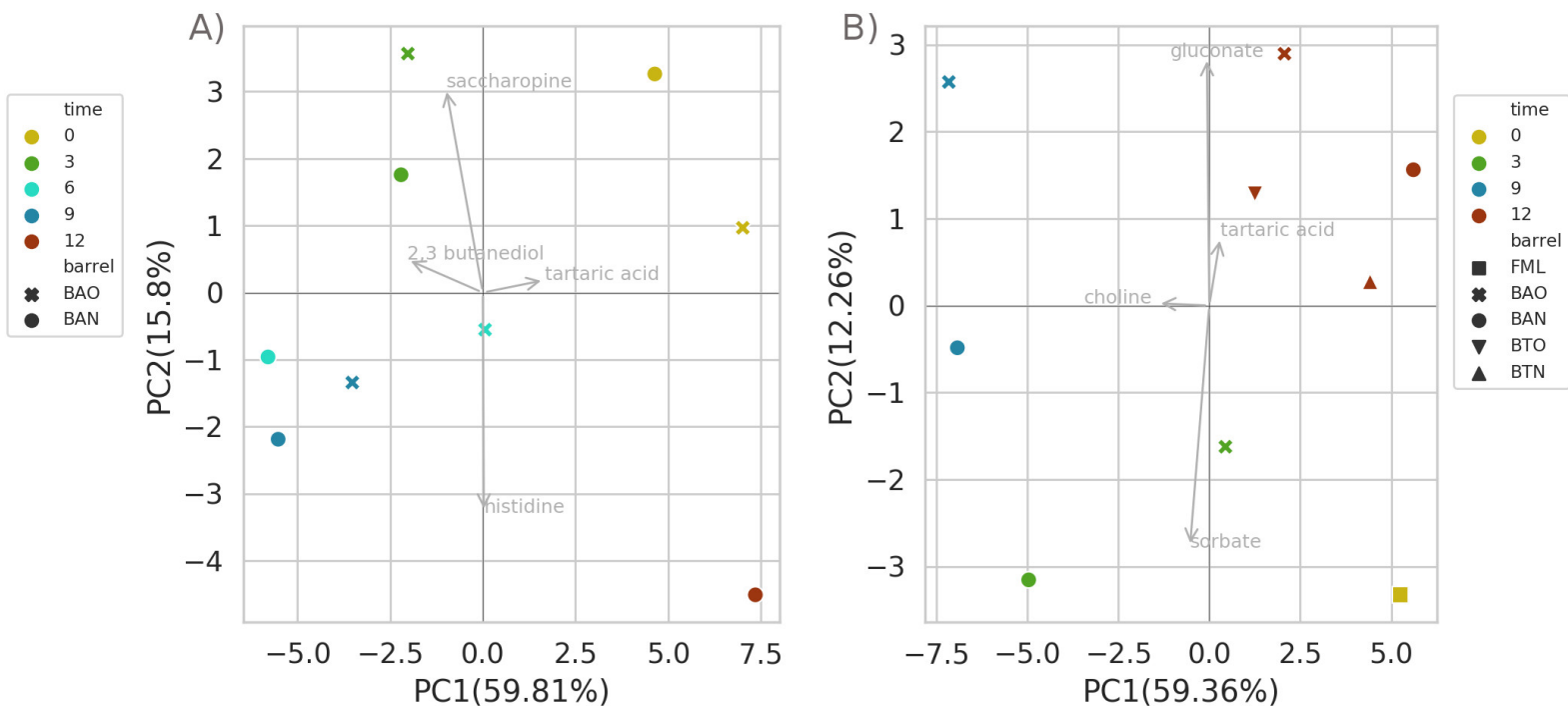


Figure S2: Log2 values of NMR metabolites with practical significance for the cellars FB (A-B) and ICVV (C-H). Acronyms BAN and BAO refer to barrel-aged wine from new and old barrel respectively, FML to final malolactic fermentation stage and BTN and BTO to bottle-aged wine from new and old barrel respectively.

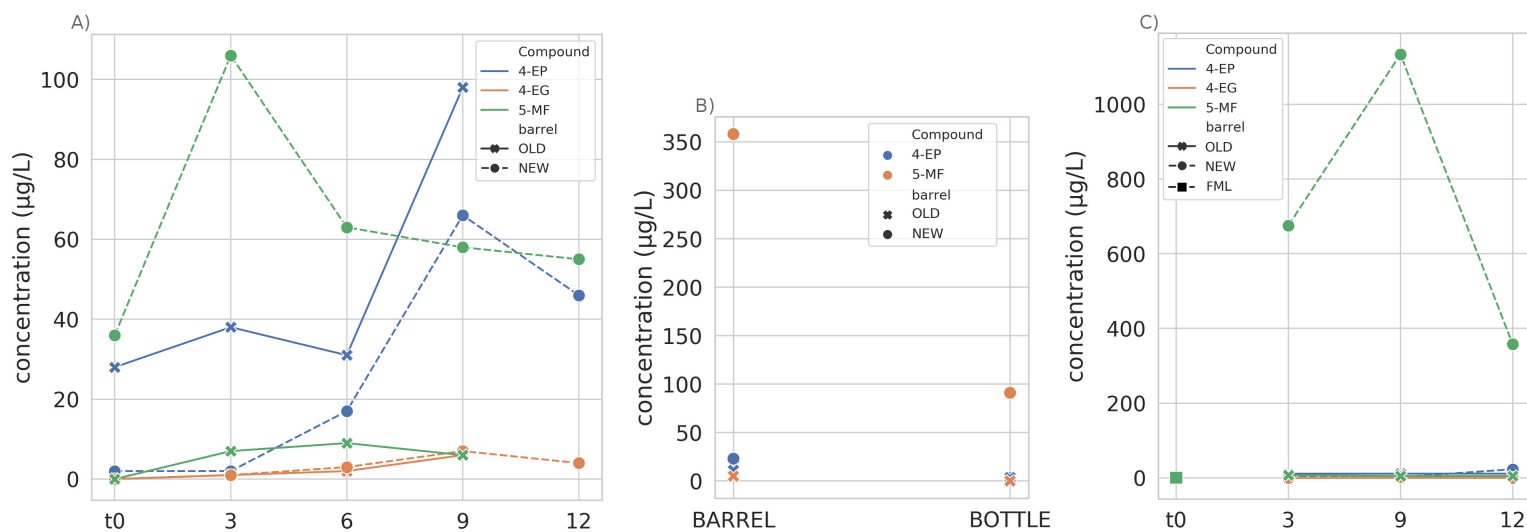


Figure S3: GC-MS targeted for the metabolites 4-ethylphenol (4-EP), 4-ethylguaiacol (4-EG) and 5-methylfurfural (5-MF) based on the factors barrel-type and time for cellar FB (A) and ICVV (C). Figure B concerns the comparison between the 12th month bottle and barrel-aged wine from ICVV cellar. For these samples the concentration of the 4-ethylguaiacol (4-EG) metabolite was zero.

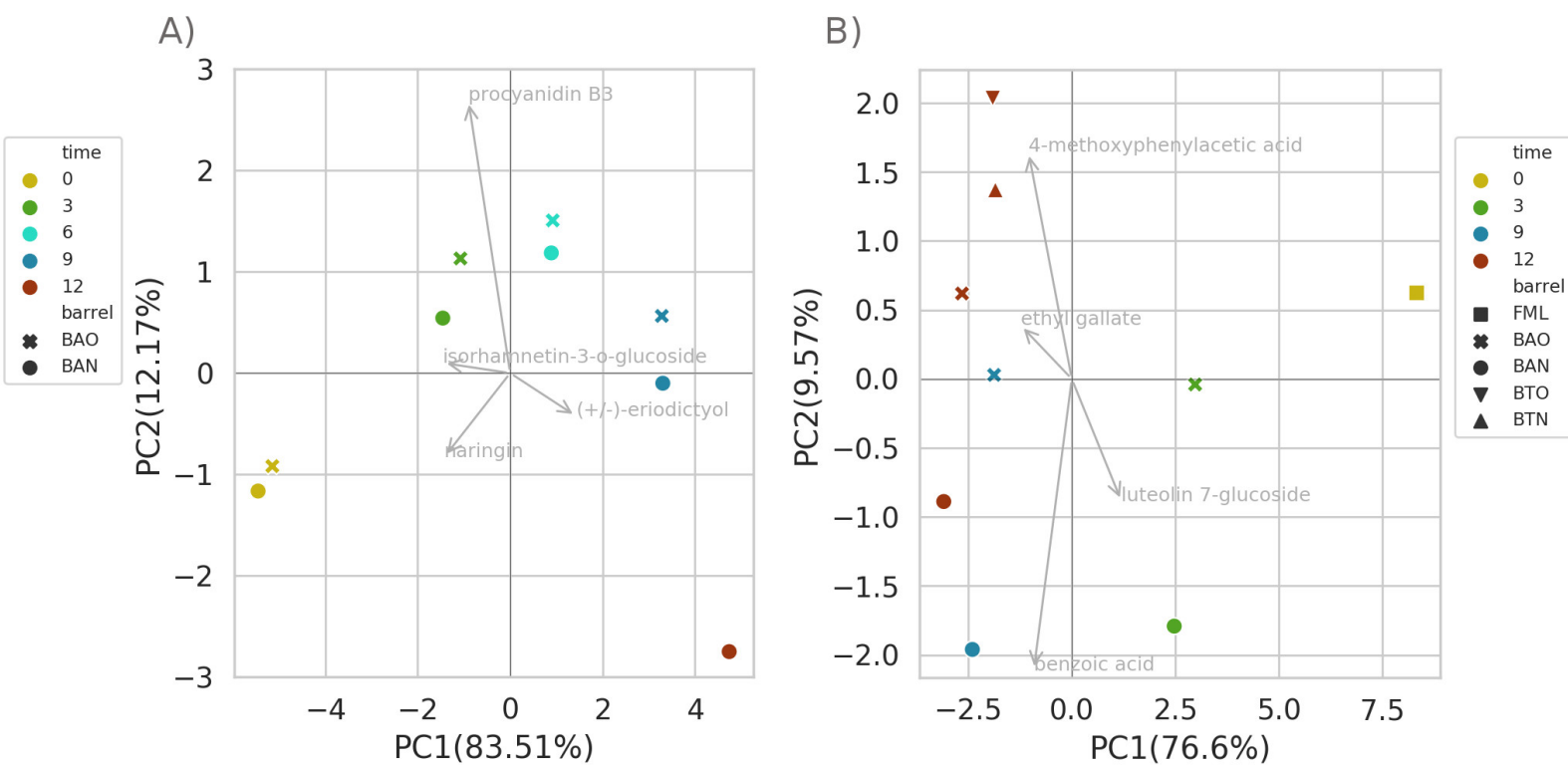


Figure S4: PCoA for cellars FB (A) and ICVV (B) based on the LC-MS metabolites. Metabolites with highest loadings across the principal components are shown. Acronyms BAN and BAO refer to new and old barrel respectively, FML to final malolactic fermentation stage and BTN and BTO to bottle-aged wine from new and old barrel respectively.



Figure S5: LC-MS log2 values of metabolites for cellar FB. Acronyms BAO and BAN refer to barrel-aged wine from old and new barrel respectively. Barplots of metabolites with blue background represent the group of metabolites whose concentration has an increasing trend whereas in orange background the group of metabolites with decreasing tendency.

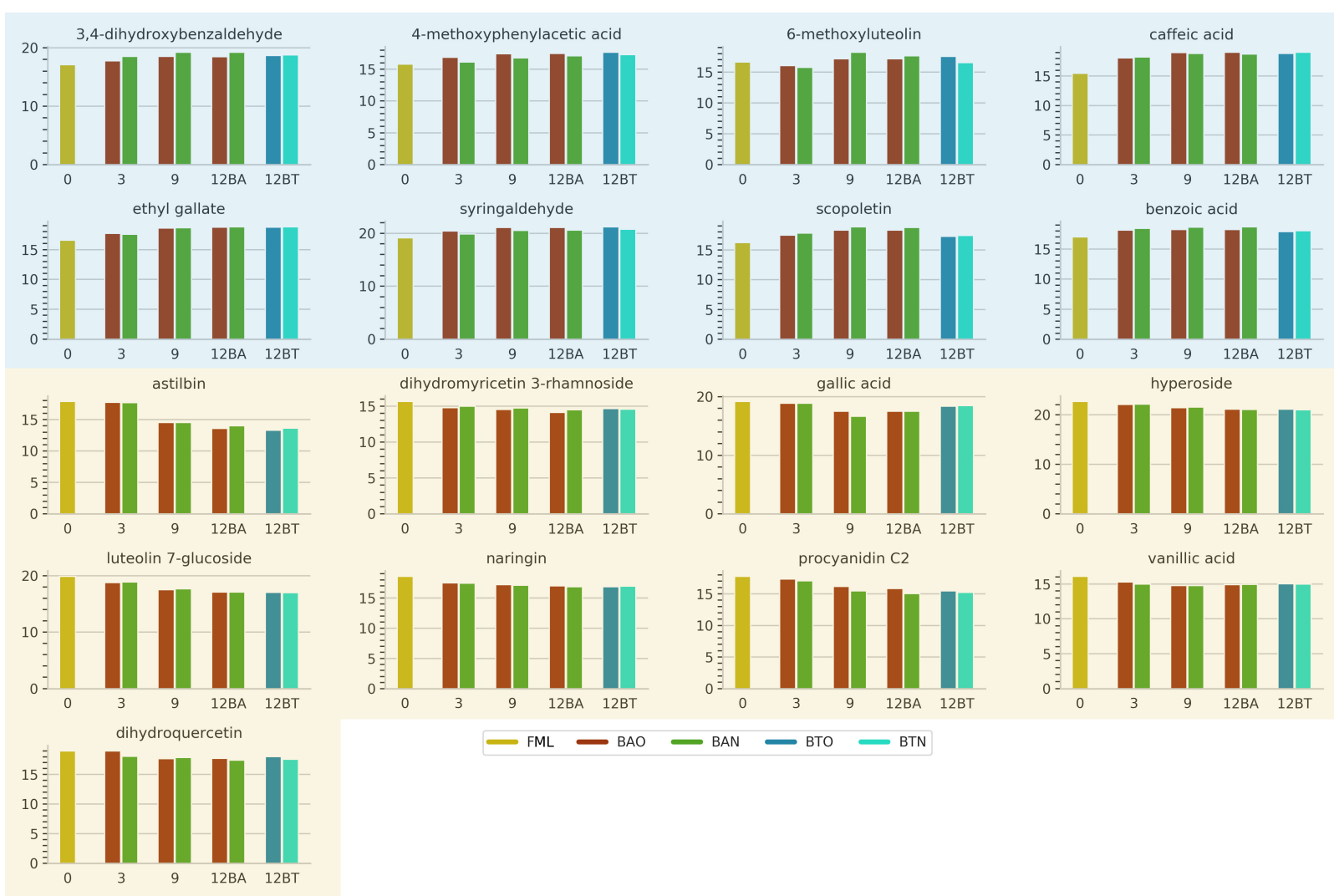


Figure S6: LC-MS log₂ values of metabolites for cellar ICVV. Acronyms BAN and BAO refer to new and old barrel respectively, FML to final malolactic fermentation stage and BTN and BTO to bottle-aged wine from new and old barrel respectively. Barplots of metabolites with blue background represent the group of metabolites whose concentration has an increasing trend whereas in orange background the group of metabolites with decreasing tendency.

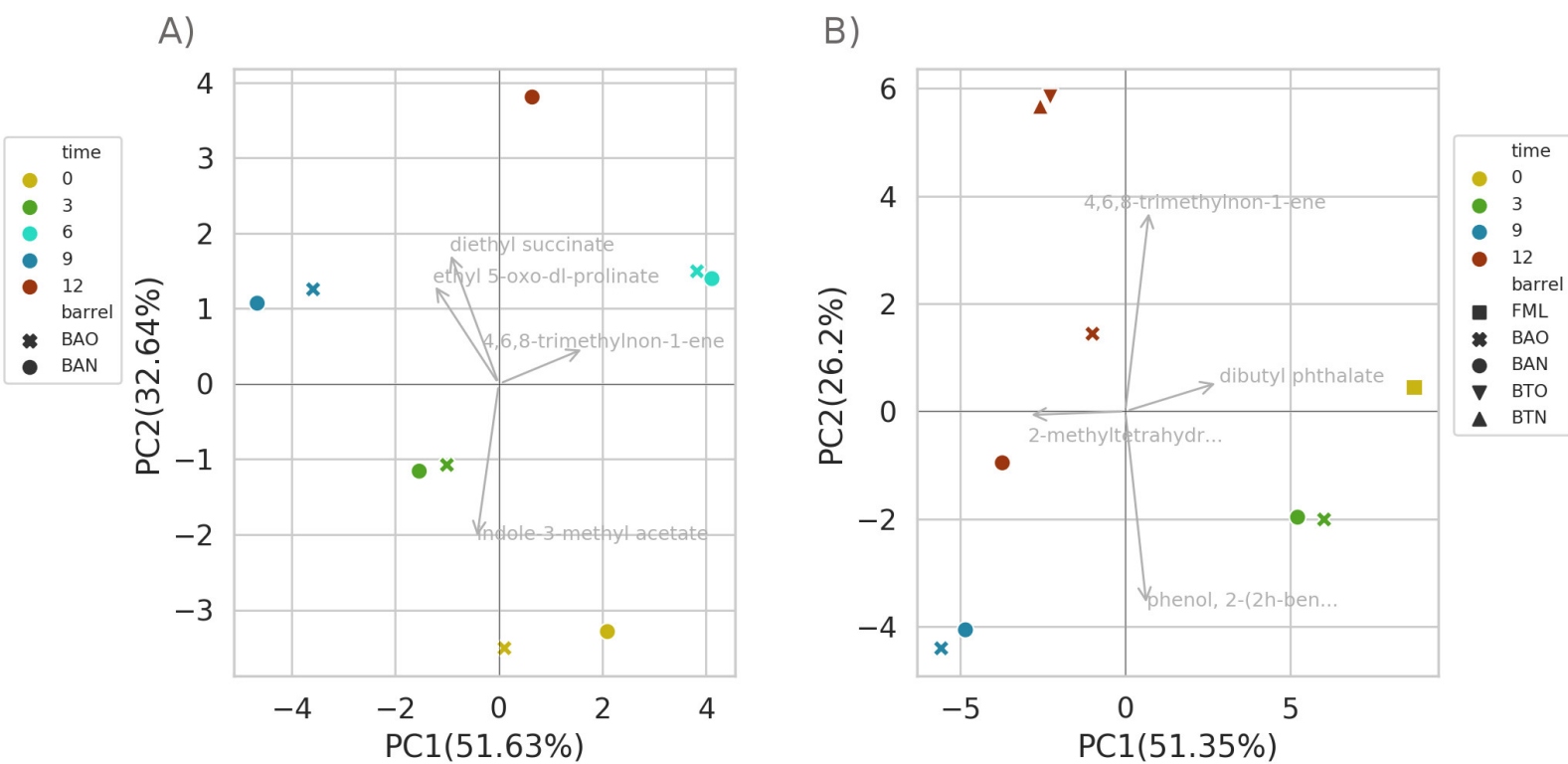


Figure S7: PCoA for cellars FB (A) and ICVV (B) based on the GC-MS metabolites. Metabolites with highest loadings across the principal components are shown. Acronyms BAN and BAO refer to new and old barrel respectively, FML to final malolactic fermentation stage and BTN and BTO to bottle-aged wine from new and old barrel respectively.

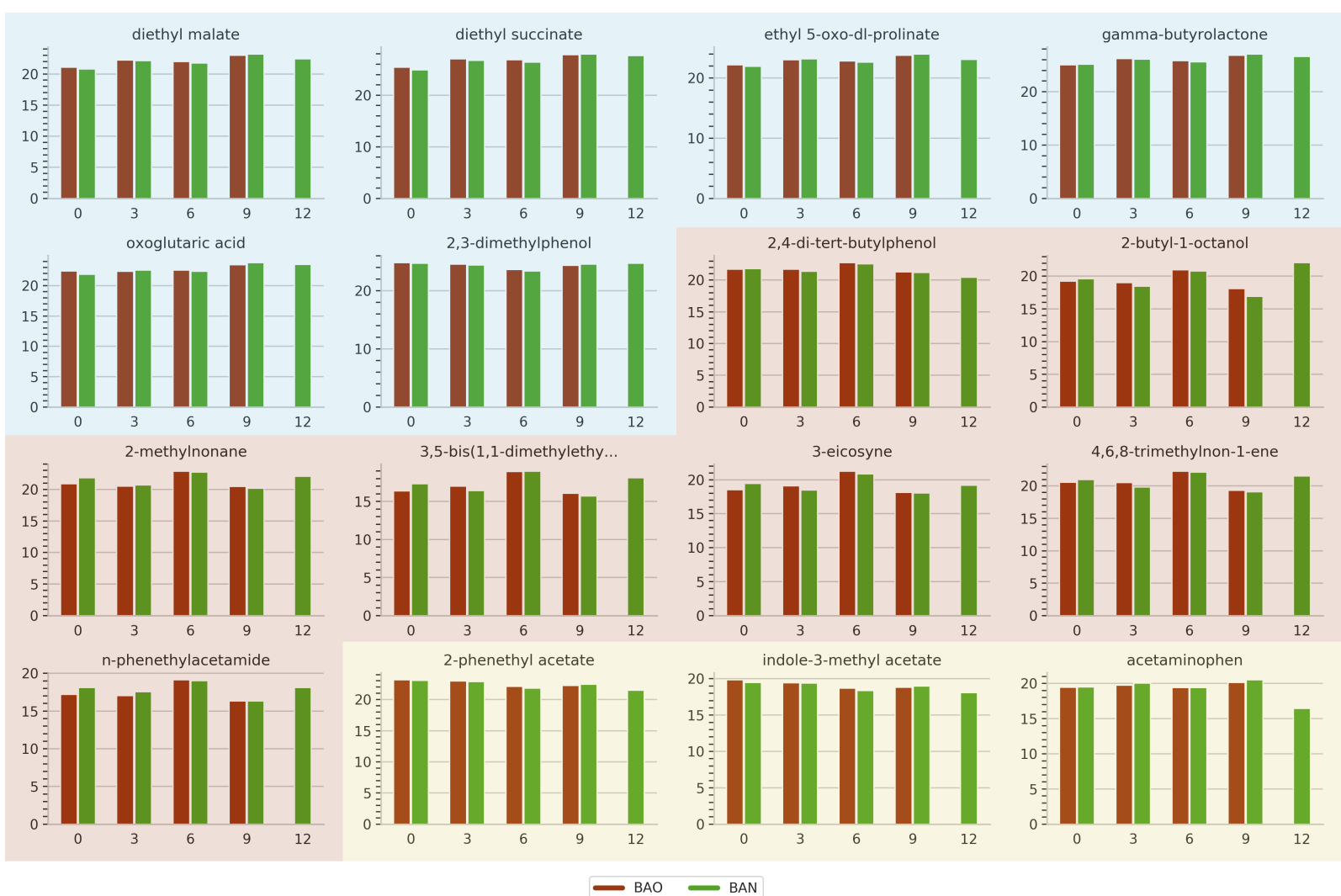


Figure S8: GC-MS log₂ values of metabolites for cellar FB. Acronyms BAO and BAN refer to barrel-aged wine from old and new barrel respectively. Barplots of metabolites with blue background represent the group of metabolites whose concentration has an increasing trend, in orange background the group of metabolites with decreasing tendency and in red background the group of metabolites showing differences during the 6th and 12th month.



Figure S9: GC-MS log₂ values of first 25 out of 48 metabolites for cellar ICVV. Acronyms BAN and BAO refer to new and old barrel respectively, FML to final malolactic fermentation stage and BTN and BTO to bottle-aged wine from new and old barrel respectively. Barplots of metabolites with blue background represent the group of metabolites whose concentration has an increasing trend whereas in orange background the group of metabolites with decreasing tendency.



Figure S10: GC-MS log₂ values of last 23 out of 48 metabolites for cellar ICVV. Acronyms BAN and BAO refer to new and old barrel respectively. Barplots of metabolites with blue background represent the group of metabolites whose concentration has an increasing trend whereas in orange background the group of metabolites with decreasing tendency.

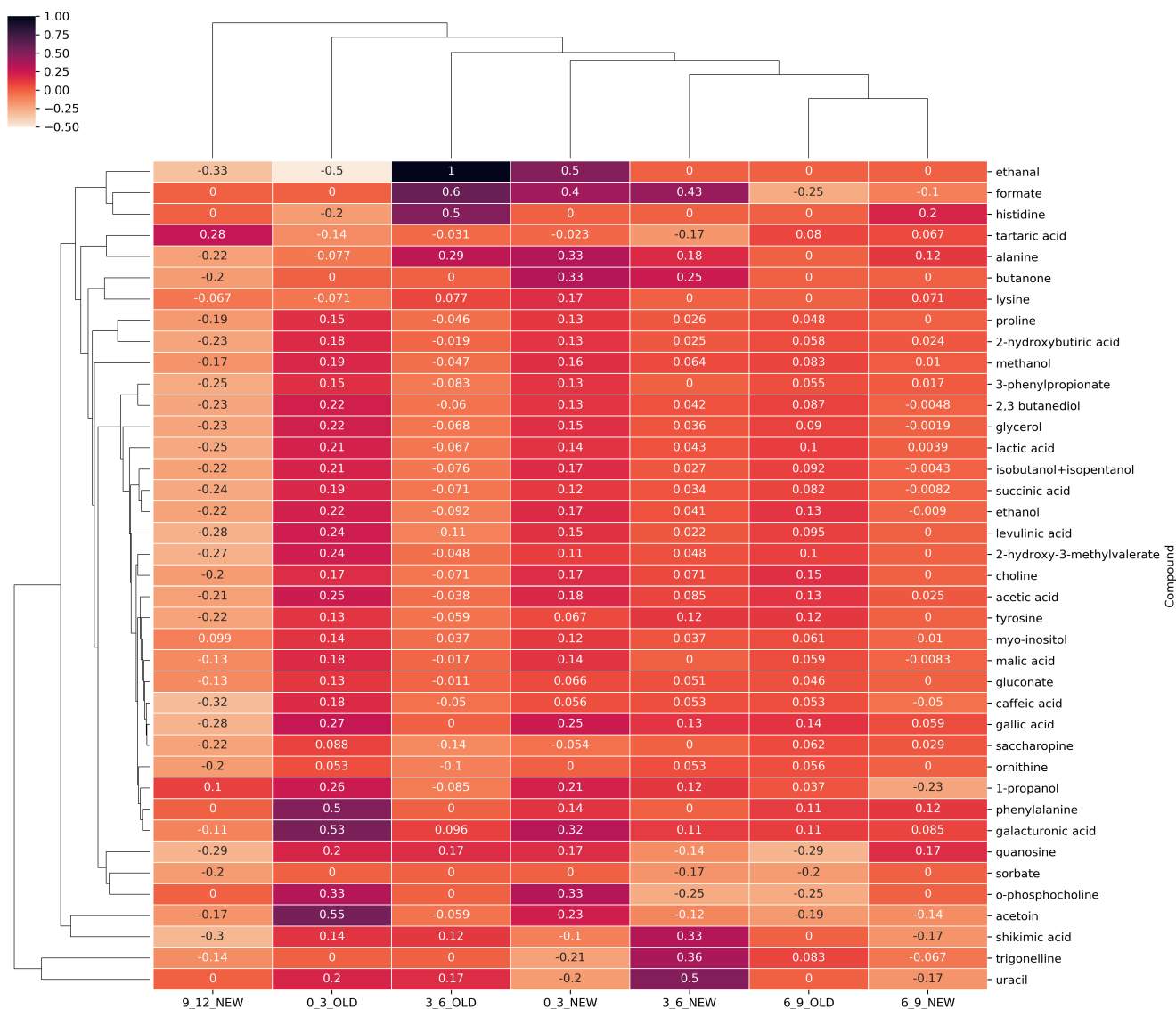


Figure S11: NMR growth rates heatmap for periods 0-3, 3-6, 6-9, and 9-12 based on barrel-type (OLD or NEW) for cellular FB. Values represent percentage of increase or decrease for each metabolite for the given period.

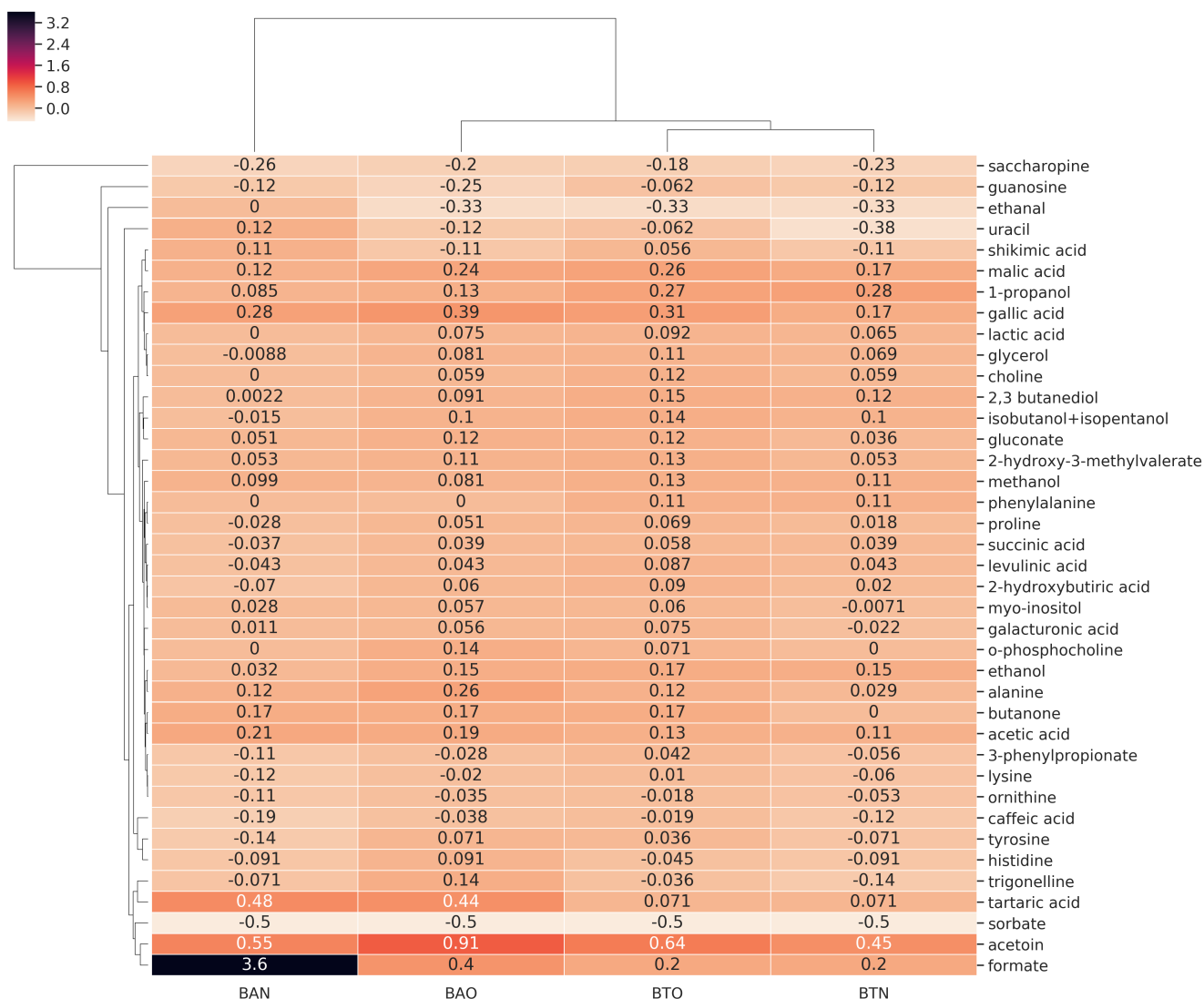


Figure S12: NMR growth rates for period 0-12 of barrel-aged wine from new (BAN) and old (BAO) barrel as well as of bottle-aged wine from new (BTN) and old (BTO) barrel for cellar ICVV. Values represent percentage of increase or decrease for each metabolite for the given period.

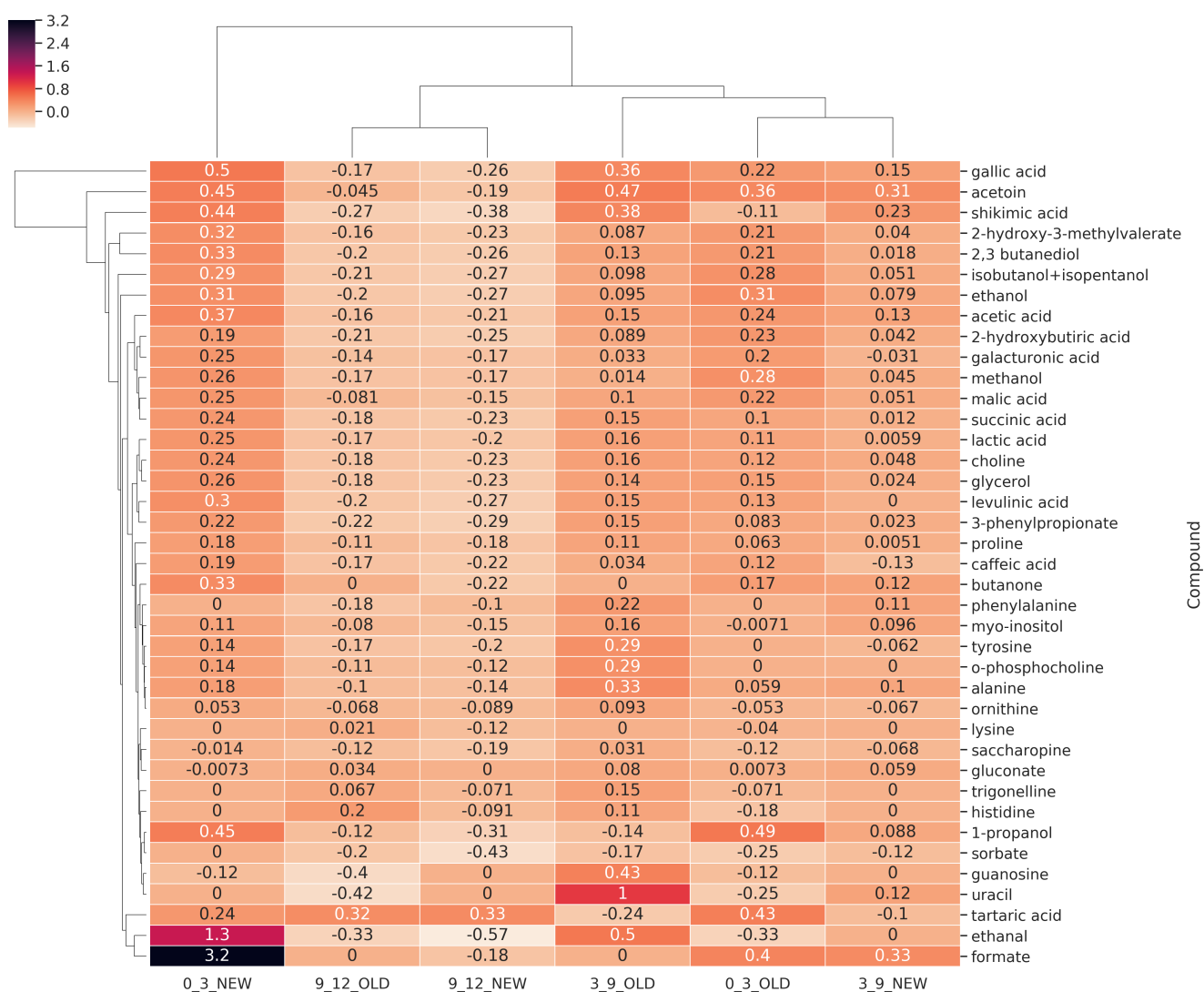


Figure S13: NMR growth rates for period 0-3, 3-9 and 9-12 based on barrel-type (OLD or NEW) for cellular ICVV. Values represent percentage of increase or decrease for each metabolite for the given period.

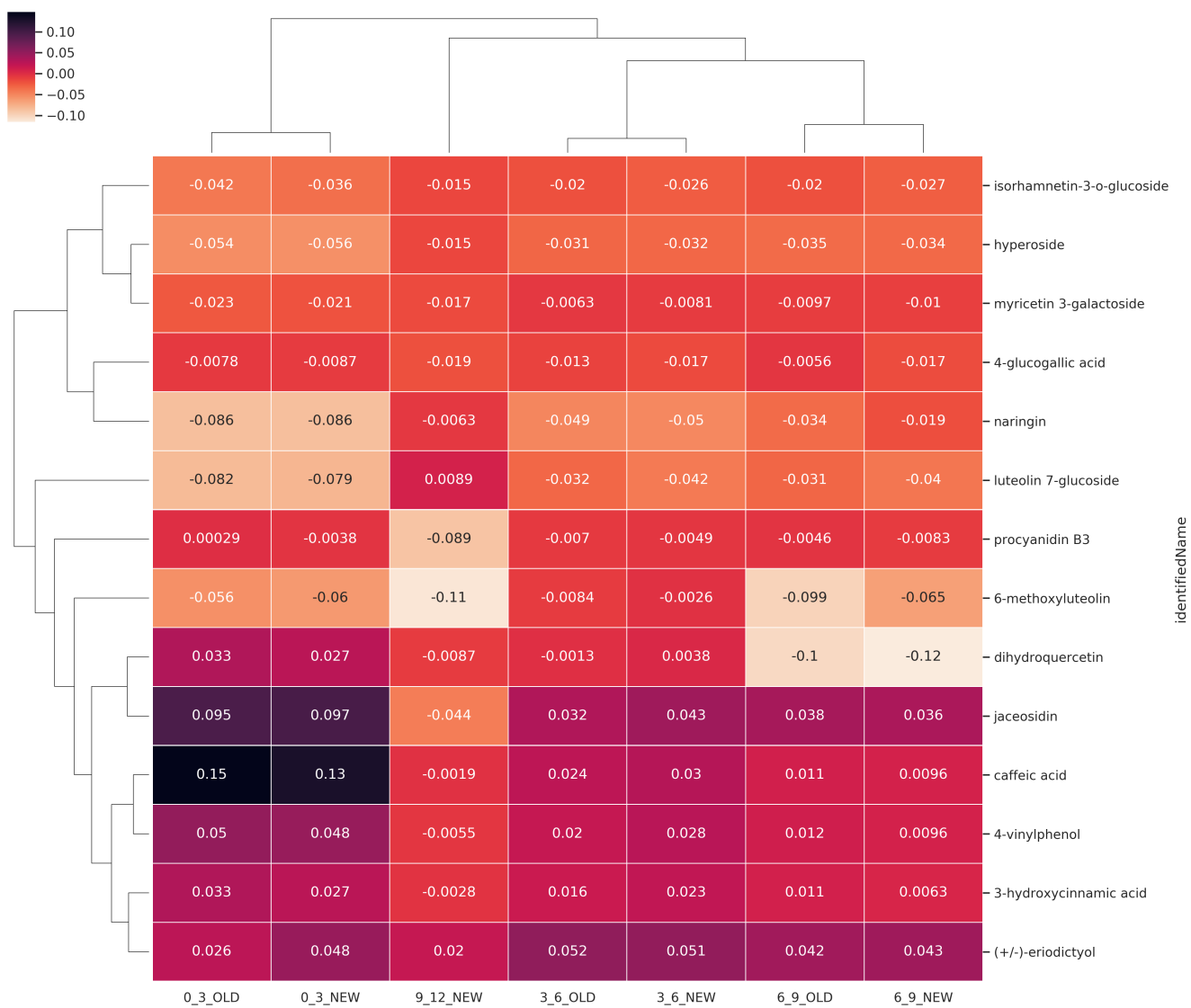


Figure S14: LC-MS growth rates heatmap for periods 0-3, 3-6, 6-9, and 9-12 based on barrel-type (OLD or NEW) for cellular FB. Values represent percentage of increase or decrease for each metabolite for the given period.

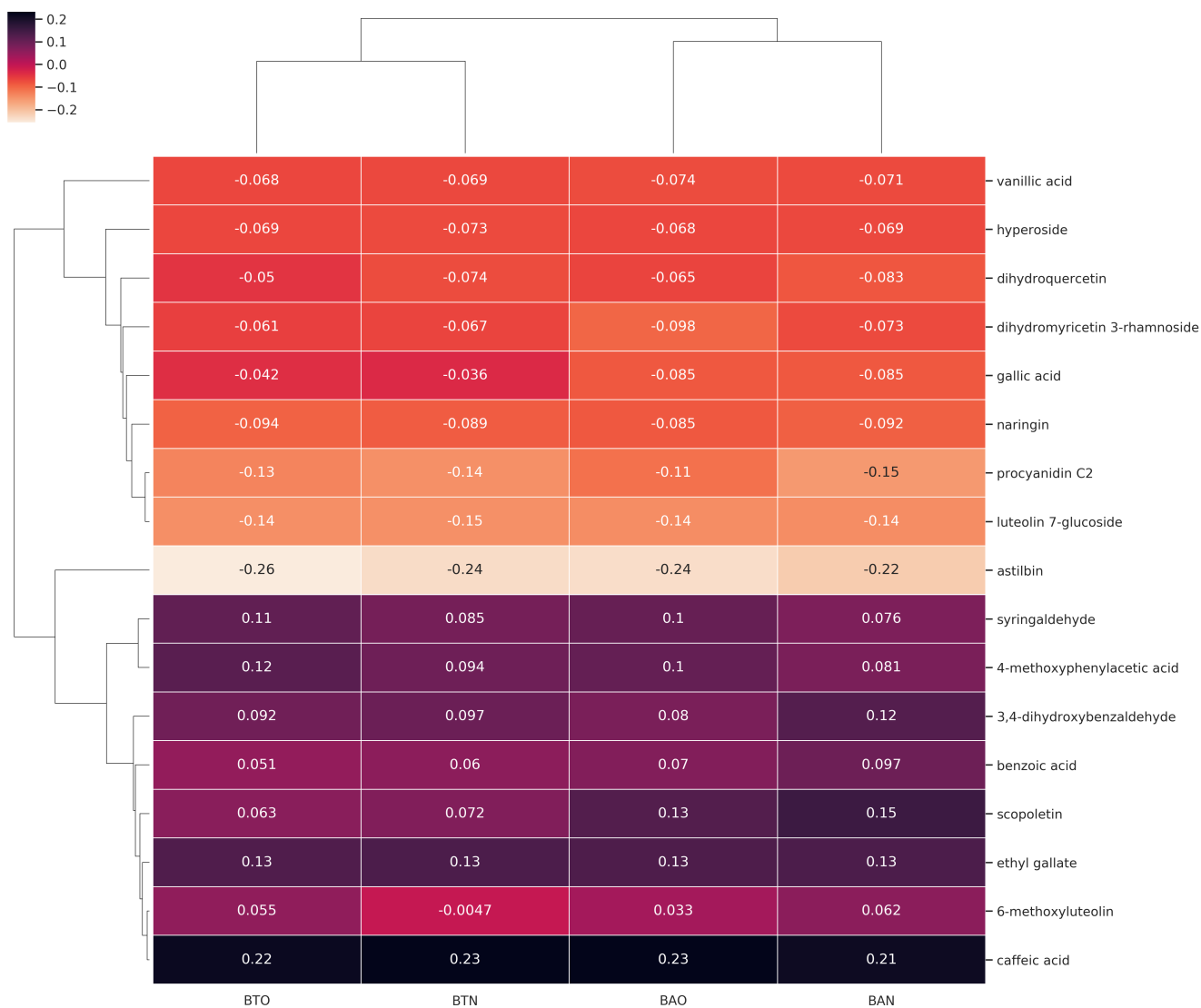


Figure S15: LC-MS growth rates for period 0-12 of barrel-aged wine from new (BAN) and old (BAO) barrel as well as of bottle-aged wine from new (BTN) and old (BTO) barrel for cellar ICVV. Values represent percentage of increase or decrease for each metabolite for the given period.

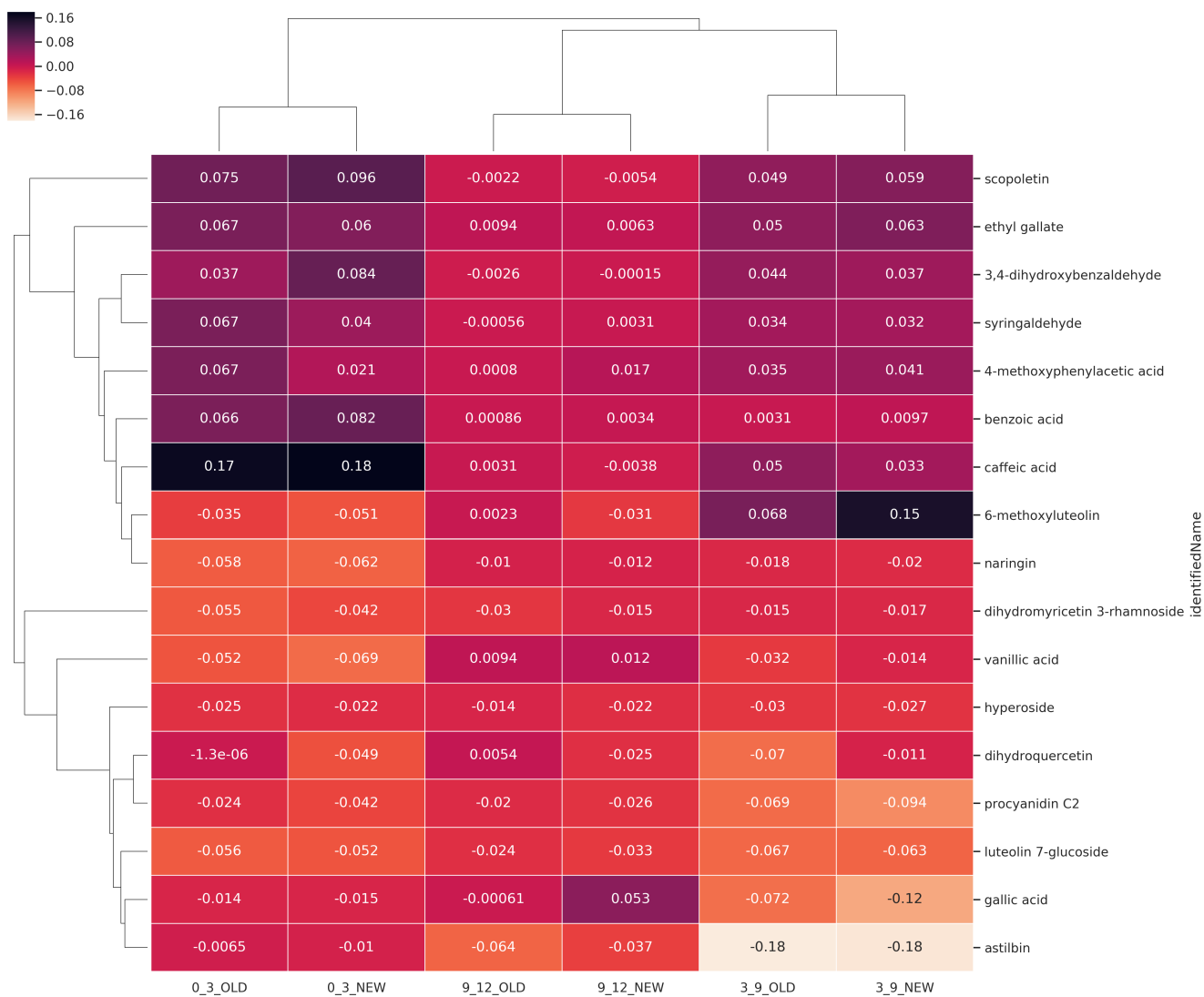


Figure S16: LC-MS growth rates for period 0-3, 3-9 and 9-12 based on barrel-type (OLD or NEW) for cellular ICVV. Values represent percentage of increase or decrease for each metabolite for the given period.

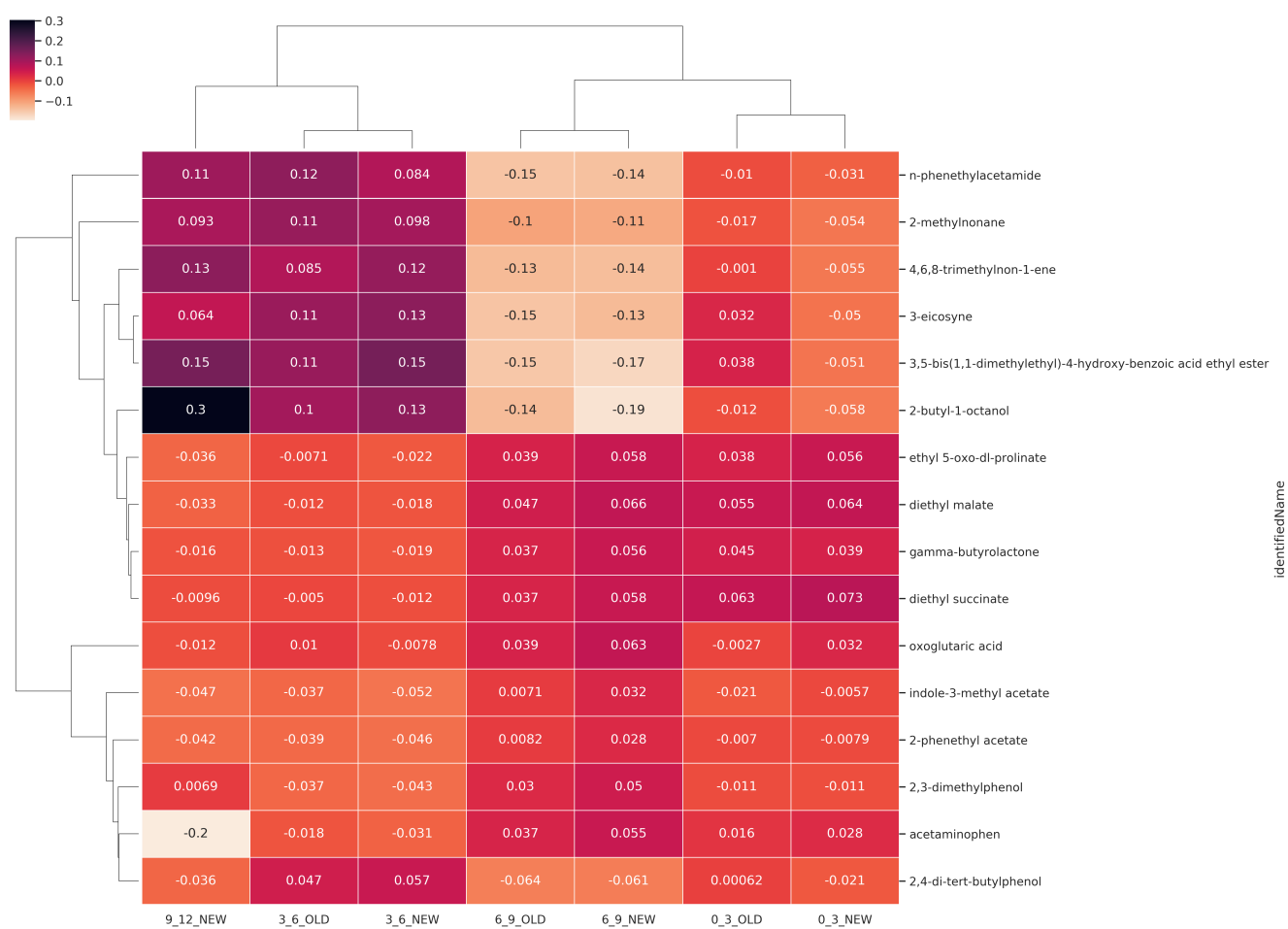


Figure S17: GC-MS growth rates heatmap for periods 0-3, 3-6, 6-9, and 9-12 based on barrel-type (OLD or NEW) for cellular FB. Values represent percentage of increase or decrease for each metabolite for the given period.

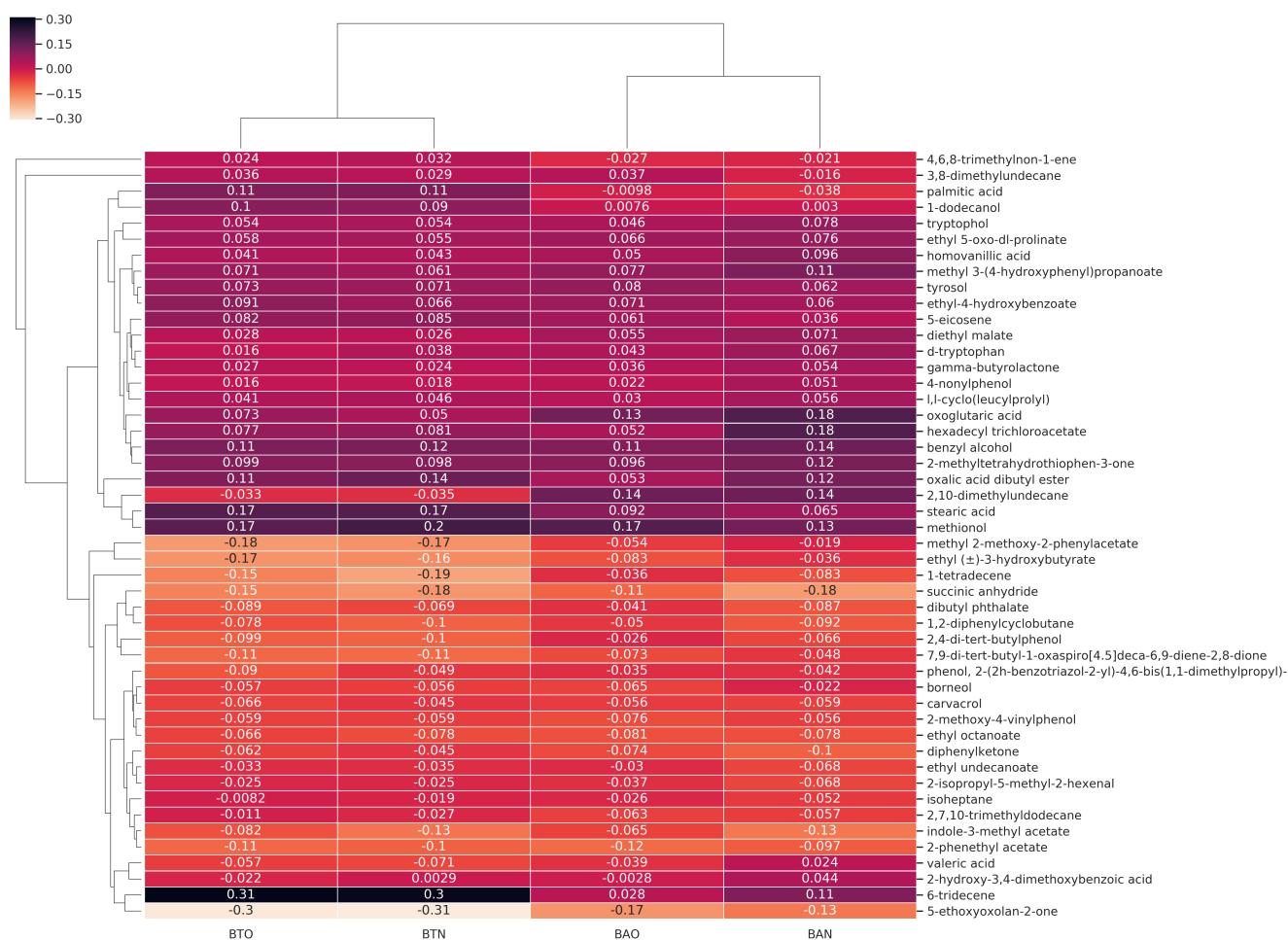


Figure S18: GC-MS growth rates for period 0-12 of barrel-aged wine from new (BAN) and old (BAO) barrel as well as of bottle-aged wine from new (BTN) and old (BTO) barrel for cellar ICVV. Values represent percentage of increase or decrease for each metabolite for the given period.

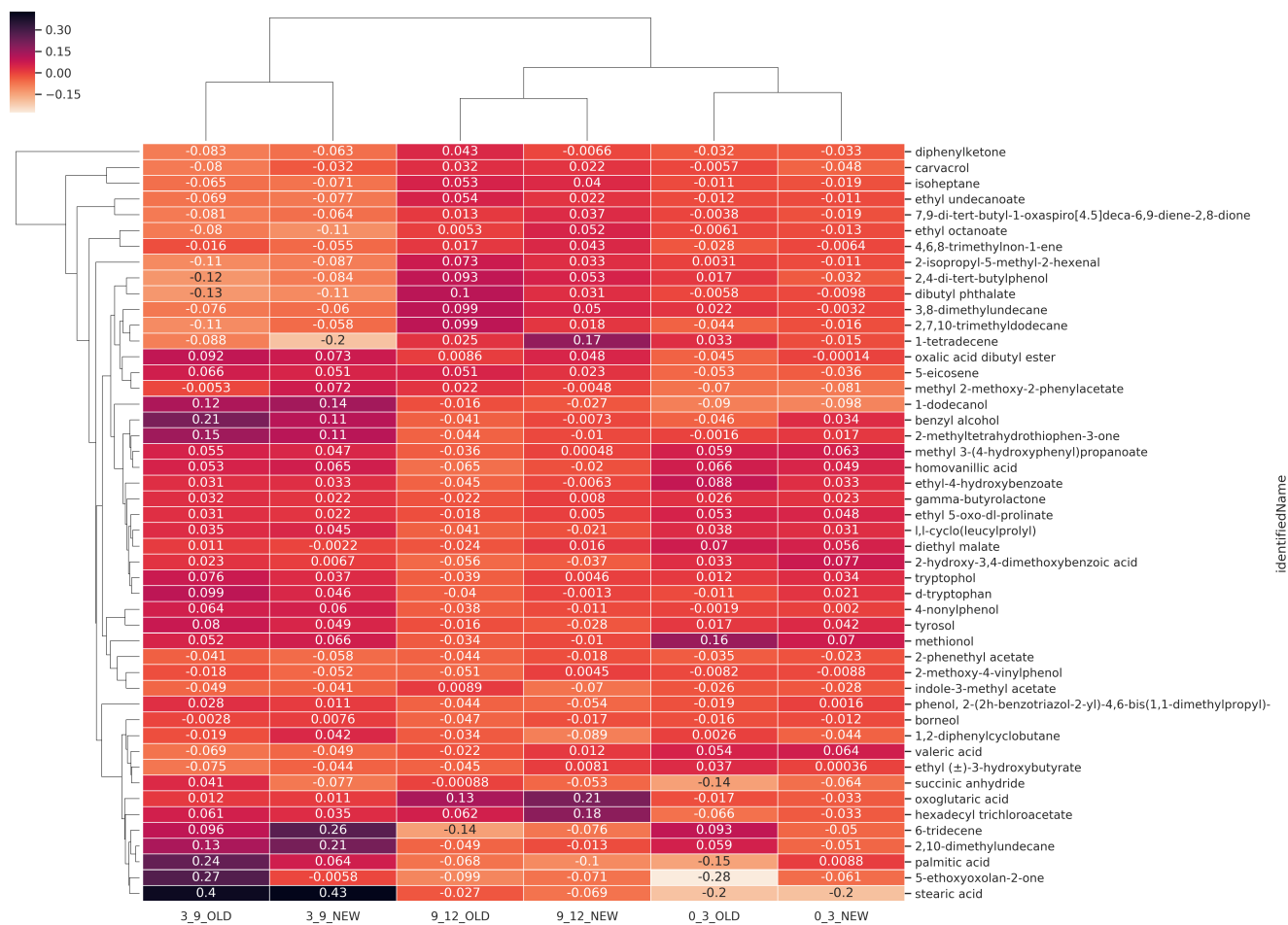


Figure S19: GC-MS growth rates for period 0-3, 3-9 and 9-12 based on barrel-type (OLD or NEW) for cellular ICVV. Values represent percentage of increase or decrease for each metabolite for the given period.