Supplemental Data for:

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Supplemental Table 1 Retention indexes (RI) (on BP21 column), odors, and olfactory perception thresholds, boiling point (BP), partitioning coefficients, and ions monitored in SIM detection for each compound (adapted from Antalick et al. 2010).

Compound	RI	Odors	Perception threshold (µg/L)[a]	BP	Log p	Selected ions[b]
Ethyl propionate	987	solvent, ripe strawberry	2100 (1)	99°C	1.21	**102**/57/75
Ethyl isobutyrate	992	strawberry, kiwi, fruity, solvent	0.1 (2)	112°C	1.77	**116**/88/71
Propyl acetate	995	solvent, fruity		102°C	1.24	**61**/43
Methyl butyrate	1022	ripe kiwi, ripe strawberry, cheese		102°C	1.29	**74**/87/71
Isobutyl acetate	1017	solvent, fruity	1600 (4)	116°C	1.78	**56**/43
Ethyl butyrate	1034	ripe kiwi, ripe strawberry, cheese	1 (2)	120°C	1.85	**88**/71/60
Ethyl 2-methylbutyrate	1046	fruity, kiwi	0.3 (2)	133°C	1.59	**102**/57/85
Ethyl isovalerate	1064	cheese, fruity	3 (3)	132°C	2.26	**88**/85/57
Butyl acetate	1070	solvent, fruity	65 (2)	125°C	1.78	**56**/43
Isoamyl acetate	1114	banana	2 (2)	142°C	2.26	**70**/55/43
Methyl hexanoate	1175	pineapple, fruity, apple		151°C	2.34	**74**/87/99
Ethyl hexanoate	1226	pineapple, fruity, apple	1 (2)	167°C	2.83	**88**/99/60
Isoamyl butyrate	1250	banana, apple, pineapple, fruity		179°C	3.25	**71**/70/55
Hexyl acetate	1258	pear	2 (2)	171°C	2.83	**56**/43
Ethyl heptanoate	1320	pineapple, fruity	220 (5)	189°C	3.32	**88**/101
Ethyl *trans*-2-hexenoate	1331	pineapple, fruity		183°C	2.91	**99**/97/55
Isobutyl hexanoate	1340	fruity, waxy		177°C	3.71	**99**/56/71
Methyl octanoate	1363	waxy, apple skin, fruity		195°C	3.32	**74**/87/127
Ethyl octanoate	1420	waxy, apple skin, fruity	580 (5)	207°C	3.81	**88**/101/127
Isoamyl hexanoate	1437	banana, pineapple, fruity		220°C	4.23	**99**/70
Octyl acetate	1450	waxy, fruity	800 (1)	210°C	3.81	**56**/43
Ethyl nonanoate	1508	waxy, fruity		229°C	4.43	**88**/101
Methyl decanoate	1542	waxy, soap, fruity		224°C	4.41	**74**/87/
Ethyl decanoate	1591	waxy, soap, fruity	200 (2)	243°C	4.96	**88**/101
Isoamyl octanoate	1607	wax, soap, pear		268°C	5.31	**127**/70
Ethyl phenylacetate	1753	flowery, rose, winy	73 (6)	229°C	2.50	**91**/105
Phenylethyl acetate	1789	flowery, mimosa, fruity, olive	250 (7)	239°C	2.27	**104**/91/43
Ethyl dodecanoate	1832	wax, soap		271°C	5.71	**88**/101
Ethyl dihydrocinnamate	1871	fruity, pineapple, almond	1.6 (3)	248°C	2.73	**104**/91/178
Ethyl cinnamate	2122	cherry, fig, fruity, flowery	1.1 (3)	272°C	2.99	**176**/131

[a]Reference from which the value has been taken is given in parentheses:
(1) Dearomatized red wine: Pineau, B., J.C. Barbe, C. Van Leeuwen, and D. Dubourdieu. 2009. Examples of perceptive interactions involved in specific red-and-black-berry aromas in red wines. J. Agric. Food Chem. 57:3702-3708.
(2) Water: Buttery, R.G., R.M. Seifert, L.C. Ling, E.L. Soderstrom, J.M. Ogawa, and J.G. Turnbaugh. 1982. Additional aroma components of honeydew melon. J. Agric. Food Chem. 30:1208-1211.
(3) 11% water/ethanol solution containing 7 g/L glycerol and 5 g/L tartaric acid, pH adjusted to 3.4 with 1 M NaOH: Ferreira, V., R. Lopez, and J.F. Cacho. 2000. Quantitative determination of the odorants of young red wines from different grape varieties. J. Sci. Food Agric. 80:1659-1607.
(4) 10% water/ethanol mixture containing 5 g/L tartaric acid at pH 3.2: Aznar, M., R. Lopez, J.F. Cacho, and V. Ferreira. 2001. Identification and quantification of impact odorants of aged red wines from Rioja. GC-olfactometry, quantitative GC-MS, and odor evaluation of HPLC fractions. J. Agric. Food Chem. 49:2924-2929.
(5) Wine: Etievant, P.X. 1991. Wine. *In* Volatile Compounds in Foods and Beverage. H. Maarse (ed.), pp. 483-586. Dekker, New York.
(6) Red wine: Tat, L., P. Comuzzo, F. Battistutta, and R. Zironi 2007. Sweet-like off-flavor in Aglianico del Vulture wine: Ethyl phenylacetate as the mainly involved compound. J. Agric. Food Chem. 55:5205-5212.
(7) 10% water/ethanol solution: Guth, H. 1997. Quantitation and sensory studies of character impact odorants of different white wine varieties. J. Agric. Food Chem. 45:3027-3032.
[b]Quantitative ions are marked in bold font and qualitative ions are marked in regular font.

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Supplemental Table 2 Linearity, limits of detection (LOD) and quantification (LOQ), repeatability, reproducibility, and accuracy of the method.

	Internal standard	Concn range	Mean r^2	Slope reproducibility (RSD %) (n = 3)	LOD (µg/L)	LOQ (µg/L)	Repeatability (RSD %) (n = 10)	Reproducibility (RSD %) (n = 5)	Recovery[a]			
									Red (%)	Dry white (%)	Sweet white (%)	Model solution[b] (%)
Ethyl propanoate	ethyl-d_5 butyrate	1.22-609 µg/L	0.9949	2.7	1.22	4.05	3.9	3.3	105	110	93	96
Ethyl isobutyrate	ethyl-d_5 butyrate	1.11-554 µg/L	0.9966	5.6	0.2471	0.8235	3	1.5	106	109	101	95
Propyl acetate	ethyl-d_5 butyrate	1.08-541 µg/L	0.9987	3.6	0.4518	1.5060	4.3	4.8	92	107	120	85
Isobutyl acetate	ethyl-d_5 butyrate	1.01-505 µg/L	0.9988	4.9	0.1618	0.5392	5.8	6.1	99	103	92	97
Methyl butyrate	ethyl-d_5 butyrate	1.08-541 µg/L	0.9979	3.1	0.3254	1.0846	2.5	4.2	98	96	100	85
Ethyl butyrate	ethyl-d_5 butyrate	8.14-4070 µg/L	0.9985	9.1	0.0346	0.1154	3	3.6	100	106	107	94
Ethyl 2-methylbutyrate	ethyl-d_5 butyrate	0.61-307 µg/L	0.9978	5.1	0.0172	0.0575	6.3	7.3	95	109	103	100
Ethyl isovalerate	ethyl-d_5 butyrate	0.58-291 µg/L	0.9966	7.9	0.0146	0.0485	4.9	2.1	103	94	106	93
Butyl acetate	ethyl-d_5 butyrate	1.01-503 µg/L	0.9959	6.7	0.3051	1.0169	5.8	15.0	106	95	98	95
Isoamyl acetate	ethyl-d_5 butyrate	5.37-2685 µg/L	0.9984	4.5	0.1097	0.3658	3.6	3.4	104	97	120	89
Methyl hexanoate	ethyl-d_5 hexanoate	0.11-55 µg/L	0.9984	2.2	0.0064	0.0213	3.4	3.9	91	105	94	85
Ethyl hexanoate	ethyl-d_5 hexanoate	5.58-2790 µg/L	0.9970	6.8	0.0025	0.0083	4.7	6.1	94	114	85	102
Isoamyl butyrate	ethyl-d_5 hexanoate	0.10-51.2 µg/L	0.9988	2.8	0.0056	0.0188	2.5	3.3	104	95	95	95
Hexyl acetate	ethyl-d_5 hexanoate	0.55-276 µg/L	0.9989	1.4	0.0115	0.0384	3.2	5.2	105	91	97	95
Ethyl heptanoate	ethyl-d_5 hexanoate	0.12-58.3 µg/L	0.9977	6.3	0.0009	0.0030	2.4	6.2	95	106	98	101
Ethyl *trans*-2-hexenoate	ethyl-d_5 hexanoate	0.10-52.1 µg/L	0.9975	4.2	0.0138	0.0461	4.1	3.3	95	93	78	92
Isobutyl hexanoate	ethyl-d_5 hexanoate	0.10-49.4 µg/L	0.9980	5.7	0.0014	0.0048	7.8	8.0	97	115	83	106
Methyl octanoate	ethyl-d_5 hexanoate	0.11-55.8 µg/L	0.9986	2.5	0.0005	0.0016	6.6	6.8	95	110	94	103
Ethyl octanoate	ethyl-d_5 octanoate	5.6-2800 µg/L	0.9990	7.0	0.0009	0.0031	5	9.0	95	83	97	99
Isoamyl hexanoate	ethyl-d_5 octanoate	0.11-54.4 µg/L	0.9973	4.4	0.0011	0.0038	3.2	4.2	102	112	95	93
Octyl acetate	ethyl-d_5 octanoate	0.12-58.7 µg/L	0.9953	8.7	0.0044	0.0148	11.2	11.8	103	112	111	87
Ethyl nonanoate	ethyl-d_5 octanoate	0.12-59.8 µg/L	0.9963	4.0	0.0004	0.0013	3	6.2	99	102	111	107
Methyl decanoate	ethyl-d_5 octanoate	0.12-60.4 µg/L	0.9982	4.5	0.0001	0.0004	4.6	11.4	94	124	101	106
Ethyl decanoate	ethyl-d_5 octanoate	5.32-2660 µg/L	0.9976	3.7	0.0002	0.0006	6.4	8.8	94	120	130	107
Isoamyl octanoate	ethyl-d_5 octanoate	0.56-278 µg/L	0.9966	13.9	0.0021	0.0070	5.4	12.7	92	117	90	97
Ethyl dodecanoate	ethyl-d_5 octanoate	5.27-527 µg/L	0.9924	9.1	0.0001	0.0004	8.6	12.9	109	116	106	114
Ethyl phenylacetate	ethyl-d_5 cinnamate	0.64-322 µg/L	0.9951	1.6	0.0071	0.0238	3.7	4.0	105	92	101	91
Phenylethyl acetate	ethyl-d_5 cinnamate	0.59-295 µg/L	0.9985	4.4	0.0050	0.0166	4.1	4.8	100	96	107	89
Ethyl dihydrocinnamate	ethyl-d_5 cinnamate	0.59-297 µg/L	0.9987	6.6	0.0030	0.0100	7.4	2.6	102	102	113	97
Ethyl cinnamate	ethyl-d_5 cinnamate	0.64-319 µg/L	0.9990	1.5	0.0136	0.0453	2.1	4.0	96	102	108	100

[a]For recovery calculations, wine samples were spiked at 50 µg/L for ethyl esters of fatty acids, higher alcohol acetates, ethyl esters of branched acids, and ethyl propionate. Cinnamates, methyl esters, isoamyl esters, ethyl esters of odd carbon number fatty acids, ethyl *trans*-2-hexenoate, and isobutyl hexanoate were spiked at 5 µg/L.
[b]Model solution (ethanol in water, 12% vol).

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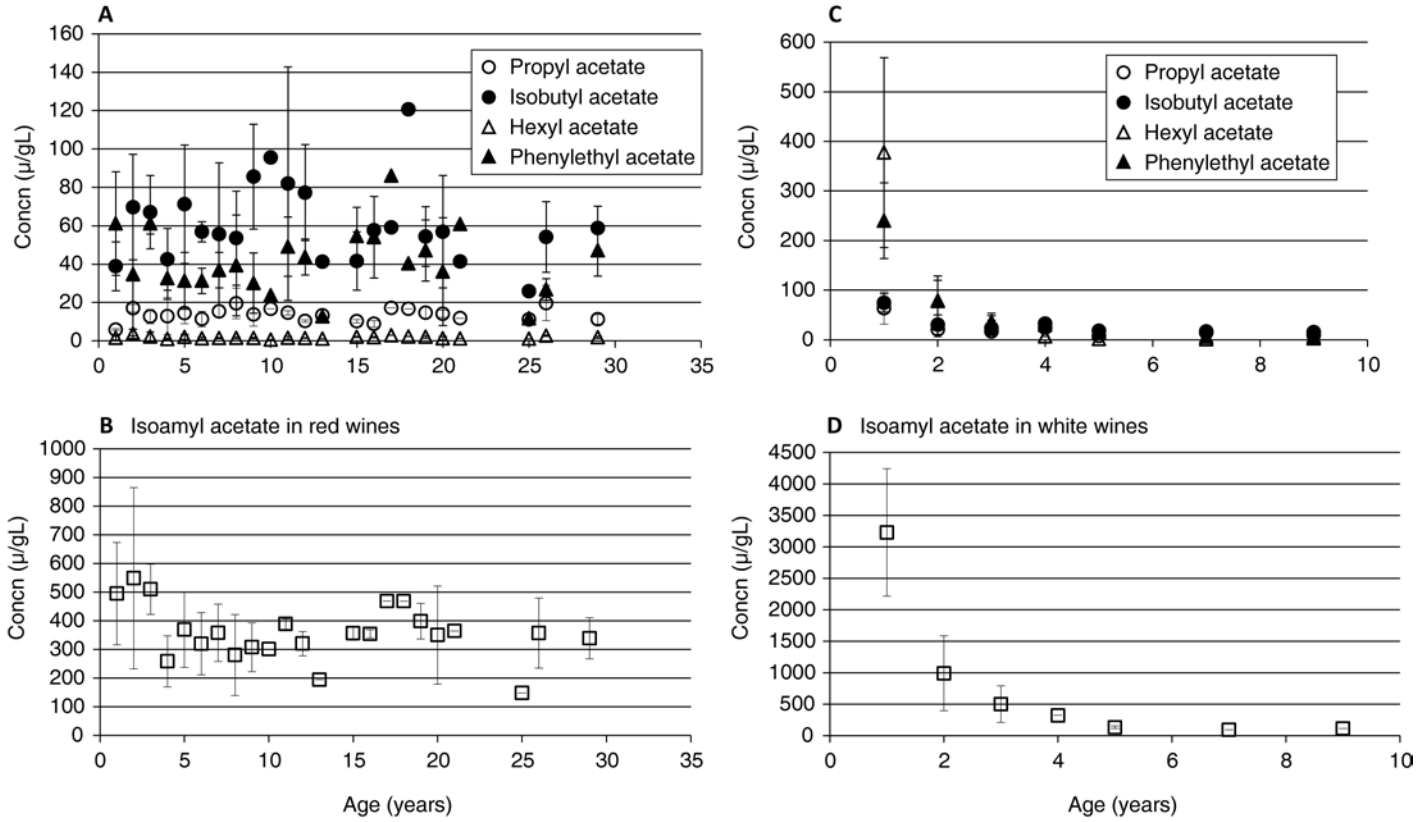

Supplemental Figure 1 Evolution of mean concentrations of higher alcohol acetates with standard deviations according to wine age. Propyl, isobutyl, hexyl, and phenylethyl acetates in red wines (**A**) and white wines (**C**); isoamyl acetate in red wines (**B**) and white wines (**D**).

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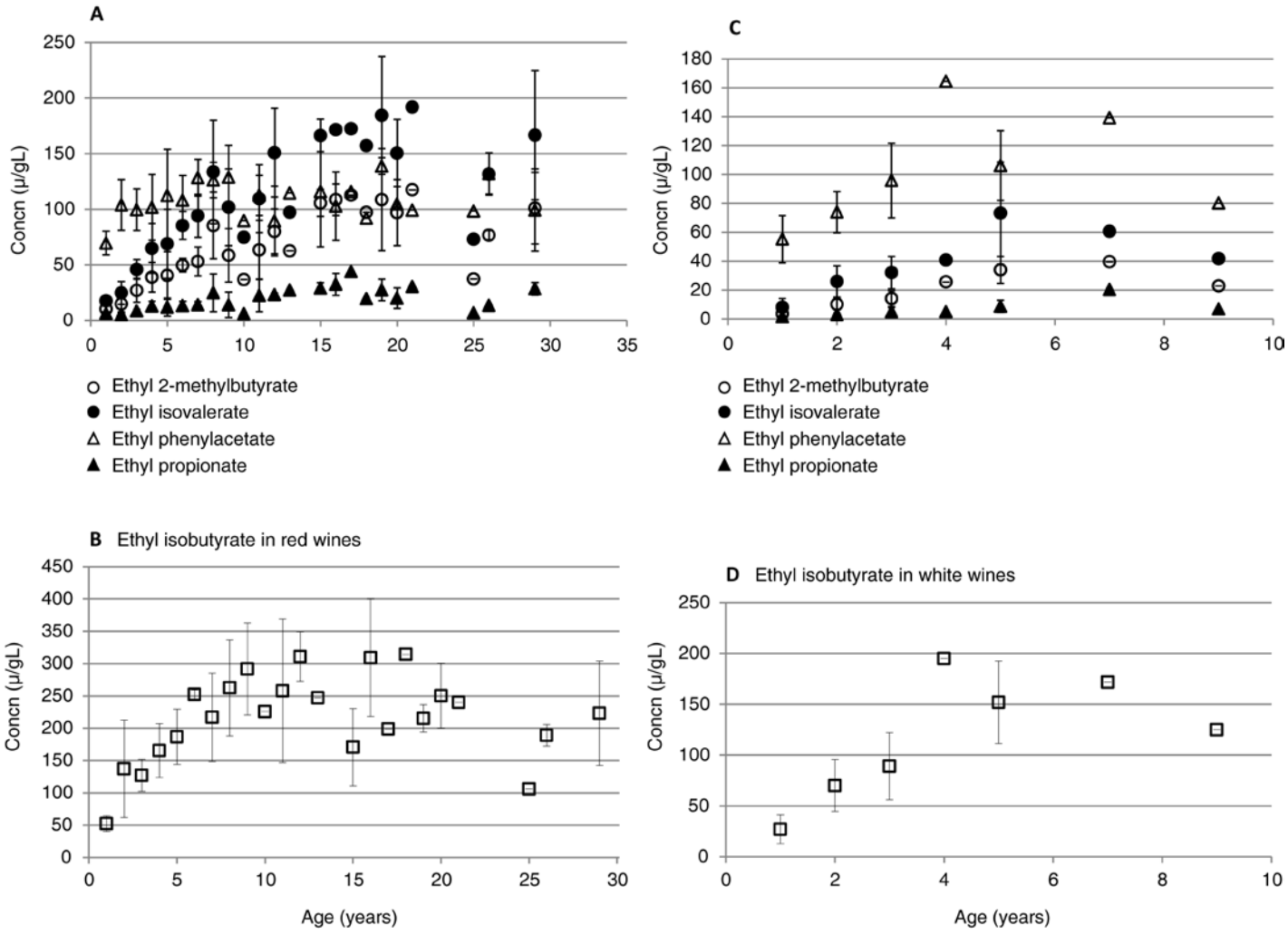

Supplemental Figure 2 Evolution of mean concentrations of ethyl esters of branched acids with standard deviations according to wine age. Ethyl 2-methylbutyrate, isovalerate, phenylacetate, and propionate in red wines (**A**) and white wines (**C**); ethyl isobutyrate in red wines (**B**) and white wines (**D**).