Volatile compounds release from oak chips in model wine media: combined influence of toasting degree, size, time of contact and ethanol content

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Supporting information

Table S1: extracted compounds grouped by the main factor size.

Size	Furfural	5-methylfurfural	Furfuryl alcohol	Maltol	Cyclotene	Whiskey lactones	Guaiacol	Eugenol	Vanillin
Large	1'069.68 ± 152.15	106.10 ± 12.32	8.82 ± 1.12	20.67 ± 2.59	2.80 ± 0.42	62.22 ± 5.46	23.91 ± 2.47	14.34 ± 1.13	579.62 ± 72.17
Small	703.76 ± 103.03	108.04 ± 18.62	8.22 ± 1.85	27.88 ± 3.94	4.96 ± 0.75	64.23 ± 5.97	31.31 ± 3.57	14.99 ± 1.35	595.14 ± 67.98
Sign.	***	ns	***(log1p)	*** (log1p)	***	ns	NA	ns	ns

Data are reported as mean [µg · L^{-1}] plus and minus standard error. Sign. = significance of ANOVA on linear mixed model fitted; ns = not significant, *** = 99.9 % significant. log1p = model fitted applying $\log_{10}(x_i+1)$ transformation due to meet the statistical assumptions. NA = not available due to statistical assumptions not fulfilled.

Table S2: extracted compounds grouped by the main factor toasting degree.

Toasting degree	Furfural	5-methylfurfural	Furfuryl alcohol	Maltol	Cyclotene	Whiskey lactones	Guaiacol	Eugenol	Vanillin
Light	33.99 ± 6.28 c	1.25 ± 0.13 d	1.94 ± 0.58 d	< LOQ d	< LOQ c	77.71 ± 1.83 b	7.13 ± 0.72	19.62 ± 1.23 a	38.98 ± 4.34 d
Medium	1'222.50 ± 77.53 a	216.31 ± 10.79 a	8.28 ± 2.20 c	23.25 ± 2.20 c	3.34 ± 0.32 b	91.90 ± 2.98 a	22.33 ± 1.56	19.44 ± 1.47 a	590.89 ± 26.98 c
Medium plus	970.49 ± 53.31 b	147.65 ± 5.66 b	15.71 ± 2.73 a	42.30 ± 4.37 a	3.88 ± 0.48 b	69.16 ± 4.86 b	38.03 ± 2.36	12.53 ± 1.07 b	986.57 ± 53.52 a
High	1'319.91 ± 265.74 b	63.06 ± 11.46 c	8.14 ± 0.60 b	31.55 ± 2.59 b	8.30 ± 0.83 a	14.13 ± 1.73 c	42.94 ± 4.49	7.06 ± 0.84 c	733.08 ± 70.30 b
Sign.	*** (log1p)	***	*** (log1p)	*** (log1p)	***	***	NA	***	***

Data are reported as mean [µg · L^{-1}] plus and minus standard error. Sign. = significance of ANOVA on linear mixed model fitted; ns = not significant, *** = 99.9 % significant. log1p = model fitted applying $\log_{10}(x_i+1)$ transformation due to meet the statistical assumptions. NA = not available due to statistical assumptions not fulfilled. < LOQ = lesser than limit of quantitation.

Table S3: extracted compounds grouped by the interaction between size and time of maceration.

Size:Time	Furfural	5-methylfurfural	Furfuryl alcohol	Maltol	Cyclotene	Whiskey lactones	Guaiacol	Eugenol	Vanillin
				Post hoc test subgroup Large size					
Large:First	776.48 ± 210.36 b	87.40 ± 21.99	6.66 ± 1.79 c	20.49 ± 4.90 ab	2.89 ± 0.77 a	49.69 ± 10.83 b	14.55 ± 2.83	10.13 ± 1.87 c	377.86 ± 98.20 d
Large:Second	994.87 ± 276.15 b	106.67 ± 25.85	8.38 ± 2.18 b	23.05 ± 6.02 ab	3.06 ± 0.92 a	64.64 ± 12.03 a	23.49 ± 4.46	13.22 ± 2.21 b	551.78 ± 137.77 c
Large:Third	1'170.75 ± 325.34 a	113.81 ± 26.92	9.56 ± 2.42 ab	20.11 ± 5.30 ab	2.62 ± 0.90 a	64.72 ± 11.07 a	27.44 ± 5.11	16.13 ± 2.39 a	639.42 ± 154.08 b
Large:Fourth	1'336.63 ± 398.73 a	116.51 ± 27.17	10.67 ± 2.64 ab	19.05 ± 5.38 b	2.62 ± 0.91 a	69.83 ± 10.50 a	30.17 ± 5.83	17.86 ± 1.95 a	749.42 ± 171.28 a
				Post hoc test subgroup Small size					
Small:First	555.76 ± 172.77 c	96.30 ± 36.31	4.89 ± 1.84 d	27.66 ± 7.63 b	5.10 ± 1.30 b	52.01 ± 10.15 d	20.75 ± 4.10	11.59 ± 2.03 c	442.45 ± 95.44 c
Small:Second	643.00 ± 185.42 b	108.25 ± 39.16	6.37 ± 2.04 c	31.68 ± 8.42 b	5.83 ± 1.61 c	68.47 ± 13.13 b	28.29 ± 5.52	15.74 ± 2.79 b	600.91 ± 136.52 b
Small:Third	711.99 ± 214.08 b	106.15 ± 37.82	7.73 ± 2.66 b	14.58 ± 3.60 c	2.52 ± 0.66 d	59.67 ± 11.40 c	30.75 ± 6.72	12.77 ± 2.37 c	579.30 ± 128.52 b
Small:Fourth	904.29 ± 261.83 a	121.45 ± 42.59	13.90 ± 6.26 a	37.60 ± 9.58 a	6.38 ± 1.99 a	76.79 ± 13.30 a	45.44 ± 9.33	19.88 ± 2.96 a	757.92 ± 174.46 a
Sign.	*(log1p)	n.s.	*** (log1p)	*** (log1p)	***	***	NA	***	**

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Table S4: extracted compounds grouped by the interaction between toasting degree and time.

Toasting degree:Time	Furfural	5-methylfurfural	Furfuryl alcohol	Maltol	Cyclotene	Whiskey lactones	Guaiacol	Eugenol	Vanillin
Post hoc test subgroup Light toasting									
Light:First	29.34 ± 11.32 b	1.09 ± 0.27 a	0.73 ± 0.42 c	< LOQ a	< LOQ a	72.10 ± 3.14 b	3.44 ± 0.34	14.93 ± 1.59	27.47 ± 2.90 a
Light:Second	23.46 ± 8.23 b	1.31 ± 0.37 a	1.94 ± 1.13 b	< LOQ a	< LOQ a	82.29 ± 3.93 a	6.75 ± 0.22	20.20 ± 1.31	31.73 ± 2.97 a
Light:Third	40.43 ± 16.11 a	1.25 ± 0.27 a	2.29 ± 1.34 ab	< LOQ a	< LOQ a	76.21 ± 3.10 ab	8.16 ± 1.01	20.33 ± 3.33	47.29 ± 8.74 a
Light:Fourth	42.71 ± 15.83 a	1.37 ± 0.25 a	2.79 ± 1.61 a	< LOQ a	< LOQ a	80.23 ± 3.44 a	10.19 ± 1.12	23.04 ± 1.90	49.43 ± 12.74 a
Post hoc test subgroup Medium toasting									
Medium:First	940.43 ± 136.64 c	193.62 ± 25.39 b	6.56 ± 3.79 b	26.22 ± 3.82 a	3.90 ± 0.58 a	75.31 ± 2.22 c	16.98 ± 2.56	15.39 ± 2.27	465.22 ± 15.21 c
Medium:Second	1'152.42 ± 103.13 b	219.22 ± 21.44 a	7.96 ± 4.66 ab	24.71 ± 4.69 a	3.87 ± 0.69 ab	98.47 ± 1.15 ab	21.36 ± 1.97	19.91 ± 2.87	570.92 ± 25.20 b
Medium:Third	1'299.73 ± 97.20 ab	218.17 ± 18.27 a	8.95 ± 5.20 ab	18.20 ± 2.12 b	2.42 ± 0.32 c	91.10 ± 5.00 b	22.16 ± 1.76	18.93 ± 1.68	598.68 ± 21.31 b
Medium:Fourth	1'497.42 ± 161.62 a	234.22 ± 24.69 a	9.65 ± 5.61 a	23.88 ± 6.59 ab	3.16 ± 0.83 bc	102.73 ± 0.92 a	28.81 ± 3.36	23.54 ± 3.98	728.72 ± 38.52 a
Post hoc test subgroup Medium Plus toasting									
Medium plus:First	764.01 ± 63.63 c	129.36 ± 7.76 b	10.25 ± 1.33 c	44.70 ± 6.65 a	4.41 ± 0.87 a	48.67 ± 5.63 c	27.05 ± 1.46	8.64 ± 1.02	728.52 ± 12.97 c
Medium plus:Second	875.14 ± 57.67 bc	147.33 ± 11.34 ab	12.08 ± 1.55 b	50.40 ± 7.20 a	4.55 ± 1.02 a	72.85 ± 7.74 b	36.29 ± 0.77	12.16 ± 1.51	1'007.28 ± 43.37 b
Medium plus:Third	1'024.17 ± 41.99 ab	150.38 ± 7.79 a	14.35 ± 2.75 b	26.71 ± 1.83 b	2.21 ± 0.27 b	67.34 ± 4.47 b	38.86 ± 1.17	11.47 ± 0.76	1'032.60 ± 105.24 b
Medium plus:Fourth	1'218.66 ± 94.66 a	163.55 ± 13.90 a	26.18 ± 9.24 a	47.41 ± 13.01 a	4.34 ± 1.22 a	87.80 ± 10.00 a	49.93 ± 4.30	17.84 ± 2.02	1'177.89 ± 94.41 a
Post hoc test subgroup High toasting									
High:First	930.71 ± 390.43 c	43.32 ± 16.66 b	5.55 ± 0.11 c	25.38 ± 2.22 c	7.68 ± 1.11 c	7.33 ± 0.53 b	23.14 ± 3.57	4.46 ± 0.11	419.39 ± 69.66 c
High:Second	1'224.72 ± 489.51 b	61.98 ± 23.43 ab	7.52 ± 0.45 b	34.35 ± 2.43 b	9.36 ± 1.54 b	12.59 ± 1.63 b	39.14 ± 3.77	5.65 ± 0.55	695.46 ± 91.23 b
High:Third	1'401.16 ± 616.74 b	70.14 ± 27.69 a	8.99 ± 0.95 a	24.48 ± 6.87 c	5.64 ± 0.55 d	14.13 ± 3.17 b	47.19 ± 5.28	7.07 ± 1.63	758.86 ± 70.41 b
High:Fourth	1'723.05 ± 728.04 a	76.79 ± 28.67 a	10.52 ± 1.27 a	42.01 ± 2.74 a	10.51 ± 2.34 a	22.47 ± 2.81 a	62.29 ± 9.06	11.06 ± 1.66	1'058.63 ± 109.08 a
Sign.	** (log)	*	*** (log1p)	*** (log1p)	***	***	NA	n.s.	***

Data are reported as mean [µg · L^{-1}] plus and minus standard error. Sign. = significance of ANOVA on linear mixed model fitted; ns = not significant, * = 95 % significant, ** = 99 % significant, *** = 99.9 % significant. log1p = model fitted applying $\log_{10}(x_i+1)$ transformation due to meet the statistical assumptions. NA = not available due to statistical assumptions not fulfilled. < LOQ = lesser than limit of quantitation.

Table S5: extracted compounds grouped by the interaction between size and toasting degree.

Size:Toasting degree	Furfural	5-methylfurfural	Furfuryl alcohol	Maltol	Cyclotene	Whiskey lactones	Guaiacol	Eugenol	Vanillin
Large:Light	2'268.47 ± 211.18 e	1.76 ± 0.06 d	< LOQ e	< LOQ d	< LOQ e	78.72 ± 3.26 ab	7.31 ± 0.82	22.81 ± 1.49 a	48.41 ± 7.28 d
Large:Medium	371.34 ± 31.15 bc	181.65 ± 8.41 b	16.56 ± 1.04 a	16.21 ± 1.12 c	2.31 ± 0.19 d	93.59 ± 3.57 a	18.21 ± 1.44	15.01 ± 0.90 bc	590.49 ± 40.23 c
Large:Medium plus	56.11 ± 5.32 c	136.67 ± 6.36 bc	9.51 ± 0.40 b	31.81 ± 2.05 b	2.51 ± 0.15 d	59.20 ± 5.32 b	35.90 ± 2.67	10.82 ± 1.16 cd	1'087.94 ± 83.12 a
Large:High	11.86 ± 0.96 a	104.32 ± 8.54 c	9.19 ± 1.03 bc	34.69 ± 1.84 b	6.37 ± 0.26 b	17.36 ± 2.72 c	34.22 ± 4.27	8.70 ± 1.35 de	591.63 ± 80.09 c
Small:Light	1'025.26 ± 79.56 f	0.75 ± 0.05 d	3.87 ± 0.59 d	0.00 ± 0.00 d	0.00 ± 0.00 e	76.69 ± 1.86 ab	6.96 ± 1.25	16.44 ± 1.19 b	29.55 ± 1.55 d
Small:Medium	1'419.74 ± 91.19 b	250.97 ± 9.24 a	0.00 ± 0.00 e	30.30 ± 2.31 b	4.37 ± 0.33 c	90.22 ± 4.95 a	26.45 ± 1.87	23.87 ± 1.69 a	591.28 ± 38.73 c
Small:Medium plus	928.89 ± 62.72 bc	158.64 ± 7.90 bc	21.92 ± 4.55 a	52.80 ± 6.80 a	5.24 ± 0.65 c	79.13 ± 6.68 ab	40.17 ± 3.92	14.23 ± 1.65 bc	885.20 ± 49.30 b
Small:High	1'012.10 ± 88.03 d	21.80 ± 1.82 d	7.09 ± 0.41 c	28.42 ± 4.75 b	10.23 ± 1.35 a	10.90 ± 1.59 c	51.65 ± 6.82	5.42 ± 0.64 e	874.54 ± 95.14 b
Sign.	*** (log)	***	*** (log1p)	*** (log1p)	***	*	NA	***	***

Data are reported as mean [µg · L^{-1}] plus and minus standard error. Sign. = significance of ANOVA on linear mixed model fitted; ns = not significant, * = 95 % significant, ** = 99 % significant, *** = 99.9 % significant. log1p = model fitted applying $\log_{10}(x_i+1)$ transformation due to meet the statistical assumptions. NA = not available due to statistical assumptions not fulfilled. < LOQ = lesser than limit of quantitation.