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Different coatings for the HS-SBSE grape volatile analysis in model solution: Preliminary results

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Table 1. Compounds analysed and their concentrations in the model solution ($\mu\text{g/L}$), retention time (RT, min), quantification ion (Q ion, m/z) and Log K_{ow} .

Compounds	$\mu\text{g/L}$	RT (min)	Q ion (m/z)	Log K_{ow} *
Benzaldehyde	186	31.1	105	1.71
β -citronellol	180	43.4	69	3.56
Eugenol	300	58.2	164	2.73
Geraniol	300	46.7	69	3.47
1-hexanol	80000	24.7	56	1.82
(E)-2-hexenal	6000	14.6	41	1.58
(E)-2-hexen-1-ol	76410	27.0	57	1.61
(Z)-3-hexen-1-ol	4000	25.4	67	1.61
α -ionone	19	45.9	121	4.29
β -ionone	19	49.5	177	4.00
D-limonene	150	13.1	68	4.83
Linalool	250	33.5	71	3.38
Nerolidol	150	52.6	69	3.78
Nerolidol 2	150	54.1	69	3.78
α -terpineol	2500	40.1	59	3.33

*Log K_{ow} according to SRC K_{ow} Win v1.67.

Table 2. Mean values (relative area) of seven replicates \pm standard errors for each coating setting CIS temperature at 0 °C. Recovery (%) compared to PDMS.

CIS Temperature 0 °C

Compounds	PDMS	EG SILICONE		PA	
	Relative Area	Relative Area	%Recovery	Relative Area	%Recovery
Benzaldehyde	0.14 \pm 0.007	0.16 \pm 0.011 *	110.1%	0.19 \pm 0.024 *	131.3%
β -citronellol	0.25 \pm 0.024	0.107 \pm 0.030 *	42.8%	0.12 \pm 0.025 *	49.9%
Eugenol	0.044 \pm 0.005	0.004 \pm 0.001 *	9.5%	0.007 \pm 0.002 *	16.7%
Geraniol	0.17 \pm 0.017	0.098 \pm 0.026 *	57.8%	0.092 \pm 0.021 *	54.7%
1-hexanol	41.17 \pm 0.232	54.24 \pm 9.400 *	131.7%	38.50 \pm 4.367	93.5%
(E)-2-hexenal	2.13 \pm 0.119	2.02 \pm 0.172	95.0%	1.65 \pm 0.127 *	77.9%
(E)-2-hexen-1-ol	20.91 \pm 0.105	33.89 \pm 3.854	162.0%	33.35 \pm 3.313 *	159.5%
(Z)-3-hexen-1-ol	0.83 \pm 0.040	1.41 \pm 0.173 *	169.4%	1.28 \pm 0.115 *	153.9%
α -ionone	0.26 \pm 0.029	0.045 \pm 0.015 *	17.2%	0.028 \pm 0.004 *	10.9%
β -ionone	0.22 \pm 0.025	0.018 \pm 0.004 *	8.0%	0.012 \pm 0.002 *	5.3%
D-limonene	3.76 \pm 0.513	1.36 \pm 0.439 *	36.0%	0.22 \pm 0.062 *	5.8%
Linalool	0.96 \pm 0.082	0.62 \pm 0.124 *	64.4%	0.33 \pm 0.065 *	33.9%
Nerolidol	0.096 \pm 0.014	0.002 \pm 0.002 *	2.4%	0.003 \pm 0.001 *	3.4%
Nerolidol 2	0.090 \pm 0.013	0.003 \pm 0.002 *	3.8%	0.007 \pm 0.001 *	7.3%
α -terpineol	1.69 \pm 0.121	0.88 \pm 0.167 *	52.2%	0.58 \pm 0.123 *	34.2%

For easier data comparison, we used grey bars in the cells: grey bars visually represent the relative areas detected with the different coatings (longest bars for highest values of relative areas; shortest bars for shortest values of relative areas).

*Significant differences at the 95% of probability level compared with PDMS coating.

Table 3. Mean values (relative area) of seven replicates \pm standard errors for each coating setting the CIS temperature at 25 °C. Recovery (%) compared to PDMS.

Compounds	CIS Temperature 25 °C				
	PDMS	EG SILICONE		PA	
	Relative Area	Relative Area	%Recovery	Relative Area	%Recovery
Benzaldehyde	0.17 \pm 0.007 Δ	0.23 \pm 0.016 Δ	139.0%	0.21 \pm 0.016 *	127.6%
β -citronellol	0.29 \pm 0.010 Δ	0.17 \pm 0.021 Δ	60.5%	0.11 \pm 0.013 *	39.4%
Eugenol	0.06 \pm 0.002 Δ	0.008 \pm 0.002 Δ	12.9%	0.007 \pm 0.003 *	11.6%
Geraniol	0.19 \pm 0.008 Δ	0.16 \pm 0.020 Δ	84.9%	0.10 \pm 0.013 *	54.2%
1-hexanol	47.13 \pm 0.152 Δ	72.30 \pm 0.610 Δ	153.4%	55.33 \pm 0.350 Δ	117.4%
(E)-2-hexenal	2.70 \pm 0.090 Δ	2.89 \pm 0.265 Δ	107.3%	2.38 \pm 0.125 Δ	88.3%
(E)-2-hexen-1-ol	24.60 \pm 0.075 Δ	42.56 \pm 0.294 Δ	173.0%	39.56 \pm 0.291 Δ	160.8%
(Z)-3-hexen-1-ol	0.987 \pm 0.030 Δ	1.76 \pm 0.143 Δ	178.3%	1.63 \pm 0.123 Δ	165.1%
α -ionone	0.33 \pm 0.010 Δ	0.09 \pm 0.013 Δ	27.0%	0.040 \pm 0.006 Δ	12.1%
β -ionone	0.26 \pm 0.006 Δ	0.025 \pm 0.004 Δ	9.8%	0.009 \pm 0.006 *	3.6%
D-limonene	2.57 \pm 0.348 Δ	2.40 \pm 0.475 Δ	93.3%	0.30 \pm 0.064 *	11.5%
Linalool	1.12 \pm 0.042 Δ	0.97 \pm 0.104 Δ	86.2%	0.41 \pm 0.026 *	36.2%
Nerolidol	0.142 \pm 0.006 Δ	0.006 \pm 0.001 Δ	4.4%	0.001 \pm 0.001 *	0.5%
Nerolidol 2	0.136 \pm 0.006 Δ	0.008 \pm 0.001 Δ	5.9%	0.004 \pm 0.003 *	3.0%
α -terpineol	1.88 \pm 0.068 Δ	1.17 \pm 0.224 *	62.4%	0.76 \pm 0.064 *	40.7%

For easier data comparison, we used grey bars in the cells: grey bars visually represent the relative areas detected with the different coatings (longest bars for highest values of relative areas; shortest bars for shortest values of relative areas).

*Significant differences at the 95% of probability level compared with PDMS coating.

Δ Significant differences at the 95% of probability level compared with each coating at CIS temperature of 0 °C (values are reported in Table 2).

Table 4. Relative area detection limit (ADL) and relative area quantification limit (AQL) for the three type of coatings (PDMS, EG Silicone and PA) employing CIS temperature 0 °C and CIS temperature 25 °C.

Compounds	CIS Temperature 0 °C						CIS Temperature 25 °C					
	ADL			AQL			ADL			AQL		
	EG			EG			EG			EG		
	PDMS (x10 ⁻⁶)	SILICONE (x10 ⁻⁶)	PA (x10 ⁻⁶)	PDMS (x10 ⁻⁶)	SILICONE (x10 ⁻⁶)	PA (x10 ⁻⁶)	PDMS (x10 ⁻⁶)	SILICONE (x10 ⁻⁶)	PA (x10 ⁻⁶)	PDMS (x10 ⁻⁶)	SILICONE (x10 ⁻⁶)	PA (x10 ⁻⁶)
Benzaldehyde	4.89	2.98	5.17	16.30	9.95	17.23	5.54	3.14	4.19	18.46	10.46	13.98
β -citronellol	5.28	2.01	2.65	17.59	6.70	8.84	3.24	2.33	5.88	10.80	7.78	19.58
Eugenol	5.65	1.87	1.31	18.83	6.22	4.38	3.20	4.23	3.26	10.67	14.11	10.88
Geraniol	9.61	1.85	3.21	32.04	6.18	10.69	3.49	2.79	5.85	11.62	9.30	19.49
1-hexanol	9.99	4.06	7.71	33.29	13.54	25.69	7.18	5.88	8.29	23.93	19.58	27.62
(E)-2-hexenal	5.60	3.35	3.23	18.68	11.16	10.75	4.94	1.97	5.99	16.48	6.57	19.97
(E)-2-hexen-1-ol	8.27	2.80	6.43	27.57	9.34	21.43	3.95	4.06	5.83	13.16	13.52	19.44
(Z)-3-hexen-1-ol	5.99	1.92	5.79	19.97	6.39	19.31	4.02	1.98	5.27	13.41	6.61	17.56
α -ionone	10.20	2.29	3.08	34.00	7.64	10.28	3.67	3.05	4.40	12.22	10.16	14.66
β -ionone	8.99	2.14	1.99	29.97	7.13	6.63	2.87	2.88	5.10	9.57	9.59	17.00
α -limonene	12.83	3.73	3.49	42.76	12.42	11.64	7.68	2.83	4.64	25.59	9.43	15.46
Linalool	7.24	2.76	2.25	24.15	9.20	7.49	3.68	3.79	5.60	12.28	12.62	18.65
Nerolidol	6.43	0.53	0.62	21.42	1.76	2.05	2.41	1.13	0.97	8.04	3.77	3.22
Nerolidol 2	7.42	0.97	1.60	24.74	3.24	5.35	3.73	1.64	1.97	12.42	5.48	6.56
α -terpineol	10.58	2.77	3.70	35.27	9.23	12.33	3.88	3.74	5.53	12.93	12.47	18.43

For easier data comparison, we used grey bars in the cells: grey bars visually represent the relative areas detected with the different coatings (longest bars for highest values of relative areas; shortest bars for shortest values of relative areas).

