

SUPPLEMENTAL MATERIAL FOR:

Characterization of the key odorants in goji wines in three levels of sweetness by applications of sensomics approach

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1 **Determination of Ethanol in GWs**

2 Ethanol was analyzed by a Clarus 400 gas chromatograph (PerkinElmer, UK) in connection
3 with a TurboMatrix 40 Trap Headspace-Sampler (Perkin Eimer, UK). The sample (10 mL) was
4 equilibrated in a 22 mL headspace vial with PTFE septa and clamp closure for 15 min at 60 °C.
5 With an injection time of 0.1 min, the sample was applied by splitless with a split/splitless-
6 injector at 15 mL/min, and the temperature was kept at 100 °C using nitrogen as the carrier gas
7 with a flow pressure of 65 kPa. The sample was flushed onto the Rtx-502.2 fused silica capillary
8 column (50 m × 0.32 mm inner diameter, 0.18 µm film thickness). The oven temperature
9 programs were as follows: 40 °C for 1 min and 10 °C/min up to 150 °C. At the end of the column,
10 the effluent was analyzed by FID, which was held at 250 °C. The detector gas was 45 mL/min
11 hydrogen and 450 mL/min air. A calibration factor was determined by analyzing mixtures of
12 defined amounts of *tert*-butanol and ethanol in ratios of 1:3, 1:2, 1:1, 2:1, 3:1 (**Table S1**).

14 **Determination of Sugar Contents in GWs**

15 Based on the method of Morlock and Sabir,¹ the sugar content was analysed via high-
16 performance thin-layer chromatography (HPTLC). An Automatic TLC sampler 4 (ATS 4,
17 CAMAG, Muttenz, Switzerland) was used to apply samples and standards. For analysis,
18 aliquots of 2-14 µL of samples (diluted to ~60 µg/L sugar content with 1:1 methanol/water, *v/v*)
19 and 1-20 µL of standards (two standard solutions; solution 1: sucrose; solution 2: fructose and
20 glucose, each analyte with ~60 µg/L in 1:1 methanol/water, *v/v*) were applied bandwise on a 20
21 cm × 10 cm silica gel 60 F₂₅₄ plate (Merck, Darmstadt, Germany) with a distance from the
22 lower edge of 8 mm and right edge of 10 mm. Methanol was used as the rinsing solvent. Plate
23 images were captured with the TLC Visualizer (CAMAG) under UV 254 nm, UV 366 nm, and
24 white light illumination. The plate was placed in an Automatic Development Chamber (ADC2,
25 CAMAG) equipped with a 20 cm × 10 cm twin-trough chamber (CAMAG). A mixture of *n*-
26 butanol/isopropanol/acetic acid/boric acid solution (200 mg boric acid dissolved in 10 mL of

27 water) (6:14:1:3, v/v/v/v) was used for the chamber saturation that was conducted for 15 min
28 (using a filter paper in the ADC 2) and for the development up to a migration distance of 60
29 mm. After a drying step for 10 min, plate images were captured a second time. For
30 derivatization, the plate was dipped into an aniline-diphenylamine-*o*-phosphoric acid reagent
31 (mixture of 2 g aniline and 2 g diphenylamine in 200 mL of methanol with an additional 20 mL
32 of *o*-phosphoric acid (85%, w/w)), with a TLC Chromatogram Immersion Device III (CAMAG,
33 immersion speed 3.5, immersion time 0). Then, the plate was dried under cold air steam until
34 dryness and heated for 5-10 min at 110 °C. Plate images were captured under UV 254 nm, UV
35 366 nm, and white illumination. Afterward, a TLC Scanner 4 (CAMAG) was used to scan the
36 plate in absorption mode at UV 380 nm. Quantification was done via a five-point calibration
37 (60-1200 ng/zone), and the standard addition technique was used to verify the results. Control
38 of HPTLC instruments and data analysis were done with winCATS software, version
39 1.4.6.2002 (CAMAG).

40 **Table S1.** Ethanol Calibration Curve and Concentrations in Three Goji Wines

sample	calibration curve	R ²	concentration (µg/L)				RSD ^b
			exp.1 ^a	exp.2	exp.3	average	
SGW			84727	101384	77017	87710	14%
SDGW	$y = 0.2351x + 0.0451$	0.9977	79463	83841	99518	87606	12%
DGW			109020	93961	93177	98719	9%

41 ^aexp., experiment. ^bRSD, relative standard deviation.

42 **Table S2.** Sugar Compositions and Concentrations in GWs

	concentration (g/L)		
	SGW	SDGW	DGW
glucose	12	4.4	0.20
fructose	21	8.4	0.40
total sugar concentration	33	13	0.60

43

44 **Table S3.** Odor Thresholds (OTs) of Odorants

odorant	OT (µg/L)	odorant	OT (µg/L)
(<i>E</i>)-β-damascenone	0.05 ^a	2-methoxyphenol	10 ^a
<i>cis</i> -whisky lactone	0.01 ^a	phenylacetic acid	2 500 ^c
<i>trans</i> -whisky lactone	0.01 ^a	2-methoxy-4-vinylphenol	40 ^a
3-methyl-2,4-nonanedione	0.046 ^h	eugenol	5 ^a
ethanol	990 000 ^h	acetic acid	200 000 ^a
ethyl 2-methylbutanoate	1 ^a	vanillin	200 ^a
ethyl octanoate	2 ^a	ethyl propanoate	5 500 ^d
decanal	1 ^f	<i>p</i> -cresol	60 ^e
ethyl 3-methylbutanoate	3 ^a	<i>m</i> -cresol	68 ^b
ethyl hexanoate	5 ^a	2, and 3-methylbutanoic acid	3 000 ^a
(<i>E</i>)-2-nonenal	0.6 ^d	2-methylpropyl acetate	1 605 ^c
3-methyl-1-butanol	30 000 ^a	α-terpineol	250 ^b
octanal	3.4 ^h	acetophenone	500 ^a
2, and 3-methylbutyl acetate	30 ^a	4-hydroxy-2,5-dimethyl-3(2 <i>H</i>)-furanone	500 ^a
ethyl 3-phenylpropanoate	1.6 ^b	methionol	500 ^a
6-methyl-5-hepten-2-one	0.16 ^g	hexanoic acid	3 000 ^a
ethyl butanoate	20 ^a	ethyl 2-phenylacetate	650 ^f
nonanal	1 ^f	2-phenylethyl acetate	250 ^a
3-hydroxy-4,5-dimethyl-2(5 <i>H</i>)-furanone	5 ^a	(<i>Z</i>)-3-hexen-1-ol	400 ^a
phenylacetaldehyde	1 ^d	decanoic acid	15 000 ^a
nonanoic acid	26 ^h	heptanoic acid	13 300 ^e
γ-nonalactone	7 ^f	butanoic acid	10 000 ^a
ethyl cinnamate	1 ^a	linalool	15 ^a
2-phenylethanol	10 000 ^a	3-phenylpropanoic acid	120 ^h
octanoic acid	500 ^b	pentanoic acid	11 000 ^h
ethyl 2-methylpropanoate	15 ^a		

45 ^aOrthonasal odor threshold in 10% ethanol/water solution as reported in ref.² ^bOrthonasal odor threshold in 11%
46 ethanol/water solution containing 7 g/L glycerol, 5 g/L tartaric acid, pH 3.2 with 1 M sodium hydroxide in ref.³
47 ^cOrthonasal odor threshold in 10% ethanol/water solution at pH 3.2 in ref.⁴ ^dOrthonasal odor threshold in 10%
48 ethanol/water solution containing 5 g/L tartaric acid at pH 3.2 in ref.⁵ ^eOrthonasal odor threshold in 46%
49 ethanol/water solution in ref.⁶ ^fOrthonasal odor threshold in 11% ethanol/water solution in ref.⁷ ^gOrthonasal odor
50 threshold in water in ref.⁸ ^hOrthonasal odor threshold in water obtained from the Leibniz-LSB@TUM Odorant
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