

1 Supplementary Materials

2 **From Extra Virgin Olive Oil to Refined Products:**
 3 **Intensity and Balance Shifts of the Volatile**
 4 **Compounds versus Odor**

5 **Jing Yan^{1,2}, Martin Alewijn², Saskia M. van Ruth^{1,2,*}**

6 ¹ Food Quality and Design Group, Wageningen University and Research, P.O. Box 17, 6700AA Wageningen,
 7 The Netherlands; jing.yan@wur.nl

8 ² Wageningen Food Safety Research, Wageningen University and Research, P.O. Box 230, 6700 AE
 9 Wageningen, The Netherlands; martin.alewijn@wur.nl

10 * Correspondence: saskia.vanruth@wur.nl; Tel.: +31-317-480250

11 **Table S1.** List of the air/liquid partition coefficients (K) and the calculated odor thresholds (OTs) in
 12 air (ppbv) of volatile organic compounds.

Compounds	K×10000 ^a	OT1 ^b	OT2 ^c	OT3 ^d	OT4 ^e	OT5 ^f	OT6 ^g	OT ^h
Methanol		24745255			100000			100000
Acetaldehyde			825		210			210
Formic acid				27925				27925
Ethanol		273766			10000			10000
2-Propenal			1564		210			210
Propanal			419					419
Acetone		17618249			100000			100000
Acetic acid			2435	162	1000	562		162
Dimethyl sulfide			1179		1			1
Butan-2-one	48	59624	149168		10000			10000
Propanoic acid			1881	33				33
Methyl acetate			561124					561124
Dimethyl sulfoxide			940		1			1
Ethyl acetate	53	1269	241973					1269
Butanoic acid			53	4	1			1
trans-2-Pentenal						437		437
Pentanal			117			11		11
Ethyl propionate			1682					1682
3-Methylbutanoic acid			19					19
Pentanoic acid			9					9
Cyclohexane		727665						727665
trans-2-Hexenal						1		1
Hexanal	6	11	69			12	0.27	0.27
4-Methylpentan-2-one					470			470
Butyl acetate	5	29	3385					29
Ethyl butyrate			8					8
Ethyl isobutyrate			5					5
Hexanoic acid			127			635		127

Compounds	K×10000 ^a	OT1 ^b	OT2 ^c	OT3 ^d	OT4 ^e	OT5 ^f	OT6 ^g	OT ^h
Toluene			87827		2140-4680			2140
Ethenyl benzene			8250		47-100			47
Ethyl benzene			39323				39323	
2,4-Heptadienal					8			8
trans-2-Heptenal					19			19
Heptanal	3	30	39			10	0.19	0.19
Heptan-2-one	5	30	1463				1	1
1,2,4-Trimethylbenzene			24545				24545	
trans-2-Octenal					4		1	1
3-Octen-2-one							1	1
Octanal	2	11	2			2	0.08	0.08
1-Octen-3-ol						1		1
Octan-2-one	3	27					27	
Propyl butanoate			2078				2078	
α-Pinene			3251				3251	
β-Pinene			5961				5961	
Limonene			6864			130		130
trans,trans-2,4-								
Nonadienal						0.04	0.04	
tran-2-Nonenal						0.02	0.02	
Nonanal			59			4	0.45	0.45
Nonan-2-one							5	5
Hexyl acetate			307				307	
trans, trans-2,4-								
Decadienal						0.37	0.37	
trans-2-Decenal					1	0.43	0.43	
Decanal			63			1	0.41	0.41

13 ^a van Ruth, et al. [1]; ^b Morales, et al. [2]; ^c Nagata and Takeuchi [3]; ^d Nielsen, et al. [4]; ^e Leonardos, et al. [5]; ^f Xu,
14 et al. [6]; ^g Yang, et al. [7]; ^h The lowest OT selected from publications was used in this study.

15 References:

1. van Ruth, S. M.; Grossmann, I.; Geary, M.; Delahunty, C. M., Interactions between artificial saliva and 20
17 aroma compounds in water and oil model systems. *J. Agr. Food Chem.* **2001**, *49*, (5), 2409-2413.
2. Morales, M. T.; Luna, G.; Aparicio, R., Comparative study of virgin olive oil sensory defects. *Food Chem.*
18 **2005**, *91*, (2), 293-301.
3. Nagata, Y.; Takeuchi, N., Measurement of odor threshold by triangle odor bag method. *Odor measurement
21 review* **2003**, *118*, 118-127.
4. Nielsen, G. D.; Hansen, L. F.; Andersen, B.; Poulsen, N.; Melchior, O., Indoor air guideline levels for
23 formic, acetic, propionic and butyric acid. *Indoor Air* **1998**, *8*, (S5), 8-24.
5. Leonardos, G.; Kendall, D.; Barnard, N., Odor threshold determination of 53 odorant chemicals. *J. Air
24 Pollut. Control Assoc.* **1969**, *19*, (2), 91-95.

- 26 6. Xu, L.; Yu, X.; Li, M.; Chen, J.; Wang, X., Monitoring oxidative stability and changes in key volatile
27 compounds in edible oils during ambient storage through HS-SPME/GC-MS. *Int. J. Food Prop.* **2017**, 20,
28 (sup3), S2926-S2938.
- 29 7. Yang, D. S.; Shewfelt, R. L.; Lee, K.-S.; Kays, S. J., Comparison of odor-active compounds from six
30 distinctly different rice flavor types. *J. Agr. Food Chem.* **2008**, 56, (8), 2780-2787.

31