Supplementary Material

Key aroma compounds in two Bavarian gins

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2.1. Materials

A homologues series of the alkanes C_6-C_{26} (Fluka and Sigma-Aldrich, Steinheim, Germany), diluted in pentane (Th. Geyer, Renningen, Germany) was used for determining (linear) retention indices (RIs). Anhydrous sodium sulfate, freshly distilled dichloromethane (Th. Geyer), dipropylenglycole (Sigma Aldrich), ethanol (VWR international GmbH, Darmstadt, Germany) and liquid nitrogen (Linde Gas, Pullach im Isartal, Germany) and sodium chloride (Fluka) were used in sample preparation/extraction procedures, as described in the main text. The following pure reference compounds were used: 4-hydroxy-3-methoxybenzaldehyde (vanillin) ≥99% (ABCR, Karlsruhe, Germany); 2-acetyl-1-pyrroline ≥95%; (*Z*)-2-nonenal ≥90% (aromaLAB, Freising, Germany); 1-methyl-4-(propan-2-yl)benzene (*p*-cymene) ≥99.5%; (*E*)-2-decenal ≥95%; (*E*)-2-hexenal ≥97%; 2-isopropyl-5-methylphenol (thymol) ≥99%; 1-methoxy-4-(2-propenyl)benzene (estragole) ≥98.5; 4-methoxy-6-(2-propenyl)-1,3-benzodioxole (myristicin) ≥97%; (4*S*)-2-(2-methyl-1-propenyl)-4-methyltetrahydropyran ((*Z*)-rose oxide) ≥97%; 7-methyl-3-methylene-octa-1,6-diene (myrcene) ≥95%; nonanal ≥95%; 1-octen-3-ol ≥98% (Fluka); 4-methylene-1-(1-methylethyl)bicyclo[3.1.0]hexane (sabinene) ≥98.5% (Roth, Karlsruhe, Germany); γ-dodecalactone ≥97%; 3,7,7-trimethylbicyclo[4.1.0]hept-3-en (δ-carene) ≥95% (SAFC, Steinheim, Germany); 1,2-benzopyrone (coumarin) ≥99%; (*E*,*E*)-2,4-decadienal ≥85%; decanal ≥98%; 3,7-dimethyl-1,6-octadien-3-ol (linalool) ≥97%; 6,6-dimethyl-2-methylidenebicyclo[3.1.1]heptane (β-pinene) ≥99%; 3,7-dimethyl-2,6-octadienal (mixture of cis/trans) (citral) ≥96%; 3,7-dimethyl-6-octenal (citronellal) ≥95%; 3,7-dimethyl-trans-2,6-octadien-1-ol (geraniol) ≥96%; ethyl-2-methylbutanoate ≥98%; hexanal ≥98%; *trans*-1-methoxy-4-(1-propenyl)benzene (*trans*-anethole) ≥99%; 2-methoxy-4-(2-propenyl)phenol (eugenol) ≥99%; 4-methoxybenzaldehyde (*p*-anisaldehyde) ≥98%; 3-methylbutanal ≥97%; 4-methyl-1-(1-methylethyl)-1,4-cyclohexadiene (γ-terpinene) ≥97%; 1-methyl-4-(1-methylethenyl)-cyclohexene ((*R*)-limonene) ≥97%; 2-methylpropyl acetate ≥98%; (*E*,*E*)-2,6-nonadienal ≥95%; (*E*,*Z*)-2,6-nonadienal ≥95%; octanal ≥99%; 1-octen-3-one ≥50%; 1,3-trimethyl-2-oxabicyclo[2.2.2]octane (1,8-cineole) ≥99%; (1*R*,4*R*)-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one (1-(*R*)-fenchone) ≥98%; 2,6,6-trimethylbicyclo[3.1.1]hept-2-ene (α-pinene) ≥97%; 2,3,5-trimethylpyrazine ≥99% (Sigma Aldrich) and 2,2-dimethyl-3-methylidenebicyclo[2.2.1]heptane (camphene) ≥96% (Supelco, Bellefonte, USA). The following isotopically-labelled standards were purchased from aromaLAB (Planegg, Germany): [$^2H_6$]-7-methyl-3-methylene-octa-1,6-diene ([$^2H_6$]-myrcene); [$^{13}C_1{}^2H_2$]-1-methyl-4-(1-methylethenyl)-cyclohexene ([$^{13}C_1{}^2H_2$]-limonene); [$^2H_6$]-3,7-dimethyl-1,6-octadien-3-ol ([$^2H_6$]-linalool); [$^2H_3$]-*trans*-1-methoxy-4-(1-propenyl)benzene ([$^2H_3$]-*trans*-anethole); [$^2H_4$]-1-methoxy-4-(2-propenyl)benzene ([$^2H_4$]-estragole); [$^2H_4$]-nonanal; [$^2H_3$]-1,3-trimethyl-2-oxabicyclo[2.2.2]octane ([$^2H_3$]-cineole).

2.7. Quantitation of selected aroma compounds by stir-bar sorptive extraction (SBSE) and gas chromatography-mass spectrometry

Table S1. Selected ions (*m*/*z*) of analytes, stable isotopically labeled standards, and response factors.

odorant	isotope label	ion (*m*/*z*)[a]		response factor[b]
		analyte	standard	
myrcene	[$^{2}H_{6}$]	136	142	1.07
limonene	[$^{13}C_{1}{}^{2}H_{2}$]	136	139	0.82
1,8-cineole	[$^{2}H_{3}$]	154	157	0.95
nonanal	[$^{2}H_{4}$]	114	118	1.19
linalool	[$^{2}H_{5}$]	136	141	1.15
estragole	[$^{2}H_{4}$]	148	152	1.11
trans-anethole	[$^{2}H_{3}$]	148	151	1.25

[a] single ions used to determine the peak areas of analyte and standard in EI mode (70 eV)
[b] response factor determined by analyzing mixtures of known amounts of analyte and internal standard

3.2. Identification of Aroma Compounds

Table S2. Aroma-active compounds and their occurrence in botanicals used in the production of the gins investigated in the present study. Botanicals marked grey were only used for the production of *Kini*.

odorant	determined in botanical
terpenes and terpenoids	
sabinene	juniper (1-40 %) [1], angelica [2], citrus fruits like lemon and lime [3]
δ-carene	juniper [1], oranges [4]
myrcene	mainly in hops[a] [5], juniper [1] and ginger [6], also in angelica [2], cinnamon [7], various citrus fruits [3]
limonene	lime and lemon (50 and 70 %) [3], orange-peel (95 %) [4], juniper [1], coriander [8], ginger [6]
1,8-cineole	laurel (up to 50 %) [9], rosemary (up to 55 %) [10] and sage (18-24 %) [11], ginger[6] [6], fennel [12], cinnamon [7]
γ-terpinene	lime [3], spice plants such as coriander [8]
p-cymene	coriander [8], cinnamon [7], sage [11], in traces in star anise [13], anise [14], juniper [1] and lemon [15]
linalool	coriander (up to 75 %) [8], cinnamon [7], orange [4]
(Z)-rose oxide	roses [16]
aldehydes (saturated, unsaturated)	
octanal	orange peels [4], oranges (up to 1.1 %) [17], lemon (0.1 %) [15]
nonanal decanal	lemon [15] and orange [4,17]
(*E*,*E*)-2,4-decadienal	lemon [4] and orange [18]
phenylpropanoids	
estragole	tarragon leaves (2900 μg/g) [14], anise [14], fennel [12]
trans-anethole	anise (16000 μg/g) [14], fennel (23000 μg/g) [12], star anise (approx. 95 %) [13]
eugenol	cloves (over 80 %) [19], cinnamon (4 %) [7], laurel leaves [9], vanilla [20], star anise [13], anise and tarragon [14]
others	
1-octen-3-one 1-octen-3-ol	orange [4]
coumarin	tonka beans [21], in small quantities in cinnamon [7]
vanillin	vanilla (11 mg/g) [20]

[a] Hops were used for the production of *Gspusi* only.

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