Decoding the unique peaty aroma of Islay scotch single malt whisky by means of the sensomics concept

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Abstract

After application of an Aroma Extract Dilution Analysis and Stable Isotope Dilution Assays, 39 odorants with Odour Activity Values ≥ 1 were mixed in their natural concentrations in 40 % ABV (alcohol by volume) ethanol for a recombination experiment to verify the correct characterisation of all aroma impact compounds. The smoky, clove-like and phenolic character of the peaty whisky was caused by a set of 14 phenol derivatives, such as 3-ethylphenol with an Odour Activity Value up to 940. Comparing the concentrations of phenol derivatives in the raw whisky with the matured ready to drink product, it seems that the maturation process also contributes to the smoky aroma by increasing the concentrations of 4-allyl-2-methoxyphenol and 2-ethylphenol, while the other phenol derivatives mainly originated from the special kilning process with peat reek.

Introduction

Whisky making has a long tradition in Scotland and its islands. After mashing barley malt with yeast, a double-batch distillation yields the raw spirit, which is then aged for at least 3 years in second hand oak casks before bottling as single malt whisky. Especially, whiskies from the island Islay are particularly known to elicit a peaty odour. The malting process on Islay contains the traditional step of kilning with so-called peat reek (peat smoke) which is responsible for the typical smoky and phenolic aroma of the spirit. It is already suggested that this "peatiness" is caused by a spectrum of phenolic compounds including phenol, methylphenol and dimethylphenol derivatives and 2-methoxyphenol with a total amount up to 80 ppm [1-5]. Early studies could correlate the cumulated concentrations of all phenolic compounds to the degree of peatiness [1,2] or identified some phenol derivatives, such as 4-ethyl-2-methoxyphenol and 2-, 3-, and 4-methylphenol in Scotch and Japanese whiskies as aroma impact compounds based odour activity values (OAV) calculated, however, using threshold data in 10 to 20 % ABV ethanol [3-5]. Poisson and Schieberle were the first to fully characterise an American Bourbon whiskey by means of the Sensomics concept. Their investigations resulted in a set of 26 impact aroma compounds, including ethyl (*S*)-2-methylbutanoate, 3-methylbutanal, 4-hydroxy-3-methoxybenzaldehyde and (*E*)-β-damascenone with highest OAV [6,7]. They also investigated a peaty whisky from Islay and could trace back the distinctive smoky aroma to the high OAVs of several phenol derivatives, such as 2-methoxyphenol, 4-allyl-2-methoxyphenol and 5-methyl-2-methoxyphenol. However, their recombination experiments did not lead to a satisfying outcome [8] as not all phenol derivatives could be identified. In order to decode the unique aroma with focus on the peatiness of Scotch Single Malt whiskies from Islay on a molecular basis, a whisky from the Ardbeg distillery was investigated by means of the Sensomics concept [9]. Additionally, selected aroma compounds were quantitated in a sample of the corresponding raw whisky to investigate the impact of the maturation process to the smoky aroma of the whisky.

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Experimental

Samples. The whisky "Uigeadail" from the distillery Ardbeg was purchased at a local spirit shop. The shop owner also kindly provided a sample of the raw whisky, intended to be matured into an "Uigeadail" whisky.

Workup. After solvent extraction and SAFE (solvent assisted flavour evaporation) distillation and Vigreux column distillation, the concentrated distillate was subjected to aroma extract dilution analysis (AEDA), which was carried out by two panellists to assure the detection of the whole set of important odorants. Impact aroma compounds with high FD factors were quantitated by means of stable isotope dilution assays (SIDA), using ^{13}C or ^{2}H-labelled analogues. OAVs were then calculated by using the respective odour threshold concentration in 40 % ABV ethanol from the literature [7,8,10].

Sensory trials. Unavailable odour threshold concentrations were newly determined in 40 % ABV ethanol by a sensory trained panel according to the method reported previously [10]. For a descriptive analysis of the recombinate and the original whisky, the sensory panel was asked to rate the intensities of nine aroma attributes from 0 (no perception) to 10 (very strong intensity) on an unscaled line.

Results and discussion

AEDA and identification experiments resulted in 36 aroma active compounds with FD factors ranging from 32 to 4096. Next to (*E*)-*β*-damascenone, *cis*-whisky lactone and 4-hydroxy-3-methoxybenzaldehyde with high FD factors, a group of phenol derivatives with FD factors ranging from 4 to 4096 with smoky, phenolic or clove-like odour attributes were identified (data not shown). Based on these data quantitations followed by the determination of OAVs of 44 aroma compounds were carried out. Highest OAVs were found for 3-ethylphenol (940), followed by 3-methybutanal (640), (*S*)-ethyl 2-methylbutanoate (410), ethanol (390), 2-methoxy-5-methylphenol (590) und 2-methoxyphenol (280). Altogether, 39 aroma compounds with an OAV $\geq$ 1 (Table 1), including 14 phenol and 2-methoxyphenol derivatives, contributed to the complex aroma of the peaty single malt whisky. A recombination experiment with all 39 impact aroma compounds in their natural concentration could mimic the original whisky very well (Figure 1) confirming their correct characterisation as impact aroma compounds. The typical smoky and phenolic aroma of the whisky was generated by the set of phenol and 2-methoxyphenol derivatives with high to very high OAVs, such as 3-ethylphenol, 2-methoxy-5-methylphenol, 4-ethyl-2-methoxyphenol, 4-methylphenol, 2-methoxy-4-propylphenol, 2-methylphenol und more.

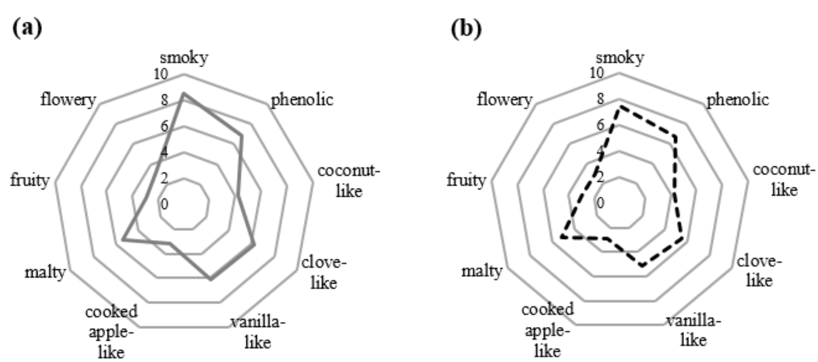

Figure 1: Aroma profiles of the original whisky (a) and the corresponding aroma recombinate (b)

Table 1: Impact aroma compounds with OAV ≥ 1 of the peaty single malt whisky from Islay.

odorant	*OAV*[1]	odorant	*OAV*[1]
3-ethylphenol	940	2-phenylethyl acetate	29
3-methylbutanal	640	(*E*)-2-nonenal	29
(*S*)-ethyl 2-methylbutanoate	410	3-methylbutyl acetate	25
ethanol	390	4-allyl-2-methoxyphenol	20
2-methoxy-5-methylphenol	380	ethyl cinnamate	18
2-methoxyphenol	280	4-ethylphenol	16
ethyl octanoate	250	3-methyl-1-butanol	15
(*E*)-*β*-damascenone	220	2-phenylethanol	14
4-ethyl-2-methoxyphenol	200	3-methylphenol	12
ethyl methylpropanoate	160	2-ethylphenol	10
vanillin	140	decanoic acid	9
ethyl 3-methylbutanoate	120	ethyl 3-phenylpropanoate	9
4-methylphenol	97	2-methoxy-4-methylphenol	7
ethyl hexanoate	80	methyl-1-propanol	5
1,1-diethoxyethane	68	*γ*-nonalactone	5
ethyl butanoate	67	phenol	4
2-methoxy-4-propylphenol	52	acetaldehyde	3
2-methylphenol	46	2,3-dimethylphenol	3
2-methylbutanal	43	3,5-dimethylphenol	1
cis-whisky lactone	30		

[1] OAV; odour activity value using odour threshold concentrations in 40 % ABV ethanol.

In order to investigate the impact of the maturation process on the smoky aroma of the whisky, a sample of the raw spirit intended for the production of “Uigeadail” with 69 % ABV ethanol was investigated focussing on known maturation derived compounds, such as *cis*-whisky lactone and 4-hydroxy-3-methoxybenzaldehyde, as well as on the previously identified phenol derivatives. Since the investigated whisky had cask strength (59 % ABV) meaning the spirit did not undergo dilution after the maturation process, the concentrations of the selected compounds in the raw spirit and final whisky were directly compared without conversion.

Next to the typical maturation derived compounds, only two phenol derivatives, such as 2-ethylphenol and 4-allyl-2-methoxyphenol showed noteworthy concentration increases after oak cask maturation. The remaining phenol derivatives were already present in the raw whisky, thus confirming their origin from the peat smoke used for kilning the malt. Minor concentration differences could be explained by the use of different starting material and vintage.

Table 2: Concentrations of impact aroma compounds in the raw and matured whisky.

odorant	concentration [µg/L] raw whisky	matured whisky	increase/ decrease [%]
maturation compounds			
cis-whisky lactone	< 1.3	2000	+150000
vanillin	23.1	3140	+ 13500
phenol derivatives			
2-ethyphenol	411	870	+ 112
4-allyl-2-methoxyphenol	89.2	139	+ 56
3-ethylphenol	444	537	+ 21
2-methoxy-4-propylphenol	88.6	97.6	+ 10
4-ethyl-2-methoxyphenol	1380	1370	- 1
2-methylphenol	4290	4120	- 4
2-methoxy-4-methylphenol	2010	1790	- 11
4-methylphenol	3260	2900	- 11
4-ethylphenol	3330	2740	- 18
3-methylphenol	1770	1400	- 21
2-methoxyphenol	3480	2600	- 25
2-methoxy-5-methylphenol	236	122	- 48

Conclusions

By applying the Sensomics concept to the Single Malt Scotch whisky from Islay, its aroma could be successfully characterised. The typical smoky and phenolic aroma was traced back to the multiplicity of phenol and 2-methoxyphenol derivatives with high OAVs. The additional investigation of the raw spirit confirmed their origin mainly from the peat reek used for malt kilning in the making process of these especially peaty whiskies.

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