Creating an artificial wine taster: Inferring the influence of must and yeast from the aroma profile of wines using Artificial Intelligence

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Abstract

The human brain is able to compute information from very complex olfactorical impressions. The special pattern of the concentrations of hundreds of aroma constituents allows an experienced wine taster to determine special features of the wine, for instance grape variety or vintage.

Artificial Neural Networks are often used to recognize shapes and patterns like faces or finger prints. Here we use Artificial Neural Networks to mimic the abilities of a wine taster to deal with very complex olfactorical patterns. We produced 120 unique wines combining twelve different grape musts and ten yeast strains and determined the aroma profile (83 aroma constituents) of all wines. We analyzed the ability of a well trained neural network to recognize the used must variety and the fermenting yeast strain from unknown aroma profiles. Furthermore we investigated the capability to predict the aroma profile of a wine with a must variety / yeast strain combination that is new to the neural network.

In 96% of all trials the neural network identified the must that was used for wine production correctly (expected random propability: 8%). An accurate identification of the yeast strain, used for fermentation, occurred in 67% of all trials (propability by chance: 10%).

The aroma profiles of the must/yeast combinations new to the neural network were forecasted with a divergence of only 2,1% compared to the actual wine of this production characterization. Thus we conclude that a comprehensive description of wines using neural networks is possible.

Key words

Artificial Neural Network, Artificial Neuronal Network, wine, wine taster, grape must, yeast, aroma profile.

Introduction

Artificial Neural Networks (ANN) were invented to mimic the extraordinary ability of the brain to recognize ‘gestalten’ (shapes and patterns). An ANN has the ability to learn and the skill to abstract. This is very important for analysis if the abstraction rules of the process of recognization are unknown to the user. In this case no tool that doesn’t have the power to learn is applicable and in this situation ANNs are very advantageous.

Common applications of Feedforeward-Backpropagation-ANNs are in statistics, e.g. as a nonlinear alternative to principal component, cluster or discriminant analysis. They are used for forecasting in medicine (diagnosis) (Stephan et al. 2005) and economy (Pino et al., 2008), to predict human behaviour (Marchiori et al. 2008) and furthermore in pattern recognition - such as identification of finger prints, faces, signatures (Marinai et al., 2005) and – to give an example with vine association – leaf shapes of grapevine varieties (Mancuso, 1999, 2002). In pattern recognition ANNs are already widely used.

The human brain is not only excellent in recognizing of visual patterns, but is also able to deal successfully with highly complex olfactorical ones. The typical flavour and taste, e.g of wine, consist of hundreds of different constituents in varying concentrations. Nevertheless to a certain extent an experienced wine taster is enabled to sense out the information about grape variety, vintage, and so on. In this article we analyse whether ANNs can be trained to do the same and even more:

The aroma spectra of wines are influenced by the used must, the fermenting yeast, the technique of wine making and the way, how and how long the wine is stored. During alcoholic fermentation, the yeast uses grape juice components to create a lot of aroma constituents (acids, alcohols, esters, terpenes and others) and hence the yeast is by no means less important for the flavour and taste of the wine, than the grape that gives the basic constituents (Cole & Noble, 1997; Lambrechts and Pretorius 2000, Fleet, 2003). Although the influence of the must - and thus of the grape variety - is a primary one and therefore dominating, it is likely that each yeast strain as well has a typical way to change the aroma composition of the fermentation product - although we do not exactly know the abstraction rules of this process.

If this idea is correct, it should be possible to recognize the yeast that was used to produce the wine out of its aroma profile. Furthermore, going far beyond human abilities, an ANN should be able to predict the aroma composition of a wine to a certain degree, if it knows which must and which yeast were used to produce it. It is worth analyzing whether it is even possible to forecast the aroma profile of a wine, if the fermenting yeast but not the used must is already known to the artificial taster. In this case information about the aroma profile of a yet unknown must should help the ANN to construct the aroma profile of the resulting wine.

Material and Methods

Yeast strains

With one exception we used yeast strains that are filed at the Institution of Applied Mikrobiology (IAM), University of Agriculture, Vienna. Ten different yeast strains were used in this experiment, seven strains of *Saccharomyces cerevisiae*, one of *S. bayanus* var *uvarum*, one hybrid with the parental species *S. cerevisiae* and *S. kudriavzevii*, and one where the species is unknown to us. All yeasts were isolated in Austrian vinegrowing regions by the Federal Office of Viticulture. Isolation was done during a monitoring in 2003 and 2004.

The *S. cerevisiae* strains are HA 1834, isolated from a Grüner Veltliner in the winegrowing region Thermenregion, HA 1919 from a Zweigelt of Neusiedlersee – Hügelland, HA 1863 - HA 1864 from Blaufränkisch of the same winegrowing region, HA 2170 from a Welschriesling of this region. HA 2198 and HA 2195 are from a Zweigelt of South Styria. HA 2245 is from the same winegrowing region, but was isolated from Sauvignon blanc. HA 1836 is the interspecies hybrid, isolated from St. Laurent of the Thermenregion. HA 2139 is a *S. bayanus* var *uvarum* strain that originates from a Zweigelt of Neusiedlersee – Hügelland. N. i. (not identified) is from the same region and was isolated from a Cuvee.

Grape musts

12 varieties of grape juice, harvested in 2005 or 2006, were used cleared and pasteurized for vinification. All juices - with one exception - are from *Vitis vinifera*. Two musts are of the grape variety Grüner Veltliner (GV I and GV II), two of Welschriesling (Wr I and Wr II). These and the following are musts from white grape varieties: Müller Thurgau, Muskat Ottonell, Bouvier, Weissburgunder and Rheinriesling. Blauburger and Zweigelt are musts of red grape varieties. One must originates from a red hybrid of different *Vitis* - species (variety Ripatella). 25 aroma constituents of all musts were analyzed, not the same as for the wines, because different components are frequent in musts and wines.

Fermentations

For the production of wines sterile 300 ml Erlenmeyer-flasks were used. To each flask 250 ml of must was added under sterile conditions and the adequate yeast was inoculated in a concentration of 10^6 cells/ml of pure yeast culture. No auxiliary substances were added. Vinification occurred at 22℃. Fermentations were observed by determining the weight loss, caused by CO_2 - production. Weight loss was measured once a day. Altogether the fermentation process of 130 wines was registered. 110 wines were unique in the combination of must variety and used yeast strain. The wines produced with the must of Grüner Veltliner I (GV I) were made in two replicas (20 wines), to analyze wine variability under identical conditions.

Analysis of aroma components

The aroma composition was analyzed, 83 aroma components from 130 resulting wines were determined and furthermore 25 aroma constituents of 12 musts.

The wine (or must, respectively) sample (5 ml) with 2 g sodium chloride and 50 µl 3-decanol (48,8 ppm) as internal standard, were placed in a 10 ml headspace vial equipped with a magnetic bar and capped with a PTFE-coated silicone septum. For the headspace SPME process a 2 cm Car/PDMS/DVB (Supelco) fibre was chosen to adsorb aroma compounds. The fibre was exposed in the headspace of sample vials for 30 min. at 30℃. After extraction, the fibre was immediately inserted into the GC injector port for 2 min. at 250℃ for thermal desorption. For determination of different aroma compounds a CP-WAX 52 CB capillary column (50 m x 0.32 mm, 0.4 µm df; Varian) was used. The oven temperature was held at 50℃ for 3 min. before being increased by 4℃ per min. to 180℃, and afterwards to 230℃ at a rate of 25℃/min. and then kept at this temperature for a further 7,5 min. The whole cycle lasts 45 min. Helium was used as carrier gas with the constant flow rate of 1.0 ml/min.

Neural Network

A three layer Feedforeward-Backpropagation-ANN was developed using Borland Developer Studio 2006, written in Delphi Pascal (Borland International, Scott's Valley CA, USA).

- Forecasting

In dependence of its task, the network was designed using a total of 22 inputs (10 for the yeast and 12 for the must) or 35 inputs (10 for the yeasts and 25 for the aroma constituents that were used to determine the must). In the latter case, the values of the SIM (single ion mode) areas of each aroma component were minimum – maximum – scaled and thus the input data ranged between 0 and 1. 48 hidden neurons were positioned in the inner layer. If there are too much hidden neurons, the ANN starts to learn by heart instead to abstract. The output layer consisted of 83 neurons, one for each aroma constituent. The activation function of the neurons was a sigmoidal function, $1/(1+e^x)$. Backpropagation of error was performed using the sum of the squared differences between measured and prospected (output-) SIM areas. Details about learning with the backpropagation algorithm can be found in Rumelhart et al., 1986. Learning was performed until a minimum error was reached. Learn items were taken from a subset of the 130 wine aroma profiles, the remaining profiles, that were not previously used for training the network, were taken as test items (Fig. 1).

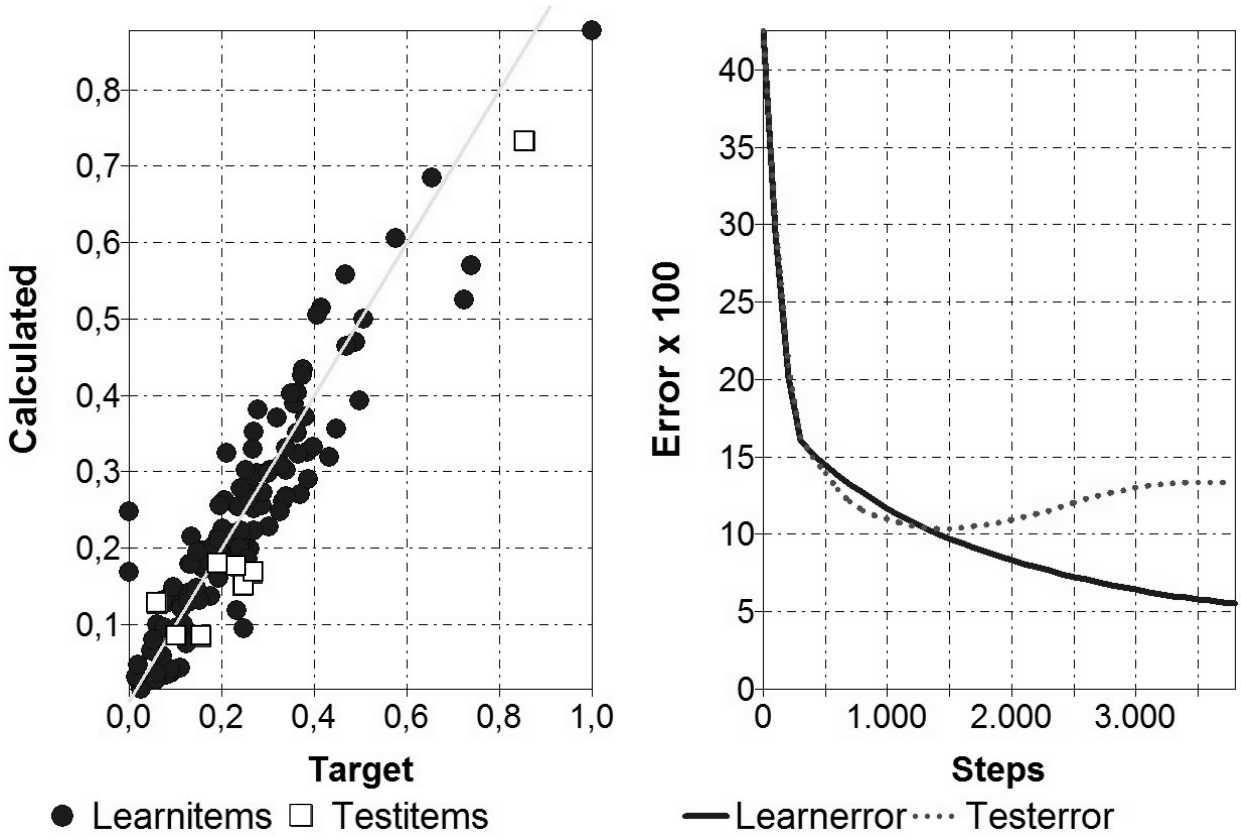

Fig. 1: Example of ANN – learning. Learning target is the abstraction rules that are necessary to calculate the SIM (single ion mode) -area of an aroma constituent (in this case isoamylacetat
) of a wine, where the must/yeast-combination is unknown to the ANN (test items). Learning occurs by comparison of known aroma profiles of wines (learn items). Target: SIM – area of the aroma constituent. Calculated: Predicted SIM area of the same aroma compound. The best result was reached after less than 1500 steps.

- Identification

Three layer Feedforeward-Backpropagation-ANNs were constructed, either with 93 input neurons (83 for the aroma constituents of the wine and 10 for the yeast strains) or with 95 (83 for the aroma constituents of the wine and 12 for the must varieties). In the first case, 12 output neurons were used to identify the must, in the second 10 output neurons had to identify the yeast strain. The hidden layer consisted of 11 or 9 neurons, respectively. Learning was performed as in the forecasting ANNs.

Data analysis

The ANN was used for the forecasting of the aroma profile of a – for the network – yet unknown wine, a new combination of must and fermenting yeast. Only the combination was new to the ANN, because the learn set contained other wines created from this special must or fermented by the special yeast, but not in the combination that was used as learn singleton.

Absolute values of differences between expected and measured aroma SIM areas were taken to quantify the forecasting quality.

Furthermore the ANN was utilized to identify either the must, or the yeast that was used to produce an unknown test wine. The highest output value was taken as identified must variety or yeast strain, respectively.

Statistical analysis (PCA) was performed using Statgraphics Centurion Version XV software (Manungistics, inc. USA, 1998).

Results and discussion

- **Description of the wines**

Most peculiar of all wines are the ones of the variety Muskat Ottonell, white wines with extremely high amounts of terpenes (see aromagram fig. 2). Compared with Muskat Ottonell, all other have only low terpene concentrations, with the exception of the Rheinriesling wines that exhibit moderate concentrations of these substances.

Relatively high concentrations of alcohols others than ethanol can be found in the wines of Grüner Veltliner I, Müller Thurgau, Blauburger and also Ripatella. Ethylester rich are Rheinriesling, Muskat Ottonell, Bouvier and Blauburger. The highest acetate concentrations can be found in Grüner Veltliner I, surprisingly the lowest in Grüner Veltliner II.

We performed a Principal Component Analysis (PCA) to see whether it's possible to obtain a small number of linear combinations of the 83 variables which account for most of the variability in the data. The procedure extracted 22 components that account together for 82% of the total variability of the original data. Thus a good simplification with this linear method is not possible. The 3D plot using the first three components as axis (not shown) separates Muskat Ottonell wines from all others and creates no further clusters. The wines which were produced by one yeast never grouped together (the first three principal components account for 34% of the total variability). From this analysis we can assume that identifying the must or the yeast is by no means trivial, nor is the forecasting of the aroma profile of an yet unknown combination of must and fermenting yeast.

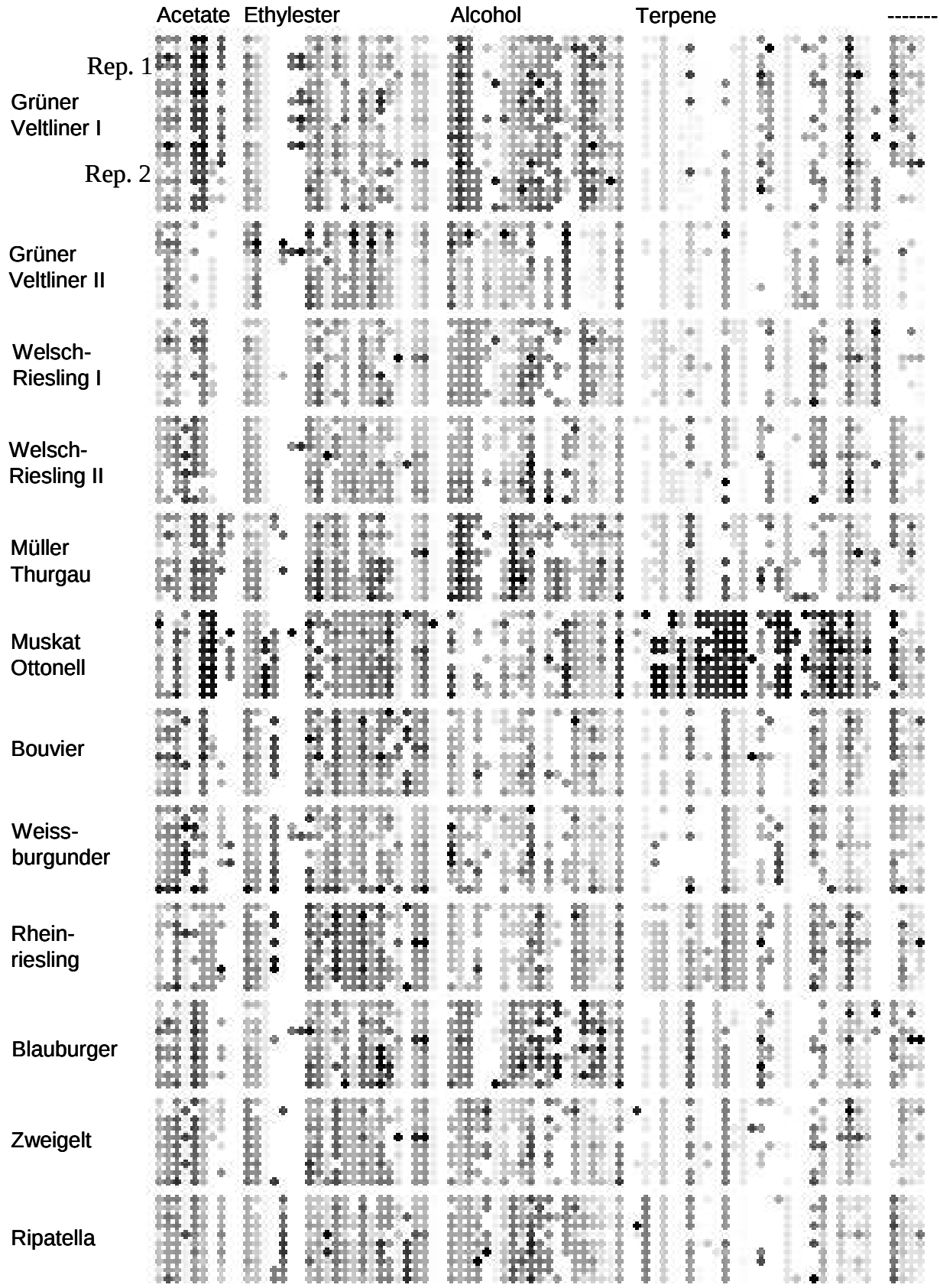

Fig. 2: Aromagram of all 130 wines. The rows represent wines, the columns single aroma constituents. The data (square root of the SIM – areas or the concentrations, respectively)

are column-wise minimum – maximum scaled, where minimum ist a white circle and maximum a black one. Wines are sorted row-wise after: 1st) must; 2nd) yeast strain (*S. cerevisiae* HA 1834
; *S. cerevisiae* x *S. kudriavzevii* HA 1836; *S. cerevisiae* HA 1919; *S. cerevisiae.* HA 1863; *S. bayanus* var *uvarum* HA 2139; *S. cerevisiae* HA 2170; n. i (not identified).; *S. cerevisiae* HA 2198; *S. cerevisiae* HA 2195; *S. cerevisiae* HA 2245
).

- **Difference between wines produced under identical conditions**

Forecasting of random processes is not possible and therefore we had to see how determined the fermentation process is. Thus we had to find out the difference between the concentrations (or SIM-areas, respectively) of the aroma constituents of wines produced under identical conditions, e.g. produced of the same must fermented by the same yeast and of course all other basic conditions as similar as feasible.

To get an impression of this difference we made two replicas of each of the wines produced from Grüner Veltliner I with the ten yeast strains. For each aroma compound we determined the absolute value of the difference of the concentrations (or SIM-areas, respectively) of the two wines created under identical conditions and compared this value with the whole production range of the aroma constituent within the 130 wines. On average the difference between the two wines accounts 6,7%. In general, terpenes are produced with the highest constancy (mean difference 4%), followed by esters (6%). Acetate and alcolhol production differ more (about 9%). The 'worst' constituents were Citronellylacetat (21%), 3-Hexen-1-ol, acetat (21%), 2-Decanol (27%), 3-Hexenioc acid,ethylester (29%) and 2-Nonanone (43%). Concerning these compounds, certainly no forecasting is possible. In wines of other grape varieties almost certainly other constituents are weakly determined but all in all we conclude that random is not too important.

Reproducibility is different in the yeast strains. It was best in HA 1919 (5% difference), good in HA 1834 (6%), HA 2195 (below 7%), and HA 1863 (also below 7%), all *S. cerevisiae*, and worst in HA 2170 (*S. cerevisiae*) and HA 2139 (*S. bayanus*), both 15% difference.

- **Forecasting of GV I wines**

To check the quality of forecasting we choose a situation that allows a comparison of the difference between the forecasting result and actual wines on one hand and the difference of wines produced under identical conditions on the other.

For this experiment the ANN got a learn set of 120 wines, that means, all wines except of the replications of the Grüner Veltliner I ones. Test items (ten forecasted wines) were those with Grüner Veltliner I must and all used yeast strains (the replications). Because the ANN got more information than the ten GV I wines and because it abstracts, the resulting aroma profiles were not identical to the corresponding GV I learn wines. The forecasted wines were compared with the corresponding replications of GV I (the wines, the ANN didn't know). On average the difference between the corresponding wines accounted 7,2%, about the same value that was reached by comparing the two replicas. Thus the forecasting at least didn't lead to loss of information.

- **Forecasting under ideal conditions**

To teach wine forcasting to the ANN we used a learn set of 129 wines. The remaining wine and hence a combination of must and fermenting yeast strain unknown to the neural network was used as singleton test set. This procedure was repeated - starting always with an untold ANN - so that all 130 wines were used as test item (leaving-one-out or jackknife method).

Compared with the whole range of the aroma constituents within the 130 wines, on average (per wine and aroma compound) the difference between original and forcasted wine was only

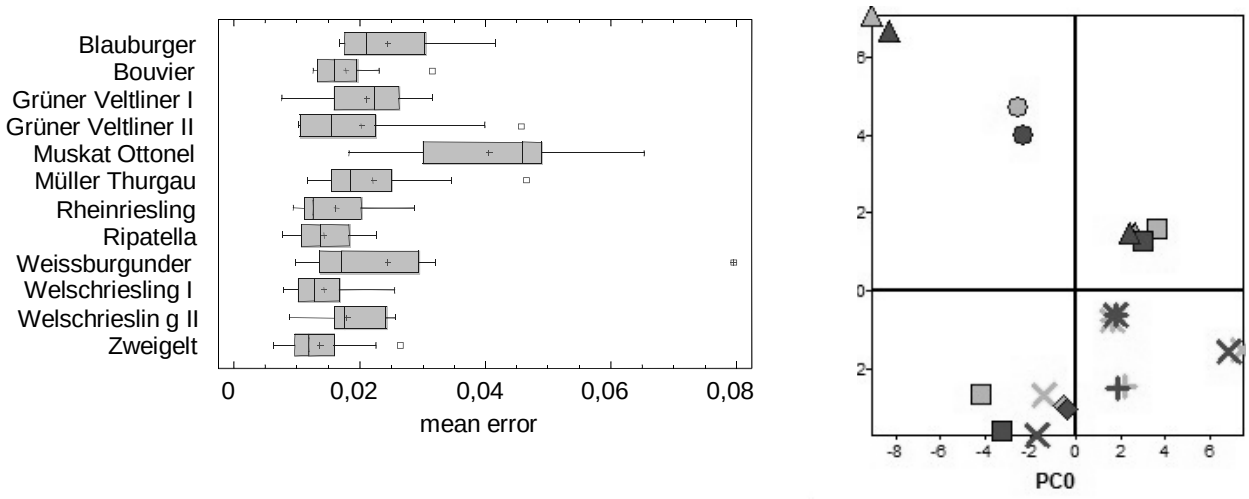

Fig. 3: Left: Average forecasting error for the wines, sorted after grape must. Right: Comparison of predicted (dark) and actual (lightgrey) Zweigelt wines using Adaptive Principal Component Analysis. Corresponding wines (same symbol) are often "paired", indicating a high aroma profile similarity of actual and predicted wines.

2,1% (fig. 3). The wines that were worst predicted are the ones that originated from Muskat Ottonell must. Here the mean error was 4,1%. Especially the forecasting of the terpenes was erroneous in these wines. This is of course understandable, because the concentration of terpenes in these wines are extremely high compared to the others. In Blauburger wines bad forecasting concerned mainly the alcohols, especially methanol and benzylalcohol. These two alcohols were found in relatively high concentrations in all Blauburger wines created in this experiment. In Weissburgunder the wine produced of HA 2245, *S. cerevisiae* of South Styria, was predicted with low quality (appendix A). The same is true for the GV II wines produced by HA 1836, the hybrid strain from the vinegrowing region Thermenregion and, to a minor extent, HA 1919, *S. cerevisiae* from Neusiedlersee – Hügelland.

- **Forecasting if the must is not known**

We simulated a situation, where the neuronal net should predict the aroma profile of a wine produced from a certain must, without knowing any wine created from this must. In this study the learn set contains must aroma profiles as an input and wine aroma profiles of wines produced from those musts as output. The ANN should abstract the special features of a must by its aroma spectrum. Hence in this study the input data were yeast index (10 different input combinations for the 10 yeasts) and concentrations (SIM-areas) of the 25 aroma constituents that were used to determine the must. 83 output neurons determined the predicted wine. During the experiment, the ANN was not allowed to learn the aroma profiles of the wines produced from that must of the twelfe, where the wines should be predicted, but of course from all other wines.

Under these circumstances the ANN was not able to forecast aroma profiles better than under random conditions (e.g. random input data for aroma constituents). It may be that the 25 aroma components of the must did not comprise enough information to forecast the 83 constituents of the wines.

- **Recognition of the must variety**

Must recognition - that means the identification of the must that had been used to produce a wine - is one of the abilities an experienced taster should have to a certain extent. To teach must recognition to the ANN, here we used the maximum possible learn set of 129 wines and the last wine remained unknown to the neural network and was used as singleton test set. Starting always with untold ANNs, this procedure was repeated 130 times, so that each wine was used once to find out, whether a correct assignement occurred (jackknife method, fig. 4).

In eight out of 130 cases (6%) the assignement was wrong and in 94% it was successful. By pure chance, we would appreciate a mean success rate of 8%. Thus we can say that the ANN is a very good taster under ideal conditions and is able to learn the general abstraction rules of the influence of must on wine aroma.

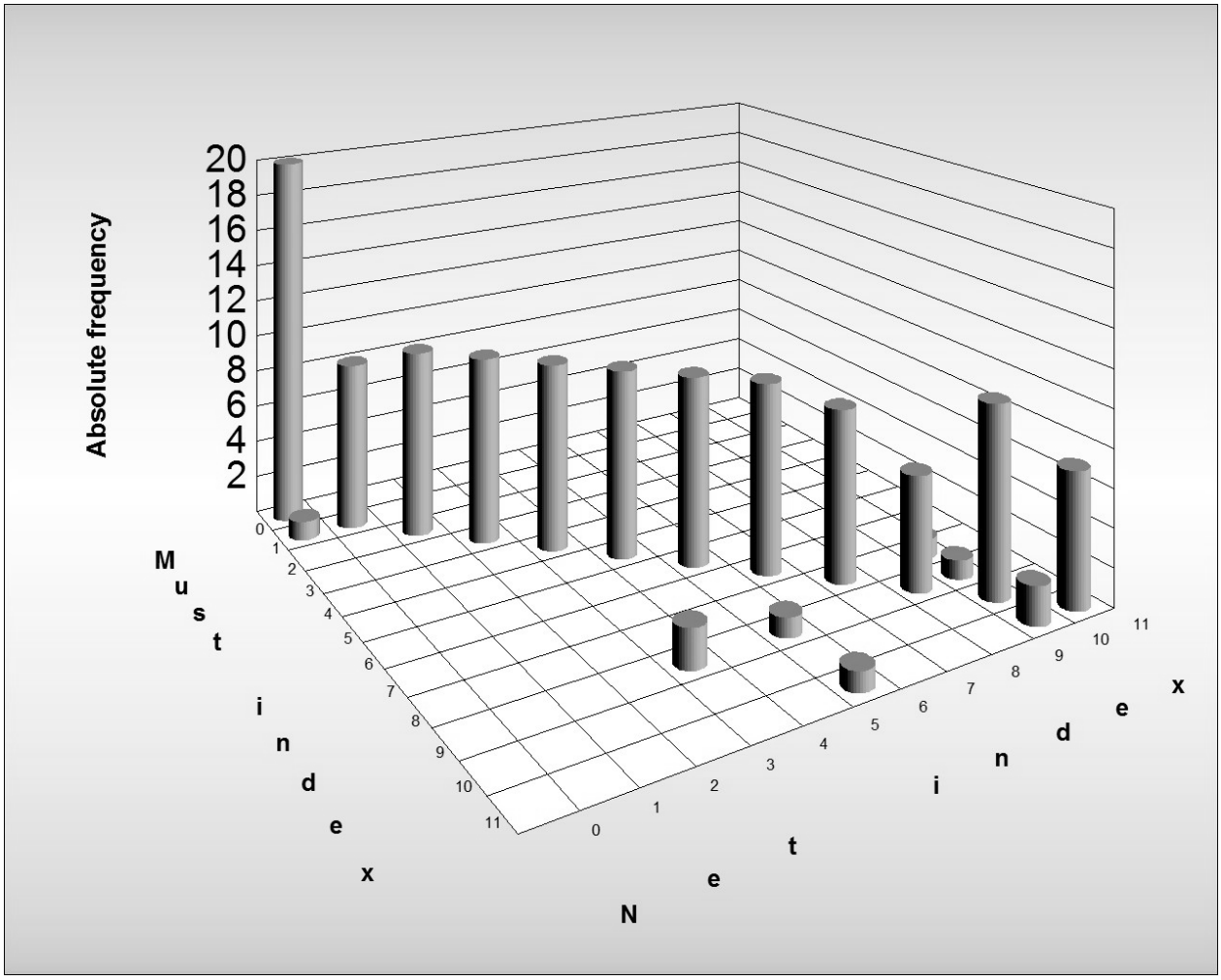

Fig. 4: Graphical representation of the confusion matrix concerning the must identification experiment. The columns in the diagonal represent correct identifications (94%).

Most erroneous identifications occurred concerning only two wines, Weissburgunder (index 9), that was confused with Grüner Veltliner (GV II, index 4), Welschriesling (Wr II, index 6) or Rheinriesling (Rr, index 10); and Zweigelt (index 11), that was (surprisingly) confused with Welschriesling (Wr II) or Rheinriesling (Rr). ‘Rheinriesling’ was the most frequent incorrect output.

- **Recognition of the yeast strain**

To identify the yeast strain that was used for fermentation from the aroma profile of a wine is certainly more difficult than must recognition. Not the basic constituents but fundamental metabolic pathways must be detected. The conditions of this experiment were similar to the one for recognizing the must. In this case we appreciate an identification rate of 10% by pure chance.

In 87 out of 130 cases the assignement was correct, which gives an accurate identification of 67%. The identification ability of the ANN differed depending on the yeast strain:

HA 2245, a *S. cerevisiae* strain isolated in South Styria and HA 2139, a *S. bayanus* var *uvarum* strain from the north of Burgenland (index 9 and 4 from fig. 5) were always correctly identified. HA 2198 (index 7), *S. cerevisiae* from South Styria and HA 1836 a hybrid (*S. cerevisiae x S. kudriavzevii*, index 1),isolated in Lower Austria were only once erroneously identified and HA 1919 (*S. cerevisiae* strain from the north of Burgenland, index 2) only three times. Most confusions occured within the yeasts of the vinegrowing region Neusiedlersee-Hügelland, especially the ones isolated in St. Georgen. In contrast no confusion occured in yeasts isolated in the Thermenregion and only one in the yeasts of South Styria. Yeasts of different winegrowing regions were frequently confused too.

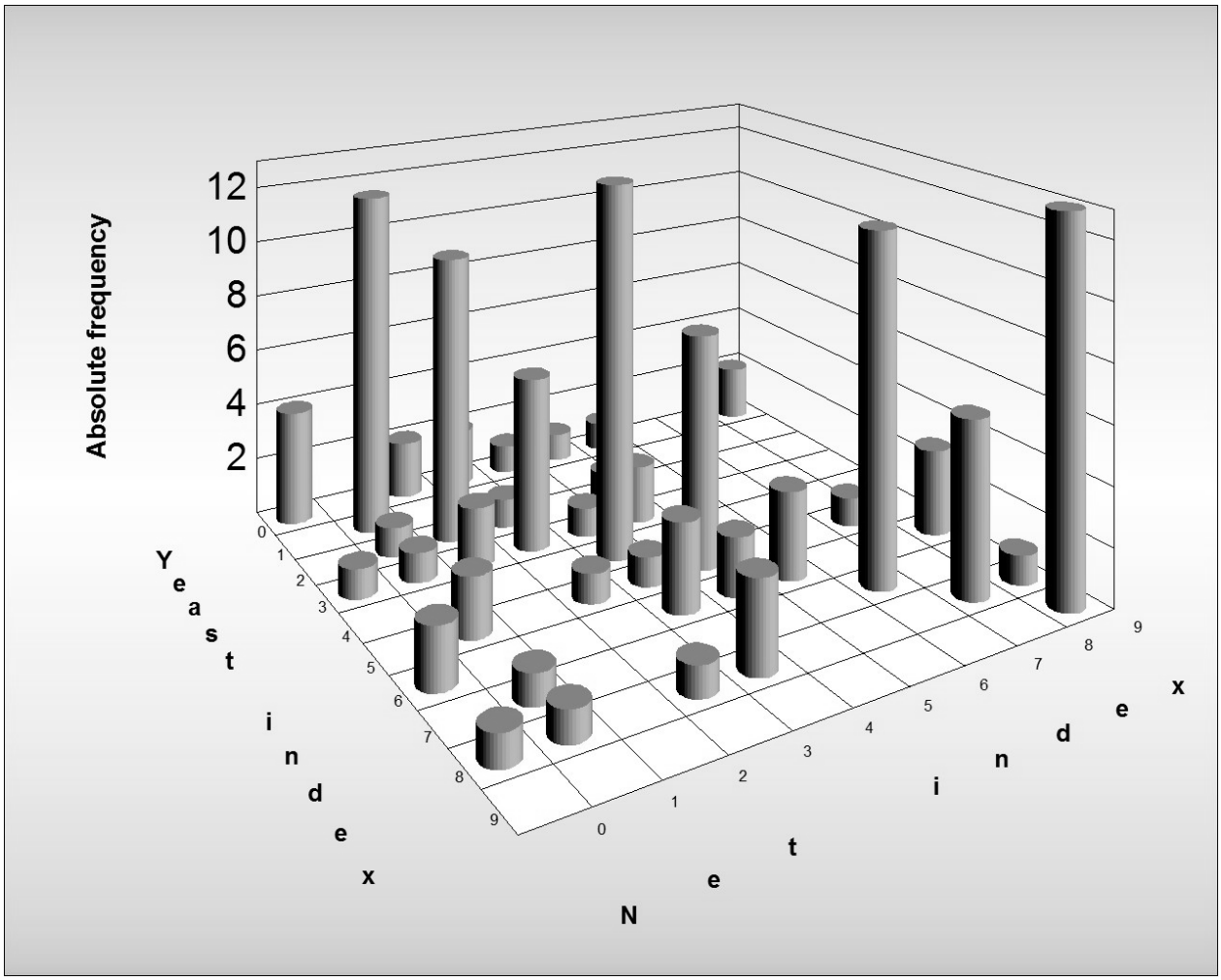

Fig. 5: Graphical representation of the confusion matrix concerning the yeast strain identification experiment. The columns in the diagonal represent correct identifications (67%).

The most frequent incorrect output concerns HA 2139 (*S. bayanus* var *uvarum*, index 4) that was ten times errouneosly chosen to have been the fermenting yeast strain from the ANN. HA 1836 (*S. cerevisiae* x *S. kudrivzevii*, index 1) and HA 2170 (*S. cerevisiae*, index 5) were both six times incorrectly chosen. So we may conclude that the most “exotic” yeast strains can be identified easily if the must is really fermented by this yeast but on the other hand in the case of a doubtful decision the ANN choose these strains especially frequently, even if the actual fermenting yeast was a different one.

Our study validates the utility of ANNs for recognizing the basic must and the fermenting yeast of wines and for the prediction of aroma constituents of yet unknown combinations of the wine producing agents. The high quality especially of the must recognition even when data extent is relatively low shows that ANNs are very likely excellent tools for wine characterization. Other wine characteristics, like vintage, localization of the grape and of course grape variety may as well leave their marks within the aroma profile of a wine and hence a comprehensive description of wines using ANNs seems possible.

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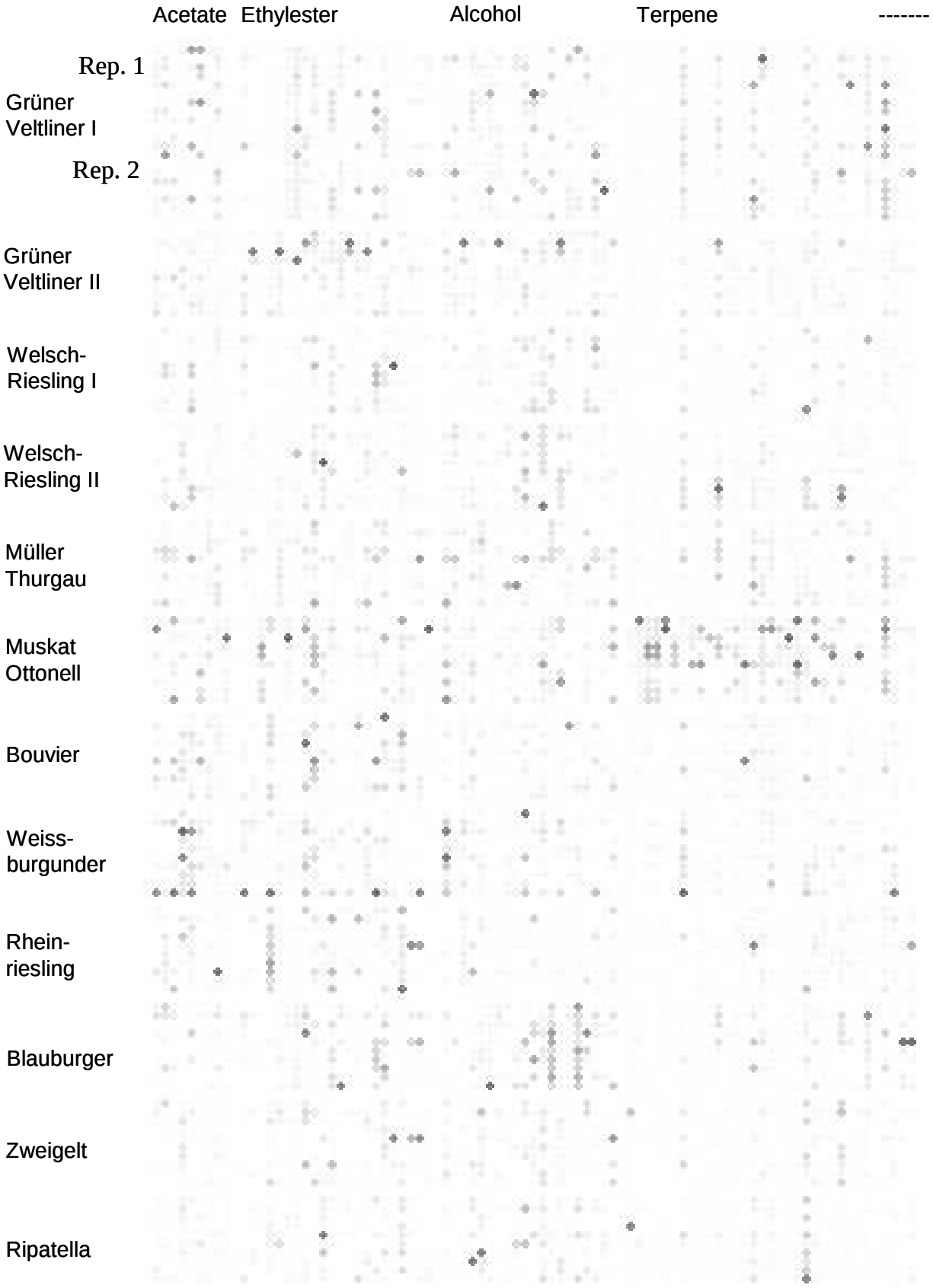
Appendix A: Difference between original and predicted wine for all wines and aroma constituents. For further explanation see legend of fig. 2 and appendix B.



Appendix B: Aroma constituents. Sequence as in fig. 2 and appendix A (from left to right).

Acetate

1 Acetat-i-Butyl
2 Acetat-n-Butyl
3 Acetat-i-Amyl
4 Hexylacetat
5 3-Hexen-1-ol, acetat (I)
6 3-Hexen-1-ol ,acetat (II)
7 Acetat-n-Heptyl
8 Acetat-i-Octyl
9 Acetat-n-Octyl

Ethylester

10 Ethylbutyrat
11 Butanoic acid,3-methyl,-ethylester
12 Ethyl-2-Butenoat
13 Ethylhexanoat
14 Ethyl-4-hexenoat
15 2-Hexenoic acid,ethylester
16 3-Hexenioc acid,ethylester
17 Ethylheptanoat
18 Ethyllactat
19 Ethyl-2-Hexenoat
20 Ethyloctanoat
21 Ethylnonanoat
22 Ethylfuroat
23 Ethyldecanoat
24 Diethylsuccinat
25 Ethyl-8-decenoat
26 Ethylundecanoat
27 Ethyldodecanoat
28 Ethyltridecanoat
29 Ethyltetradecanoat
30 Ethylhexadecanoat
31 Ethylacetat

Alcohol

32 iso-Hexanol
33 n-Hexanol
34 3-Hexen-1-ol (I)
35 3-Hexen-1-ol (II)
36 3-Octanol
37 1-Octen-3-ol
38 n-Heptanol
39 n-Hexanol-2-ethyl
40 2-Octanol
41 n-Octanol
42 2-Decanol
43 n-Decanol
44 Benzylalkohol
45 Whiskeylactone
46 4-Ethylguaiacol
47 Methanol
48 n-Propanol
49 i-Butanol
50 n-Butanol
51 i-Pentanole

Terpene

52 ß-Pinene
53 p-Myrcene
54 iso- Terpinolen
55 D-Limonene
56 ß-Thujene
57 α -Terpinen
58 o-Cymol
59 p-Caren
60 iso-Terpinolen
61 Geranylethylether 1.
62 α-Ionon
63 Linalool
64 Hotrienol
65 alpha-Fenchen
66 Citronellylacetat
67 ß-Farnesen
68 α-Fencon
69 α-Terpineol
70 Spiro-substances
71 Geranylacetat
72 Nerylacetat
73 ß-Citronellol
74 Nerol
75 2-Phenylethylacetat
76 ß-Damascenon
77 Geraniol
78 2-Phenylethanol
79 Nerolidol

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80 2-Nonanone
81 Furfural
82 Benzaldehyd
83 Hexanoic acid