# Application of Artificial Aging Techniques to Samples of Rum and Comparison with Traditionally Aged Rums by Analysis with Artificial Neural Nets

J. Quesada Granados,*,† J. J. Merelo Guervós,‡ M. J. Oliveras López,†
J. González Peñalver,‡ M. Olalla Herrera,† R. Blanca Herrera,† and
M. C. López Martinez†

Departamento de Nutrición y Bromatología, Facultad de Farmacia, Universidad de Granada,
Campus Universitario de Cartuja s/n, 18071 Granada, Spain, and Departamento Arquitectura y
Tecnología de Computadores, Facultad de Ciencias, Universidad de Granada,
Campus Fuentenueva s/n, 18071 Granada, Spain

Artificial aging techniques were applied to samples of rum. These samples were then compared, by artificial neural nets, with traditionally aged rums. Analysis was based on the phenolic and furanic composition of each sample. There were found to be few statistical differences between samples, thus confirming the possibility of applying artificial aging techniques to obtain rum with phenolic and furanic characteristics that are similar to those of rum obtained by traditional methods.

## INTRODUCTION

**Considerations about Rum Aging.** Rum is a cane spirit obtained by the distillation of sugar cane molasses, after fermentation with various types of yeast, and subsequent aging in wooden casks, normally of American oak, where the spirit acquires its special characteristics of flavor and aroma during the time it is in contact with the wood (*1*). During this stage, also termed maturation, the spirit extracts a series of compounds from the wood that have a positive influence on the organoleptic characteristics of the final product (*2*, *3*). The physical and chemical process that occurs during aging is the hydrolysis of the lignin in the wood of the cask (*4*−*6*), from which various phenolic compounds are extracted; by oxidation, these form aldehydes and acids with radicals, together with aromatic agents such as vanillin and syringaldehyde (*7*−*9*). Another group of compounds, the furanic aldehydes, which are extracted by cask distilling, do not directly intervene in the final characteristics of aroma, color, and bouquet of the beverage (*10*−*13*).

The fundamental process by which the beverage acquires its unique organoleptic characteristics, however, incurs substantial maintenance overheads, arising from nonsaleable stocks, the annual rotation of casks, insurance of premises and merchandise, storage costs, and, above all, evaporation losses (*10*).

Therefore, the alcoholic beverages group within the Department of Nutrition and Bromatology at the Pharmacy Faculty, University of Granada, since 1990, has been investigating the artificial aging of all alcoholic beverages that are subjected to aging in wooden casks (*14*). Rum is one such beverage.

**Neural Nets for Rum Composition Visualization and Analysis.** Neural nets (NNs) are statistical techniques that are commonly used for pattern recognition, forecasting, and scientific visualization (*15*). It is impossible to generalize about NNs, so we will focus only on the algorithm used in this study: Kohonen's self-organizing map (SOM) (*16*).

Kohonen's SOM can be described as a single-layer, feedforward, nonsupervised neural net. Like all NNs (and many statistical algorithms) SOMs must be "trained" before being able to perform whatever they were designed to do. Training means presenting a set of vectors to the NN, so that it changes its internal values. In this case, the values by which each sample is classified need not be set in advance, which is why it is called nonsupervised.

An SOM is basically a set of *N*-dimensional vectors in which a neighborhood relation has been defined. These vectors are arranged in a two-dimensional grid in such a way that each vector or unit is the neighbor of another six; that is why each unit is represented as a hexagon (another possibility is for each unit to be a neighbor of another eight, in which case each unit is represented as a square and the map itself is rectangular). An SOM must be trained for each task; the vector in each unit changes its values. Initially, all vectors are set to a small random quantity; training means selecting one vector fom the training set, computing the unit closest to it, and changing that unit's vector and those of all its neighbors to make them closer to the input vector. The neighborhood arrangement makes the map self-organize, so that nearby units respond to contiguous zones

* Corresponding author (telephone +34-958243863; fax +34-958243869; e-mail quesadag@ugr.es).
† Departamento de Nutrición y Bromatología.
‡ Departamento Arquitectura y Tecnología de Computadores.

Application of Artificial Aging Techniques to Rum

*J. Agric. Food Chem.*, Vol. 50, No. 6, 2002 **1471**

in the input space, and because the neighborhood decreases during training, each unit becomes fine-tuned to a particular zone in the input space.

SOMs that have been trained with a particular training set, such as the compositions of artificially and naturally aged rums in this case, perform several tasks at the same time:

(i) Clustering. By analysis, clusters, that is, natural groups within the data, can be discovered.

(ii) Nonlinear projection, which, in addition, preserves metric distances.

With these considerations in mind, we have attempted to apply artificial aging techniques in order to avoid, at least in part, some of the problems implicit in "classical" aging methods for rum. So, the objective for this project was to compare the phenolic and furanic composition of artificially aged and traditionally aged rums to check if the artificial aging techniques are adequate for obtaining rums with phenolic and furanic characteristics similar to those of rum obtained by traditional methods.

## MATERIALS AND METHODS

**Samples Analyzed.** The following samples were analyzed:

(a) Eighteen samples of commercially available brands of rum, manufactured by traditional aging techniques, were grouped according to the aging time stated on the label and to the denominations established by the pertinent legislation in Spain [white rum, golden rum, aged (not less than one year in the cask) rum. and old rum (not less than three years in the cask)]. The commercial brands analyzed comprised two samples of white rum, five of golden rum, five of aged rum, and six of old rum (*17*).

(b) Thirty-six samples of rum were manufactured by 18 methods of artificial aging, such that two samples of each method were available (a and b), identified as methods 0(V0)−17(V17).

Each sample was analyzed three times, obtaining the arithmetic median for each of them.

Finally, we obtained a sample of white cane spirit, the raw material used to manufacture the noncommercial rums.

**Analytical Method.** High-performance liquid chromatography (HPLC) was used to determine the phenolic and furanic composition of the different types of rum by direct injection of the samples. Prior to HPLC, as is standard practice, the samples were filtered through cellulose membranes of 0.45 $\mu$m pore diameter. The chromatographic technique applied was based on that developed by Gimenez et al. (*6*) for samples of brandies. The liquid chromatograph was a Perkin-Elmer Binary LC Pump 250, with a Waters 717 plus autosampler and a vis−UV Perkin-Elmer diode array detector 235 set at 280 nm. The column used was a Spherisorb ODS, 20 cm long and having an internal diameter of 4.7 mm. Two solvents were used: A, bidistilled water containing 0.15% of trifluoroacetic acid; and B, bidistilled water containing 70% of methanol and 0.15% of trifluoroacetic acid, with a flow rate of 1 mL/min. A correct separation was obtained with the following elution gradient: time 0 min, 100% of A and 0% of B; time 5 min, 95% of A and 5% of B; time 10 min, 75% of A and 25% of B; time 18 min, 70% of A and 30% of B; time 33 min, 60% of A and 40% of B; and time 53 min, 0% of A and 100% of B.

For computer analysis of the results, the statistical software packages Statgraphics v5.0 (STSC) and SOM-PACK v3.1 and 3.2 (Technological University of Helsinki) were used.

**Artificial Aging Treatments.** Artificial aging treatments are based on previous studies carried out in our laboratories (*14*), but, in general, all of them were based upon the use of 5 mm diameter oak chips.

White cane spirit was used to manufacture rum, which was then subjected to the artificial aging treatments described in **Table 1**.

## RESULTS AND DISCUSSION

A chromatographic study was made of 13 compounds, 11 of which were phenolic and 2 of which were furanic: gallic acid,

**Table 1.** Treatments of Artificial Aging Characteristics[a]

| treat-ment | alcoholic strength (% v/v) | washing of toast oak shaving in boiling water (h) | | shaving (%) | treatment time (days) |
|---|---|---|---|---|---|
| | | previous | current | | |
| V0 | 55.0 | | | 2 | 30 |
| V1 | 55.0 | | 2 | 0.5 | 30 |
| V2 | 55.0 | | 2 | 0.8 | 15 |
| V3 | 55.0 | | 2 | 2 | 30 |
| V4 | 55.0 | | 2 | 2 | 330 |
| V5 | 55.0 | 2 | | 1 | 330 |
| V6 | 55.0 | | 2 | 1 | 60 |
| V7 | 55.0 | 3 | | 1 | 330 |
| V8 | 55.0 | | 2 | 1 | 90 |
| V9 | 55.0 | | 2 | 1 | 120 |
| V10 | 55.0 | | 2 | 1 | 150 |
| Vll | 55.0 | | 2 | 0.5 | 10 |
| V12 | 40.0 | | 2 | 0.8 | 20 |
| V13 | 37.5 | | 2 | 0.8 | 20 |
| V14 | 40.0 | | 2 | 0.8 | 30 |
| V15 | 40.0 | | 2 | 0.8 | 25 |
| V16 | 40.0 | | 2 | 0.8 | 10 |
| V17 | 75.0 | | 2 | 0.8 | 20 |

[a] Toast oak shaving temperature, 180 °C; toast time, 3 h; kind of maceration, static.

5-(hydroxymethyl)furfural, protocatechuic acid, furfural, *p*-hydroxybenzoic acid, *p*-hydroxybenzaldehyde, vanillic acid, caffeic acid, syringic acid, vanillin, *p*-coumaric acid, syring-aldehyde, and sinapaldehyde. All of these are related to the process of aging in oakwood casks. Although the chromatographic development of other phenolic compounds appears to be isolated, we decided to study only the ones previously described, due to the fact that they are most frequently found in the literature closely related to the processes of aging in wood (*12−14*).

**Commercial Rum Samples.** The commercial brands analyzed were grouped into the four categories described above, according to their aging characteristics (**Table 2**). The reference-level phenolic and furanic concentrations for each category were taken as the arithmetic mean of the concentrations obtained within each of the groups (**Table 3**).

**Tables 2** and **3** illustrate the results obtained by HPLC analysis of the samples. It is apparent from these results that the differences between the means are sufficient to distinguish the different categories of rum. Furthermore, the concentration of these compounds tends to increase with aging time, which in this case is equivalent to the transition from white rum to golden rum, to aged, and finally to old rum, as the difference between the various categories is precisely the aging time spent in the cask. This increase is especially apparent in the cases of syringaldehyde and vanillin, as these aromatic compounds are characteristic of aging in oakwood casks. On the other hand, levels of sinapaldehyde, which is equally characteristic and thus might be expected to show a similar behavior pattern, actually fall with increased cask storage time. These results have been confirmed after the application of Fisher's least significant difference (LSD) procedure (**Table 4**), where we can observe, apart from the comments above, that there are significant statistical differences between the phenolic and furanic concentrations found in the different categories of commercial rum studied.

**Rum, Subjected to Artificial Aging Techniques, and White Cane Spirit.** The samples thus obtained (**Table 1**), together with those of white cane spirit, were analyzed under chromatographic conditions identical to those described for the com-

**1472** *J. Agric. Food Chem.,* Vol. 50, No. 6, 2002

Quesada Granados et al.

**Table 2.** Concentrations (Milligrams per Liter) of Phenolic and Furanic Compounds Found in the Samples of Commercially Available Rums

| | GA | 5HMF | PA | F | pHBAC | pHBAD | VA |
|---|---|---|---|---|---|---|---|
| RB1 | 4.09 ± 0.03 | 0.11 ± 0.32 | 0 | 0.17 ± 0.89 | 0 | 0 | 0 |
| RB2 | 4.91 ± 0.04 | 0 | 0.25 ± 0.72 | 0.17 ± 1.23 | 2.78 ± 0.52 | 3.80 ± 1.12 | 4.55 ± 0.76 |
| RD1 | 7.77 ± 0.44 | 5.75 ± 0.27 | 2.46 ± 0.06 | 1.41 ± 1.25 | 3.24 ± 0.85 | 0 | 4.38 ± 0.08 |
| RD2 | 4.95 ± 0.99 | 3.27 ± 0.86 | 1.34 ± 0.04 | 0.50 ± 1.59 | 2.06 ± 0.04 | 1.87 ± 0.65 | 4.49 ± 0.24 |
| RD3 | 6.27 ± 2.24 | 1.84 ± 0.53 | 2.72 ± 0.95 | 1.02 ± 0.16 | 6.22 ± 1.37 | 2.65 ± 0.75 | 0 |
| RD4 | 6.76 ± 2.30 | 7.11 ± 0.62 | 0.68 ± 0.12 | 0 | 0 | 0 | 0 |
| RD5 | 6.30 ± 0.38 | 2.39 ± 0.47 | 1.12 ± 0.35 | 0.66 ± 0.73 | 0 | 0 | 0.70 ± 1.30 |
| RA1 | 4.64 ± 0.05 | 0.13 ± 0.78 | 2.13 ± 0.03 | 1.65 ± 0.15 | 2.27 ± 0.04 | 1.95 ± 0.07 | 4.85 ± 0.83 |
| RA2 | 6.61 ± 0.38 | 1.21 ± 0.59 | 1.41 ± 0.42 | 1.85 ± 0.88 | 3.77 ± 0.24 | 3.76 ± 0.05 | 4.70 ± 0.37 |
| RA3 | 7.01 ± 0.58 | 0.58 ± 1.45 | 0.39 ± 0.12 | 0.33 ± 0.89 | 3.94 ± 0.78 | 4.46 ± 0.03 | 9.97 ± 0.73 |
| RA4 | 5.12 ± 0.94 | 1.67 ± 0.27 | 1.22 ± 0.33 | 0.68 ± 0.05 | 6.04 ± 0.57 | 4.09 ± 0.12 | 7.05 ± 0.06 |
| RA5 | 0 | 0 | 1.64 ± 0.09 | 0 | 4.43 ± 0.05 | 6.41 ± 0.31 | 0 |
| RV1 | 8.30 ± 2.60 | 1.35 ± 0.58 | 4.43 ± 2.98 | 5.07 ± 1.45 | 5.07 ± 2.89 | 2.42 ± 0.43 | 6.76 ± 1.97 |
| RV2 | 5.63 ± 0.84 | 1.65 ± 0.34 | 1.73 ± 0.67 | 0.51 ± 0.09 | 3.46 ± 40.97 | 5.51 ± 0.92 | 17.83 ± 0.61 |
| RV3 | 6.29 ± 0.57 | 2.04 ± 0.34 | 6.33 ± 1.73 | 1.64 ± 0.07 | 6.34 ± 0.76 | 5.83 ± 0.14 | 6.75 ± 0.32 |
| RV4 | 5.61 ± 0.44 | 0.40 ± 0.83 | 0.50 ± 0.26 | 0.48 ± 0.72 | 4.41 ± 0.19 | 5.68 ± 0.37 | 4.88 ± 0.47 |
| RV5 | 9.83 ± 2.56 | 2.11 ± 1.34 | 0 | 1.37 ± 0.53 | 5.33 ± 1.27 | 0 | 10.91 ± 1.21 |
| RV6 | 9.09 ± 1.61 | 8.61 ± 2.51 | 1.90 ± 0.97 | 3.60 ± 0.41 | 24.85 ± 0.52 | 10.85 ± 3.15 | 14.86 ± 1.02 |

| | CA | SA | pCA | SY | VN | SN |
|---|---|---|---|---|---|---|
| RB1 | 0 | 1.39 ± 0.18 | 2.55 ± 0.15 | 0 | 0 | 0 |
| RB2 | 3.34 ± 0.42 | 3.23 ± 0.32 | 2.42 ± 0.23 | 2.32 ± 0.46 | 6.20 ± 0.78 | 8.16 ± 4.08 |
| RD1 | 3.80 ± 0.49 | 4.37 ± 0.79 | 3.61 ± 0.04 | 3.70 ± 0.94 | 6.83 ± 0.55 | 8.04 ± 0.03 |
| RD2 | 3.48 ± 0.37 | 3.31 ± 0.14 | 2.41 ± 0.07 | 1.71 ± 0.02 | 6.15 ± 0.11 | 0 |
| RD3 | 2.92 ± 0.51 | 2.62 ± 0.71 | 3.09 ± 0.53 | 1.92 ± 0.72 | 3.56 ± 0.54 | 0 |
| RD4 | 7.46 ± 0.90 | 3.97 ± 0.56 | 1.64 ± 0.33 | 1.39 ± 0.08 | 6.69 ± 0.55 | 0 |
| RD5 | 4.11 ± 0.40 | 4.50 ± 0.98 | 3.83 ± 0.46 | 4.05 ± 0.81 | 6.97 ± 0.60 | 8.04 ± 0.03 |
| RAI | 4.03 ± 1.24 | 4.47 ± 0.29 | 2.00 ± 0.04 | 3.66 ± 0.61 | 7.30 ± 0.58 | 3.98 ± 0.63 |
| RA2 | 3.74 ± 0.09 | 3.74 ± 0.16 | 3.41 ± 0.68 | 2.55 ± 0.53 | 6.79 ± 0.39 | 4.12 ± 0.83 |
| RA3 | 3.62 ± 0.99 | 3.62 ± 2.35 | 2.43 ± 0.23 | 1.69 ± 0.28 | 7.24 ± 0.81 | 0 |
| RA4 | 10.42 ± 0.31 | 8.94 ± 0.76 | 8.59 ± 0.49 | 6.39 ± 0.86 | 11.03 ± 0.15 | 0 |
| RA5 | 0 | 8.03 ± 1.54 | 3.14 ± 2.24 | 1.46 ± 0.98 | 10.13 ± 0.62 | 0 |
| RV1 | 7.17 ± 1.28 | 5.36 ± 1.48 | 5.36 ± 0.95 | 4.40 ± 0.78 | 8.69 ± 0.94 | 7.89 ± 0.40 |
| RV2 | 4.96 ± 0.23 | 6.18 ± 0.49 | 2.64 ± 0.16 | 7.36 ± 0.56 | 8.46 ± 2.47 | 0 |
| RV3 | 7.09 ± 0.04 | 7.86 ± 0.55 | 4.40 ± 0.38 | 11.07 ± 0.94 | 8.27 ± 0.82 | 0 |
| RV4 | 6.87 ± 0.31 | 5.57 ± 0.20 | 3.12 ± 0.04 | 12.27 ± 0.99 | 7.92 ± 0.76 | 0 |
| RV5 | 9.67 ± 0.10 | 3.47 ± 3.01 | 5.38 ± 42.34 | 6.28 ± 0.52 | 6.23 ± 0.31 | 0 |
| RV6 | 11.05 ± 0.13 | 12.57 ± 0.41 | 4.65 ± 0.16 | 12.07 ± 0.08 | 11.27 ± 0.73 | 9.67 ± 1.07 |

**Table 3.** Mean Concentrations (Milligrams per Liter ± SD) of Phenolic and Furanic Compounds Found in Samples of the Different Categories of Commercially Available Rums

| component | white rum | golden rum | aged rum | old rum |
|---|---|---|---|---|
| GA | 4.50 ± 0.04 | 6.47 ± 1.27 | 5.76 ± 0.49 | 7.45 ± 1.43 |
| 5HMF | 0.05 ± 0.32 | 3.94 ± 0.55 | 0.84 ± 0.77 | 2.69 ± 0,99 |
| PA | 0.12 ± 0.72 | 1.40 ± 0.31 | 1.62 ± 0.20 | 2.48 ± 1.10 |
| F | 0.17 ± 1.06 | 0.88 ± 0.75 | 0.73 ± 0,50 | 2.11 ± 0.55 |
| pHBAC | 1.39 ± 0.52 | 1.81 ± 0.75 | 4.58 ± 0.34 | 8.24 ± 1.10 |
| pHBAD | 1.90 ± 1.12 | 1.12 ± 0.70 | 3.91 ± 0.11 | 5.04 ± 0.84 |
| VA | 2.27 ± 0.76 | 2.85 ± 0.54 | 4.37 ± 0.50 | 9.82 ± 0.93 |
| CA | 1.67 ± 0.42 | 4.51 ± 0.54 | 4.19 ± 0.66 | 7.79 ± 0.35 |
| SA | 2.31 ± 0.25 | 3.97 ± 0.64 | 5.53 ± 1.02 | 6.83 ± 1.02 |
| pCA | 2.48 ± 0.19 | 2.98 ± 0.29 | 3.85 ± 0.74 | 4.25 ± 0.67 |
| SY | 1.16 ± 0.46 | 2.68 ± 0.51 | 3.04 ± 0.65 | 8.90 ± 0.65 |
| VN | 3.10 ± 0.78 | 6.68 ± 0.47 | 7.85 ± 0.51 | 8.47 ± 1.01 |
| SN | 4.08 ± 0.86 | 4.04 ± 0.03 | 0.79 ± 0.73 | 2.92 ± 0.74 |

**Table 4.** LSD Procedure for Commercial Rums Analyzed

| method: 95.0%LSD | count | mean | homogeneous groups |
|---|---|---|---|
| RB | 13 | 1.93846 | X |
| RD | 13 | 3.33308 | XX |
| RA | 13 | 3.62000 | X |
| RV | 13 | 5.92231 | X |

| contrast | difference | ± limits |
|---|---|---|
| RB − RD | −1.39462 | 1.66502 |
| RB − RA | −1.68154[a] | 1.66502 |
| RB − RV | −3.98385[a] | 1.66502 |
| RD − RA | −0.28692 | 1.66502 |
| RD − RV | −2.58923[a] | 1.66502 |
| RA − RV | −2.30231[a] | 1.66502 |

[a] Denotes a statistically significant difference.

mercially available brands. The phenolic and furanic concentrations are summarized in **Tables 5** and **6**.

For each of the two methods, two replicates (a and b) were analyzed to test whether the results obtained were statistically significant and thus a real consequence of the application of the technique or, on the contrary, were the product of chance and not reproducible in successive samples. First, we studied the type of distribution of the data obtained for each of the treatments applied in order to adapt the statistical tests to the distributive characteristics of these data. The Kolmogorov−Smirnov goodness-of-fit test for a normal distribution at a confidence level of 95% was applied to the sample populations (treatment data). The type of distribution found for the sample populations was normal with the exception of the distribution found for sample V16 treatment, which was not normal. The statistical software package Statgraphics v5.0 was used to perform the statistical tests described in this section.

A multivariante parametric method (*t*-test based) was used to compare the results obtained for the replicates by the same method. In the case of method 16, for which the data produced by both replicates presented a non-normal distribution, a multivariante nonparametric method (Mann−Whitney-test based), was used, at a confidence level of 95% in both cases (*18−20*).

Application of Artificial Aging Techniques to Rum

*J. Agric. Food Chem.,* Vol. 50, No. 6, 2002 **1473**

**Table 5.** Concentrations (Milligrams per Liter) of Phenolic and Furanic Compounds Found in the Samples Analyzed

| | GA | 5HMF | PA | F | pHBAC | pHBAD | VA |
|---|---|---|---|---|---|---|---|
| WCS | 3.94 ± 0.25 | 0.21 ± 0.03 | 0 | 0.30 ± 0.02 | 0 | 0 | 5.09 ± 0.23 |
| VO(A) | 16.13 ± 1.02 | 3.26 ± 0.56 | 7.13 ± 1.25 | 3.39 ± 0.36 | 7.94 ± 0.63 | 5.00 ± 0.48 | 19.10 ± 1.52 |
| VO(B) | 17.38 ± 0.98 | 3.09 ± 0.75 | 7.93 ± 1.05 | 3.39 ± 0.59 | 7.92 ± 0.34 | 5.47 ± 0.75 | 20.82 ± 1.00 |
| VI(A) | 3.48 ± 0.51 | 0.29 ± 0.05 | 1.94 ± 0.09 | 0.85 ± 0.05 | 0 | 0 | 12.56 ± 0.93 |
| VI(B) | 3.86 ± 0.60 | 0.31 ± 0.06 | 1.98 ± 0.10 | 0.86 ± 0.03 | 0 | 0 | 13.47 ± 0.81 |
| V2(A) | 2.27 ± 0.51 | 0.50 ± 0.10 | 1.33 ± 0.04 | 0.81 ± 0.09 | 0 | 1.45 ± 0.12 | 6.28 ± 0.23 |
| V2(B) | 3.42 ± 0.26 | 0.57 ± 0.08 | 1.30 ± 0.13 | 0.75 ± 0.07 | 0 | 2.29 ± 0.09 | 7.35 ± 0.85 |
| V3(A) | 5.99 ± 0.85 | 3.25 ± 0.64 | 1.33 ± 0.07 | 2.21 ± 0.21 | 3.24 ± 0.55 | 3.21 ± 0.12 | 6.75 ± 0.54 |
| V3(B) | 5.97 ± 0.76 | 3.34 ± 0.45 | 1.33 ± 0.12 | 2.26 ± 0.25 | 3.24 ± 0.24 | 4.80 ± 0.26 | 7.26 ± 0.13 |
| V4(A) | 5.84 ± 0.42 | 0.21 ± 0.12 | 1.24 ± 0.21 | 0.64 ± 0.10 | 0 | 0 | 2.27 ± 0.22 |
| V4(B) | 5.52 ± 0.53 | 0.19 ± 0.22 | 1.24 ± 0.25 | 0.61 ± 0.12 | 0 | 0 | 2.61 ± 0.14 |
| V5(A) | 10.24 ± 0.99 | 3.17 ± 0.43 | 7.53 ± 0.42 | 3.39 ± 0.32 | 7.93 ± 0.61 | 3.23 ± 0.65 | 7.32 ± 0.72 |
| V5(B) | 16.36 ± 1.21 | 8.13 ± 0.75 | 4.21 ± 0.67 | 9.25 ± 1.12 | 9.13 ± 0.78 | 8.31 ± 0.78 | 8.96 ± 0.21 |
| V6(A) | 13.52 ± 1.02 | 3.63 ± 0.26 | 8.98 ± 1.02 | 3.48 ± 0.43 | 3.58 ± 0.52 | 5.51 ± 0.63 | 14.63 ± 1.45 |
| V6(B) | 12.74 ± 0.95 | 3.89 ± 0.31 | 8.89 ± 1.04 | 3.45 ± 0.51 | 3.53 ± 0.24 | 4.30 ± 0.69 | 13.72 ± 1.28 |
| V7(A) | 8.28 ± 1.12 | 4.26 ± 0.35 | 4.89 ± 0.84 | 3.28 ± 0.25 | 6.51 ± 0.71 | 7.28 ± 0.87 | 5.28 ± 0.76 |
| V7(B) | 11.48 ± 1.43 | 8.40 ± 0.88 | 2.97 ± 0.36 | 9.72 ± 0.67 | 9.15 ± 0.35 | 10.52 ± 1.21 | 1.95 ± 0.10 |
| V8(A) | 13.00 ± 1.28 | 3.43 ± 0.50 | 7.63 ± 0.68 | 2.82 ± 0.31 | 3.41 ± 0.46 | 5.20 ± 0.25 | 10.71 ± 0.98 |
| V8(B) | 14.27 ± 1.16 | 3.45 ± 0.39 | 7.67 ± 0.69 | 2.82 ± 0.25 | 3.39 ± 0.31 | 5.30 ± 0.43 | 9.62 ± 0.45 |
| V9(A) | 15.36 ± 1.25 | 4.15 ± 0.76 | 10.05 ± 0.98 | 4.25 ± 0.56 | 9.10 ± 1.00 | 4.36 ± 0.61 | 15.45 ± 1.22 |
| V9(B) | 15.73 ± 1.56 | 4.22 ± 0.69 | 10.22 ± 0.87 | 4.23 ± 0.55 | 9.17 ± 1.09 | 5.55 ± 0.28 | 16.51 ± 1.31 |
| VI0(A) | 17.50 ± 0.67 | 4.19 ± 0.21 | 14.43 ± 0.97 | 3.91 ± 0.14 | 1.46 ± 0.10 | 6.10 ± 0.45 | 20.12 ± 1.14 |
| VIO(B) | 17.28 ± 0.99 | 4.17 ± 0.25 | 14.21 ± 0.91 | 3.93 ± 0.22 | 1.43 ± 0.09 | 5.43 ± 0.38 | 21.60 ± 1.08 |
| V11(A) | 4.13 ± 0.32 | 0.08 ± 0.05 | 0.75 ± 0.13 | 0.34 ± 0.09 | 1.11 ± 0.13 | 0 | 0 |
| V11(B) | 4.25 ± 0.23 | 0.09 ± 0.05 | 0.72 ± 0.16 | 0.30 ± 0.08 | 1.10 ± 0.19 | 0 | 0 |
| V12(A) | 9.43 ± 0.87 | 2.35 ± 0.21 | 2.44 ± 0.20 | 1.16 ± 0.12 | 4.92 ± 0.25 | 22.14 ± 1.32 | 6.96 ± 0.55 |
| V12(B) | 9.12 ± 0.98 | 2.20 ± 0.15 | 2.50 ± 0.32 | 1.14 ± 0.21 | 4.92 ± 0.31 | 28.42 ± 1.12 | 7.75 ± 0.42 |
| V13(A) | 4.11 ± 0.55 | 0.18 ± 0.05 | 0.36 ± 0.14 | 0.67 ± 0.07 | 4.25 ± 0.43 | 4.49 ± 0.27 | 20.30 ± 1.02 |
| V13(B) | 3.90 ± 0.13 | 0.15 ± 0.06 | 0.34 ± 0.15 | 0.64 ± 0.09 | 4.14 ± 0.46 | 4.54 ± 0.29 | 22.89 ± 1.25 |
| V14(A) | 5.13 ± 0.21 | 2.30 ± 0.31 | 13.20 ± 1.15 | 4.22 ± 0.36 | 5.92 ± 0.61 | 9.78 ± 0.58 | 7.10 ± 0.39 |
| V14(B) | 5.61 ± 0.43 | 2.28 ± 0.30 | 13.29 ± 1.21 | 4.25 ± 0.29 | 5.86 ± 0.54 | 8.90 ± 0.78 | 8.52 ± 0.49 |
| V15(A) | 9.75 ± 0.83 | 3.14 ± 0.27 | 18.16 ± 1.29 | 4.24 ± 0.32 | 7.32 ± 0.48 | 9.27 ± 0.76 | 10.01 ± 0.88 |
| V15(B) | 9.47 ± 0.78 | 3.22 ± 0.35 | 18.15 ± 1.32 | 4.21 ± 0.35 | 7.38 ± 0.57 | 14.47 ± 1.05 | 10.29 ± 0.99 |
| V16(A) | 0 | 0.99 ± 0.10 | 9.34 ± 0.45 | 0 | 16.84 ± 1.10 | 8.75 ± 0.64 | 0 |
| V16(B) | 0 | 0.92 ± 0.09 | 9.30 ± 0.53 | 0 | 16.86 ± 1.09 | 9.75 ± 0.43 | 0 |
| V17(A) | 5.46 ± 0.42 | 0.15 ± 0.12 | 1.21 ± 0.19 | 0.18 ± 0.05 | 2.22 ± 0.26 | 3.81 ± 0.23 | 0 |
| V17(B) | 5.86 ± 0.52 | 0.11 ± 0.09 | 1.20 ± 0.16 | 0.16 ± 0.06 | 2.24 ± 0.21 | 3.86 ± 0.43 | 0 |

Significance levels greater than the 0.05 required by these tests were obtained in every case except those of methods 5 and 7. **Table 7** summarizes these results. The data reflect the absence of statistically significant differences between the replicates obtained by the same method (except methods 5 and 7). In other words, the phenolic and furanic concentrations found for the replicates did not vary and thus are truly indicative of the consequences of the aging technique applied.

In the case of methods 5 and 7, the statistically significant differences that were found between the replicates show that the sample populations were not homogeneous. It cannot be unequivocally claimed that the phenolic and furanic characteristics determined for these replicates are the real consequence of the method employed, and therefore these samples have been excluded from the study to prevent anomalous factors from influencing the conclusions reached.

Having identified and eliminated the methods that did not present a real and reproducible effect on phenolic and furanic concentrations within the samples studied, the remaining methods were studied by means of artificial NNs.

In this study, the SOM (neural net map) was used with the following objectives: (1) to visualize the relationships between the naturally and artificially aged rums; (2) to confirm which components of the rum are most influenced by aging; (3) to create an analytical method to automatically compute the commercial type (which broadly corresponds to age) from the composition of naturally and artificially aged rums; and (4) to illustrate statistical (and thus flavor) similarities between naturally and artificially aged rums.

*Visualizing Rums.* To get an idea of how naturally and artificially aged rums are distributed, we trained Kohonen's SOM 10 times using all of the samples as the training set. The map with the smallest test error, using the same set as the test error, was chosen. A procedure called Umatrix (*21*) was then applied to the resulting map. This procedure measures the distances between each neuron and its neighbors and plots them as grayscale, darker with increasing distance. The results are shown in **Figure 1**.

**Figure 1** was computed as follows: after training, the best-matching unit for each sample waas computed; that is, for each vector in the training set, the distances to all units in the map were computed, and the closest one noted. Sometimes, several samples corresponded to the same unit, in which case only one was noted. If the samples corresponded to different classes, the class that appeared the most was used.

By calibrating the map, that is, by computing the closest unit to an input vector, we are effectively projecting high-dimensional vectors onto a two-dimensional space. Kohonen maps have the property that, due to the training process, distance relations are maintained in such a way that if two vectors are close in the high-dimensional space, they correspond to nearby units in the two-dimensional map; that is why it is also called a topology-preserving map. Overlaying the Umatrix distances onto the map allows us to determine not only which input vectors are nearby but also how close they are and how they are organized in clusters.

In **Figure 1**, we plot the Umatrix representation of the naturally and artificially aged rums. Two clusters can be
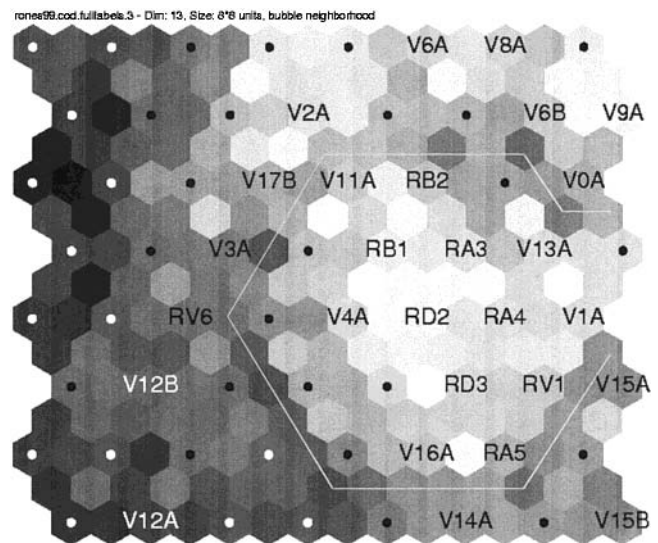
**Table 6.** Concentrations (Milligrams per Liter) of Phenolic and Furanic Compounds Found in the Samples Analyzed

|         | CA           | SA           | pCA          | SY           | VN           | SN           |
|---------|--------------|--------------|--------------|--------------|--------------|--------------|
| WCS     | 0            | 2.96 ± 0.12  | 0            | 0            | 0            | 0            |
| VO(A)   | 6.62 ± 0.45  | 7.01 ± 0.59  | 4.50 ± 0.13  | 8.91 ± 0.78  | 10.37 ± 0.85 | 19.99 ± 1.16 |
| VO(B)   | 6.03 ± 0.54  | 8.65 ± 0.75  | 4.86 ± 0.29  | 7.41 ± 0.23  | 13.33 ± 1.03 | 18.36 ± 1.07 |
| VI(A)   | 5.10 ± 0.43  | 6.25 ± 0.28  | 6.85 ± 0.75  | 8.26 ± 0.39  | 7.95 ± 0.66  | 11.72 ± 0.75 |
| VI(B)   | 5.52 ± 0.23  | 7.19 ± 0.39  | 7.46 ± 0.69  | 9.39 ± 0.54  | 8.12 ± 0.45  | 12.96 ± 0.86 |
| V2(A)   | 3.42 ± 0.13  | 6.75 ± 0.53  | 0            | 11.98 ± 1.04 | 8.10 ± 0.42  | 17.00 ± 0.59 |
| V2(B)   | 4.43 ± 0.32  | 5.29 ± 0.51  | 0            | 10.15 ± 0.86 | 9.50 ± 0.51  | 18.85 ± 0.89 |
| V3(A)   | 3.95 ± 0.56  | 8.98 ± 0.66  | 0            | 8.75 ± 0.25  | 12.01 ± 0.95 | 35.10 ± 1.27 |
| V3(B)   | 5.27 ± 0.25  | 11.77 ± 0.99 | 0            | 11.11 ± 0.43 | 13.16 ± 0.97 | 40.60 ± 1.12 |
| V4(A)   | 12.65 ± 0.31 | 4.26 ± 0.38  | 6.65 ± 0.36  | 6.98 ± 0.27  | 8.69 ± 0.62  | 7.95 ± 0.25  |
| V4(B)   | 9.71 ± 0.67  | 4.37 ± 0.45  | 6.01 ± 0.48  | 5.24 ± 0.49  | 10.04 ± 0.92 | 9.28 ± 0.36  |
| V5(A)   | 0.91 ± 0.43  | 0.92 ± 0.13  | 0.57 ± 0.57  | 0.27 ± 0.09  | 1.26 ± 0.14  | 6.27 ± 0.42  |
| V5(B)   | 3.33 ± 0.34  | 3.83 ± 0.28  | 4.68 ± 0.25  | 2.30 ± 0.21  | 7.86 ± 0.35  | 10.00 ± 0.25 |
| V6(A)   | 4.12 ± 0.67  | 7.65 ± 0.42  | 3.85 ± 0.52  | 11.21 ± 0.98 | 10.25 ± 0.27 | 22.11 ± 0.99 |
| V6(B)   | 5.39 ± 0.32  | 6.61 ± 0.38  | 4.46 ± 0.29  | 13.85 ± 1.18 | 13.59 ± 1.10 | 26.27 ± 0.84 |
| V7(A)   | 1.01 ± 0.15  | 0.97 ± 0.17  | 0.96 ± 0.13  | 0.81 ± 0.25  | 1.26 ± 0.21  | 4.51 ± 0.28  |
| V7(B)   | 5.26 ± 0.27  | 2.10 ± 0.26  | 4.28 ± 0.53  | 3.95 ± 0.22  | 7.27 ± 0.14  | 10.91 ± 0.23 |
| V8(A)   | 8.81 ± 0.86  | 7.52 ± 0.29  | 3.96 ± 10.36 | 12.76 ± 1.21 | 12.99 ± 1.05 | 19.00 ± 0.97 |
| V8(B)   | 7.46 ± 0.25  | 7.09 ± 0.41  | 5.07 ± 0.63  | 13.92 ± 1.02 | 11.98 ± 0.83 | 20.23 ± 0.82 |
| V9(A)   | 8.10 ± 0.53  | 8.70 ± 0.28  | 5.35 ± 0.25  | 17.10 ± 1.26 | 15.73 ± 1.02 | 28.13 ± 0.79 |
| V9(B)   | 9.45 ± 0.67  | 7.23 ± 0.33  | 6.06 ± 0.42  | 18.77 ± 0.98 | 17.32 ± 1.05 | 33.03 ± 1.21 |
| V10(A)  | 12.85 ± 0.93 | 1.45 ± 0.09  | 4.26 ± 0.25  | 22.13 ± 1.12 | 16.97 ± 0.88 | 32.80 ± 1.23 |
| V10(B)  | 14.39 ± 0.83 | 1.56 ± 0.10  | 4.77 ± 0.36  | 14.10 ± 1.03 | 16.08 ± 0.74 | 24.69 ± 1.18 |
| V11(A)  | 0            | 1.45 ± 0.05  | 0            | 0            | 0            | 8.27 ± 0.69  |
| V11(B)  | 0            | 1.56 ± 0.19  | 0            | 0            | 0            | 9.06 ± 0.35  |
| V12(A)  | 9.81 ± 0.75  | 7.96 ± 0.40  | 6.14 ± 0.41  | 1.78 ± 0.12  | 7.12 ± 0.56  | 19.10 ± 1.01 |
| V12(B)  | 12.05 ± 0.74 | 8.52 ± 0.25  | 7.73 ± 0.63  | 2.61 ± 0.29  | 8.62 ± 0.42  | 20.28 ± 0.98 |
| V13(A)  | 4.88 ± 0.43  | 7.56 ± 0.38  | 2.26 ± 0.29  | 2.50 ± 0.21  | 9.94 ± 0.28  | 0            |
| V13(B)  | 5.68 ± 0.59  | 6.59 ± 0.27  | 2.63 ± 0.25  | 2.36 ± 0.19  | 11.94 ± 0.95 | 0            |
| V14(A)  | 4.95 ± 0.35  | 10.10 ± 0.91 | 3.02 ± 0.42  | 2.10 ± 0.34  | 29.31 ± 1.16 | 0            |
| V14(B)  | 4.30 ± 0.27  | 11.61 ± 0.62 | 3.14 ± 0.16  | 3.58 ± 0.16  | 33.31 ± 1.08 | 0            |
| V15(A)  | 5.01 ± 0.39  | 10.95 ± 0.54 | 4.82 ± 0.29  | 6.58 ± 0.52  | 18.95 ± 0.98 | 22.13 ± 0.85 |
| V15(B)  | 5.62 ± 0.45  | 12.35 ± 0.79 | 4.04 ± 0.31  | 5.57 ± 0.66  | 20.80 ± 1.23 | 18.70 ± 0.73 |
| V16(A)  | 0            | 0            | 0            | 0            | 0            | 0            |
| V16(B)  | 0            | 0            | 0            | 0            | 0            | 0            |
| V17(A)  | 2.96 ± 0.14  | 4.32 ± 0.27  | 0            | 6.96 ± 0.27  | 7.68 ± 0.45  | 20.18 ± 1.06 |
| V17(B)  | 4.15 ± 0.18  | 4.66 ± 0.36  | 0            | 5.36 ± 0.36  | 8.39 ± 0.34  | 23.10 ± 1.13 |

**Table 7.** Levels of Significance Found by Comparing Replicates Obtained by the Same Artificial Aging Treatment

| variation | multivariante method based | P value | results |
|-----------|---------------------------|---------|---------|
| V0  | t test | 0.280000 ($p > 0.05$) | not SSD |
| V1  | t test | 0.803649 ($p > 0.05$) | not SSD |
| V2  | t test | 0.884460 ($p > 0.05$) | not SSD |
| V3  | t test | 0.761260 ($p > 0.05$) | not SSD |
| V4  | t test | 0.899304 ($p > 0.05$) | not SSD |
| **V5**  | **t test** | **0.025931 ($p < 0.05$)** | **SSD** |
| V6  | t test | 0.797186 ($p > 0.05$) | not SSD |
| **V7**  | **t test** | **0.021970 ($p < 0.05$)** | **SSD** |
| V8  | t test | 0.968819 ($p > 0.05$) | not SSD |
| V9  | t test | 0.764731 ($p > 0.05$) | not SSD |
| V10 | t test | 0.747723 ($p > 0.05$) | not SSD |
| V11 | t test | 0.942107 ($p > 0.05$) | not SSD |
| V12 | t test | 0.691976 ($p > 0.05$) | not SSD |
| V13 | t test | 0.887354 ($p > 0.05$) | not SSD |
| V14 | t test | 0.855365 ($p > 0.05$) | not SSD |
| V15 | t test | 0.900446 ($p > 0.05$) | not SSD |
| V16 | Mann–Whitney | 0.974980 ($p > 0.05$) | not SSD |
| V17 | t test | 0.895714 ($p > 0.05$) | not SSD |



**Figure 1.** Umatrix representation of the naturally (R) and artificially (V) aged rums. Although not very clearly, two clusters can be observed in the figure; one is the group of clear hexagons marked with "R" samples, and the other corresponds to the rest of the samples. The two clusters are separated by a group of dark hexagons (which indicate greater distance). As is to be expected, naturally aged rums cluster together, although some artificially aged rums are also found in the same cluster.

observed in the figure: one for naturally aged rums, and another for artificially aged rums. Other than that, we find the results to be as expected: white rum lies close to golden rum (because they are next to each other in the age sequence), and golden and aged rums are close to old rum, except for one case, RV6, which is probably an unusual rum. There are some artificially aged rums that also lie close to some of the former group, and then there is a group of artificially aged rums that are distant from each other and from the naturally aged rums. This confirms

one of our initial hypotheses: the artificial aging process is capable of producing rums that are similar to the naturally aged ones.

Application of Artificial Aging Techniques to Rum

*J. Agric. Food Chem.,* Vol. 50, No. 6, 2002    **1475**

This initial study is similar to the "whiskey map" shown in the Introduction to Deboeck (*22*), except that in this case we wished to obtain a predictive value from the map, that is, to determine whether the artificially aged rums were close enough, in compositional terms, to the naturally aged rums; moreover, in our case only composition was used, whereas many more components, some of them subjective, were used for the whiskey map.

*Visualizing Components.* Using the same map, and taking into account the clusters that were observed, the component values that define those clusters can also be investigated. The objective of this is to confirm which components are the most important in making a rum look like, or be of, a certain type, irrespective of the aging process applied. We took a special interest in three components: vanillin, syringaldehyde, and sinapaldehyde. These components are extracted from the cask wood in the aging process and are what give aged rums their quality and flavor. The results of applying the plane program to the map analyzed in the previous section are shown in **Figure 2**. The structure of the map is the same as in **Figure 1**, whereas the gray shading of each circle represents the relative value of the component in the unit. These three components (vanillin, syringaldehyde, and sinapaldehyde) were chosen because they pass from the wood in the cask to the rum during aging; this makes them the most difficult to reproduce artificially and the most critical factor in obtaining good, albeit artificially aged, rums.

In fact, the value of all three components is high across the aged rums cluster and is higher still with the old rums (RV). These values fall somewhat with the artificially aged rums, which border the non-aged rums cluster, but are still quite good. This leads us to conclude that what defines the cluster of aged rums, that is, a high concentration of vanillin, syringaldehyde, and sinapaldehyde, is also included in some of the samples of artificially aged rums.

Analysis of the rest of the planes, not shown here, gives similar results. For instance, plane 10, which corresponds to *p*-coumaric acid, shows a low value for the aged rums but a high value for the others.

*Estimating Rum Type from Composition.* Finally, we were interested in using SOMs not only for their descriptive value but also for their predictive properties. An SOM calibrated as described enables us to classify unknown samples depending on the unit they correspond to. In the first map, two zones were defined, but these were created to minimize the distance from the input vectors to the map and thus were not valid as predictive maps for a given sample with the composition of an artificially aged rum. That is why we performed a jackknife procedure (*15*) on the V samples: each pair of samples V × A and V × B was extracted in turn. Five maps were trained with the rest of the R and V samples, and the map with the smallest distortion (or square root of the squared distance from the input vectors to the weight vectors, or vectors in the map) was chosen.

We established a criterion to classify a V sample as "indistinguishable" from a naturally aged, or R, sample: this criterion was whether the samples that were previously unused during training corresponded to the same unit as a naturally aged one. The samples that met this requirement are shown in **Table 8**

**Table 8** shows that some samples correspond to the same unit as, or share a unit with, naturally aged samples; nevertheless, there are differences. In the case of samples 6 and 16, only one of the samples obtained using the same method shares a unit with R samples; thus, it will be discarded, because the method does not guarantee R-type samples will be obtained. In
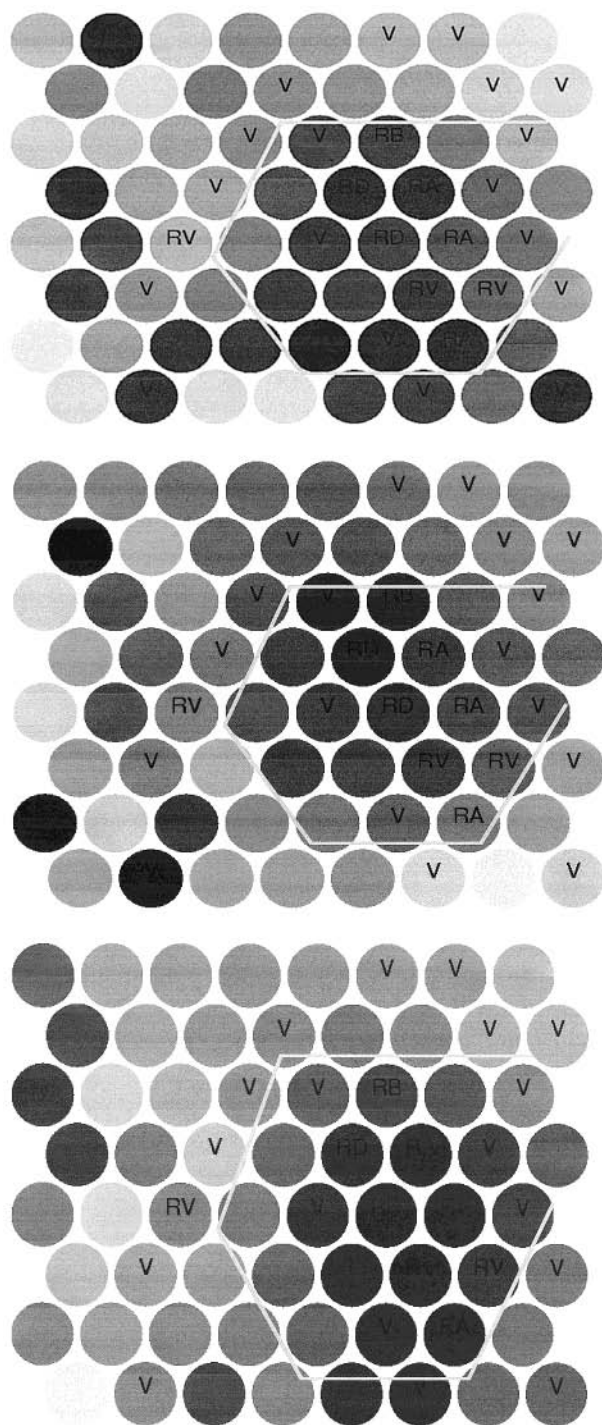


**Figure 2.** (A, Top) Plane 11, which corresponds to syringaldehyde. The "aged rum" clusters present a uniform coloration, reflecting a high concentration of syringaldehyde. (B, Middle) Plane 12, which corresponds to vanillin. Again, the "aged rum" clusters present a uniform, dark coloration, reflecting a high concentration of the component. (C, Bottom) Plane 13, which corresponds to the concentration of sinapaldehyde. The coloration indicates that concentration is higher in the older rums (golden, aged, and old) and lower in the young rums (white rum), whereas it is lower still in some artificially aged samples.

another case, sample 4, it corresponds to a unit shared by all kinds of rums and thus cannot clearly be classified as any specific one; in this case, it could be classified as the youngest type of rum, that is, white rum. Nevertheless, this also shows that naturally aged rums are fairly similar, especially in the case of white and golden rums and in the case of aged and old rums.

**1476** *J. Agric. Food Chem.,* Vol. 50, No. 6, 2002

Quesada Granados et al.

**Table 8.** Artificially Aged Rum Samples as They Correspond to the Naturally Aged Ones[a]

| artificially aged sample | classified as |
|---|---|
| V4A, V4B | RA, RB, RD, RV |
| V6A | RV |
| V8A, V8B | RV |
| V11A, V1IB | RD |
| V13A, VI3B | RV |
| V14A, V14B | RV |
| V16A | RA, RB, RD |

[a] In some cases, only one of the two samples obtained with the same method, although considered statistically similar, corresponded to the same unit, and thus should probably be discarded. After this, only samples 4, 8, 11, 13, and 14 would be left.
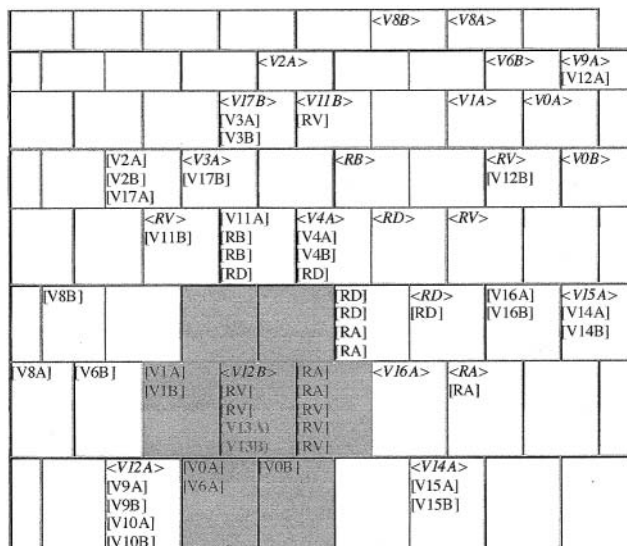


**Figure 3.** Jackknife evaluation for sample 13. This map was trained with all samples except V13A and V13B. Distribution of samples is plotted as follows: In each cell, the samples within angular brackets, in italics, represent the class label (computed using the VCAL program, which is part of the SOM_PAK package), that is, the unit closest to each sample in the training set. The samples in square brackets represent the rest of the samples that correspond to the same unit (computed using the VISUAL program, also a part of the same package). The sample in boldface, in parentheses, is the sample that was omitted from training. The cells shaded in gray represent the neighborbood of the cell that won for the omitted samples. In this case, V13 not only corresponds to a unit shared by old rum (RV) but is surrounded by other units in which aged and old rums are also represented. This means that, from a pattern recognition point of view, the characteristics of the V13A and V13B samples are indistinguishable from those of an old rum.

The third case is probably the most interesting: samples were clearly classified as R samples, that is, samples 8, 11, 13, and 14. Three of these have the same characteristics as "old" rum, which is the most valuable, and sample 11 is similar to "golden" rum. Thus, it is shown that three samples (each of them comprising two replicates) are statistically similar to the best kind of rum, old rum, which was one of the goals of this study. **Figure 3** shows one of the maps obtained using this procedure, the one corresponding to probably the best artificially aged sample, V13.

**Figure 3** shows the shape of the map computed, which is similar to the one used in the previous subsections; in this case, however, we were not interested in clusters but only in the unit that was closest to the samples that were omitted during training, V13A and B, in this case. Even so, we could say that V13 is

on the boundary between naturally and artificially aged rums but shares many characteristics with "old" rum (because they correspond to the same unit) and also some with "aged" rum (which corresponds to the unit to its right). Similar maps were computed for all the samples but for the sake of brevity are not shown here.

Therefore, an alcoholic beverage such as rum can be artificially aged by means of methods of artificial aging. By these means, and in a relatively short period, we obtained samples of rum with phenolic and furanic characteristics similar to those of commercially available brands labeled as golden or old rum. Nevertheless, for a higher reliability of the results obtained, it will be necessary to develop a study based on sensorial analysis for the same samples treated here.

### ABBREVIATIONS USED

CA, caffeic acid; F, furfural; GA, gallic acid; 5HMF, 5-(hydroxymethyl)furfural; HPLC, high-perfomance liquid chromatography; NNs, neural nets; PA, protocatechuic acid; pCA, *p*-coumaric acid; pHBAC, *p*-hydroxybenzoic acid; pHBAD, *p*-hydroxybenzaldehyde; RA, aged rum; RB, white rum; RD, golden rum; RV, old rum; SA, syringic acid; SD, standard deviation; SN, sinapaldehyde; SOM, self-organizing map; SSD, statistically significant differences; SY, syringaldehyde; VA, vanillic acid; VN, vanillin; WCS, white cane spirit.

### ACKNOWLEDGMENT

### LITERATURE CITED

(1) Johnson, H. *Atlas Mundial de Vinos y Licores*; Blume, Ed.; Barcelona, Spain, 1986.

(2) Villalón, M.; Montilla, J. Determinación espectrofotométrica de vainillina y siringaldehído en ron. *An. Bromatol.* **1987**, *39*, 271–279.

(3) Giménez, R.; Quesada, J.; Villalón, M.; López, H.; López, M. C. Influencia del sistema de maduración en la calidad de los brandies: envejecimiento por soleras, envejecimiento tradicional. *Ars Pharm.* **1992**, *19*, 957–962.

(4) Chatonnet, P.; Boidrons, J. N.; Pons, M. Incidence du traitement thermique du bois de chêne sur sa composition chimique. 2 partie: évolution de certains composés en function de l'intensité de brûlage. *Connaiss.Vigne Vin* **1989**, *23*, 223–250.

(5) Artajona Serrano, J. Caracterización del roble según su origen y grado de tostado, mediante la utilización de GC y HPLC. *Vitic./ Enol. Professional* **1991**, *114*, 61–72.

(6) Giménez Martinez, R.; Villalón Mir, M.; López G×bb Serrana, H.; López Martinez, M. C. Simultaneous determination of vanillin and syringaldehyde using high perfomance liquid chromatography. Application to static and soleras aged brandies. *J. Liq. Chromatogr.* **1993**, *16*, 4079–4094.

(7) Boidron, J. N.; Chatonnet, P.; Pons, M. Influence du bois sur certaines substances odorantes des vins. *Connaiss. Vigne Vin* **1988**, *22*, 275–294.

(8) Puech, J. L.; Jouret, C. Dosage des aldéhydes aromatiques des eaux-de-vie conservées en fûts de chêne: détection d'adulteration. *Ann. Falsif. Exp. Chim.* **1982**, *75*, 81–90.

(9) Giménez, R.; López, H.; Villalón, M.; Quesada, J.; López, M. C. Influence of wood heat treatment temperature and maceration time on vanillin, syringaldehyde, and gallic acid contents in oak wood and wine spirit mixtures. *Am. J. Enol. Vitic.* **1996**, *47*, 441–446.

(10) Quesada, J. *Determinación de Furfural y 5-Hidroximetilfurfural en Aguardientes de Vino y su Relación con el Proceso de Envejecmiento en Roble*; Servicio de Publicaciones de la Universidad de Granada: Granada, Spain, 1996.

Application of Artificial Aging Techniques to Rum

*J. Agric. Food Chem.,* Vol. 50, No. 6, 2002 **1477**

(11) Quesada, J.; Villalón, M.; López G×bb Serrana, H.; López Martinez, C. Influence of aging factors on the furanic aldehyde contents of matured brandies: aging markers. *J. Agric. Food Chem.* **1996**, *44*, 1378−1381.

(12) Goldberg, D. M.; Hoffman, B.; Yang, J.; Soleas, G. J. Phenolic constituents, furans, and total antioxidant status of distilled spirits. *J. Agric. Food Chem.* **1999**, *47*, 3978−3985.

(13) Canas, S.; Leandro, M. C.; Spranger, M. I.; Belchior, A. P. Low molecular weight organic compounds of chestnut wood (*Castanea sativa* L.) and corresponding aged brandies. *J. Agric. Food Chem.* **1999**, *47*, 5023−5030.

(14) Monedero, L.; Olalla, M.; Quesada, J.; Villalón, M.; López, H.; López, M. C. Exhaustion techniques in the selection and description of phenolic compounds in Jerez wine extracts obtained by an accelerated aging technique. *J. Agric. Food Chem.* **1998**, *46*, 1754−1764.

(15) Ripley, B. D. *Pattern Recognition and Neural Networks*; Cambridge University Press: Cambridge, U.K., 1996.

(16) Kohonen, T. *The Self-Organizing Maps*, 2nd ed.; Springer: Berlin, Germany, 1997.

(17) Reglamentación Especial para la elaboración, circulación y comercio del ron. Decreto 1228/75 de la Presidencia del Gobierno de 5 de Junio (BOE no. 136 de 7 de Junio de 1975).

(18) Porreta, S.; Sandei, L. Determination of 5-HMF in tomato products: proposed of a rapid HPLC method and its comparison with the colorimetric method. *Food Chem.* **1991**, *16*, 51−57.

(19) Quesada, J.; Villalón, M.; López G×bb Serrana, H.; López Martinez, C. Comparison of spectrophotometric and chromatographic methods of determination of furanic aldehydes in wine distillates. *Food Chem.* **1995**, *52*, 293−298.

(20) Fernández Izquierdo, M. E.; Quesada Granados, J.; Villalón Mir, M.; López Martinez, M. C. Comparison of methods for determining coumarins in distilled beverages. *Food Chem.* **2000**, *70*, 251−258.

(21) Ultsch, A. Self-organized neural networks for visualization and classification. In *Information and Classification*; Opitz, O., Lausen, B., Klar, R., Eds.; Springer-Verlag: Berlin, Germany, 1993.

(22) DeBoeck, G.; Kohonen T. *Visual Explorations in Finance with Self-Organizing Maps*; DeBoeck, G., Kohonen, T., Eds.; Springer Finance: London, 1998.