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Rapid Discrimination of Scented Rice by Solid-Phase Microextraction, Mass Spectrometry, and Multivariate Analysis Used as a Mass Sensor

MICKAËL LAGUERRE,[†] CHRISTIAN MESTRES,*[,†] FABRICE DAVRIEUX,[‡] JOHANNY RINGUET,[†] AND RENAUD BOULANGER[‡]

UPR Qualité des Aliments Tropicaux and UPR Qualité Produits Pérennes, CIRAD, 73 Rue J.F. Breton, Montpellier F-34398 France

This study describes a new and suitable method for the rapid evaluation of rice (*Oryza sativa*, L.) aroma by analysis of the volatile fraction using solid-phase microextraction coupled with mass spectrometry (SPME/MS). The abundance list of unresolved mass fragments of the SPME extracted volatile fraction formed the "fingerprint" of a rice sample. Fingerprints of 61 rice samples were recorded in duplicate. Pollutants originating from the extraction system induce fingerprint background that could be lowered by careful cleaning of vials and caps and by exclusion of specific mass fragments. A good discrimination between scented and nonscented rice samples was obtained using the SIMCA procedure. Most of the discriminating mass fragments could be directly or indirectly assigned to potential aromatic molecules present in rice.

KEYWORDS: Scented rice; aroma; 2-acetyl-1-pyrroline; solid-phase microextraction; mass spectrometry; fingerprint

INTRODUCTION

Scented rice (*Oryza sativa*, L.) that exhibits a special aroma when cooked is very popular in Southeast Asia and has recently gained wider acceptance in Europe and the United States. Few varieties are scented; they are mainly produced in Asia and marketed all around the world. Characterizing the aroma is thus an important challenge for rice buyers to control quality and for rice breeders who want to develop new aromatic rice cultivars.

Among the numerous volatile compounds identified in scented rice, very few possess an odor activity enough to be detected by consumers (*1*). 2-Acetyl-1-pyrroline (2AP), a "popcorn"-like flavor compound, has been reported (*2*, *3*) and confirmed (*4*) as the most important compound contributing to the aroma of scented rice and as being the most discriminant compound between scented and nonscented varieties (*5*). Although only scented rice cultivars possess the genetic potential (*6*, *7*) for accumulating 2AP, nongenetic factors can also modulate scented rice aroma and particularly the agroecological conditions (*8*, *9*) that limit the extension of scented rice production. In addition, drying, milling, and storage can deteriorate the flavor of rice by two mechanisms: losses of desirable volatile constituents, in particular 2AP (*10*−*12*), and the generation of undesirable volatile components, due particularly to lipid oxidation (*13*).

There is indeed a growing need to find rapid and reliable methods for assessing the aroma of rice and particularly the content of 2AP. The sensory method used by breeders (*14*) is rapid but insufficiently sensitive and reproducible. The extraction and the quantification of 2AP have been the object of numerous studies (*15*−*17*). It can be assessed after (i) extraction by various techniques (*18*), (ii) separation using gas chromatography (GC), and (iii) quantification by a flame ionization detector (FID) (*19*) or by mass spectrometry (*17*, *18*, *20*). These analytical studies are focused on the assessment of the few components of the aroma but cannot represent the diversity encountered in the various scented rices (*1*). GC type methods are, in addition, tedious, and potential errors are associated with identification and tracking the large numbers of peaks. There is therefore a need for a simpler and faster method that would provide a direct and reliable evaluation of global aroma of rice.

Recent studies on milk and cheese have shown that direct coupling of MS with static headspace (SHS), dynamic headspace (DHS) (*21*), or solid-phase microextraction (SPME) (*22*−*24*) can lead to the development of fast methods of food characterization. The mass spectrum obtained without prior chromatographic separation forms a "spectral fingerprint"; each *m*/*z* variable of the fingerprint can be considered as a potential chemical descriptor of the sample. The fingerprint is subjected to a multivariate analysis [principal component analysis (PCA), linear discriminant analysis, partial least squares, soft independent modeling of class analogy (SIMCA), etc.] in order to extract the qualitative or quantitative information that can predict food quality. Among the headspace methods used to extract aroma

* To whom correspondence should be addressed. Tel: +33 4 67 61 44 73. Fax: +33 4 67 61 44 44. E-mail: christian.mestres@cirad.fr.
[†] UPR Qualité des Aliments Tropicaux.
[‡] UPR Qualité Produits Pérennes.

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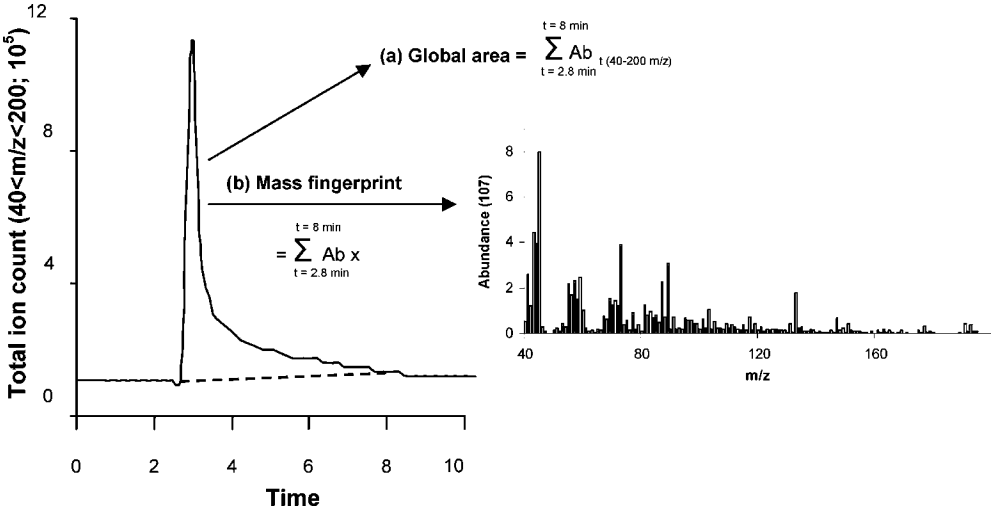

Figure 1. Total ion count (between 40 and 200 *m*/*z*) as a function of time obtained by SPME-MS system. (**a**) The global area is integrated between 2.8 and 8 min. (**b**) The mass fingerprint is the mean abundance values of all of the mass fragments recorded between 2.8 and 8 min.

compounds, SPME has the advantage of requiring less complex equipment than SHS and DHS (gas extractor, numerous valves, and double gas circuit) and seems to give better results (*25*). Moreover, several groups (*12*, *15*) including ours (*26*) have already applied SPME to analyze aroma compounds of scented rice.

This study describes the optimization and application of a nonseparative method to distinguish scented and nonscented rices by using SPME-MS as a mass sensor.

MATERIALS AND METHODS

Rice Samples. The optimization of SPME conditions was achieved using two scented samples: One cultivar (Aychade) was harvested in 2004 in the Camargue (Centre Français du Riz, CFR, France), and one commercial-milled Basmati rice was purchased in a French supermarket. The Aychade sample was dehulled (THU 35B, Satake Engineering Co., Tokyo) and milled (Olmia Testing Abrasive Polisher, Vercelli, Italy) in the laboratory to remove 12% bran. Broken kernels and impurities were removed by manual sorting.

For the rice discrimination experiment, a set of 61 rice cultivars were collected from CFR experimental fields in the Camargue in 2004. Paddy grains were sun-dried and dehulled in the laboratory as previously described.

All samples were stored in an air-conditioned room (20 °C, 70% relative humidity) for at least 1 month before use; they were hence equilibrated at 13% water content (wet basis). Grinding was performed using a 3100 Perten (Sweden) mill with a 0.8 mm sieve.

Chemical Products. Hexanal, 2,3,5-trimethylpyrazine, isoamyl acetate, benzyl alcohol, and ethanol, all of analytical grade, were purchased from Sigma (Saint Quentin, France). Synthetic 2AP was a kind gift of Dr. Yoshihashi (Japan).

SPME-MS Analysis. *SPME General Conditions.* The SPME fibers used were 1 cm long divinylbenzene/carboxen/polydimethylsiloxane (DVB/Car/PDMS) from Supelco (Bellefonte, PA). They were conditioned in a GC injector with Supelco SPME liner (0.75 mm d.i.) at 270 °C under a helium flux for 1 h before use. Prior to each extraction, the fiber was cleaned in the same GC injector for 10 min at 250 °C to remove contaminants. SPME sampling was performed by exposing the fiber in the headspace surrounding the sample placed in a 10 mL GC glass vial capped with a 20 mm PTFE/Silicon septum (Interchim, France). For this, the setting of the SPME holder assembly (57330-U, Supelco) was adjusted to 1.0 unit to ensure that the fiber was always in the same position in the headspace above the sample (the extremity of the fiber was at 1 cm over the rice bead). The setting was changed to 5.0 units prior to injection or cleaning in the GC injector.

SPME Optimization. To select the optimum conditions of SPME sampling, a complete factorial design of 80 treatment combinations was performed: All combinations of the four temperature values (40, 50, 60, and 80 °C), five preincubation durations (5, 15, 30, 45, and 60 min), and four adsorption durations (15, 30, 45, and 60 min) were tested in a random order. Each extraction was performed once on 3.5 g of milled Basmati rice. A single fiber was used for the experimental design while its repeatability was controlled every 10 extractions by extracting the same sample under standard conditions: 50 °C, preincubation for 15 min, and then extraction for 30 min.

The presence of pollutants was first evaluated by sampling the headspace of empty closed vials with different septa (butyl/teflon, PTFE/silicon, and viton). In a second test, vials were washed with ethanol and acetone, and septa were washed with ethanol. Both were heated at 150 °C for 2 h and then stored in a glass desiccator with light vacuum until use. Each extraction was performed in triplicate with the same fiber.

SPME Procedure for Mass Fingerprinting. Vials and septa were washed and heated as previously described. A 3.5 g amount of brown rice kernel was placed into a 10 mL vial, 500 μL of ultrapure water was added, and the vial was capped with PTFE/silicon septum. It was heated at 80 °C for 5 min before the SPME fiber was introduced into the headspace surrounding the rice and left in at the same temperature for 15 min. Each extraction was duplicated. A SPME fiber control was performed using a mixture of standards prepared by dissolving 51 mg of 2,3,5-trimethylpyrazine, isoamyle acetate, and benzyl alcohol in 100 mL of ethanol. It was aliquoted in 6 mL glass flasks that were stored at −20 °C. Three milliliters of this solution was extracted every 20 extractions at 80 °C with a preincubation duration of 15 min and an adsorption duration of 30 min.

MS Conditions. Mass spectra were registered using an Agilent 6980 (Agilent Technologies, Palo Alto, CA) gas chromatograph coupled with an Agilent 5973N quadrupole mass spectrometer (Agilent Technologies). The volatiles were thermally desorbed from the fiber in the GC-MS injector at 250 °C operating in split/pulsed splitless mode for 4 min. They were quickly transferred to the mass detector through a DB-Wax fused silica capillary column (60 m × 0.32 mm i.d.; film thickness = 0.25 μm) operating at 220 °C with helium (2 mL/min) as the carrier gas. The MS source temperature was 150 °C, and the mass spectra were scanned in EI+ mode with a current of 70 eV. The *m*/*z* range used was from 40 to 200 at a rate of 8.17 scans/s. The global signal registered between 2.8 and 8 min was transformed by using Pirouette software v 3.1. (Infometrix Inc., Woodinville, WA) (**Figure 1**). The global area was the mean abundance values of the mass fragments recorded between 2.8 and 8 min.

When GC separation was necessary, the initial oven column temperature was set at 40 °C for 4 min, ramped to 250 °C at a rate of 6 °C/min, and then held at 250 °C for 5 min. The helium flux was set at 1.5 mL/min. The *m*/*z* ranged in this case from 40 to 350 at a rate of

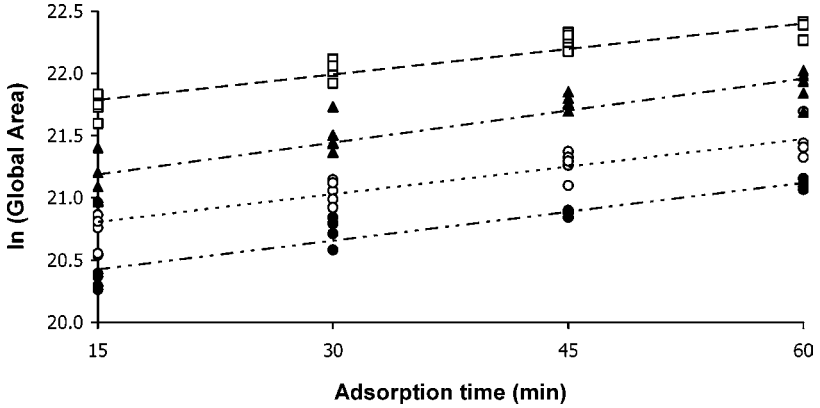

Figure 2. Evolution of ln of the global area with extraction time and temperature: ●, 40 °C; ○, 50 °C; ▲, 60 °C; and □, 80 °C.

2.89 scans/s. Volatile compounds were identified using the Wiley Mass Spectral library and by comparison with GC-MS analysis of authentic standards.

SPME-GC-FID Analysis. *SPME Procedure for 2AP Assessment.* In parallel to the fingerprinting, the 2AP content of each rice sample was assessed by SPME coupled with GC-FID. The general procedure for SPME sampling was similar as for fingerprinting, but 1.5 g of rice was used in the presence of 200 μL of ultrapure water. The vial was preheated at 80 °C for 5 min, and then, the SPME fiber was exposed to the headspace for 15 min. Each extraction was performed in duplicate using two different fibers.

GC-FID Conditions. A Hewlett-Packard 5890 Series II gas chromatograph equipped with a DB-5 fused silica capillary column (60 m $\times$ 0.32 mm i.d.; film thickness = 0.25 μm, J&W Scientific), and FID was used. The volatiles were desorbed from the fiber at 250 °C in the GC inlet operating in splitless mode for 5 min. The GC oven temperature was held at 40 °C for 45 min, ramped to 115 °C at a rate of 3 °C/min, then to 220 °C at 30 °C/min, and held at 220 °C for 5 min. Helium at 1.9 mL/min was used as the carrier gas. 2AP was identified and assessed by comparison with Kovats retention index and response coefficient of an authentic standard.

Statistical Analysis. For the SPME optimization, analysis of variance (ANOVA) and mean comparison (Student) tests were performed using SAS v.9,1 software (SAS Institute Inc., Cary, NC).

For rice discrimination, PCA and the SIMCA procedure of Pirouette software v 3.1 were used on mean-centered and standardized variables. The original data set was randomly divided in two subsets: One group was used to build the model (training set, 55 samples), and the other was used to validate it (external test set, six samples, representing 10% of the original data set). Unknown samples were compared with the class models and assigned to classes according to their analogy with the training samples. Finally, discriminating powers were calculated; they indicated the weight of a variable (mass fragment) in the discrimination model.

RESULTS AND DISCUSSION

SPME Optimization. SPME, with in particular PDMS/Car/DVB fibers suitable for analyzing aroma compounds of food products, has already been used to evaluate the 2AP content of rice (*15*) after GC. It was, however, crucial to optimize the extraction procedure for obtaining the best image of the whole volatile fraction by MS fingerprint.

Grinding Test. Extractability of the volatile compounds can be affected by a modification of the matrix, such as grinding. To study this effect, the global areas recovered from 3.5 g of whole milled kernels and rice flour (particle size lower than 200 μm) were compared. A Student *t* test performed on the mean values for five replications of each treatment showed that the global area was significantly higher by 30% for whole milled rice kernels. Grimm et al. (*15*) also recovered more 2AP from whole kernels as compared to flour. This appeared quite surprising, as the extraction/diffusion process of volatile compounds should normally have been favored by matrix size reduction. It can, however, be inferred that, due to the lack of stirring during the extraction, volatile compounds diffused slowly from the closely packed flour bed, whereas they more easily pass to the headspace of the loosely packed whole kernel bed. The extraction will thus be performed on whole rice kernels in the following experiments.

Experimental Design. Basmati milled rice was extracted at four temperatures (40, 50, 60, and 80 °C) with five preincubation durations (5, 15, 30, 45, and 60 min) and four adsorption durations (15, 30, 45, and 60 min). The fiber repeatability control performed every 10 extractions showed that the global area varied only slightly with a coefficient of variation of 8.8%. No age effect of the fiber (number of injections) was found during the course of the experiment. It was hence unnecessary to perform any correction of the data during the whole experiment.

An ANOVA of the raw global areas showed that a Neperian logarithmic (ln) transformation of the data was necessary in order to meet the homoscedasticity hypothesis (variance is similar for all factor levels)—a prerequisite condition of ANOVA. After this transformation, no interaction effect was evidenced. The preincubation duration factor was also not significant, which means that an preincubation duration of 5 min was sufficient to reach an equilibrium between sample and headspace. This condition was thus adopted in the following experiment. Temperature and adsorption duration had on the contrary significant effects on the ln of global area. It increased linearly with time with similar slopes whatever the temperature (**Figure 2**): The Global area almost doubled when the adsorption duration increased from 15 to 60 min, but the equilibrium was not achieved after 60 min. The equilibrium is, however, not necessary for accurate and precise analysis by SPME, because of the linear relationship between the amount of analyte adsorbed by the SPME fiber and its initial concentration in the sample matrix (*27*). To minimize the sampling period, we thus adopted the shortest adsorption period of 15 min, which is broadly enough to obtain a satisfactory intensity for mass spectra fingerprints. Concerning the temperature, the release of volatile compounds from the matrix to the headspace will normally increase with temperature, whereas an excessive temperature can cause a premature desorption of analytes from the fiber or the formation of new compounds. We observed a regular increase of global area with temperature and chose the highest one that ensured the largest extraction yield of 2AP (*15*).

Water Addition Test. The effect of water addition was first tested by comparing global areas recovered from 3.5 g of milled Basmati grain rice without or with the addition of 250, 500,

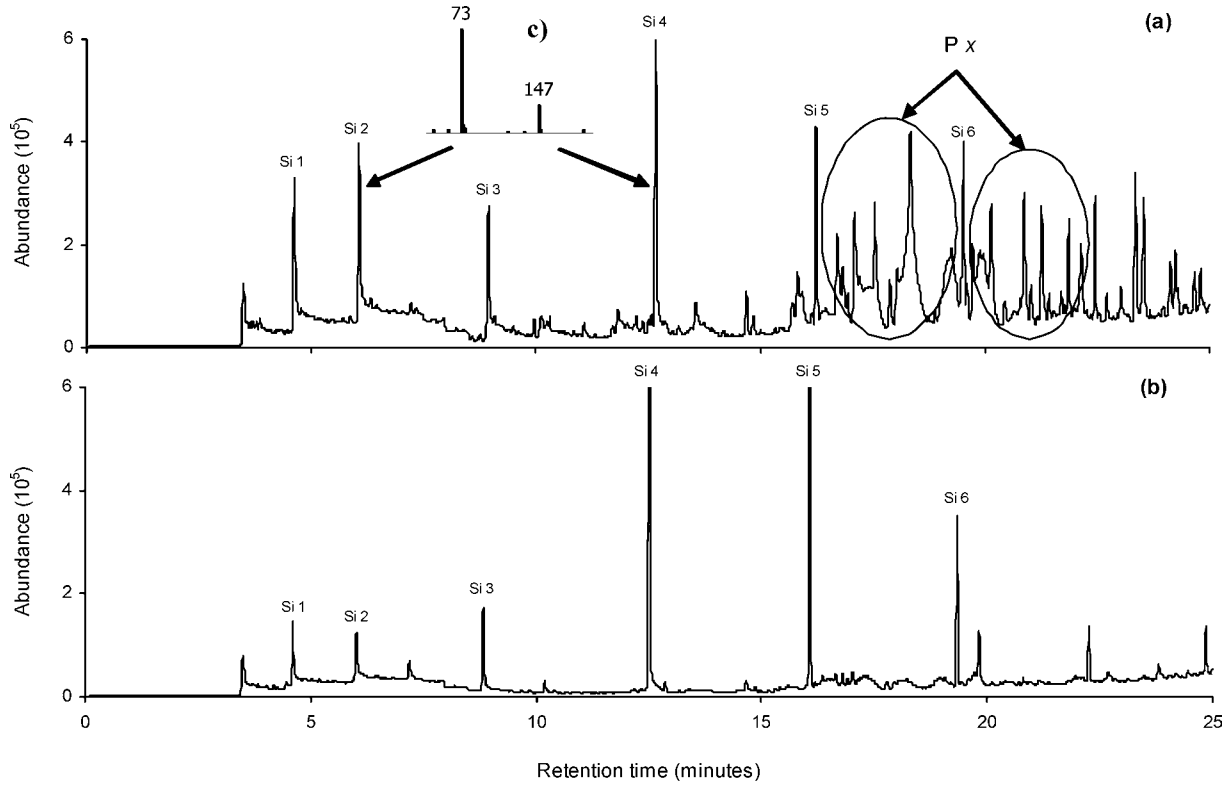

Figure 3. Chromatogram obtained for a fiber previously equilibrated in the headspace of an empty vial capped with a PTFE/silicon septum without (**a**) or with precleaning and preheating (**b**). (**c**) Mass spectrum of Si_x peaks.

750, or 1000 μL of water (quantitative optimization). Each extraction was performed in triplicate with two SPME fibers. An ANOVA of the data showed that neither the water addition nor the fiber had any significant effect on the global area (data not shown).

Nevertheless, this factor must also be optimized on the basis of the chemical composition of the volatile fraction (qualitative optimization), especially upon 2AP and hexanal abundance, two key volatile compounds of rice (*5*, *20*). We thus compared the recovery of 2AP and hexanal extracted from 3.5 g of grain rice without or with the addition of 500 μL of water. The experiment was triplicated and showed that the addition of 500 μL of water significantly increased 2AP and hexanal yields by 50 and 20%, respectively. We therefore adopted the addition of 500 μL of water in the following experiments that allows an optimal extraction of 2AP (*15*).

The observed differences could be linked to a preferential stripping of 2AP and hexanal by steam from the matrix to the headspace. A complementary hypothesis is that 2AP is present as a starch-bound form (*10*). Starch gelatinization that partly occurred in rice heated in the presence of water at 80 °C would facilitate the release of starch-bound volatile compounds.

Pollution Test. During the course of the SPME optimization experiment, it was found that GC-MS profiles of rice extracts were polluted with, in particular, silyl derivatives. SPME is indeed a very sensitive technique but is easily affected by the presence of pollutants (*28*) from the extraction system (SPME fiber, vial, and septum), the GC-MS system (column and septum), and the environment. These pollutants must be identified and removed as far as possible as they will induce a bias in the statistical interpretation of mass spectral fingerprints.

It was first checked that the pollutants did not appear on the GC profile obtained after the desorbing of a clean fiber. The chromatogram was, however, greatly altered when the fiber had been previously equilibrated in the headspace of an empty vial (**Figure 3a**). As for rice extracts, two types of compounds were found as follows: (i) components mainly fragmented in 73 and 147 *m/z* that are characteristic of silyl products (named Si_x) and (ii) components that give a high background on the chromatogram after 15 min (named Px). Six compounds, especially hexamethyl-cyclotrisiloxane (Si_1), octamethylcyclotetrasiloxane (Si_2), and decamethylcyclo-pentasiloxane (Si_3), have been already reported by Marsili (*23*) as contaminants of SPME headspace of milk.

Px contaminants were largely removed after washing the vials and septa, followed by heating at 150 °C for 2 h, before use (**Figure 3b**). This did not have, however, any significant effect on Si_x components that were not eliminated by changing septa nature. It can thus be hypothesized that the fiber (containing PDMS) releases alkylcyclosiloxans in the SHS of the closed vial during the adsorption step at high temperature (80 °C) that are subsequently readsorbed by the fiber. These components are then desorbed in the GC injector at 250 °C, which also explains why no Si_x peaks could be detected on a blank injection with a cleaned fiber.

According to this result, we adopted the following procedure: washing vials (with ethanol and acetone) and septa (with ethanol), heating both at 120 °C for 2 h, followed by storage in a desiccator under light vacuum. In spite of this cleaning procedure, the global area of empty vial and septa represented 15% of that of scented rice.

Application for Rice Discrimination. *Reference Analyses.* 2AP content was assayed by the reference method (GC-FID). It was identified by its retention time, by comparison with that of a standard, and its concentration calculated from its response coefficient.

Of the 61 samples, 29 were scented with a 2AP content ranging from 1.1 to 9.7 μg/kg. These concentrations are only relative as only a small proportion of the volatile compounds are adsorbed on the SPME fiber; Grimm et al. (*15*) evaluated

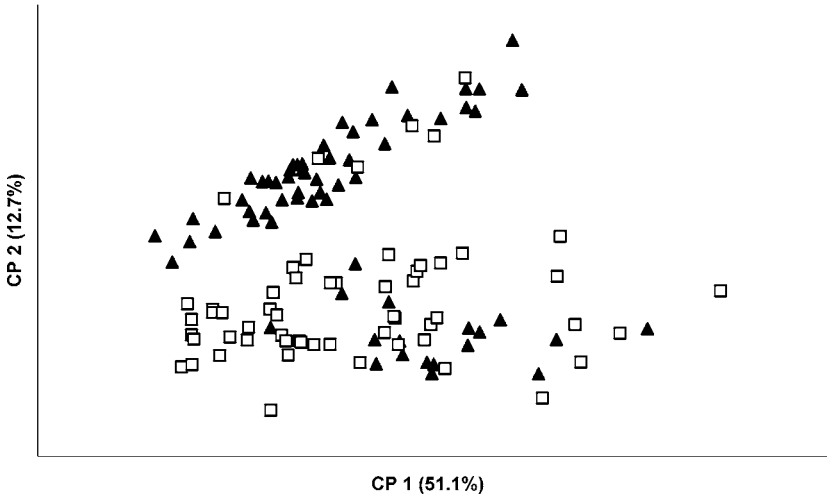

Figure 4. Score plot of nonscented (▲) and scented (□) rice fingerprints on the first plan of the PCA.

at 0.3% the recovery factor of 2AP by SPME. Thirty-two rice samples were nonscented (lack of the 2AP peak). Two classes were thus defined from these results (scented and nonscented samples) that were used as reference data for calibrating the SPME-MS method. There were approximately equal numbers in the population of both classes.

Registration and Pretreatment of Mass Spectral Fingerprints. The volatile fraction of 61 brown rice samples was extracted by SPME in duplicate, and their mass spectral fingerprints were registered (122 fingerprints) in a random order. The repeatability of the SPME fibers was evaluated in parallel by using a standard solution that was extracted (at 80 °C, preincubation period of 15 min, and adsorption period of 30 min) every 20 rice fingerprints. The global area of the standard solution did not significantly change during the course of the experiment, and no data correction was necessary.

Mass spectral fingerprints were one column tables of 160 mass fragments intensities from 40 *m*/*z* to 199 *m*/*z*. First the range between 40 and 50 *m*/*z* was removed from the table, because these ions are too common and can be considered as noise and, then, the range between 151 and 199 *m*/*z*, which contained few or no expected mass fragments of aromatic compounds of rice. Then, the 73 and 147 *m*/*z* intensities were excluded, because they are specific and intense mass peaks of Si_x contaminants. Marsili (*23*) used a similar approach to reduce the influence of silyl compounds on milk MS fingerprints, excluding the 73 and 77 *m*/*z* variables.

PCA. A PCA was first performed on the whole database of 122 fingerprints. The first two factors accounted for 63.8% of the variance in the data set; eight factors were sufficient to account for 90.6% of the initial variability. A class variable was defined by belonging to the nonscented (value of 0) or scented (value of 1) class, as defined previously. Considered as an additional variable in the PCA, it was not significantly correlated with any of the first eight factors. Another variable was constructed with the number of fiber used (four fibers were used during the course of the experiment). It was not correlated with any of the PC factors, confirming that the fiber itself did not contribute significantly to the variability of the fingerprints.

Duplicates were generally close when plotted against the two first factors. One fingerprint was considered an outlier based on its Mahalanobis distance to the centroid of the database. We hence excluded two fingerprints from the database: the outlier and its duplicate. Scented and nonscented rice fingerprints were not clearly separated on PCA sample plots (**Figure 4**) for any combination of factors. This agreed with the lack of correlation of sample class variable with PC factors. The aromatic value thus did not appear to contribute a lot on whole volatile mass spectral fingerprint. The aromatic compounds, and particularly 2AP, are indeed present in rice at a very low level, and a supervised multivariate analysis method is necessary to specifically extract the information in the fingerprints related to the aromatic attribute.

SIMCA. A SIMCA analysis was performed on the training data set (108 fingerprints), corresponding to 54 duplicated samples. Each fingerprint was assigned to the scented or nonscented class (that is to say 25 scented and 29 nonscented rice samples). The SIMCA algorithm performs a PCA for each class with the number of principal components adjusted to account for most of the variation within each class. An interclass distance is then calculated as the H value between the centroids of each population. We chose the optimal number of PCs that allowed the highest interclass distance with the minimum PC number. It was 19 for both scented and nonscented classes, achieving an interclass distance of 2.09. An interclass distance of three or greater indicates a good separation between the groups. Considering the relatively small number of samples (54 × 2), an interclass distance of 2.09 seems promising. All fingerprints of the training data set were indeed correctly assigned by the model to their proper class, except one fingerprint as seen on the Cooman's plot (*29*) (**Figure 5**).

The reliability of the model was tested with the validation subset, which consisted of three scented and three nonscented rice samples randomly selected and duplicated, representing 9.2% of the initial set. All nonscented rice fingerprints were correctly assigned; one fingerprint of a scented rice could not be assigned to any class (**Figure 5**). This represents a percentage recognition of 91.6%.

Molecular Basis of Discrimination. One of the advantages of the SIMCA procedure is that it gives structural information based on the discriminating power (DP). DP indicates how much each variable (mass fragment abundance) contributes to the discrimination between scented and nonscented rice classes; the higher the DP, the higher its contribution is. **Figure 6a** shows that 145, 83, 52, 111, 66, and 68 *m*/*z* mass units are, by decreasing order, the most discriminating variables. Among them, 68, 83, and 111 *m*/*z* mass fragments are typical of the 2AP mass spectrum (**Figure 6b**). This confirmed that the discrimination was meaningful and based on 2AP content.

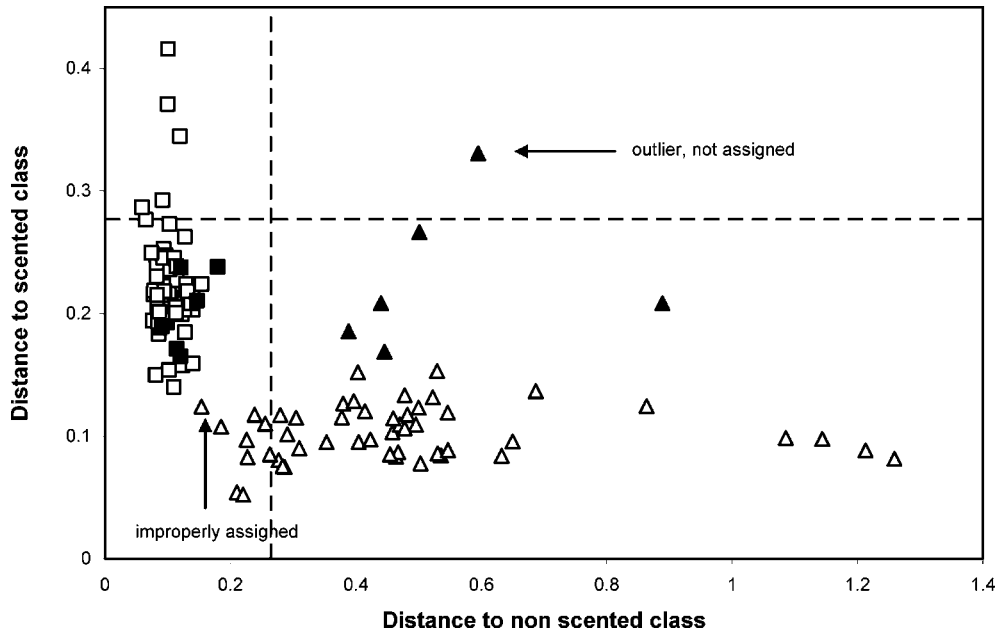

Figure 5. Coomans' plot of nonscented (■, □) and scented rice (▲, △) fingerprints; open symbols, model set; closed symbols, validation set.

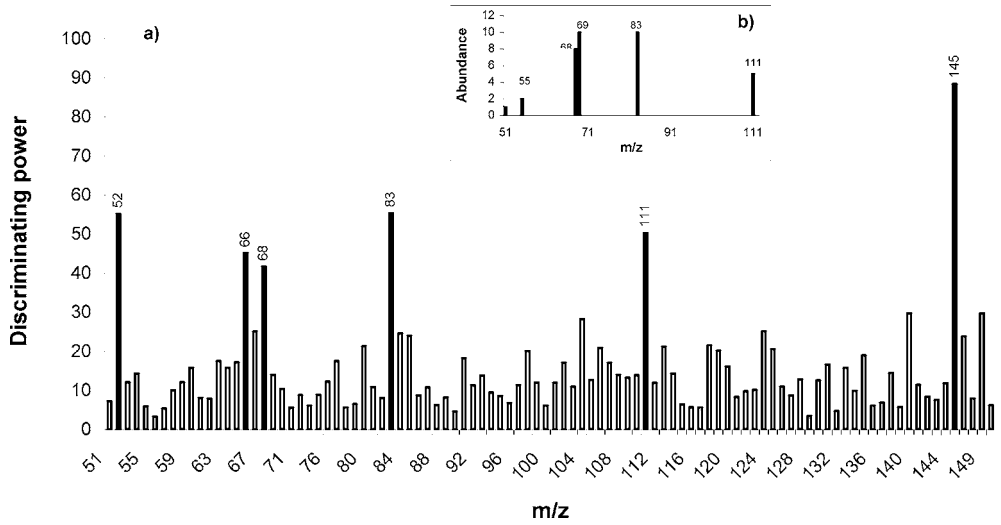

Figure 6. (**a**) Discriminating powers of the SIMCA model. (**b**) Mass spectrum of 2AP.

The discriminating power of 145, 52, and 66 *m*/*z* variables showed that besides 2AP other volatile compounds contribute to the discrimination. The molecular origin of these mass fragments can be looked for on single ion monitoring (SIM) chromatograms. The 52 *m*/*z* fragment is preponderant in the mass spectrum of pyridine and is the most important substance contributing to SIM chromatograms of Aychade and Fidji, two scented rice samples. Pyridine has been indeed already identified in several scented and nonscented rice cultivars (*11*, *30*−*32*). Widjaja and co-workers reported that the pyridine content was higher in a nonscented rice (28 μg/kg) than in four scented rice cultivars (7−13 μg/kg). We, however, observed that 52 *m*/*z* abundance was higher in scented rice than in nonscented rice fingerprints. Pyridine may therefore be an indicator for differentiating scented rice, but its odor threshold (2 μL/L in water; *33*) seems too high for it to play a significant role in rice aroma.

The 66 *m*/*z* fragment is present in the mass spectrum of 2-acetylpyrrole, which is the main substance detected in SIM chromatograms of Aychade and Fidji. This compound is structurally close to 2AP, but in contrast to the latter, its odor threshold in water solution is high (170 μL/L against 0.1 nL/L for 2AP; *33*). Hence, it should not contribute significantly to rice aroma but may act, as for pyridine, as an indirect indicator. Finally, the 145 *m*/*z* fragment remains unidentified.

In conclusion, SPME-MS coupled with SIMCA statistical analysis appears to be a potential tool for the rapid discrimination of scented and nonscented rice samples. Twenty-five samples a day can be routinely analyzed in manual mode. The procedure will be implemented soon on an automatic sampler in order to analyze up to 60 samples per day. The technique can be considered as a mass sensor or as an electronic-nose system; each ion, generated by the mass spectrometer, can be viewed as a virtual sensor, the whole system being composed of 160 "pseudo-sensors". It has the advantage of not suffering from drift problems with respect to the classical electronic nose and affords, in addition, the possibility of interpreting the significance of the discriminating variables.

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