Assessment of aromatic quality of rice samples using fingerprinting methods

C. Mestres, M. Laguerre, F. Gay, R. Boulanger, F. Davrieux
CIRAD
TA 70/16, 73 avenue JF BRETON,
Montpellier Cedex 05
E-mail :christian.mestres@cirad.fr

Perfumed rice account for 30% of rice consumption in France. Their aromatic character is linked mainly to the presence of 2-acetyl-1-pyrole (2AP) in the grain. The objective of our work is to establish a quick method for discrimination of rice sample according to their aromatic quality. We investigate the possibility of using fingerprints obtained from whole grain with Near InfraRed Spectrometry (NIRS) or Mass Spectrometry of the entire volatile fraction (MS). Spectral data are analyzed using the discriminant method SIMCA (Soft Independent Modeling of Class Analogy).

Experimental design

SM : we used 61 rice samples from Camargue harvested in 2004: 29 aromatic, 32 non aromatic. The entire volatile fraction of a 3.5g sample of brown rice was trapped by SPME (Solid Phase Micro Extraction) at 80°C then analyzed by SM (EI+ 70 eV) with a Agilent spectrometer (5973N model). Mass range used was included between 40 and 200 uma. Global fingerprints were obtained twice with a total randomization. By this way, we had 122 fingerprints: 58 from perfumed rice and 64 from non perfumed rice.

SPIR : we used 117 rice samples from Camargue (61) and Vietnam (56) harvested in 2004. Amongst them 65 were perfumed and 52 non perfumed. 6 g of brown rice were analyzed by diffuse reflection from 400 to 2500nm with a 2nm increment using a spectrometer Foss- NIRsystem 6500. Spectral data were processed with the software NIRS 2 version 4.11 (InfraSoft International). Every sample was analyzed twice and the average spectrum was kept.

Mass spectrometry

Six samples were extracted randomly out of the 61 analyzed with SM for validation. The model developed with the SIMCA method keep 23 CPs for the perfumed rice class and 22 for the non perfumed one. The distance H between classes is 1.95 and the classification rate of samples used for validation is 100 % (fig. 1). This rate is 83 % for the validation set : two samples of perfumed rice are not affected to any classes.

The discriminative power of each variable, it means their contribution to discrimination of non-perfumed and perfumed classes, was calculated. Abundance of ions 68, 83 and 111 uma have a discriminative power above 40 (fig. 2). These ions are characteristics of 2AP's mass spectrum (fig. 2). The aromatic character of rice do contribute to discrimination of spectral fingerprints.

Results

Near Infrared Spectrometry

The SIMCA model has been calibrated over 97 samples and validated on 20 samples randomly extracted from the initial pool of 117 samples. 12 CPs are kept for the non aromatic class and 13 for the aromatic one. The distance H between classes is 0.83 and the classification rate of samples used for calibration is 100 %.

The discriminative power of each variable, it means their contribution to discrimination of non-perfumed and perfumed classes, was calculated. Abundance of ions 68, 83 and 111 uma have a discriminative power above 40 (fig. 2). These ions are characteristics of 2AP's mass spectrum (fig. 2). The aromatic character of rice do contribute to discrimination of spectral fingerprints.

Conclusion

Results show that both global fingerprinting methods combined with the SIMCA statistical analysis make it possible to discriminate rice according to their aromatic characteristic (83% of match with MS and 84% with NIRS). Moreover, the SIMCA analysis shows that discrimination is directly linked to the molecules involved in rice aroma. This interpretation is more difficult with NIRS method which is based on the response of the whole matrix of the grain and not only on the volatile fraction. Joint analysis of the datasets obtained with the two methods might improve the discrimination.