The Recognition and Characterization of the Quality and Origin of Botrytized Wines Vintaged by Various Appellations based on Excitation-Emission-Matrix

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1. Backgrounds

Wine frauds are always disrupting the whole wine market order. Finding wine fraud from sets of suspicious wines is a challenging subject with conventional methods such as ~~（~~sophisticated physical-chemical analysis or sensual evaluation. ~~, which are time-consuming and requires high cost and skilled personnel, and sometimes is risky to perform sensual evaluation when the wine frauds are suspected of using harmful additives.)~~

In this study, the botrytized wine (BW) was used as the case example accompanied with the Excitation-Emission-Matrix (EEM) aim to develop a rapid and objective method that can predict BW's quality and appellations. Multi-way analysis methods were used to ~~t~~Tentatively ~~separating~~ separate fluorophores in the spectra ~~by means of multi-way analysis method, trying to correlate the fluorophores with specific chemical compounds in the samples. And expecting ~~t~~~~T~~his approach is expected to have a potential to ~~could~~ be applied as an alternative method to measure other types of beverages.

2. Materials & Methods

17 different classed BWs from 4 appellations and 7 control group samples were selected in this study and their EEMs were measured using a fluorescence spectrometer (F-7000, Hitachi High-Tech Corp.). Measurement parameters were set as ~~e~~Excitation/~~e~~Emission detection ranges: 200-700 nm; ~~s~~Sampling interval: 10 nm; ~~v~~Voltage: 700 V; ~~t~~The angle of incidence:45 degrees; ~~s~~Sample preparation: none.

The analytical methods, Principal Component Analysis (PCA), Parallel Factors Analysis (PARAFAC), and Partial Least Square Discriminant Analysis (PLS-DA), were used to analyze sample spectra's relationship with ~~origin~~ quality and ~~class~~ appellations in this study.

3. Results

【Fluorescence profiles of samples】

All of the BW samples have ~~three~~3 maxima, the first maximum appears in 220/350; the second maximum appears in 280/350; the third maximum appears in 350/450. (Unit: nm; Ex/Em)

Compared to the BW, the control group (white wines) has a close fluorescence profile of the first ~~two~~2 maxima and a significantly weaker third maximum with BW.

【PCA】

According to the PCA result~~,~~ when using ~~4 Principal Components (PCs) with~~ class centroid centering preprocessing, the distribution of samples dots shows a clear separation in the case of setting principal component (PC) 1 and PC2 as X and Y-axis. (Fig.1) ~~And~~ In addition, higher-class samples tend to have a lower PC1 score but a higher PC 2 score. PC loading suggests that the PC1 is related to the first ~~two~~2 maxima of the original spectra and PC2 is related to the third maxima, suggesting that the higher-class sample has higher intensity at the third maximum~~a~~ but ~~the~~ lower intensity in the first ~~two~~2 maxima.

【PARAFAC】

PARAFAC decomposed and extracted 4 fluorophores from the original spectra. ~~And found that t~~The fluorophore located in Ex 360 nm to 490 nm, Em 420 nm to 530 nm has a good separation of samples' class. (Fig.2) ~~And t~~This area also emerged in PCA, which related to the third maximum of the original spectra.

【PLSDA】

PLS-DA reached 86.2% of accuracy on fitting sample's appellat (47 corrects of total 51 fittings, 4 latent variables were used, total d usage was 89.19%, preprocessing was auto-scale.)

PLS-DA reached 94.4% of accuracy on fitting sample's quality (34 corrects of total 36 fittings. 2 latent variables were used, total data usage was 80.88%, preprocessing was auto-scale.)

PLS-DA model got 76 % accuracy (16 corrects of total 21 fittings) on predicting control group samples, it correctly arranged non-botrytized wines (class 0), and the botrytized wine from South Africa (class 1)

4. Summary

In this study, EEM combined with multivariate analysis has successfully been applied on recognizing the appellation and quality of BW, also exhibits good performance on discriminating the authenticity of BW. ~~But~~ However, the model requires further refinement to reach better performance and ~~the~~ investigations on~~f~~ the compounds that are related to the fluorescence profile of the sample need to be performed.

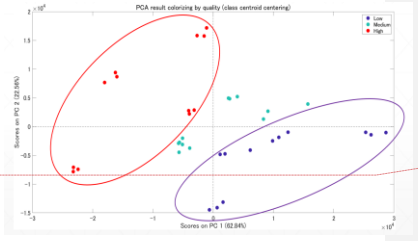

Fig.1. PCA result

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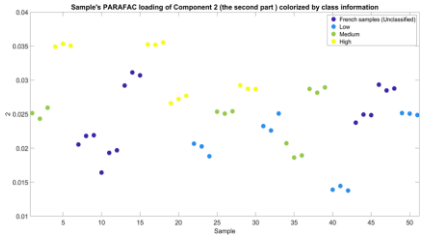

Fig.2 PARAFAC loading of fluorophore