Accepted Manuscript

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PII: DOI: Reference:	S1386-1425(18)30708-X doi:10.1016/j.saa.2018.07.054 SAA 16323
To appear in:	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy
Received date: Revised date: Accepted date:	10 April 2018 16 July 2018 17 July 2018

Please cite this article as: Leqian Hu, Chunling Yin, Shuai Ma, Zhimin Liu, Rapid detection of three quality parameters and classification of wine based on Vis-NIR spectroscopy with wavelength selection by ACO and CARS algorithms. Saa (2018), doi:10.1016/j.saa.2018.07.054

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Rapid detection of three quality parameters and classification of wine based on Vis-NIR spectroscopy with wavelength selection by ACO and CARS algorithms

Leqian Hu*, Chunling Yin, Shuai Ma, Zhimin Liu

College of Chemistry, Chemical and Environmental Engineering, Henan University of Technology, Zhengzhou 450001, China

*Corresponding author. Fax: +86-371-67756718 E-mail address: leqianhu@163.com

Abstract: The feasibility of rapid detection of three quality parameters and classification of wines based on visible and near infrared spectroscopy (Vis-NIRs) was investigated. A modified ant colony optimization (ACO) algorithm for wavelength selection in Vis-NIR spectral analysis was proposed to improve the prediction performance of partial least squares regression (PLSR) model. The result proved that feature wavelengths/variables can be selected by the proposed method for building a high performance PLSR model. The root mean square error of total acid, total sugar and alcohol obtained by ACO-PLS were 0.00122 mol/l, 0.0893 g/l and 0.206 (v/v), respectively. Their correlation coefficients obtained by ACO-PLS reach to 0.973, 0.994 and 0.928, respectively. Compared with full-spectral PLS and PLS based on competitive adaptive reweighted sampling (CARS-PLS) method, the application of ACO wavelength selection provided a notably improved regression model. The prediction results were significantly better than the full-spectral PLS model and slightly better than the CARS-PLS method. Meanwhile, a classification study was also constructed based on the ACO-Principal component analysis (ACO-PCA) model showed that Vis-NIR spectra could be used to classify wines according to the geographical origins. Therefore, it can be concluded that the Vis-NIR spectroscopy technique based on ACO wavelength selection has high potential to differentiate the wine origins and predict the quality parameters in a nondestructive way.

Keyword: Visible and near infrared spectroscopy; Wine; Quality parameters; Wavelength selection; Modified ant colony optimization algorithm.

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