以揮發性化合物辨別食品詐欺

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大綱

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摘要

食品詐欺 (food fraud) 是為了謀取經濟利益，而在食品性質、成分、來源標示故意欺騙的行為。本報告旨在探討利用食品中獨特的揮發性化合物(Volatile Organic Compounds ,VOCs)作為指紋圖譜,結合化學計量學能作為快速識別食品真實性的工具。研究彙整三種不同複雜度實驗模型,如下:芝麻油精摻入低價食用油、不同豆種與產地之醬油混和,以及烘焙研磨咖啡與其常見摻假物。使用頂空氣相層析離子遷移譜 (HS-GC-IMS)及頂空固相微萃取氣相層析質譜法 (HS-SPME/GC–MS) 分析，結合主成分分析 (PCA)、正交偏最小二乘判別分析 (OPLS-DA)、偏最小二乘判別分析 (PLS-DA) 和隨機森林 (RF) 等機器學習模型分析。結果顯示真偽芝麻油利用 OPLS-DA 成功區分，並鑑定出 5 種芝麻油精標記物 (markers) ，如 2-甲基丁酸、2-呋喃甲硫醇、甲基吡嗪、甲硫醛和 2,5-二甲基吡嗪。並成功區分黑豆與黃豆醬油及臺灣與日本產地，且發現 15 種關鍵揮發物，而模型能偵測出低比例摻假。另成功發現阿拉比卡咖啡與其常見摻假物的 11 種獨特揮發性化合物作為潛在標記物。綜上所述，分析食品中的揮發性化合物，經由化學計量統計能展現良好的分類能力，其高效率及高靈敏度能有效區分食品真實性，而標記物的發現因其準確性和可追溯性，能夠用於市場仲裁檢驗。

Volatile compounds analysis for food fraud detection

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outline

1.Introduction

2. Coffee Adulteration Detection

3. Discrimination the Soy Sauce of Bean Species and Geographical Origin

4. Adulteration detection of essence in sesame oil

5.Conclusion

Abstract

Food fraud involves intentional deception of food nature, ingredients, or origin for economic gain. This study explores using volatile organic compounds (VOCs) as unique fingerprints combined with chemometrics for rapid food authenticity verification. Three complex models were tested: premium sesame oil adulterated with cheaper oils, soy sauce blends from different bean varieties and origins, and roasted coffee mixed with common adulterants. Analysis employed HS-GC-IMS and HS-SPME/GC–MS techniques coupled with PCA, OPLS-DA, PLS-DA, and Random Forest algorithms. Results demonstrated successful discrimination of authentic sesame oil with five identified markers, clear distinction between black and yellow soybean soy sauces and their origins with fifteen key VOCs, and differentiation of Arabica coffee from adulterants via eleven unique VOCs. Overall, VOC analysis combined with chemometrics shows high accuracy and sensitivity in food authenticity, providing precise and traceable markers useful for market inspection.

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