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Food Control

journal homepage: www.elsevier.com/locate/foodcont

Rapid determination of geographical authenticity of *Gastrodia elata* f. *glauca* using Fourier transform infrared spectroscopy and deep learning

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ARTICLE INFO

Keywords:

Gastrodia elata f. *glauca*
Fourier transform infrared spectroscopy
Deep learning
Data driven version of soft independent
modeling of class analogy

ABSTRACT

For quality evaluation of *Gastrodia elata* f. *glauca* (GEFG), it's crucial to develop an analytical method to determine the geographical origin. Herein, 371 GEFGs are collected from five provinces, focusing on analysis of dry matter content (DMC), origin identification, geographical indication (GI) production area discrimination by using a combination of Fourier transform infrared (FTIR) spectroscopy and deep learning, data driven version of soft independent modeling of class analogy (DD-SIMCA). A significant difference in DMC of GEFG between Yunnan and other origins, which may be related to precipitation, altitude, temperature, and soil. The residual neural network (ResNet) model based on synchronous two-dimensional correlation spectroscopy (2DCOS) images has stable performances, its accuracy is 100%. The DD-SIMCA model can differentiate GI production areas of GEFG, while for non-GI areas, the model specificity is 71.38%. This study provides a promising approach for GEFG geographical traceability and GI production area differentiation.

1. Introduction

Gastrodia elata blume (GEB), known as Tianma in China, is a genus of perennial saprophytic herbs in the family Orchidaceae that grows in symbiosis mainly with fungus *Armillaria mellea* (Zhan, Yang, Lu, Deng, & Yang, 2022). GEB has been used as a significant traditional Chinese medicine, which has been recorded in Divine Farmer's Classic of Materia Medica (Shen Nong Ben Cao Jing) more than 2000 years ago. It is mainly used for the treatment of neurological disorders, such as headache, dizziness, epilepsy, neuralgia, and paralysis (Wang et al., 2018; Yang et al., 2023). Though modern pharmacological analysis and identification, it was found that this plant is rich in aspalathin, *p*-hydroxybenzyl alcohol, polysaccharides, vanillin, parishin and other compounds (Sun et al., 2023). Based on its medicinal value, GEB has been listed in the pharmacopoeias of China, Japan, the United Kingdom and Europe (Yang et al., 2023). In 2023, GEB was classified by the State Administration of Market Supervision and Administration of China as a plant that is both a traditional food and a traditional Chinese medicine (<http://www.nhc.gov.cn/wjw/index.shtml>). It is of great significance for affirming its nutritional and medicinal value, as well as enhancing its economic value. There are five species of GEB widely grown in China, including

G. elata f. *glauca* S. Chow (GEFG), *G. elata* f. *elata*, *G. elata* f. *viridis* Makino, *G. elata* f. *flavida* S. Chow, and *G. elata* f. *alba* S. Chow (Wang et al., 2018). Among them, GEFG is an excellent GEB variety in China and is widely planted in Yunnan, Guizhou, Hubei, Sichuan and Tibet provinces.

Effective differentiation of GEFG's origin is essential for the success in commercial trade, as the quality of GEFG varies depending on the region in which it is grown, and this variance in quality is reflected in various pharmacological activities and economic values (Chen et al., 2015). The origins can be the main basis for judging the quality of GEFG. Owing to the unique climate and geographical characteristics, GEB in Zhaotong, Yunnan Province has good quality, and Zhaotong has been registered as a National Geographical Indication (GI) production area (Zheng, Li, Liu, & Wang, 2023). Driven by economic competition, the issue of geographical authenticity in the GEFG trade process has attracted the attention of consumers, mainly in the form of origin confusion trafficking (Li, Shen, Li, & Wang, 2024). However, it is challenging for professionals to discern GEFG from distinct origins. Traditionally, varieties of GEB have been identified mainly from differences in flower stem color, discrepancy in rhizome length, width and thickness for traditional character divergence analysis (Yang et al., 2023). It is not

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<https://doi.org/10.1016/j.foodcont.2024.110810>

Received 16 July 2024; Received in revised form 4 August 2024; Accepted 12 August 2024

Available online 13 August 2024

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全国大学英语四级考试(CET4)成绩报告单

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笔试成绩

准考证号：

总 分：**427**

听 力：**128**

阅 读：**169**

写作和翻译：**130**

考试时间：2020年12月

口试成绩

准考证号：--

等 级：--

考试时间：--

5、学术能力证明材料

LWT - Food Science and Technology 201 (2024) 116243



Contents lists available at ScienceDirect

LWT

journal homepage: www.elsevier.com/locate/lwt



A fast method for predicting adenosine content in porcini mushrooms using Fourier transform near-infrared spectroscopy combined with regression model

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ARTICLE INFO

Keywords:

Fourier transform near-infrared spectroscopy
Porcini mushrooms
Adenosine
Partial least squares regression

ABSTRACT

Adenosine is an endogenous neuroprotective agent. It is of great importance to research the porcini mushrooms' adenosine for developing products. However, problems, such as the old for new and traditional methods for detecting adenosine content are complicated and time-consuming, seriously restrict industrial development. The present study aimed to achieve a rapid quantification of adenosine content in porcini mushrooms on the market using Fourier transform near-infrared (FT-NIR) spectroscopy combined with partial least squares regression (PLSR) model. Herein, the nucleoside content and spectral characteristics of the large-scale dataset ($n = 242$) were analyzed, which was used as the calibration set for constructing the PLSR model. The PLSR model had an R^2_c of 0.907 and a residual predictive deviation (RPD) of 2.726. For random samples with different origins, the R^2_p was 0.768 and the RPD was 1.326, for the storage period, the R^2_p was 0.952 and the RPD was 3.069, and for various collection years, the R^2_p was 0.927 and the RPD was 2.548. It was demonstrated that the established method offers a rapid and reliable prediction strategy for adenosine content of random porcini mushrooms samples, which has the potential to be applied in the market.

1. Introduction

Boletus sect. *Boletus* (porcini mushrooms) are one of the most significant fungal groups due to their ecological and economic importance, and this group of fungi forms ectomycorrhizal symbioses with plants of many families, including Pinaceae, Fagaceae and Dipterocarpaceae (Cui, Feng, Wu, Xu, & Yang, 2015). They are one of the most collected species in the world, being consumed 20–100 tons per year (Rivas-Ferreiro, Otero, & Morán, 2023). According to public databases, the export value of porcini mushrooms in China exceeded \$66.06 million in 2023 years (<http://www.customs.gov.cn/>). Porcini mushrooms are beneficial for increasing income in rural areas due to their high economic value. Additionally, the nutritional and medicinal values for porcini mushrooms are the main reasons for popularity. Porcini mushrooms are high in protein, polyunsaturated fatty acids, minerals and vitamins, making them one of the most popular foods for vegetarians (Tan, Zeng, & Xu, 2022). Modern pharmacological research has shown that some bioactive

substances, such as phenolic compounds and polysaccharides, have antihyperglycemic and antioxidant properties (Wei et al., 2024). Mushroom's polysaccharides have great medicinal potentials that can manage cardiovascular diseases, cancers, and diabetes mellitus (Zhang, Lei, Zhou, Ye, & Zhao, 2022). On the other hand, nucleosides have been showed to strengthen brain function, influence immune modulation, affect fatty acids metabolism, contribute to absorption of intestinal function, and enhance gastrointestinal tract repair after damage (Phan et al., 2018). Nucleosides are involved in the regulation of several physiological processes in the human body, mainly through purinergic and/or pyrimidine receptors. Nucleosides, for instance uridine, adenosine and guanosine are precursor molecules for the production of DNA and RNA (Phan et al., 2018). Adenosine is necessary for the normal function of all cells within the human body. It acts as a neurotransmitter for P1 and P2 purine receptors in its native state (Solakov et al., 2022). Adenosine has various pharmacological effects, including anti-inflammatory, immunomodulatory and neuroprotective effects. It is

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<https://doi.org/10.1016/j.lwt.2024.116243>

Received 3 January 2024; Received in revised form 5 May 2024; Accepted 22 May 2024

Available online 22 May 2024

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Fingerprinting of *Boletus bainiugan*: FT-NIR spectroscopy combined with machine learning a new workflow for storage period identification

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ARTICLE INFO

Keywords:

Boletus bainiugan

Fourier transform near infrared spectroscopy

Machine learning

Storage period identification

ABSTRACT

Food authenticity and food safety issues have threatened the prosperity of the entire community. The phenomenon of selling porcini mushrooms as old mixed with new jeopardizes consumer safety. Herein, nucleoside contents and spectra of 831 *Boletus bainiugan* stored for 0, 1 and 2 years are comprehensively analyzed by high performance liquid chromatography (HPLC) coupled with Fourier transform near infrared (FT-NIR) spectroscopy. Guanosine and adenosine increased with storage time, and uridine has a decreasing trend. Multi-conventional machine learning and deep learning models are employed to identify the storage time of *Boletus bainiugan*, in which convolutional neural network (CNN) and back propagation neural network (BPNN) models have superior identification performance for distinct storage periods. The Data-driven soft independent modelling of class analogy (DD-SIMCA) model can completely differentiate between new and old samples, and partial least squares regression (PLSR) can accurately predict the three nucleoside compounds with an optimal R^2 of 0.918 and an excellent residual predictive deviation (RPD) value of 3.492. This study provides a low-cost and user-friendly solution for the market to determine, in real time, storage period of *Boletus bainiugan* in the supply chain.

1. Introduction

The twenty-first century, marked by technological evolution and big data, has reshaped many aspects of human society. Simultaneously, the sustainability challenges posed by social development have also increased (Li et al., 2024a). The issue of food authenticity has become a critical and highly discussed issue in terms of the modern food industry. Food authenticity is defined as the quality of a food product that is genuine and indisputable in its nature, origin, identity, and claims, as well as to meet the desired characteristics (Deng et al., 2024b). The proposal of food authenticity reveals vulnerabilities in the food system, there is an urgent need for a low-cost, rapid, and stable detection method to detect and prevent food fraud problems.

Boletus bainiugan, a fungus of the genus *Boletus* widely distributed in southwestern China, which has rich nutritional value, unique flavor and potential pharmacological activity. The pharmacological and nutritional effects of nucleoside components as one of the quality components of porcini mushrooms have been widely studied. Adenosine can inhibit

platelet aggregation, with anti-angiogenic and anti-inflammatory effects, uridine is related to nerve synapse growth stimulation activity. The guanosine is involved in various metabolic activities in the human body, and may be related to the formation of porcini mushrooms taste flavor (Phan et al., 2017). Due to its high moisture content and rapid respiratory metabolism, fresh *Boletus bainiugan* is prone to stipe elongation, cap opening, softening and browning after collection (Deng et al., 2023). To extend the storage period, *Boletus bainiugan* dried to dry slices and sold. Nevertheless, dried slices are characterized by non-perishable and unrecognisable appearance with the naked eye (Fig. S1 a, b), which creates challenges for appraisal of storage time. Meanwhile, the increase in storage time may lead to the production of harmful substances, such as the amines, mercaptans, and indole compounds, as well as results in the degradation of nutrients including proteins and polysaccharides (Yan et al., 2023). The authorities in Yunnan Province, China, have set the storage period of dried porcini mushroom slices at two years. However, the global economic recession and the backlogs of products in the marketplace provide motives for

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<https://doi.org/10.1016/j.fm.2025.104743>

Received 14 November 2024; Received in revised form 20 January 2025; Accepted 5 February 2025

Available online 6 February 2025

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Volatile compounds and aroma characteristics of mushrooms: a review

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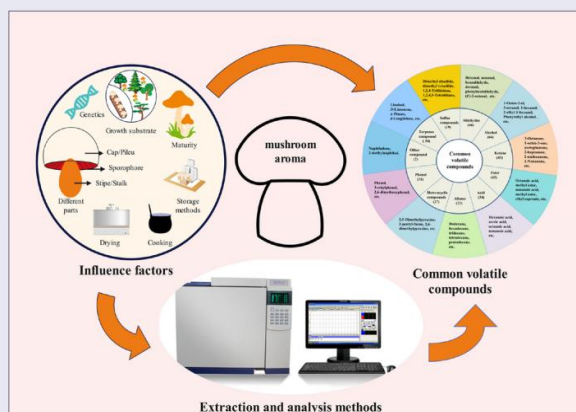
ABSTRACT

Mushrooms are popular due to their rich medicinal and nutritional value. Of the many characteristics of mushrooms, aroma has received extensive attention and research as a key determinant of consumer preference. This paper reviews the production, role and contribution of common volatile compounds (VCs) in wild and cultivated mushrooms, and explores the methods used to characterize them and the factors influencing aroma. To date, more than 347 common VCs have been identified in mushrooms, such as aldehydes, ketones, alcohols and sulfur-containing compounds. Extraction and identification of VCs is a critical step and combining multiple analytical methods is an effective strategy in mushroom aroma studies. In addition, the VCs and the aroma of mushrooms are affected by a variety of factors such as genetics, growing conditions, and processing methods. However, the mechanism of influence is unknown. Further studies on the production mechanisms of VCs, their contribution to aroma, and the factors influencing their formation need to be determined in order to fully elucidate aroma and flavor of mushrooms.

KEYWORDS

characteristic aroma; identification techniques; influence factors; mushrooms; volatile compounds

GRAPHICAL ABSTRACT




Introduction

Mushrooms, a large fungal organism, has been used since ancient times as a source of medicine and as a health food (Hamza, Ghanekar, and Santhosh Kumar 2023). It has been widely studied due to its pharmacological activities such as anti-tumour (Niu et al. 2021), anti-diabetic (Xiao et al. 2019), anti-viral (He et al. 2020) and as a rich nutrient substance due for instance protein, minerals and vitamins content (Zhang et al. 2021b). In nature, 22,000 known species of mushrooms have been identified, including more than 2,000 edible species, of which exceed 20 are cultivated species (Zhang et al. 2021b). Wild mushrooms are an important

source of rich protein and their consumption is gradually increasing (Agrahar-Murugkar and Subbulakshmi 2005). Five species dominate the cultivated mushrooms and their commercial value is very remarkable. They are *Agaricus bisporus*, *Lentinus edodes*, *Pleurotus spp*, and *Flammulina velutipes*, etc. (Kalac 2013). There has been a significant increase in mushrooms production and economic value in a global scale (Lu et al. 2020). The global edible mushrooms market is expected to be USD 62.19 billion by 2023 due to the increasing demand for mushrooms (Niego et al. 2021).

The attributes of flavor of mushrooms like aromatic, delicious, meaty, sweet is a crucial reason for their popularity (Zhu

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 Supplemental data for this article can be accessed online at <https://doi.org/10.1080/10408398.2023.2261133>.

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Contents lists available at ScienceDirect

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

journal homepage: www.journals.elsevier.com/spectrochimica-acta-part-a-molecular-and-biomolecular-spectroscopy

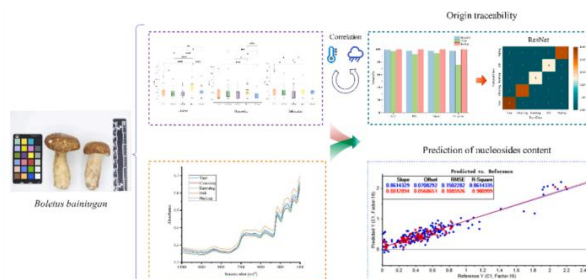
Rapid prediction of nucleosides content and origin traceability of *Boletus bainiugan* using Fourier transform near-infrared spectroscopy combined with chemometrics

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HIGHLIGHTS

- First analysis of the correlation between climatic factors and nucleoside content.
- ResNet model successfully traced the origin of *Boletus bainiugan*.
- PLSR model smoothly predicts three nucleoside compounds.

GRAPHICAL ABSTRACT



ARTICLE INFO

Keywords:

Fourier transform near-infrared spectroscopy
Nucleoside compounds
Climatic factors
Two-dimensional correlation spectroscopy
Residual neural networks

ABSTRACT

Boletus bainiugan has high nutritional and economic values. As one of the potential medicinal active ingredients, nucleosides have important research significance. Porcini mushrooms fraud is frequently detected on the market, including substitute inferior into superior and lack of geographical origin's certification. This behavior results in economic loss and health damage to consumers. Fourier transform near-infrared (FT-NIR) spectroscopy is a fast, efficient and reliable analytical tool. In the present study, the effect of source environment (climatic factors) on nucleoside content is analyzed for the first time. Then, the FT-NIR spectroscopy to study the origin traceability and content prediction of *Boletus bainiugan* are utilized. The results indicate that the nucleoside content is associated with precipitation and temperature. The combination of synchronous two-dimensional correlation spectroscopy (2DCOS) with residual neural networks (ResNet) model obtains the precise identification of the origin of *Boletus bainiugan*, with an accuracy of 100%. In the prediction models of content for uridine, guanosine, and adenosine, the optimal coefficient of determination of predictive set (R_p^2) is 0.901, and the optimum residual prediction deviation (RPD) is 3.178. FT-NIR spectroscopy has proven to be an environmentally friendly and non-destructive analytical tool for accurate origin traceability and content prediction.

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Received 17 May 2024; Received in revised form 6 November 2024; Accepted 7 November 2024

Available online 10 November 2024

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我国天麻研究态势问题分析及未来发展对策研究 ——基于 20 年专利数据为例

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摘 要: 天麻 (*Gastrodia elata* Blume) 是一种药食同源植物, 具有极高的药用和食用价值。专利文献具有创造性、新颖性和实用性, 为了解目前我国天麻专利的研究方向及重点, 以 Patentics 数据库为数据源, 检索公开日为 2003 年以来国内天麻专利, 利用 Excel 2019、Origin 2021 工具以及专利计量学, 对申请数量、申请地区、申请人、主要发明人、技术领域分布、法律状态和专利地图等方面进行分析。结果发现: 近 20 年天麻专利申请数量呈波浪形变化; 不同地区申请数量与地理位置和科技发展水平有关; 申请人呈现较强地域性, 重点关注领域也有所不同; 所属单位相同的发明人存在合作关系; 国内天麻专利技术领域分布重点集中于人类生活需要方面; 专利地图呈现了天麻专利研究热点以及未来发展方向, 具有一定参考意义。研究揭示近 20 年天麻专利技术分布和研发重点, 为天麻未来研究领域和专利布局提供参考和新思路。

关键词: 天麻; 专利计量学; 专利分析; 专利地图; Patentics 数据库

中图分类号: S-1

文献标志码: A

DOI: 10.19754/j. nyyjs. 20240315038

引言

天麻 (*Gastrodia elata* Blume) 原名赤箭, 始记载于《神农本草经》, 被列为上品^[1]; 天麻之名始载于宋代《开宝本草》, 后被李时珍合并于《本草纲目》, 统称为天麻^[2]。天麻为兰科天麻属多年生草本植物, 被列为国家二级保护植物 (详见国家重点保护野生植物名录)。天麻在《神农本草经》中被记载为“天麻味辛, 温。主杀鬼精物, 蛊毒恶气。久服益气力, 长阴, 肥健, 轻身增年”^[3], 是中国珍贵中草药之一, 其药用部位为块茎。现代药理学表明, 天麻具有抗氧化、抗衰老、抑菌抗炎、抗惊厥、抗抑郁、增加血流量、降血压等作用^[4,5]。除药用价值外, 天麻还有食用价值。据报道, 天麻已经有 2000 多年食用历史, 是一种较高档次的绿色保健食品^[6]。此外, 天麻作为一种传统中药材, 《化妆品原料目录 (2021 年版)》已经将天麻提取物纳入其中^[5]。目前, 天麻在药品、保健品、食品及化妆品方面的研究日益增多^[7]。

专利文献具有创造性、新颖性和实用性, 受到研究人员重视, 据欧洲专利局统计, 世界 80% 的技术信息都可以在专利文献中找到^[8]。近年来, 人们对天麻相关研究和发明已逐渐增加, 通过对专利文献进行计量分析, 可掌握科技发展最新态势。目前关于天麻专利文献分析的文章较少。在近期发表文章中, 上官晨虹等^[9]对国内外天麻药品专利进行分析, 并预测了未来天麻药品研究热点方向, 具有很好的借鉴作用。肖兴娟等^[10]对贵州省天麻专利进行分析, 揭示了贵州省利用开发天麻的产业方向。以上文章研究范围有一定局限性, 未能站在全国视角下对以天麻和天麻提取物为原料的相关专利进行解析。众所周知, 天麻与蜜环菌共生, 种植条件要求苛刻, 市场需求量大^[11]。关于天麻种植以及蜜环菌改良相关专利不断涌现。对天麻相关专利进行全面分析, 能够确保更深入了解天麻研究热点、研究难题以及未涉及的研究领域, 为开发新的研究方向提供思路。冯培松^[12]曾对国内天麻专利现状进行分析, 但研究年份较为久远, 仅对专利

收稿日期: 2024-01-05

基金项目: 云南省重大科技专项“航天育种和航天食品研发与示范” (项目编号: 202202AE090001)

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