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Environmental Friendly Coffee Ground (SCG) Essential Oil Extraction and Predictive Analysis of Its Efficacy Biomarkers

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Abstract: In recent years, the growing demand and consumption of coffee have led to increasing pressure on coffee residue processing. As the largest byproduct of the coffee industry, coffee waste residue is often incinerated or landfilled as solid waste, potentially releasing approximately 5.04 billion kilograms of carbon dioxide annually. Studies indicate that coffee residue contains polyphenols, caffeine, and certain organic acids, and direct disposal poses environmental hazards. Literature review reveals that the value of coffee waste residue remains underutilized, with limited research reported on essential oil extraction from it. Through extensive literature review, this study proposes an environmentally friendly essential oil extraction process for coffee waste residue (SCG) and evaluates the feasibility of functional marker prediction using network pharmacology. Additionally, the paper identifies current technical challenges and research trends in coffee residue essential oil extraction to facilitate innovative eco-friendly extraction processes, providing new insights for the application of coffee waste residue (SCG) in pharmaceutical and health product development.

Keywords: Coffee Grounds; Essential Oils; Extraction; Resource Recycling; Efficacy Biomarkers.

1. Introduction

Coffee (*Coffea arabica L*) is a brown beverage produced by roasting and grinding coffee beans to varying degrees, renowned for its stimulating effects and rich flavor profile. As one of the world's most popular beverages and the second-largest traded commodity after petroleum, coffee has seen continuously rising demand and consumption in recent years, leading to escalating pressure on coffee grounds processing. A single freshly ground coffee cup generates approximately 30 grams of coffee grounds [1]. According to a 2020 report by the International Coffee Organization, global coffee consumption reached around 9.96 million tons, with each ton of coffee beans producing 650 kilograms of grounds. Even "coffee giant" Starbucks reports an average of 10 kilograms of coffee grounds generated per store daily. With global coffee consumption continuing to rise, coffee grounds production remains rapidly increasing. As the largest byproduct of the coffee industry, coffee waste is often incinerated or landfilled as solid waste. Improper disposal causes environmental pollution and significant resource waste, potentially releasing approximately 5.04 billion kilograms of carbon dioxide annually. Additionally, coffee grounds contain polyphenols, caffeine, and organic acids, which pose environmental hazards when discarded directly.

Currently, coffee cultivation areas in regions like Yunnan are expanding rapidly in China. However, most coffee products are sold in primary processed forms, and more concerning is that coffee grounds are often discarded as waste. This not only causes environmental pollution but also prevents natural resources from being utilized effectively. If these discarded materials could be repurposed through green recycling of brewing residues from Yunnan's small-grain coffee varieties and their conversion into sustainable solid waste resources, it would significantly boost local economic development. To enhance the economic value of coffee products, leverage our province's coffee resource advantages, and reduce environmental pollution caused by waste disposal, such initiatives are crucial.

2. Current Status of Coffee Development in Yunnan

Yunnan is the earliest region in China to cultivate coffee. Due to its suitable altitude and climatic conditions, Yunnan has become one of the most suitable areas for coffee cultivation, serving as a golden zone for coffee farming. It has now developed into China's largest coffee planting base [2]. With the increasing demand for coffee, Yunnan Province, as the region with the largest coffee planting area, has its production zones widely distributed across Baoshan, Dehong, Lincang, Pu' er, and other areas [3]. Both the coffee planting area and output account for over 98% of the national total [4].

The coffee industry in Yunnan ranks first nationwide due to its unique development advantages, which include optimal planting conditions and a long history of industrial development. Coffee was introduced to Yunnan from Vietnam by French missionaries in the 1890s. After years of development, Yunnan has become China's largest coffee trading hub and export base. Yunnan coffee holds an absolute leading position domestically, driving the growth of a series of local coffee enterprises. For example, Dehong Hougu Coffee Co., Ltd., established in 1994, has grown into a coffee group company integrating coffee cultivation, deep processing, product development, and international trade. Its best-selling product is "Hougu Coffee Instant Pure Black Coffee Fresh Ground American Coffee Powder with Oil Yunnan Small Granule Coffee Powder." Through the "*cooperative+*" model, the company has established a standardized coffee planting base covering 18,000 hm^2, with an average green bean yield of 2,220 kg/hm^2, boosting local

economic development and helping over 300,000 people from 65,000 coffee farmers escape poverty. The company has an initial processing capacity of 80,000 tons and has built two of China's largest instant coffee powder production plants with an annual capacity of 13,000 tons, accounting for nearly 85% of the country's deep processing production capacity. It also operates the only freeze-drying powder production line in China [5]. Yunnan has a large coffee planting area and high coffee residue (SCG) output.

3. Current Utilization Status of Coffee Grounds (SCG)

Coffee grounds (SCG) are by-products of primary coffee processing and constitute a significant proportion of waste resources in the coffee industry. Studies indicate that approximately 1 ton of coffee beans generates 650 kg of waste coffee grounds (SCG) [6]. Vardon et al. [7] analyzed that SCG contains 45.20% neutral washing fibers (composed of hemicellulose, cellulose, and lignin-related compounds), 29.80% acidic washing fibers (composed of cellulose and lignin), 16.20% oils, and 15.40% proteins (these data are influenced by factors such as coffee tree species, tree age, geographical location, climate, and soil conditions). Internationally, coffee grounds (SCG) are primarily used as fertilizer and fuel, while domestically they are mostly discarded as waste [8].

3.1. Coffee Grounds (SCG) as a Cultivation Substrate

Edible fungi possess strong capabilities in decomposing and utilizing cellulose, hemicellulose, lignin, and other components. The raw materials are primarily agricultural, forestry, and livestock by-products as well as processing residues. Due to the abundant oil, sugar, and protein content in coffee grounds (SCG), it can be utilized for the cultivation of edible fungi [8].

3.2. Coffee Grounds (SCG) as an Adsorbent

3.2.1. Direct use as an Adsorbent.

Using coffee grounds (SCG) as an adsorbent for treating heavy metal ions in acidic mine wastewater not only facilitates the recovery of waste coffee grounds (SCG) but also provides a novel approach for acid wastewater treatment. Utomo H D et al. [9] investigated the effect of dosage on adsorption efficiency of Zn^{2+}, Pb^{2+}, Cu^{2+}, and Cd^{2+} using coffee grounds (SCG).

3.2.2. As Raw Material for the Preparation of Adsorbents.

Ren Jie et al. [10] prepared activated carbon using coffee grounds (SCG) as raw material through vacuum pyrolysis self-activation followed by phosphoric acid-assisted activation, and determined its self-activation temperature. The study focused on investigating the effects of activation temperature, vacuum degree, heating rate, activation time, and impregnation ratio on the performance of coffee grounds (SCG)-based activated carbon.

3.3. Thermal Pyrolysis and Chemical Conversion of Coffee Grounds (SCG) to Bio-oil and Biodiesel

Due to its high calorific value of approximately 1195 kJ/kg, SCG can be utilized, like other industrial and agricultural residues, for the production of biofuels such as bio-oil, biodiesel, bio-butanol, fuel pellets, bioethanol, biogas, and biochar through thermal cracking [11] or chemical conversion [12].

3.4. Biological Conversion into Mannose Oligosaccharides and other Proliferative Compounds

Guo Yueping et al. [13] utilized coffee bean dregs remaining after chlorogenic acid extraction by water methods to enzymatically produce high-value-added products such as mannose oligosaccharides, and conducted component analysis. The results revealed that the oligosaccharides exhibited a high mannose content, meeting the requirements for functional oligosaccharides as mannose oligosaccharides. In Nguyen et al.'s [14] study, SCG was employed to produce valuable bioproducts including oligosaccharides, mannose oligosaccharides, mannose, and bioethanol.

3.5. Extraction and Classification of Phenolic Compounds and Dietary Fiber from Coffee Grounds (SCG)

Under microwave irradiation for 40 seconds (80 W), total phenolic compounds in SCG were extracted using a 20% ethanol solution, achieving the highest total phenolic content (GAE) of 399 mg/g, indicating that this method is highly effective and time-efficient [15]. Coffee grounds (SCG) contain abundant crude proteins, crude fibers, rich antioxidant substances, and antimicrobial components, exhibiting multiple effects such as improving lean meat percentage in pigs and enhancing animal physiological functions, making it a promising novel feed additive [16].

However, there are currently no reports on the extraction of essential oils from coffee grounds (SCG) and their efficacy studies.

4. Current Development Status of Essential Oil Extraction Technology for Food Applications

Essential oils (also known as volatile oils) are widely found in the flowers, fruits, leaves, stems, peels, and roots of plants. Composed of various volatile aromatic compounds, they exhibit multiple bioactivities including antibacterial, insecticidal, anticancer, antimutagenic, antiviral, antidiabetic, anti-inflammatory, and antioxidant effects [17]. Numerous extraction methods exist for essential oils, with significant variations in operational conditions. Based on extraction principles, essential oils are classified into two main types: distillation and extraction methods.

4.1. Current Development Status of Distillation Methods

Hydrodistillation (HD) equipment is simple, cost-effective, and compliant with food safety requirements, making it the primary method for industrial extraction of edible essential oils [18]. Microwave-assisted hydrodistillation (MAHD) employs microwave radiation heating instead of traditional heat sources, representing a rapid and environmentally friendly approach to essential oil extraction. Yang Ting et al. [19] utilized MAHD to extract essential oil from Cinnamomum cassia leaves, achieving a 4.43% extraction rate within just 1.5 hours. Lucchesi et al. [20] developed solvent-free microwave extraction (SFME), which requires

no solvent addition. However, SFME still involves evaporation processes, leading to high energy consumption and potential loss of volatile components. To address this, Vian et al. [21] designed microwave hydrodiffusion gravity (MHG) technology, enabling essential oil collection without evaporation under gravitational force. Ultrasonic-assisted hydrodistillation (UAHD) pre-treats plant materials with ultrasound before hydrodistillation, utilizing mechanical cell disruption and cavitation effects to generate instantaneous pressures exceeding several atmospheres, thereby accelerating the diffusion of aromatic compounds from plant materials into solvents [22]. Gavahian et al. [23] pioneered the application of ohmic heating in HD essential oil extraction, developing ohmic-assisted hydrodistillation (OAHD). Cui Lijiao et al. [24] extracted lemon essential oil from fresh lemon peel using ionic liquid-assisted steam distillation, achieving an extraction rate of 0.93%.

4.2. Current Status of Extraction Methods

Organic solvent extraction (OSE) offers advantages such as low extraction temperatures and protection of heat-sensitive components from degradation, making it suitable for delicate, fragile, and heat-sensitive floral raw materials [25]. Leveraging the high solubility of essential oils in supercritical CO_2, these oils can be efficiently extracted from plant materials. Subsequent adjustments in operating pressure and temperature facilitate separation between essential oils and extraction fluid, enabling rapid and efficient extraction under mild conditions with enhanced environmental sustainability [26]. Zeng Chaoyi et al. [27] compared the effects of HD, MAHD, UAHD, and supercritical CO_2 extraction methods on Lonicera japonica flower bud oil. Results demonstrated that supercritical CO_2 extraction required the shortest processing time and achieved significantly higher extraction yields compared to the other three methods. Subcritical water extraction (SWE) features simple equipment, cost-effectiveness, and continuous operation capabilities. Khajenoori et al. [28] reported excellent extraction efficiency of chamomile essential oil using SWE technology.

4.3. Advantages of Simultaneous Distillation Extraction Method (SDE)

Simultaneous distillation extraction (SDE) is a method that extracts volatile compounds from organic solvents by simultaneously heating both the sample solution and organic solvent to boiling point. During this process, compounds in the sample's aqueous vapor and organic solvent vapor form an azeotropic mixture, which then transfers to the organic solvent. Each component in the sample can be distilled off at temperatures below its boiling point, while the mixture's boiling point remains constant throughout distillation. The temperature only rises to the boiling point of residual components in the distillation flask after complete evaporation of a specific component. Compared to traditional aqueous distillation extraction, this method reduces experimental steps, lowers solvent consumption, minimizes sample loss during transfer, and enables direct application of extracted plant essential oils to GC-MS analysis. Due to reduced sample loss during transfer, SDE achieves relatively higher oil yield rates compared to conventional atmospheric-pressure aqueous distillation extraction. The extraction of coffee grounds essential oil using SDE is therefore feasible.

4.4. Feasibility Analysis of Essential Oil Extraction from Coffee Grounds (SCG)

Coffee beans contain abundant fats that are difficult to extract through aqueous solutions, resulting in relatively low fat content in coffee beverages. These fats are primarily retained in coffee grounds [29]. Studies indicate that coffee grounds are rich in oils, and the extracted coffee essential oil serves as a natural flavoring oil that can function as a flavor enhancer and aroma additive in food products, as well as a key component in crafting coffee-flavored perfumes. The unique properties of essential oils endow coffee with significant practical applications [30], demonstrating promising market potential. However, current coffee essential oil extraction primarily relies on ground coffee powder, while reports on utilizing coffee grounds (SCG) for oil extraction to repurpose coffee remain limited. Particularly, there are no documented cases of obtaining high-quality coffee refined residue oil through safe, environmentally friendly, efficient, and economical methods.

Coffee grounds extract contains high concentrations of phenolic compounds, including chlorogenic acid, caffeic acid, ferulic acid, p-coumaric acid, gallic acid, protocatechuic acid, and rutin. The predominant compounds are chlorogenic acid, protocatechuic acid, and flavonoids, which exhibit significant biological functions such as antioxidant activity, hepatoprotective effects, hypoglycemic properties, anti-allergic actions, and antibacterial characteristics, making them suitable as natural additives. The antioxidant effects of chlorogenic acid can be utilized for colorectal cancer prevention and intestinal microbiota regulation [31]. These findings suggest that coffee grounds (SCG) essential oil is a substance with substantial practical applications.

5. Current Research Status of Network Pharmacology in Predictive Analysis of Efficacy Biomarkers

Network pharmacology is an interdisciplinary field integrating multidisciplinary technologies and content, which analyzes biological networks to elucidate complex relationships between drug components and disease targets while revealing their mechanisms of action. Deng et al. [32] investigated the potential therapeutic mechanisms of Platycodon grandiflorus in lung cancer treatment, suggesting that the herb may exert its effects through signaling pathways such as MAPK and P13K-AKT. Network pharmacology studies have also demonstrated that Taohong Siwu Decoction can treat post-articulation infections around prostheses, primarily through antibacterial effects and improved hemorheology. Research on drug-organism interactions using network pharmacology approaches has garnered significant attention [33] and emerged as a research hotspot, yet no studies have yet explored the predictive application of network pharmacology to elucidate the mechanism of action of essential oil efficacy biomarkers in coffee grounds (SCG).

6. Outlook

In recent years, coffee demand has shown a steady growth trend, generating substantial coffee by-products with coffee grounds (SCG) accounting for a significant proportion. SCG is now widely utilized as a free resource for biofuel production and chemical compound synthesis. Current research on SCG resource utilization primarily focuses on

synthetic biofuels, feed applications, and fertilizers, while studies on extracting coffee essential oils from SCG remain scarce. Volatile compounds in coffee beans—including alcohols, aldehydes/ketones, carboxylic acids, esters, pyrazines, pyrroles, pyridines, alkalis, sulfides, furans, and phenols—are not fully utilized during roasting processes, with most remaining in coffee grounds. This indicates that significant quantities of volatile components can still be extracted from SCG, suggesting its potential as a highly functional material for essential oil production. Innovations in environmentally friendly SCG essential oil extraction processes, combined with network pharmacology-based efficacy marker prediction analysis, could expand SCG applications beyond biofuels and fertilizers to pharmaceuticals and health supplements. Such approaches not only promote resource utilization and value-added processing of food waste while reducing environmental impact, but also provide theoretical foundations for developing SCG-based materials in medical and nutritional industries.

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