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Advances in the Extraction of Active Ingredients from Traditional Chinese Medicine Using Deep Eutectic Solvents

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Abstract: ***Deep eutectic solvents (DES), a class of novel green solvents, offer a promising alternative for the extraction of bioactive compounds from traditional Chinese medicinal herbs, addressing both environmental and efficiency limitations associated with conventional organic solvents. Their advantages include straightforward synthesis, low toxicity, biodegradability, and tunable physicochemical properties. This article systematically summarizes recent advances in the application of DES for extracting various active ingredients of traditional Chinese medicine, including flavonoids, saponins, alkaloids, polysaccharides, polyphenols, and volatile oils. It focuses on analyzing the structural characteristics of these compound classes and the underlying principles guiding DES selection, categorizes DES systems suitable for each class of active ingredient, and outlines the corresponding optimized process conditions. Building upon this foundation, the extraction mechanisms—particularly hydrogen bonding interactions and polarity matching between DES and target components—were investigated, and the influencing factors and underlying patterns governing DES extraction efficiency were systematically summarized. In response to current research challenges—including high viscosity, difficult separation and recovery, and the absence of a targeted design theory—future research directions were proposed to support the continued advancement of green extraction processes for traditional Chinese medicine.***

Keywords: Deep eutectic solvents, Active ingredients of traditional Chinese medicine, Process optimization, Extraction of traditional Chinese medicine**.**

1. Introduction

Efficient and environmentally friendly extraction of active ingredients of traditional Chinese medicine is a critical step in its modernization. Conventional organic solvent extraction methods commonly suffer from inherent drawbacks, including high volatility, significant toxicity, high environmental burden, and relatively low extraction efficiency, making them incompatible with the contemporary requirements of green manufacturing and clean production [1]. Meanwhile, the growing demand for developing high-value-added active ingredients from traditional Chinese medicinal resources has raised higher expectations for extraction solvents in terms of selectivity, safety, and functionality, thereby driving the development of novel green solvent systems.

Deep eutectic solvents (DES), as an emerging class of green solvents, have rapidly become a research frontier in natural product extraction since their introduction in the early 21st century, owing to their distinctive tunable physicochemical properties. Typically prepared by mixing an HBD and an HBA at a defined molar ratio, the resulting intermolecular hydrogen bond network significantly lowers the melting point, forming a stable liquid eutectic mixture at or near room temperature. This system exhibits exceptional dissolution performance comparable to that of ionic liquids [2].

By tuning the types and molar ratios of HBD and HBA, as well as water content and temperature, the viscosity, polarity, and hydrogen bond network structure of DES can be precisely tailored, thereby conferring exceptional selective dissolution capacity toward target components of diverse structural classes. Functional groups such as hydroxyl or carboxyl groups commonly present in the molecular structures of DES facilitate hydrogen bonding interactions with target components, thereby enhancing the extraction yield and preserving the stability of active ingredients—including polyphenols, flavonoids, and polysaccharides [3].

This article provides a systematic review of the application of DES in the extraction of active ingredients of traditional Chinese medicine, with a focus on analyzing extraction rules and mechanisms of action for various components. It summarizes current challenges in this field of research and outlines future directions, aiming to provide a reference for in-depth studies on green extraction processes for traditional Chinese medicine.

2. Extraction of Active Ingredients of Traditional Chinese Medicine Using Deep Eutectic Solvents

2.1 Extraction of Flavonoids Using Deep Eutectic Solvents

Flavonoids are important secondary metabolites in plants and exhibit diverse pharmacological activities, including anticancer, antioxidant, and hypoglycemic effects. Their molecular structures are rich in phenolic hydroxyl groups, which readily form strong hydrogen bonding interactions with hydrogen bond donors or acceptors in deep eutectic solvents (DES), rendering DES ideal solvents for extracting flavonoid constituents. Studies have shown that DES not only significantly enhance the extraction efficiency of flavonoids

but also better preserve their bioactivity.

DES have been applied to flavonoid extraction from various plant sources. For instance, Wang et al. [4] used a choline chloride-ethanol system (molar ratio 1:1) to extract total flavonoids from chestnut shells. Under optimal conditions — an ultrasonic temperature of 40 ℃, an ultrasonic power of 150 W, a solid-liquid ratio of 1:25 (g/mL), and an ultrasonic time of 60 min—the relative error between the theoretical and actual total flavonoid yields was only 1.49%, confirming the reliability of the process. YIMING·Gahafu et al. [5] employed a choline chloride-levulinic acid DES (molar ratio 1:2) combined with ultrasound-assisted extraction to isolate safflower total flavonoids. Under conditions of a solid-liquid ratio of 1:25, ultrasonic time of 30 min, temperature of 60 ℃, power of 300 W, and water content of 37%, the extraction efficiency reached 5.07%, and the acetylcholinesterase inhibition rate of the extract was 65.52%, indicating that DES extraction helps preserve the bioactive functionality of the extracted components.

In addition to the aforementioned studies, DES have been increasingly applied in the extraction of flavonoid constituents from traditional Chinese medicinal materials in recent years, including Albiziae Flos, Saururus chinensis, Ginkgo biloba leaves, and sea buckthorn leaves. Table 1 summarizes representative studies, including the DES systems employed, optimized extraction protocols, and corresponding extraction outcomes. As shown, the choline chloride-polyol system is the most widely used DES for flavonoid extraction. Moreover, most studies maintain the water content of the DES within the range of 20%–40% (w/w), as the addition of an appropriate amount of water reduces system viscosity and enhances mass transfer efficiency.

Table 1: Applications of DES in the extraction of flavonoids from traditional Chinese medicines

plant	Target Active Component	Composition of DES	Optimal Extraction Conditions	Result	References
Albiziae Flos	Total flavonoids	Choline chloride/1,2-propanediol (molar ratio 1:3)	Ultrasonic temperature: 65 °C; ultrasonic time: 37 min; liquid-solid ratio: 35:1 (g/mL)	Flavonoid extraction rate: 4.15%	[6]
Saururus chinensis	Total flavonoids	Choline chloride/ethylene glycol (molar ratio 1:3)	Ultrasonic temperature: 69 °C; extraction time: 20 min; liquid-solid ratio: 40:1 (mL/g); DES volume fraction: 89%	Total flavonoid extraction amount: 13.85 mg/g	[7]
Ginkgo biloba leaves	Total flavonoids	Choline chloride/urea (molar ratio 1:1.6)	Extraction temperature: 57 °C; extraction time: 60 min; liquid-solid ratio: 30:1 (mL/g); water content: 40%	Total flavonoid extraction rate: 1.062%	[8]
Chrysanthemum morifolium 'Boju'	Total flavonoids	Choline chloride/1,3-butanediol (molar ratio 1:3)	Ultrasonic extraction temperature: 40 °C; ultrasonic extraction time: 25 min; solid-liquid ratio: 1:25 (g/mL); water content: 20%; ultrasonic extraction power: 110 W	Total flavonoid yield: 51.74 mg/g	[9]
Vaccinium vitis-idaea L.	Total flavonoids	Choline chloride/1,3-butanediol (molar ratio 1:1)	Extraction temperature: 55 °C; extraction time: 20 min; liquid-solid ratio: 15:1 (mL/g); water content: 50%	Total flavonoid yield: 96.29 ± 0.62 mg/g	[10]
Hippophae rhamnoides subsp. yunnanensis leaves	Total flavonoids	Choline chloride/lactic acid (molar ratio 1:3)	Extraction time: 30 min; liquid-solid ratio: 40:1 (mL/g)	Yield: 18.70% ± 0.25%	[11]
Urtica fissa	Total flavonoids	Choline chloride/ethylene glycol (molar ratio 1:3)	Ultrasonic temperature: 61 °C; ultrasonic time: 41 min; solid-liquid ratio: 1:30 (g/mL); water content: 30%	Total flavonoid yield: 45.26 mg/g	[12]
Epimedium brevicornu Maxim.	Total flavonoids	Choline chloride/ethanolamine (molar ratio 1:4)	Extraction temperature: 70 °C; extraction time: 15 min; solid-liquid ratio: 0.5 g:25 mL; water content: 50%	Total extraction rate: (20.07 ± 0.43) mg/g	[13]
Plantago asiatica L.	Total flavonoids	Choline chloride/urea (molar ratio 2.2:1)	Extraction temperature: 34 °C; reaction time: 41 min; DES water content: 47%	Total flavonoid extraction rate: 6.28%	[14]
Forsythia suspensa	Total flavonoids	Choline chloride/glycerol (molar ratio 1:2)	Extraction temperature: 70 °C; extraction time: 125 min; liquid-solid ratio: 35 mL/g; water content: 21%	The total flavonoid extraction rates of Forsythia suspensa fruits, leaves, and stems were 20.01%, 13.50%, and 6.11%, respectively	[15]
Lonicera japonica Thunb.	Total flavonoids	Choline chloride/1,3-butanediol (molar ratio 1:2.7)	Ultrasonic time: 29 min; solid-liquid ratio: 27:1 (mL/g)	Total flavonoid yield: 7.85%	[16]
Tilia amurensis Rupr.	Total flavonoids	Choline chloride/lactic acid (molar ratio 1:2)	Extraction time: 30 min; ultrasonic power: 200 W; water content: 50%	Total flavonoid extraction rate: 10.61%	[17]
Morus alba L.	Total flavonoids	Choline chloride/fructose/ethanol (molar ratio 1:1:3)	Ultrasonic temperature: 40 °C; ultrasonic time: 40 min; liquid-solid ratio: 40 mL/g; water content: 30%; ultrasonic power: 360 W; enzyme dosage: 4%	Total flavonoid extraction amount: 46.58 mg/g	[18]
Polygonatum kingianum Coll.et Hemsl.	Flavonoids	Choline chloride/lactic acid (molar ratio 1:2)	Ultrasonic extraction temperature: 45 °C; ultrasonic extraction time: 40 min; solid-liquid ratio: 1:20 (g/mL); water content: 20%	Flavonoid extraction rate: 17.13% ± 0.25%	[19]

2.2 Extraction of Saponins Using Deep Eutectic Solvents

Saponins, an important class of phytochemicals found in Chinese herbal medicine, are widely involved in multiple physiological regulatory processes and exhibit significant bioactivities, including antioxidant, anti-inflammatory, cholesterol regulation, antiviral, anti-radiation, hypoglycemic, immunomodulatory, and neuroprotective effects [20]. In recent years, green extraction technology based on deep eutectic solvents (DES) has been progressively applied to the efficient extraction of saponin components and demonstrates promising application potential.

Dong Mingran et al. [21] employed the ultrasound-assisted deep eutectic solvent method to extract total saponins from the dried root of Brazilian ginseng (Pfaffia glomerata), optimizing the extraction process through single-factor tests and Box-Behnken response surface methodology. Results showed that urea-choline chloride at a 1:1 molar ratio was the optimal DES; under the optimized conditions—38% water content, a liquid-solid ratio of 18:1 (mL/g), and an extraction time of 37 min—the total saponin yield reached 6.26%, outperforming the ethanol ultrasound method, heat reflux method, and flash extraction method.

In another study, Tan Tianyu et al. [22] used the dried roots of Chaihu (Bupleurum chinense DC., Radix Bupleuri) as the raw material and identified lactic acid-choline chloride (2:1 molar ratio) as the most suitable DES for ultrasound-assisted extraction of saikosaponins. Under conditions of 22% water content, a liquid-solid ratio of 1:40 (g/mL), an ultrasonic time of 18 min, and an ultrasonic power of 330 W, the saikosaponin yield reached 16.25 ± 0.42 mg/g—significantly higher than that obtained by water extraction (5.84 ± 0.33 mg/g) and ethanol extraction (8.06 ± 0.16 mg/g). Moreover, the Chaihu extract obtained via ultrasound-assisted DES extraction exhibited strong scavenging capacity against both $DPPH^{\cdot}$ and $ABTS^{+}$ radicals, with IC50 values of 0.22 mg/mL and 0.16 mg/mL, respectively. Its antioxidant activity was markedly superior to that of traditional solvent extracts.

A summary of DES extraction processes for saponin components from various plant sources, along with corresponding results, is presented in Table 2.

Table 2: Application of DES in the extraction of saponin components from traditional Chinese medicines

plant	Target Active Component	Composition of DES	Optimal Extraction Conditions	Result	References
stem-leaf of Panax japonicus	Total saponins	L-proline/glycerol/sucrose (molar ratio 5:4:1)	Extraction temperature 40℃, extraction time 31 min, liquid-solid ratio 48 mL/g, water content 32%	Total saponin extraction rate 35.98%	[23]
Ginseng (Panax ginseng C. A. Mey.)	Total saponins	Choline chloride/1,4-butanediol (molar ratio 1:1)	Extraction time 20 min, liquid-solid ratio 1:44 (g/mL), water content 40%, ultrasonic power 258 W	Total saponin content 59.33 mg/g	[24]
Hawthorn (Crataegus pinnatifida Bge.)	Total saponins	Choline chloride/ethanol (molar ratio 1:3)	Ultrasonic time 25 min, liquid-solid ratio 1:8 (g/mL), water content 20%	Extraction rate of total saponin components (7.21 ± 0.15)%	[25]
leaves of Xanthoceras sorbifolium Bunge	saponins	Choline chloride/lactic acid (molar ratio 1:1)	Extraction temperature 43.00℃, liquid-solid ratio 42.00 mL/g, DES concentration 47.00%	Saponin yield (10.22 ± 0.28)%	[26]
Maca leaves (Lepidium meyenii Walp.)	saponins	Choline chloride/glycerol (molar ratio 1:2)	Extraction time 30 min, ultrasonic power 300 W, liquid-solid ratio 40 mL/g, water content 30%	Saponin content 37.07 mg/g	[27]

2.3 Extraction of Alkaloids Using Deep Eutectic Solvents

Alkaloids are a class of natural basic organic compounds widely distributed in plants and characterized by nitrogen-containing heterocyclic structures; many members exhibit significant bioactivities, including antibacterial, anti-inflammatory, and analgesic effects [28]. In recent years, deep eutectic solvents (DES) combined with assisted extraction technologies have emerged as a research focus for the efficient and green extraction of alkaloids, with notable progress reported in extraction process optimization, solvent screening, and activity retention.

Li et al. [29] used Rhizoma Coptidis as the model material and employed the ultrasound-assisted deep eutectic solvent method to extract alkaloids, systematically optimizing the extraction process using Box-Behnken response surface methodology. The results showed that the deep eutectic solvent composed of glucose and lactic acid was highly suitable for alkaloid extraction from Rhizoma Coptidis. The optimal extraction conditions were determined to be an extraction time of 35 min, a water content of 26%, and a liquid-solid ratio of 33:1 (mL/g), under which the yield of total alkaloids reached 7.22%. This study confirmed the stability and feasibility of DES in alkaloid extraction and provided a methodological reference for the green extraction of related active ingredients.

Lei Qian [30] developed an ultrasound-assisted extraction (UAE) system based on DES for the alkaloid active ingredients in Stephania tetrandra, a Jiangxi genuine medicinal material. Using response surface methodology for optimization, choline chloride–ethylene glycol (at a molar ratio of 1:2) was identified as the optimal extraction solvent; the optimal process parameters were determined to be an extraction temperature of 52 ℃, an extraction time of 82 min, a DES water content of 23% (v/v), and a liquid-solid ratio of 23:1 (mL/g). Under these optimal conditions, the extraction yield of total alkaloids reached 20.59 mg/g—2.2-fold, 3.3-fold, and 4.1-fold higher than those obtained using methanol, 95% ethanol, and the water extraction method, respectively—thereby achieving high-efficiency green extraction of alkaloids from S. tetrandra.

Mo et al. [31] employed the microwave-assisted deep eutectic solvent method to extract total alkaloids from the stems of Euchresta tubulosa Dunn, using oxymatrine, matrine, and cytisine as marker compounds; the yield was quantified by High Performance Liquid Chromatography (HPLC). Among the 18 DES evaluated, betaine–1,2-propanediol (1:3 molar

ratio) was identified as the optimal extraction solvent. Subsequently, single-factor tests combined with response surface methodology were used to refine the extraction parameters, yielding the following optimal conditions: a microwave power of 400 W, an extraction temperature of 70 °C, a DES water content of 27%, an extraction time of 30 min, and a liquid-solid ratio of 29:1 (mL/g). Under these conditions, the yield of total alkaloids reached 1.89%, closely matching the model-predicted value. Scanning electron microscopy (SEM) imaging revealed pronounced structural disruption on the surface of the herbal powder after DES treatment. Antioxidant activity assessments demonstrated that the DES extract exhibited superior scavenging capacity against both DPPH· and $ABTS^+$ free radicals compared with ethanol- and methanol-based extracts, indicating that DES extraction better preserves the antioxidant activity of alkaloids.

2.4 Extraction of Polysaccharides Using Deep Eutectic Solvents

Polysaccharides, as an important class of natural polymers, perform diverse physiological regulatory functions in biological systems. Studies have demonstrated that polysaccharides exhibit multiple bioactivities—including immunomodulation, antioxidant effects, neuroprotection, and antitumor activity—highlighting their broad application potential in pharmaceuticals and functional foods [32]. In recent years, deep eutectic solvents (DES) based strategies for polysaccharide extraction have gradually attracted attention, with related research achieving positive progress in process optimization and activity retention.

Wang Yanyan et al. [33] conducted an ultrasound-assisted DES extraction study targeting polysaccharide components from Ziziphus jujuba. Through solvent screening, choline chloride-1,2-propanediol was identified as the optimal DES; subsequently, the extraction process was systematically optimized using single-factor tests combined with Box-Behnken response surface methodology. The results showed that the optimal extraction conditions were an ultrasonic time of 41.68 min, a liquid-solid ratio of 1:20 (g/mL), and a DES water content of 19.96%. Under these conditions, the polysaccharide yield from Ziziphus jujuba reached 571.31 ± 3.84 mg/g, indicating high extraction efficiency. Song Qiaoying et al. [34] employed the ultrasound-assisted DES method to extract polysaccharides from Tremella fuciformis and optimized the process parameters using single-factor tests combined with orthogonal design. Choline chloride-urea (molar ratio 1:2) was identified as the optimal extraction solvent. Under the optimized conditions—a liquid-solid ratio of 1:35 (g/mL), DES water content of 15%, ultrasonic time of 40 min, temperature of 60 °C, and ultrasonic power of 200 W—the target component concentration in the Tremella fuciformis polysaccharide extract reached 24.47 mg/g, confirming the applicability of DES for fungal polysaccharide extraction.

The DES extraction processes and corresponding results for polysaccharides from different plant sources are summarized in Table 3.

Table 3: Application of DES in the extraction of polysaccharide components from traditional Chinese medicinesmedicines

plant	Target Active Component	Composition of DES	Optimal Extraction Conditions	Result	References
Pueraria lobata (Pueraria lobata Willd.)	Polysaccharides	Choline chloride/ethylene glycol (molar ratio 1:2)	Extraction time 35 min, extraction temperature 40°C, liquid-solid ratio 14 mL/g	Average extraction rate of Pueraria lobata polysaccharides 13.27%	[35]
Wild jujube flesh (Ziziphus jujube Mill.)	Polysaccharides	Choline chloride/urea (molar ratio 1:2)	Ultrasonic temperature 54°C, ultrasonic time 62 min, solid-liquid ratio 1:20 (g/mL), water content 24%	Yield of wild jujube flesh polysaccharides (WJFP) 5.57%	[36]
Hawthorn (Crataegus pinnatifida Bge.)	Total polysaccharides	Choline chloride/1,2-propanediol (molar ratio 1:3)	Ultrasonic time 38.98 min, solid-liquid ratio 1:20, water content 20.12%	Content of total polysaccharides from hawthorn (523.49 ± 8.79) mg/g	[37]
Artichoke (Cynara scolymus L.)	Polysaccharides	Choline chloride/malic acid (molar ratio 1:4)	Extraction temperature 70°C, extraction time 41 min, water content 40%, solid-liquid ratio 1:31, ultrasonic power 300 W	Yield of artichoke polysaccharides (163.7 ± 0.34) mg/g	[38]
Dendrobium officinale (Kimura et Migo)	Polysaccharides	Choline chloride/lactic acid (molar ratio 4:1)	Extraction temperature 80°C, liquid-solid ratio 110:1 (mL/g), DES concentration 40%	Extraction rate 33.2% ± 0.28%	[39]
Sage (Salvia japonica Thunb.)	Polysaccharides	Choline chloride/malic acid (molar ratio 1:3)	Extraction time 50 min, liquid-solid ratio 1:51 mL/g, water content 37%, ultrasonic power 370 W	Average extraction rate 25.22%	[40]

2.5 Deep Eutectic Solvents Extraction of Other Components

Phenols are a class of secondary metabolites widely distributed in plants, with chlorogenic acid, anthocyanins, isoflavones, and curcumin being common representatives. Studies have shown that polyphenols exhibit multiple bioactivities, including anti-inflammatory, antiviral, hypoglycemic, antioxidant, and antibacterial effects, and have thus attracted broad attention in the development of functional foods and pharmaceuticals.

He Ruotong et al. [41] used dried Lonicera japonica Thunb. as the raw material and systematically compared the polyphenol extraction efficiencies of five DES versus conventional solvents (60% ethanol and deionized water), using polyphenol yield as the evaluation criterion. Choline chloride-acetic acid was identified as the optimal DES. Subsequently, the extraction process was refined using response surface methodology, and the optimal conditions were determined to be a liquid-solid ratio of 1:38 (g/mL), an extraction temperature of 47 °C, and an ultrasonic time of 40 min; under these conditions, the polyphenol yield reached 121.22 mg/g.

This study achieved efficient extraction of polyphenols from Lonicera japonica Thunb. using a green solvent system and evaluated their bioactivity, thereby providing a theoretical basis for the development of honeysuckle polyphenol–based products.

Gulifeire Yilhamu et al. [42] investigated Elaeagnus moorcroftii Wall. ex Schlecht. in Xinjiang and comparatively assessed 12 DES against three conventional solvents, identifying choline chloride–malic acid (at a 1:1 molar ratio) as the optimal extraction solvent. Extraction parameters were optimized through a combination of single-factor tests and Box-Behnken response surface methodology, yielding optimal conditions of 25% water content in the DES, a liquid-solid ratio of 1:48 (g/mL), an ultrasonic time of 34 min, and an ultrasonic temperature of 57 °C. Under these conditions, the polyphenol yield reached 63.378 mg/g, with DPPH· and ABTS+ free radical scavenging capacities of 35.004 mg TE/g and 82.443 mg TE/g, respectively. The study also revealed a significant positive correlation ($P < 0.05$) between the yields of polyphenols and flavonoids and their antioxidant activity under different extraction conditions. This green extraction method simultaneously optimizes both the yield of target components and antioxidant activity, providing a scientific basis for the comprehensive development of Elaeagnus moorcroftii Wall. ex Schlecht. —a large-fruited seabuckthorn native to southern Xinjiang.

Volatile oils are a class of secondary metabolites primarily composed of terpenoids, aliphatic compounds, and aromatic compounds. They are widely distributed in plant tissues such as roots, stems, and leaves, and exhibit diverse pharmacological activities—including antibacterial, antioxidant, anti-inflammatory, and antitumor effects — making them highly valuable in pharmaceutical and health care applications [43]. Because the constituents of volatile oils are prone to thermal degradation or loss through volatilization, the choice of extraction method significantly influences both their yield and activity retention.

Yang Niuniu et al. [44] investigated essential oil from Trichosanthes kirilowii Maxim. seeds using the ultrasound-assisted deep eutectic solvent method. Preliminary screening identified betaine–glycerol (4:3 molar ratio) as the optimal DES. Subsequent optimization of the extraction process using Box-Behnken response surface methodology yielded the following optimal parameters: an ultrasonic time of 34 min, an ultrasonic power of 370 W, a liquid-solid ratio of 7:1 (mL/g), and a distillation time of 70 min. Validation experiments indicated that the average essential oil yield under these optimized conditions was 9.24%.

Luo Lanping et al. [45] used Cinnamomum cassia Presl. bark powder as the raw material and employed the deep eutectic solvent method to extract cinnamon essential oil, optimizing the extraction process with cinnamaldehyde yield as the evaluation criterion. Volatile components of the essential oil were analyzed using solid-phase microextraction–gas chromatography–mass spectrometry (SPME-GC-MS), and scanning electron microscopy (SEM) was used to observe changes in raw material surface morphology before and after extraction. Results showed that choline chloride–ethylene glycol (1:6 molar ratio) was the most suitable DES. Under the optimized conditions—a system water content of 35%, a liquid-solid ratio of 1:80 (g/mL), an extraction time of 90 min, and an extraction temperature of 100 °C—the cinnamaldehyde yield reached 11.22 mg/g. SPME-GC-MS analysis revealed that the major volatile components of the obtained essential oil were trans-cinnamaldehyde (32.91%), δ-junimone (16.58%), and α-ylangene (9.00%). SEM observations showed that the surface structure of untreated Cinnamomum cassia Presl. bark powder was compact with few pores, whereas after DES treatment, the surface became loose and porous, indicating that DES effectively disrupted the dense structural matrix of cinnamon bark and facilitated the release of essential oil constituents.

A summary of DES extraction processes and outcomes for other types of active ingredients from plant materials of different origins is presented in Table 4.

Table 4: Application of DES in the extraction of other types of components from traditional Chinese medicines

plant	Target Active Component	Composition of DES	Optimal Extraction Conditions	Result	References
Dryopteris crassirhizoma (Dryopteridis Crassirhizomatis Rhizoma)	Total phloroglucinols	Choline chloride/urea/1,4-butylene glycol (molar ratio 1:2:2)	Extraction time 60 min, liquid-solid ratio 16:1 mL/g, DES water content 62%	Total phloroglucinol yield 18.59%	[46]
Rubus crataegifolius roots (Rubus crataegifolius)	Total triterpenoids	Choline chloride/fructose (molar ratio 1:1)	Extraction temperature 60°C, ultrasonic extraction for 20 min, liquid-solid ratio 40:1 mL/g, water content 40%	Total triterpenoid extraction rate 9.42%	[47]
Dryopteris crassirhizoma (Dryopteridis Crassirhizomatis Rhizoma)	Total phloroglucinols	Choline chloride/urea/1,4-butylene glycol (molar ratio 1:2:2)	Extraction time 60 min, liquid-solid ratio 16:1 mL/g, DES water content 62%	Total phloroglucinol yield 18.59%	[46]
Rubus crataegifolius roots (Rubus crataegifolius)	Total triterpenoids	Choline chloride/fructose (molar ratio 1:1)	Extraction temperature 60°C, ultrasonic extraction for 20 min, liquid-solid ratio 40:1 mL/g, water content 40%	Total triterpenoid extraction rate 9.42%	[47]
Loquat leaves (Eriobotrya japonica (Thunb.) Lindl.)	Ursolic acid in triterpenic acid extract	Thymol/benzyl alcohol (molar ratio 2:1)	Extraction time 64 min, extraction temperature 59°C, liquid-solid ratio 14 (g/g)	Ursolic acid yield in triterpenic acid extract 17.79 ± 0.45 mg/g	[48]
Picris hieracioides L. (Picris hieracioides L.)	Organic acids	Choline chloride/urea (molar ratio 1:2)	Extraction temperature 30°C, extraction time 30 min, liquid-solid ratio 20:1 mL/g	Organic acid extraction amount 1.0929%	[49]
Litchi flesh (Litchi chinensis Sonn.)	Polyphenols	Choline chloride/lactic acid (molar ratio 1:2)	Extraction time 60 min, extraction temperature 80°C, solid-liquid ratio 1:4 (g/mL), water content 62.1%	Polyphenol extraction amount 307.50 mg/100 g	[50]
Persimmon leaves (Diospyros kaki L.)	Polyphenols	Choline chloride/citric acid (molar ratio 1:1)	Liquid-solid ratio 1:20 g/mL, extraction time 43 min, DES water content 44%, extraction temperature 64°C	Polyphenol extraction rate 51.26 mg/g	[51]
Chestnut shells	Polyphenols	Choline chloride/oxalic acid (molar ratio 1:1)	Liquid-solid ratio 42:1 mL/g, water content 32%, ultrasonic power 348 W	Total phenol yield (99.66 ± 2.63) mg/g	[52]
Lonicerae Flos (Lonicera japonica Thunb.)	Chlorogenic acid	L-proline/L-lactic acid (molar ratio 1:3)	Extraction temperature 45°C, extraction time 25 min, liquid-solid ratio 16 mL/g, water content 30%, ultrasonic power 240 W	Maximum chlorogenic acid extraction rate 4.53% ± 0.11%	[53]
Magnolia bark residues (Magnolia officinalis Rehd. et Wils.)	Lignanoids	Choline chloride/levulinic acid (molar ratio 1:2)	Extraction temperature 90°C, extraction time 1.5 h, solid-liquid ratio 1:25 g/mL, solvent water content 30%	Total extraction rate 32.87 mg/g	[54]
Lotus leaves (Nelumbo nucifera Gaertn.)	Polyphenols	Choline chloride/lactic acid (molar ratio 1:2.6)	Ultrasonic time 65 min, solid-liquid ratio 1:20 (g/mL), water content 8%	Total phenol yield (187.23 ± 14.67) mg/g	[55]

3. Problems and Prospects

Although DES show broad prospects in the field of extracting active ingredients from traditional Chinese medicine, current research still faces the following challenges:

3.1 High Viscosity Problem

Most DES exhibit high viscosity at room temperature (often exceeding 100 mPa·s), which severely limits their mass transfer efficiency and operational convenience. High viscosity not only reduces the diffusion rate of the target components but also increases energy consumption and processing time. Current main solutions include: adding an appropriate amount of water (20%–50%) to weaken the hydrogen bond network and reduce system viscosity; moderately increasing the extraction temperature; and combining auxiliary technologies such as ultrasound and microwave to enhance mass transfer. Studies have shown that water content has a significant impact on both DES viscosity and extraction efficiency—either excessive or insufficient water content may lead to a decrease in extraction yield. Future research could focus on developing novel DES systems with intrinsically low viscosity or incorporating low-viscosity functional components into DES design to fundamentally improve rheological properties.

3.2 Difficult Separation and Recovery

Due to their extremely low volatility, deep eutectic solvents (DES) present a critical bottleneck for large-scale applications — namely, the efficient separation of extracted products from the DES phase. Current separation strategies include back-extraction (using organic solvents or water to recover target compounds), solid-phase extraction, and membrane separation. However, these approaches often increase process complexity and may introduce new solvent contaminants, partially offsetting the green advantages of DES. Notably, recent studies have explored the recyclability of DES after extraction—for instance, by combining ethanol precipitation with rotary evaporation to achieve highly efficient recovery of target compounds, with recovery yields exceeding 96%. Future research directions warrant exploring include the development of functional, recyclable DESs with stimulus-responsive properties (e.g., temperature-responsive, pH-responsive, or CO_2-responsive behavior) and the design of volatile DES systems that undergo phase separation under simple post-extraction condition changes.

3.3 Lack of Theoretical Guidance

Current DES screening relies heavily on empirical trial-and-error approaches, resulting in low efficiency and limited predictive capability. With advances in computational chemistry, rationally designed DES guided by theoretical principles have become feasible. Quantum chemical calculations can elucidate interaction energies and charge distributions between hydrogen bond donors (HBDs) and hydrogen bond acceptors (HBAs), providing molecular-level insights into DES formation mechanisms. Molecular dynamics simulations enable prediction of the microscopic structure and dynamic behavior of DESs, thereby facilitating mechanistic analysis of their interactions with target components. Thermodynamic models—including the COSMO-RS model and Hansen solubility parameters—have been successfully applied to predict the solubilization capacity of DES toward specific compounds, significantly enhancing screening efficiency. Recent studies have integrated machine learning with molecular simulation to develop predictive models for DES formation based on hydrogen-bonding characteristics, offering a novel approach to high-throughput screening. Future efforts should strengthen the synergy between multi-scale simulation and experimental validation to establish accurate predictive models for DES interactions with active ingredients of traditional Chinese medicine, thereby enabling the rational design and rapid screening of DES.

3.4 Limited Application in Traditional Chinese Medicine Compound Prescriptions

Current DES extraction research predominantly focuses on single herbs or isolated active ingredients, with relatively limited exploration of traditional Chinese medicine compound prescriptions—the primary form of clinical herbal therapy in TCM. Such compound prescriptions typically contain multiple classes of chemical constituents exhibiting diverse polarities, and their synergistic interactions constitute a core tenet of traditional Chinese medicine theory. Owing to their tunable composition and adjustable physicochemical properties, DES hold promise for the construction of multicomponent solvent systems capable of simultaneously dissolving compounds across a broad polarity range—by regulating the types and molar ratios of hydrogen-bond donors (HBDs) and hydrogen-bond acceptors (HBAs). This approach enables the synchronous, high-efficiency extraction of multiple active ingredients from complex herbal formulations. Not only does this strategy align with the holistic research paradigm of traditional Chinese medicine, but it also offers a novel technical pathway for the development of compound preparations—warranting further in-depth investigation.

3.5 Insufficient Research on Industrial-scale Scaling

Current DES extraction studies are largely confined to laboratory-scale operations (milligram to gram scale), with inadequate attention paid to engineering challenges associated with process scale-up. The scale-up of DES preparation itself introduces systematic variations. Studies have shown that factors such as raw material ratios, reaction temperature, time, and water content significantly influence the physicochemical properties of the resulting DES, and these scale-up effects cannot be overlooked. Moreover, critical industrial-scale data—including economic feasibility assessment, safety evaluation, and long-term stability testing of the DES extraction process—remain severely limited. The high viscosity of DES leads to mass transfer bottlenecks, while separation and recovery steps entail increased equipment investment, solvent loss, and regeneration costs—all of which require systematic evaluation at pilot-scale and industrial-scale levels. Future efforts should focus on strengthening the engineering research of DES extraction processes, conducting systematic economic analyses and Life Cycle Assessments to provide a robust scientific foundation for the industrial application of DES technology.

4. Conclusion

Deep eutectic solvents (DES) exhibit considerable potential for the extraction of active ingredients from traditional Chinese medicine, owing to their facile preparation, eco-friendliness, and tunable physicochemical properties. By rationally designing DES composition and process parameters, efficient extraction of multiple classes of active components—including flavonoids, saponins, alkaloids, and polysaccharides—can be achieved, with certain DES systems demonstrating better preservation of component bioactivity. A substantial body of experimental data has been accumulated to date, enabling preliminary elucidation of the underlying principles and mechanisms governing DES extraction. Future efforts should prioritize the development of low-viscosity, high-selectivity DES; innovation in efficient DES recovery technologies; establishment of predictive theoretical models; and advancement of industrial scale-up studies. This will help transform DES extraction into a practical green technology for TCM and facilitate the modernization of traditional Chinese medicine and the development of a green pharmaceutical industry.

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