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Original Research Article

Network Pharmacology-based Mechanistic Exploration of Pediatric Dingchuan Oral Liquid, A Polyherbal Chinese Patent Medicine, in the Treatment of Childhood Asthma

Pharmacognosy Magazine
22(3) 925–932, 2026
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DOI: 10.1177/09731296251408896
journals.sagepub.com/home/phm
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Abstract

Background: Pediatric Dingchuan Oral Liquid (PDOL) is a traditional Chinese polyherbal formulation widely used in the clinical treatment of pediatric asthma. It comprises 11 medicinal ingredients, including *Ephedra sinica*, *Prunus armeniaca*, *Raphanus sativus*, *Lepidium apetalum*, *Perilla frutescens*, *Scutellaria baicalensis*, *Morus alba*, *Gypsum fibrosum*, *Isatis indigotica*, *Houttuynia cordata*, and *Glycyrrhiza uralensis*. Despite its established clinical efficacy, the underlying pharmacological mechanisms remain unclear.
Objectives: This study aimed to systematically explore the bioactive phytoconstituents, core protein targets, and molecular pathways through which PDOL exerts its anti-asthmatic effects, using a network pharmacology approach.
Materials and Methods: Active compounds were screened based on oral bioavailability (OB ≥ 30%) and drug-likeness (DL ≥ 0.18) criteria using the Traditional Chinese Medicine Systems Pharmacology Database and Analysis Platform (TCMSP) database. Disease targets associated with asthma were retrieved from GeneCards, DrugBank, DisGeNET, and other public databases. Network construction and protein–protein interaction (PPI) analysis were performed using Cytoscape and STRING databases. Gene Ontology (GO) and Kyoto Encyclopedia of Genes and Genomes (KEGG) pathway enrichment analyses were conducted using Metascape.
Results: A total of 207 active compounds and 104 overlapping asthma-related targets were identified. Quercetin, kaempferol, β-sitosterol, stigmasterol, and luteolin were identified as the core phytoconstituents of PDOL. Six hub genes (IL6, TNF, IL1B, JUN, IFNG, and STAT3) were screened as major therapeutic targets. GO and KEGG enrichment analysis reveal that PDOL exerts therapeutic effects through pathways related to immune regulation, inflammatory response, and the repair of lung tissue injury, such as the IL-17 and TNF signaling pathways.
Conclusion: This study provides a mechanistic foundation for the multi-component and multi-target actions of PDOL in the treatment of pediatric asthma, highlighting its pharmacological potential as a plant-based therapeutic agent. These findings support further experimental and clinical studies on the PDOL and other traditional Chinese herbal formulations for respiratory disorders.

Keywords

Pediatric Dingchuan Oral Liquid, childhood asthma, traditional Chinese medicine, network pharmacology, herbal formulation

Received 04 September 2025; **revised** 25 November 2025; **accepted** 03 December 2025

Introduction

Childhood asthma is a common chronic inflammatory disease of the respiratory system in the field of pediatrics, and it falls under the category of "asthma" in traditional Chinese medicine (TCM). It includes clinical subtypes such as bronchial asthma and cough variant asthma. The primary symptoms involve recurrent wheezing, coughing, shortness of breath, and chest tightness. Recent data indicate a continuous upward trend in the incidence of childhood asthma, making it a growing public health concern (Asthma Group of Chinese Thoracic Society, 2020).

Modern medical research suggests that asthma is a heterogeneous disease caused by the synergistic action of immune cells—including airway epithelial cells, eosinophils, and

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mast cells—and the inflammatory mediators they release. It is characterized by chronic airway inflammation and hyperresponsiveness (Chinese Thoracic Society, Chinese Medical Association, 2025). Despite existing therapies such as β_2-adrenergic agonists, glucocorticoids, and anti-cholinergic agents, these drugs are often associated with limitations, including high recurrence rates and adverse effects (Asthma Group of Chinese Thoracic Society, 2020; Asthma Workgroup, Chinese Thoracic Society, & Chinese Society of General Practitioners, 2013; Editorial Board, Chinese Journal of Pediatrics, Subspecialty Group of Respiratory Diseases, the Society of Pediatrics, Chinese Medical Association, & Children's Respiratory Professional Committee, the Society of Pediatrics of Chinese Medical Doctor Association, 2020; Lü et al., 2011).

In recent years, traditional Chinese herbal formulas, particularly those derived from medicinal plants, have demonstrated promising therapeutic effects in pediatric respiratory diseases due to their safety, efficacy, and good patient compliance (Han et al., 2022). Pediatric Dingchuan Oral Liquid (PDOL) is a well-known polyherbal formulation comprising eleven traditional medicinal herbs, including *Ephedra sinica*, *Prunus armeniaca* (bitter apricot kernel), *Raphanus sativus* (radish seed), *Lepidium apetalum*, *Perilla frutescens* (perilla seed), *Scutellaria baicalensis*, *Morus alba* (mulberry root bark), *Gypsum fibrosum* (raw gypsum), *Isatis indigotica* (indigo leaf), *Houttuynia cordata*, and *Glycyrrhiza uralensis* (licorice). Clinical observations suggest that PDOL exhibits significant anti-asthmatic effects, but its pharmacological mechanisms remain to be elucidated.

Network pharmacology, a systems-level approach integrating bioinformatics and pharmacology, is particularly suitable for exploring the pharmacodynamic mechanisms of traditional herbal formulas due to their multi-component and multi-target nature (Li et al., 2023). It enables the systematic investigation of the interactions between bioactive plant-derived compounds and their associated disease targets.

In this study, we employed a network pharmacology strategy to explore the potential mechanisms of PDOL in the treatment of pediatric asthma. By identifying its active phytoconstituents, potential protein targets, and involved biological pathways, this work aims to elucidate the systemic therapeutic effects of this classical Chinese herbal medicine. The findings are expected to contribute to the scientific understanding of PDOL and provide a theoretical foundation for further experimental validation and clinical application.

Materials and Methods

Target Collection

The active phytochemical constituents of PDOL were identified using the TCM Systems Pharmacology Database and Analysis Platform (TCMSP v3.0, https://www.tcmspe.com/load_intro.php?id=43). Eleven medicinal herbs in the formulation—excluding *G. fibrosum* due to its mineral nature and lack of bioactive small molecules—were used as search terms. Each herb's chemical components were filtered based on absorption, distribution, metabolism, and excretion (ADME)-related pharmacokinetic parameters, with thresholds set at oral bioavailability (OB) ≥ 30% and drug-likeness (DL) ≥ 0.18.

The selected active compounds were then mapped to their corresponding protein targets using the "Related Targets" function in TCMSP. The resulting target data were standardized to the gene symbol format and deduplicated using the UniProt database (https://www.uniprot.org/). These data were used to construct a comprehensive compound-target database representing the pharmacological content of PDOL.

To identify disease-associated targets, multiple publicly available biomedical databases were searched using "asthma" as the keyword. These included: DisGeNET (Lazzara et al., 2024) (https://www.disgenet.org/), GeneCards (Gao et al., 2024) (https://www.genecards.org/), DrugBank (Wang et al., 2020) (https://go.drugbank.com/), the Comparative Toxicogenomics Database (CTD) (Dave et al., 2025) (http://ctdbase.org/), Online Mendelian Inheritance in Man (OMIM) (Chen et al., 2022) (https://www.omim.org/), Pharmacogenomics Knowledge Base (PharmGKB) (Luo et al., 2023) (https://www.pharmgkb.org/), and the Therapeutic Target Database (TTD) (Davis et al., 2023) (http://db.idrblab.net/ttd/). Targets common to both PDOL constituents and asthma-related genes were retained as candidate therapeutic targets.

Construction of the Compound-target Network

The intersecting targets derived from PDOL active components and asthma-related genes were compiled into a pharmacological interaction table detailing compound-target relationships. This dataset was imported into Cytoscape software (version 3.10.2) to construct a visualized network representing the multi-component, multi-target interactions of the PDOL formulation. A topological analysis was conducted to evaluate node connectivity and identify hub compounds and targets with high degrees, which may play key roles in the therapeutic effects.

Construction of the Protein–Protein Interaction (PPI) Network

The putative therapeutic targets of PDOL were input into the STRING database (https://string-db.org/) for PPI analysis. The species was set to Homo sapiens, and the minimum required interaction score was set at >0.9 (high confidence). The resulting interaction data were exported in tab-separated values (TSV) format and visualized in Cytoscape 3.10.2. Further topological analysis and modular clustering were performed using the molecular complex detection (MCODE) plugin to identify densely connected modules, with a cutoff of K-core ≥ 4 applied to highlight core functional subnetworks.

Gene Ontology (GO) and Kyoto Encyclopedia of Genes and Genomes (KEGG) Pathway Enrichment Analysis

To further elucidate the biological roles and mechanisms of PDOL targets, GO and KEGG enrichment analyzes were conducted using the Metascape database (https://metascape.org/). Target species were limited to Homo sapiens, and enrichment significance was set at $p < .05$. GO terms were categorized into biological processes (BP), cellular components (CC), and molecular functions (MF). The top enriched terms and pathways were visualized using Cytoscape to identify major pharmacological activities and signaling cascades modulated by the herbal constituents of PDOL.

Results

Screening of Active Compounds and Potential Targets

A total of 207 active phytochemical compounds from the 10 herbal components of PDOL met the screening criteria of OB ≥ 30% and DL ≥ 0.18, as retrieved from the TCMSP database. These compounds were associated with 306 putative protein targets. Meanwhile, 484 asthma-related targets were collected from multiple disease databases. By performing an intersection analysis between the compound-associated and disease-related targets, a total of 104 common targets were identified, representing potential therapeutic targets of PDOL in the treatment of asthma.

Construction of the Compound-core Target Network of PDOL

Based on the identified chemical components and their mapped targets, a compound-target interaction network was constructed using Cytoscape (v3.10.2), as shown in Figure 1. This network included 207 compound nodes, 104 target nodes, and 1,562 edges, visually illustrating the complex interactions between multi-component herbal compounds and multiple biological targets. The network topology analysis revealed several key hub compounds with high degrees of connectivity, including quercetin, kaempferol, β-sitosterol, stigmasterol, and luteolin. According to network pharmacology theory, these five compounds may represent the core bioactive constituents contributing to the pharmacological efficacy of PDOL.

Identification of Core Targets and Construction of the PPI Network

The 104 overlapping targets were imported into the STRING database for PPI analysis, with the confidence threshold set to >0.9 and species restricted to Homo sapiens. After excluding isolated nodes, the resulting PPI network contained 74 nodes and 244 edges, which were visualized and analyzed using Cytoscape 3.10.2 (Figure 2). Topological analysis identified

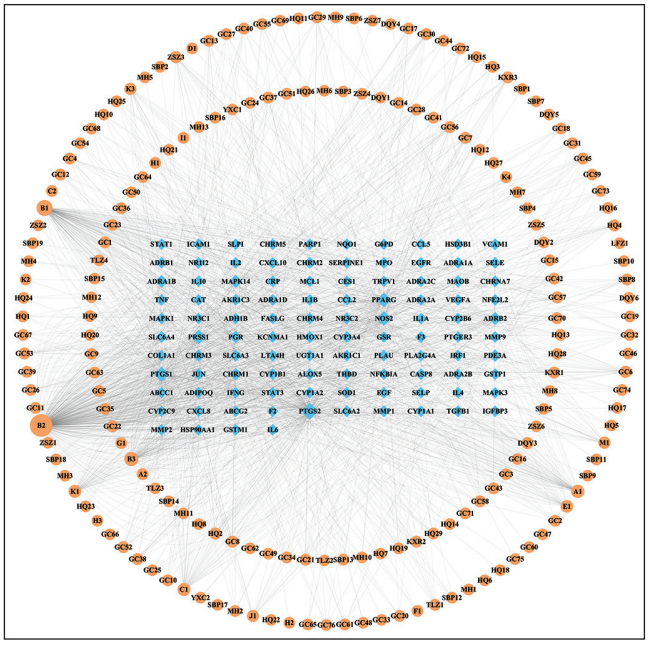


Figure 1. Construction of the Active Ingredient—Potential Target Network.

Note: The yellow nodes in the figure are Pediatric Dingchuan Oral Liquid (PDOL) compounds, and the blue nodes are potential targets.

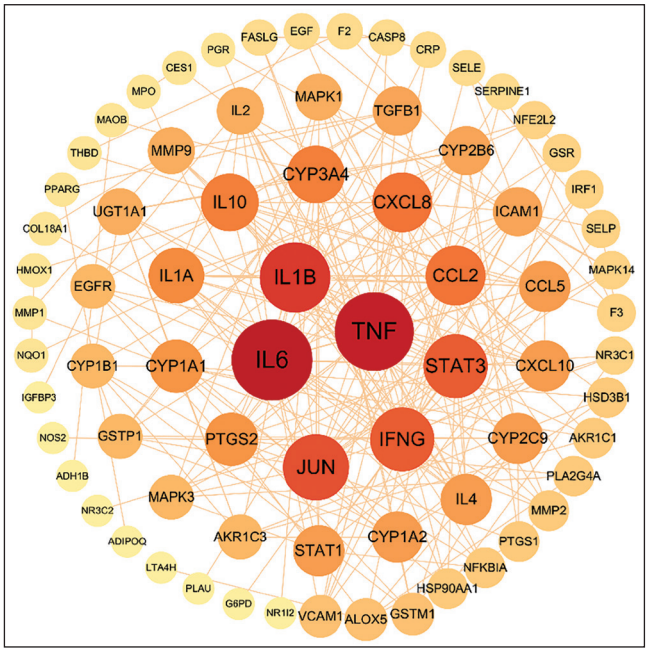


Figure 2. Protein–Protein Interaction (PPI) Network of the Core Target.

Note: The size of the nodes represents, and the color from cold to warm represents the degree.

Table 1. Cluster Data of Related Protein Targets.

Cluster	Node	Edge	Target Protein
1	12	61	IL2, IL1A, IL1B, CXCL8, CCL5, IL4, IL6, CXCL10, CCL2, IL10, IFNG, TNF
2	6	11	AKR1C1, CYP3A4, CYP1B1, CYP1A2, HSD3B1, CYP1A1
3	5	8	ALOX5, PTGS1, CYP2B6, CYP2C9, UGT1A1

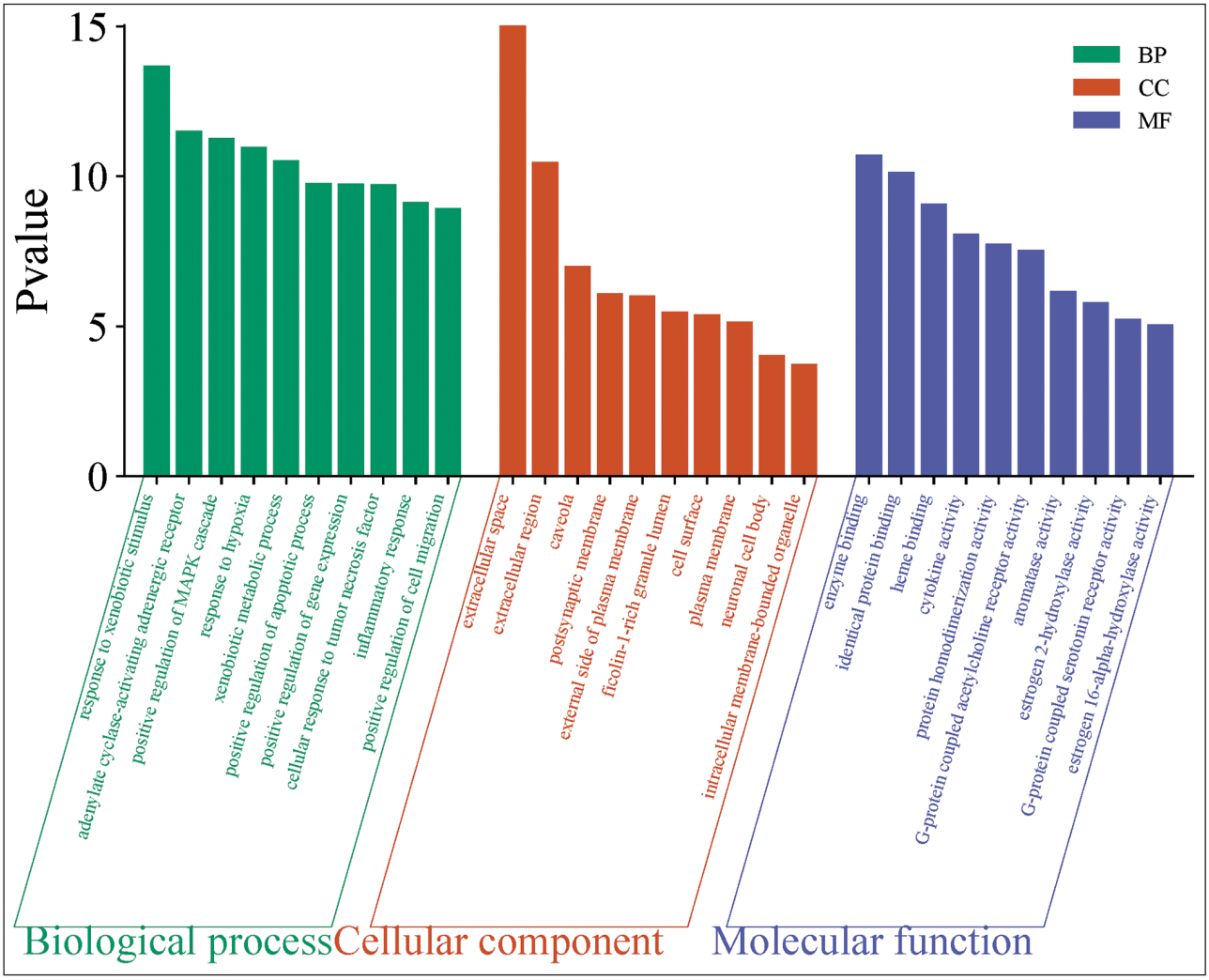


Figure 3. Gene Ontology (GO) Analysis of the Target of Pediatric Dingchuan Oral Liquid (PDOL) for Treating Asthma Diseases.

six highly connected hub proteins—IL6, TNF, IL1B, JUN, IFNG, and STAT3—suggesting their central role in mediating PDOL's therapeutic effects on asthma.

Furthermore, modular clustering of the PPI network using the MCODE plugin (K-core ≥ 4) identified three functional modules: Cluster 1 included targets involved in cytokine-mediated signaling, inflammatory response, leukocyte activation, and adhesion regulation. Cluster 2 was associated with xenobiotic metabolism, chemical carcinogenesis, and hematopoietic disorders. Cluster 3 comprised targets related to endogenous metabolism, detoxification processes, and biotransformation. The composition of each module and associated protein targets is summarized in Table 1.

GO and KEGG Pathway Enrichment Analysis

To further elucidate the biological roles of PDOL's therapeutic targets, GO and KEGG enrichment analyzes were performed using the Metascape platform. GO enrichment results were categorized into BP, CC, and MF. A total of 493 BP terms, 45 CC terms, and 93 MF terms met the significance threshold of $p < .05$. Representative enriched terms included:

BP: Response to exogenous stimuli, adenylate cyclase activation via adrenergic receptor signaling, positive regulation of the mitogen-activated protein kinase (MAPK) cascade, and hypoxia response. CC: Extracellular space, extracellular region, caveola, postsynaptic membrane, lateral plasma membrane, and ficolin-1-rich granule lumen. MF: Enzyme binding, protein homodimerization, heme binding, cytokine activity, and G protein-coupled acetylcholine receptor activity (Figure 3). KEGG pathway analysis identified 146 significantly enriched signaling pathways ($p < .05$), many of which are closely related to inflammatory and immune responses. These included: Disease-related pathways: Pertussis, COVID-19, tuberculosis, and influenza A. Immune-inflammatory pathways: IL-17 signaling, TNF signaling, Toll-like receptor signaling, C-type lectin receptor signaling, nucleotide-binding oligomerization domain (NOD)-like receptor signaling, cytokine-cytokine receptor interaction, Th1/Th2 cell differentiation, and HIF-1 signaling (Figure 4).

These enrichment results support the hypothesis that PDOL exerts its anti-asthmatic effects primarily through modulation of inflammation-related and immunoregulatory pathways, consistent with the pharmacological actions of its herbal constituents. The chemical components in TCM compound prescriptions exert anti-asthmatic effects by exerting their pharmacological actions.

Discussion

PDOL is a widely used traditional Chinese patent medicine for the treatment of pediatric asthma. Its formulation is rooted in classical principles of TCM, integrating herbs that promote lung function, relieve asthma, clear heat, and resolve phlegm. Clinically, PDOL has shown favorable outcomes in alleviating symptoms during asthma attacks through multiple mechanisms, including modulation of respiratory immune responses, inhibition of bronchial smooth muscle contraction, and attenuation of oxidative stress (Ling et al., 2023).

According to the Huangdi Neijing, "Yin contends within, while Yang disturbs outside... When it starts, it fumigates the lungs, causing wheezing and dyspnea." This classical statement encapsulates the pathogenesis of asthma in TCM, wherein phlegm and fluid retention disrupt lung functions. Contemporary TCM theory attributes childhood asthma to

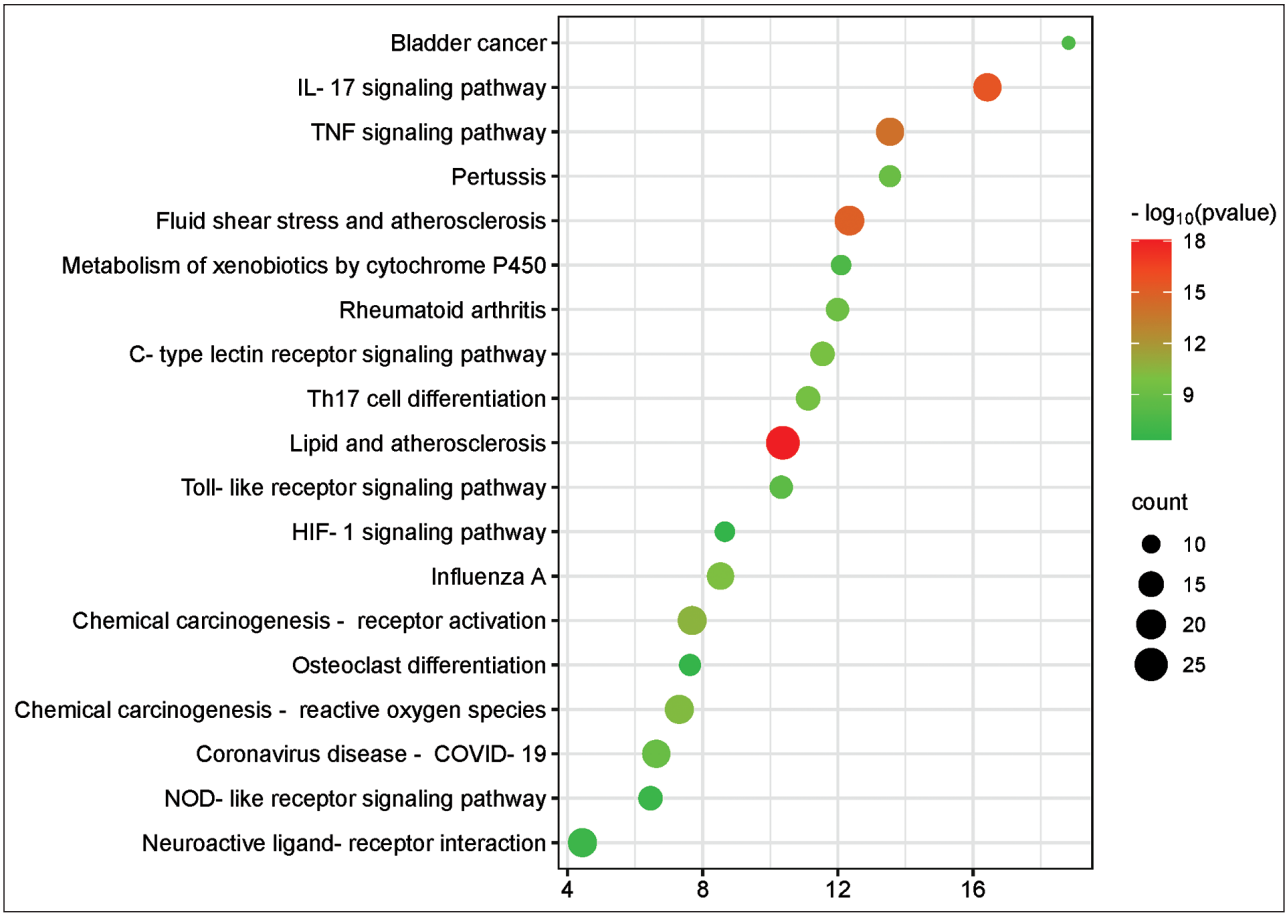


Figure 4. Kyoto Encyclopedia of Genes and Genomes (KEGG) Analysis Bubble Chart of Pediatric Dingchuan Oral Liquid (PDOL)'s Target for Treating Asthma Diseases.

internal accumulation of phlegm, invasion by exogenous pathogenic factors, dietary imbalance, and emotional disturbances—all of which contribute to the blockage of qi flow in the lung and loss of descending function (Jeong & Choi, 2022). The PDOL formulation reflects this pathophysiological understanding, combining 11 medicinal ingredients, including *E. sinica*, *P. armeniaca*, and *G. fibrosum*. *E. sinica* and *P. armeniaca* are the sovereign medicines. One disperses lung qi, and the other descends it, rapidly alleviating the primary symptoms of cough and wheezing in children. *G. fibrosum*, *R. sativus* L. (seed), and *Descurainia sophia* (L.) Webb ex Prantl serve as ministerial medicines, supporting the sovereign medicines to strengthen the effects of "clearing heat, resolving phlegm, and relieving asthma." *S. baicalensis* Georgi, *P. frutescens* (L.) Britt. (fruit), *Citrus reticulata* Blanco (pericarp), *H. cordata* Thunb., and *Mentha haplocalyx* Briq. act as assistant medicines: *S. baicalensis* Georgi clears lung heat; *P. frutescens* (L.) Britt. (fruit) enhances phlegm-resolving; *C. reticulata* Blanco (pericarp) addresses children's spleen weakness to prevent internal phlegm-damp accumulation; *H. cordata* Thunb. targets sore throat caused by lung heat; *M. haplocalyx* Briq. relieves sore throat and nasal congestion associated with cough and wheezing, supplementing the deficiency of the sovereign and ministerial medicines. *G. uralensis* Fisch. functions as the envoy medicine, tonifying qi and benefiting the middle energizer, clearing heat and detoxifying, and harmonizing all medicines. It protects children's delicate zang-fu organs, coordinates the cold-heat properties of the entire formula, and promotes the synergistic effect of all ingredients.

The formulation demonstrates a balanced therapeutic strategy. Ephedra is pungent and warm, dispersing cold and facilitating lung qi to relieve asthma; Apricot kernel is bitter and descending, easing the lung; the cold-natured Gypsum clears heat, while *M. alba* root bark further purges fire. Perilla seed and *L. apetalum* reduce qi and eliminate phlegm. *H. cordata* and *I. indigotica* detoxify and resolve inflammation, while *S. baicalensis* dries dampness and clears heat. *R. sativus* aids digestion and relieves stagnation, and *G. uralensis* harmonizes the overall formula (Zhao et al., 2024). Together, these herbs demonstrate a synergistic action across four traditional therapeutic dimensions: clearing, promoting, reducing, and transforming.

Modern pharmacological studies support the biological activities of these herbs. The Maxing Ganshi Decoction, which shares components with PDOL, has demonstrated anti-inflammatory and anti-tussive effects via inhibition of the nuclear factor kappa B (NF-κB) signaling pathway half-maximal inhibitory concentration (IC_{50} = 12.3 μg/mL), and has showed anti-viral efficacy by reducing H1N1 viral load by 42% in murine models (Liu et al., 2022). *R. sativus* extract significantly reduced TNF-α and IL-6 levels ($p < .01$), indicating its anti-inflammatory potential (Hong et al., 2022). Herbal lignans have also been shown to activate peroxisome proliferator–activated receptor gamma (PPAR-γ) and inhibit matrix metalloproteinase-9 (MMP-9), potentially limiting airway remodeling in chronic asthma (Wyatt et al., 2024). Notably, active compounds such as baicalin (23.8 mg/g) and benzyl isothiocyanate (18.2 μg/mL) appear to modulate the Th1/Th2 cytokine balance, which may explain PDOL's superior efficacy compared to single-compound interventions.

This study adopted a network pharmacology approach to elucidate the mechanistic basis of PDOL. Based on the ADME criteria, we screened hundreds of compounds from the 10 herbal components (excluding Gypsum) and identified five core bioactive constituents—quercetin, kaempferol, β-sitosterol, stigmasterol, and luteolin—through network topological analysis. Among them, quercetin is a flavonoid with demonstrated anti-inflammatory, anti-viral, immunoregulatory, anti-tussive, and bronchodilatory activities (Li et al., 2021; Pertzborn et al., 2020). It mitigates airway hyperresponsiveness by modulating cytokines and inflammatory mediators. Previous studies have shown that such flavonoids may inhibit pathways including NF-κB and NLRP3 inflammasomes (Tian et al., 2021), while restoring Th1/Th2 immune balance, thereby reducing mucus secretion and airway constriction (Jing et al., 2020).

Interestingly, beyond herbal interventions, anti-inflammatory dietary patterns—such as the Mediterranean and Okinawan diets—have also been associated with reduced asthma risk in children, likely due to their emphasis on plant-based, antioxidant-rich foods and healthy lifestyle components (Mascarenhas, 2019). This aligns with the multi-faceted regulatory effects observed in PDOL.

Analysis of the PPI network identified IL6, TNF, IL1B, JUN, IFNG, and STAT3 as central nodes. These proteins are intimately involved in chronic airway inflammation and immune dysregulation. For instance, JUN, a proto-oncogene regulated via the JNK/SAPK cascade (a MAPK-related pathway), has been implicated in the development of respiratory inflammation (Swantek et al., 1997). The modular analysis of PPI clusters has further confirmed that PDOL's targets are concentrated in networks involved in inflammatory response, detoxification, and immune activation.

GO enrichment highlighted PDOL's influence on BP, such as response to exogenous stimuli and hypoxia—both highly relevant to asthma pathophysiology. KEGG pathway enrichment revealed regulation of inflammation-related signaling pathways (e.g., TNF, IL-17, Toll-like receptor, Th1/Th2 differentiation), as well as pathways involved in lung injury repair (e.g., HIF-1 and cGMP-PKG). These findings indicate that PDOL may exert its therapeutic effects by modulating multiple signaling axes related to lung inflammation, immune dysfunction, and tissue repair.

Despite the systematic network pharmacology analysis, this study has several limitations. First, although core targets such as IL6, TNF, and IL1B, and key pathways including IL-17 and TNF signaling were identified, the mechanistic interpretation was not deeply connected to specific pathological features of childhood asthma—such as airway epithelial injury, mucus hypersecretion, and airway remodeling.

The study did not further clarify how PDOL might regulate the IL-6, TNF, IL-1B inflammatory axis or distinguish potential effects during acute versus chronic stages of asthma. Second, as a predictive analysis, the findings lack *in vivo* or *in vitro* experimental validation, such as cytokine assays, Western blotting of hub proteins, or animal model pharmacodynamic studies, which limit the strength of causal inferences. Third, comparisons with other TCM formulations for pediatric asthma were not included, making it difficult to highlight the unique mechanistic advantages of PDOL. These limitations indicate that further experimental and comparative studies are required to substantiate and refine the mechanistic conclusions.

Conclusion

This study employed a network pharmacology approach to preliminarily explore the molecular mechanisms of PDOL, a traditional Chinese polyherbal formulation, in the treatment of childhood asthma. Ten medicinal herbs (excluding *G. fibrosum*) were found to contain active phytoconstituents that interact with inflammation- and immunity-related targets. Core bioactive compounds—including quercetin, kaempferol, and β-sitosterol—were identified as key mediators. PDOL may exert its anti-asthmatic effects by modulating multiple biological pathways involved in inflammation suppression, immune regulation, and lung tissue repair. These findings provide a scientific foundation for further pharmacological and clinical investigations into the therapeutic potential of plant-based formulations in respiratory diseases.

Abbreviations

ADME: Absorption, distribution, metabolism, excretion; BP: Biological processes; CC: Cellular components; CTD: Comparative Toxicogenomics Database; DL: Drug-likeness; GO: Gene Ontology; KEGG: Kyoto Encyclopedia of Genes and Genomes; MCODE: Molecular complex detection; MF: Molecular functions; MMP-9: Matrix metalloproteinase-9; OB: Oral bioavailability; OMIM: Online Mendelian Inheritance in Man; PDOL: Pediatric Dingchuan Oral Liquid; PPI: Protein–Protein interaction; TCM: Traditional Chinese medicine; TCMSP: Traditional Chinese Medicine Systems Pharmacology Database and Analysis Platform; TSV: Tab-separated values; TTD: Therapeutic Target Database.

Declaration of Conflicting Interests

The authors declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

Ethical Approval and Informed Consent

Not applicable.

Funding

The authors received no financial support for the research, authorship, and/or publication of this article.

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