RESEARCH PAPER

The Role of Traditional Chinese Medicine in Modern Pharmacology: A Comparative Analysis of Herbal and Synthetic Drugs

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Abstract

Traditional Chinese Medicine (TCM) is increasingly examined through modern pharmacological frameworks because of its multi-component and multi-target therapeutic characteristics. However, comparative molecular evidence between TCM herbs and synthetic drugs remains limited. The present study aimed to evaluate the role of TCM in modern pharmacology by comparing herbal and synthetic drugs through molecular target overlap, target diversity, and network pharmacology analysis. A quantitative secondary-data analysis was conducted using publicly available TCM herb-target interaction data and synthetic drug pharmacodynamic data. Herbal and synthetic drug targets were harmonized using UniProt identifiers. Shared targets were identified, target diversity was compared using descriptive statistics and the Mann–Whitney U test, and integrated herb–drug–target networks were constructed to examine pharmacological connectivity. The analysis included 85,821 herbal target interaction records, 571 unique herbs, 1,915 herbal molecular targets, 1,520 synthetic drugs, and 546 synthetic drug targets. A total of 267 shared molecular targets were identified. Key shared targets included *BCL2, PTGS2, TNF, ACHE, AKT1, PPARG*, and *PPARA*. TCM herbs showed substantially broader target diversity than synthetic drugs, with a median of 54 targets per herb compared with one target per synthetic drug. The difference was statistically significant ($U = 824{,}180$; $p = 4.45 \times 10^{-237}$). This network integration also illustrated the remarkable pharmacological convergence of herbal and synthetic drugs through their effects on inflammation, apoptosis, metabolism, endocrine function, and neuropharmacology. The results highlight the significance of TCM in contemporary systems pharmacology and drug discovery, underscoring the importance of additional experimental and clinical validation.

Keywords: Traditional Chinese Medicine, synthetic drugs, network pharmacology, molecular targets, systems pharmacology

How to cite this article: Hosamath R, Kallatti K. The Role of Traditional Chinese Medicine in Modern Pharmacology: A Comparative Analysis of Herbal and Synthetic Drugs. Int J Drug Deliv Technol. 2026;16(69s): 1833-1841. DOI: 10.25258/ijddt.16.69s.181

1. Introduction

Traditional Chinese Medicine (TCM) is one of the oldest medical practices existing today and is very much part of health care services in many different places around the world. While traditional pharmacology is mainly targeted at individual active substances and very specific molecular targets, TCM is based on a holistic therapeutic concept with complex multipolyherbs and the regulation of interconnected physiological processes. Over the years, growing interest in TCM has increased greatly, as its pharmacological diversity and the potential contribution to modern therapeutic discovery have come to light (Matos et al., 2021). Conceiving the basis of TCM, integrated physiological balance, dynamic energy interactions and individualized therapeutic approaches, are very different from the reductionist biomedical models used in synthetic pharmacology (Chen et al., 2023).

As traditional medicine becomes increasingly accepted and adopted with modern biomedical science, there has been a renewed interest in elucidating the molecular mechanisms of herbal medicines. With the development of systems biology, computational pharmacology and omics technologies, the research of TCM has entered the molecular and network biology era, and the scientific level of research has been promoted, and the therapeutic mechanism of TCM can be scientifically explained at the molecular and network level (Guo et al., 2020). All these developments have led to the emergence of multi-component and multi-target-oriented approaches with systems pharmacology that can be used to assess interactions with herbal medicines. Meanwhile, synthetic pharmacology remains predominant in modern drug development by the design of highly selective compounds for the regulation of specific biological pathways (Ezeako et al., 2025). The complexity of cancer and other diseases, including inflammatory disorders, neurodegenerative diseases and metabolic syndromes, is becoming increasingly apparent to pharmacologists, as they are often the result of multiple interconnected signaling pathways, rather than single molecular abnormalities. This recognition has led to increased interest in the development of multi-target therapeutic strategies and in drug discovery based on polypharmacology. The relevance of herbal medicines is of significance in this context, as many of the herbal formulations or medicines used in the TCM contain multiple bioactive compounds that can work

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simultaneously at multiple biological targets (Ebadi & Selamoglu, 2025). Due to such features, researchers have been interested in the possibility of finding common molecular pathways between the compounds used in TCM and synthetic drugs, despite the fact that they have different formulation strategies and therapeutic philosophies.

Naturally occurring products have significantly contributed to drug development historically. The importance of naturally occurring resources in developing therapeutics has been evidenced by some clinically relevant drugs obtained directly or indirectly from natural products (Yuan et al., 2016). With the shift in scientific focus towards the discovery of new drugs from natural products, there has been an increasing emphasis on combining the principles of traditional medicines with the concept of modern pharmacology, as well as using an integrated computational and molecular approach (Truax & Romo, 2020). With a long history of application and rich variety of herbal medicines, the TCM has drawn lots of attention in the current context, considering the opportunity of finding novel compounds with pharmacological effects.

A number of recent studies have shown that network pharmacology can be used to address the complexity associated with herbal medicine. Unlike traditional single-target drug development models, network pharmacology is applied to simultaneously assess the interaction of herbs with compounds and target proteins and biological pathway connectivity. This type of analysis has been shown to be valuable in studying TCM because it possesses systems-level properties in traditional herbal medicines (Zhao et al., 2019). Likewise, multi-component Chinese medicine formulas are also increasingly being studied for their potential in the development of new drugs, in addition to their various pharmacological effects and action on multiple molecular pathways (Zhang et al., 2023).

The philosophical and scientific differences between traditional medicine and modern biomedical pharmacology have also been emphasized in the past. In contrast to the synthetic pharmacology that traditionally takes a highly specific biochemical intervention approach, TCM treats the body as a unified system with dynamic physiological balance and interconnected regulation of the system. However, there is emerging evidence that both therapeutic systems may influence common biological systems related to inflammation, apoptosis, endocrine signaling, metabolism, and neurologic function. Molecular studies have revealed that the compounds used in TCM have the ability to modulate pharmacological targets traditionally linked to conventional synthetic drugs, which is consistent with the hypothesis of these systems being pharmacologically converged (Wang et al., 2018). Research on TCM has increased significantly in the last 20 years owing to the development of computational biology, molecular pharmacology and translational medicine. These advances have enhanced the scientific validity of the studies on TCM and promoted more active integration of TCM and modern biomedical research systems (Tian et al., 2021). With the development of emerging regulatory and translational disciplines, a scientific rigor established by scientifically sound methodologies to assess the pharmacologic basis of TCM in current healthcare systems has become increasingly important (Hua et al., 2025).

Although these developments have been made, there are still significant gaps in the comparative pharmacological studies of TCM herbs and synthetic drugs. Previous research primarily addresses single herbal molecules, disease-specific preparations or the theoretical network pharmacology models, and fails to quantify the differences and similarities in molecular target diversity and shared pharmacological connectivity between these two therapeutic systems. There have been very few studies on secondary data at a large scale to systematically analyze the coverage of molecular overlap between the formulation of TCM herbs and synthetic pharmacological substances based on integrated target interaction data sets.

Thus, the present study was conducted to comparatively assess the potential of TCM in modern pharmacology using molecular target analysis and network pharmacology methods. The study specifically focused on shared molecular targets between TCM herbs and synthetic drugs, the difference in diversity of targets between both therapeutic systems, the highly connected pathways in the Pharmacological network and the construction of the integrated interaction networks to explore the route of convergence of pharmacological pathways between the traditional herbal therapeutics and modern synthetic pharmacology.

2. Methodology

2.1 Research Design

This research design used a quantitative secondary data study to compare the pharmacological interaction between the TCM herbs and synthetic drugs. A comparative systems pharmacology framework was used to examine the interactions between the molecular targets and the pharmacological overlap and target diversity of herbal and synthetic therapeutic agents. The discussion emphasized the molecular and network-level pharmacological properties as opposed to clinical efficacy outcomes.

The research conducted an integrated computational analysis to detect the similarities of biological targets as well as assess disparities in pharmacological connections between herbal drugs and synthetic medications. Statistical and network-based comparative methods of analysis were then used to study molecular interaction patterns and combined pharmacological associations between the two therapeutic systems.

2.2 Data Sources

The following two secondary datasets available in the public domain were used in this paper. Data related to pharmaceutical drugs were obtained from the dataset compiled by Douguet (2023). The data includes pharmacodynamic and pharmacokinetic features of FDA-approved drugs and their metabolites

experimentally proven. The data provided by Douguet et al. contained information regarding the target interaction of molecular structures.

Information about TCM molecular interaction was retrieved from the dataset prepared by Fathi and Moghaddam Charkari (2024). It included heterogeneous networks related to TCM, such as herb-target interaction networks, herb-compound networks, and pharmacological interaction networks. Information contained in this database helped in analyzing the molecular targets of herbs and synthetic drugs.

2.3 Data Extraction and Preprocessing

CSV data files pertaining to interactions between herbs and targets, molecular target details, and properties of synthetic drug pharmacodynamics were selected and processed from the available downloads. Preprocessing of the data included removing duplicates, standardizing the names of variables, normalizing text formatting, and discarding those rows which contained any missing values for molecular identifiers.

The identifiers relating to targets of synthetic drugs were extracted and normalized so as to facilitate the comparison with herb targets. After that, integration of molecular targets was performed using common identifiers to allow comparison of herb medicine with synthetic drugs.

2.4 Molecular Target Integration and Comparative Analysis

The integration of molecular targets was achieved through matching between herbal and synthetic drugs using the UniProt ID numbers of the targets. The comparative study involved calculating the total number of unique molecular targets associated with each herb and each synthetic drug, respectively, and then selecting the most frequent herbs, major molecular targets, and pharmacological pathways. Focus was directed at targets involved in inflammatory responses, apoptosis, endocrinology, metabolism, and neuropharmacology because they have considerable similarities between the two classes of drugs.

2.5 Statistical and Network Pharmacology Analysis

Descriptive statistics were used to describe features of the data set, target distributions, and the number of interactions. The median numbers of target diversity of herbal medicines and synthetic drugs were determined independently, and the Mann–Whitney U test was used to compare the target diversities between the two groups because of the non-normal distribution of data.

The network pharmacology approach was used to examine patterns of herb-target interaction and drug-target interaction. A molecular network of interactions was created to determine the hub herbs and molecular targets with high connectivity from interaction frequency. Network visualization was then carried out to demonstrate the pharmacological connection between herbal medicines and synthetic drugs. The entire analytical process implemented in this paper is shown in Figure 1 below.

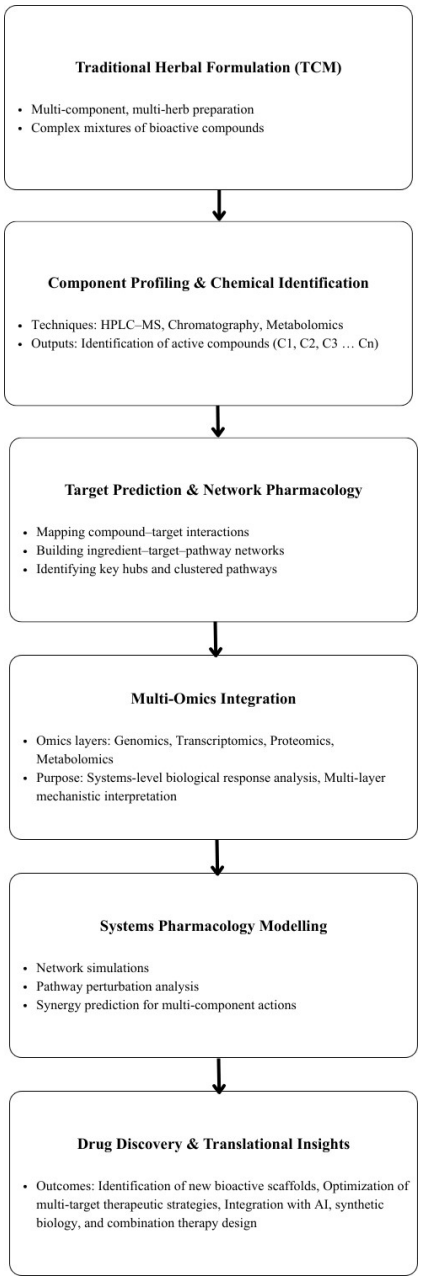

Figure 1. Systems Pharmacology and Omics Workflow for TCM Research

3. Results

3.1 Dataset Characteristics and Molecular Target Profiles

There was a total of 85,821 herb-target interactions recorded in the TCM dataset after data cleaning and standardization. This dataset included 571 distinct herbal drugs associated with 1,915 distinct molecular targets. In contrast, the synthetic drug dataset had 1,520 distinct synthetic drugs interacting with 546 molecular targets. The comparison analysis between the two datasets resulted in the identification of 267 common molecular targets among herbs and synthetic drugs (Table 1).

This result shows that there is a significant overlap at the molecular level between the molecules obtained from TCM and modern medicinal molecules. The presence of common targets means that herbs and synthetic drugs can affect similar biological processes despite their contrasting nature.

Table 1. Dataset Characteristics and Molecular Target Summary

Characteristic	Value
Total herbal target records	85,821
Unique herbs	571
Unique herbal molecular targets	1,915
Unique synthetic drugs	1,520
Unique synthetic drug targets	546
Shared molecular targets	267

Enrichment of the protein targets identified through the analysis of herbal compounds is seen with respect to those that play roles in inflammation, apoptosis, metabolic functions, and signal transduction. The most common among the protein targets include *CASP3, BCL2* apoptosis regulator, *TNF, NFKB1* (nuclear factor NF-kappa-B), *PTGS2*, and *AKT1* (RAC-alpha serine/threonine-protein kinase). They are significant to inflammatory response, cancer, and cell survival mechanisms. The drug compounds include protein targets for inflammatory processes, endocrine functions, neuronal transmission, and membrane receptors.

3.2 Shared Molecular Targets Between TCM Herbs and Synthetic Drugs

Target comparison analysis showed that there were many very well-connected molecular targets that existed in both TCM herbs and synthetic medicines. These highly connected molecular targets included *BCL2, PTGS2, TNF, ACHE, AKT1*, and *PPARG*, all of which had high connectivity frequencies within the herbal data set (Table 2).

Table 2. Top Shared Molecular Targets Between TCM Herbs and Synthetic Drugs

Gene Symbol	Protein Name	Associated Herbs	Associated Drugs	Combined Frequency
BCL2	Apoptosis regulator BCL-2	345	1	346
PTGS2	Prostaglandin G/H synthase 2	309	37	346
TNF	Tumor necrosis factor	338	2	340
ACHE	Acetylcholinesterase	299	13	312
AKT1	RAC-alpha serine/threonine-protein kinase	306	1	307
PPARG	Peroxisome proliferator-activated receptor gamma	282	3	285
TYR	Tyrosinase	250	2	252
PPARA	Peroxisome proliferator-activated receptor alpha	238	5	243
ESR1	Estrogen receptor	217	21	238
MAOA	Amine oxidase [flavin-containing] A	232	5	237
FASN	Fatty acid synthase	235	1	236
AR	Androgen receptor	197	26	223
MMP2	72 kDa type IV collagenase	218	1	219
ABCB1	ATP-dependent translocase ABCB1	213	1	214
PTGS1	Prostaglandin G/H synthase 1	181	30	211

The highest level of correlation was seen for pathways involved in inflammation and apoptosis. *PTGS2* and *TNF*, key components of the inflammation pathway, had a high degree of connectivity not only with herbal compounds but also with artificial drugs. Similarly, *BCL2* and *AKT1* demonstrated high correlations with herbal compounds, indicating the importance of TCM for the pathways that regulate apoptosis and cancer signaling. Figure 2 illustrates the pattern of the most shared molecular targets found in both datasets.

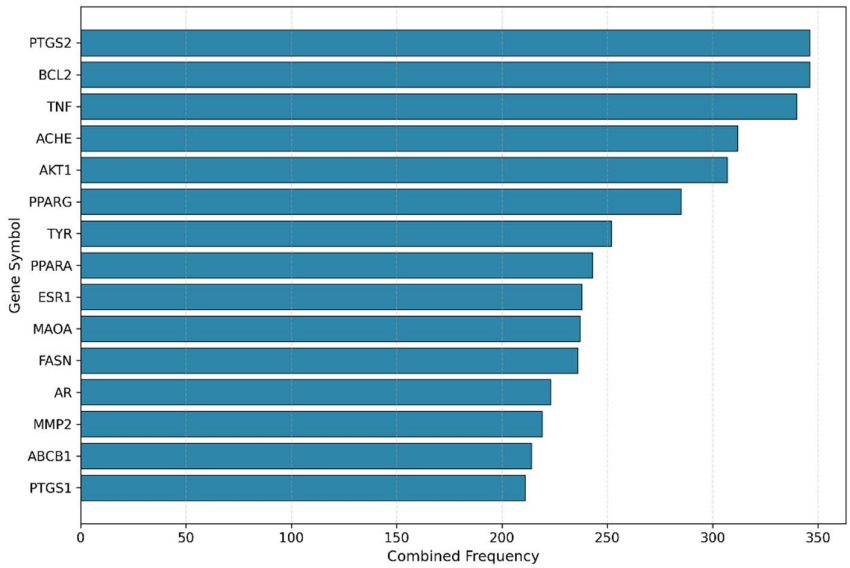

Figure 2. Top Shared Molecular Targets Between TCM Herbs and Synthetic Drugs

As seen in the graph below, it is clear that *PTGS2, BCL2, TNF*, and *ACHE* are among the highest shared pharmacological targets. It can be inferred from this information that TCM and synthetic compounds share biological targets associated with inflammatory processes, cancer development, hormonal activities, and nervous system function.

3.3 Molecular Target Diversity Among TCM Herbs

Substantial variability in target diversity was observed among the analyzed TCM herbs. Several herbs demonstrated exceptionally broad molecular connectivity, indicating extensive multi-target pharmacological behavior. Human placenta exhibited the highest number of associated molecular targets, followed by Chinese date, the root of red-rooted salvia, Japanese fleeceflower, and Ginkgo species. Figure 3 presents the herbs with the highest molecular target diversity identified within the dataset.

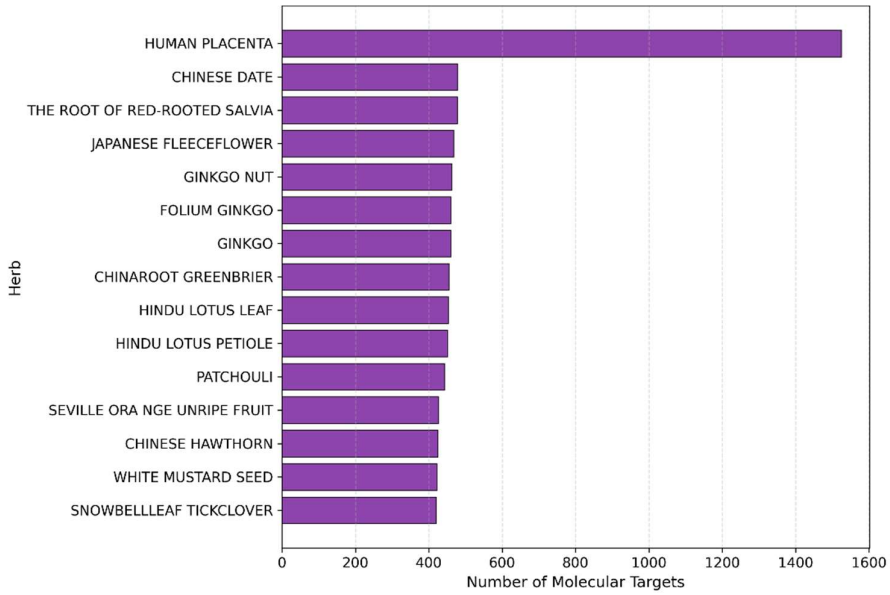

Figure 3. Top TCM Herbs by Molecular Target Diversity

According to the results, there is more than one type of herb in traditional Chinese medicine that interacts with hundreds of targets simultaneously. Ginkgo, red-rooted Salvia, and Japanese fleeceflower displayed a high number of different targets, indicating their extensive pharmacological potential related to inflammation, metabolism, neurology, and apoptosis. Multi-target interactions distinguish herbal medicine from synthesized drugs' interactions with only one specific

target; hence, systems pharmacology may be applied to herbs.

3.4 Comparative Associations of Shared Molecular Targets

In terms of the connectivity of targets for common targets evaluation, there exists a marked disparity between herbal medicine and synthetic drugs. In most cases, for all common major targets, herbal medicine has considerably greater connectivity than synthetic drugs. This is illustrated by Figure 4 below, which indicates connectivity comparison between herbal medicine and synthetic drugs.

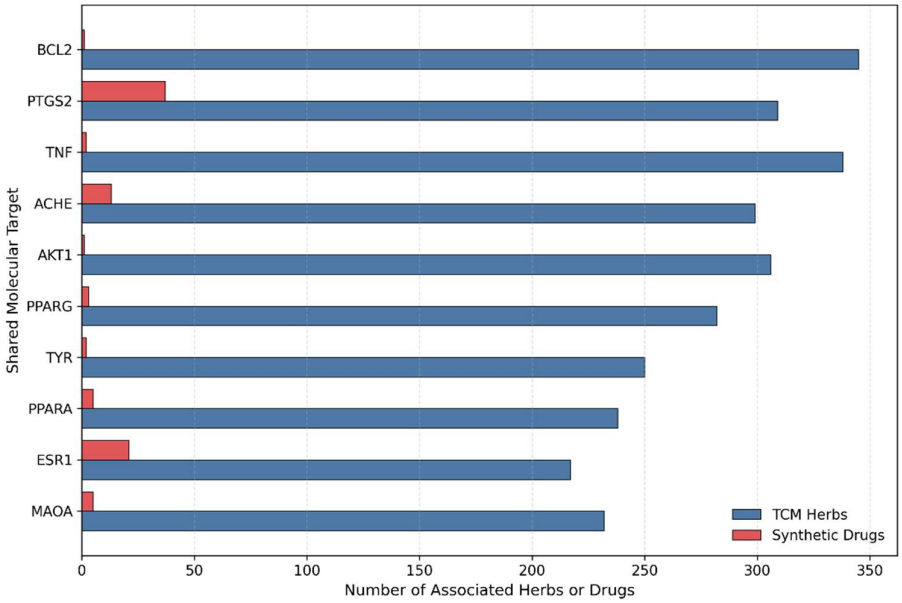

Figure 4. Comparative Associations of Shared Molecular Targets

As depicted in Figure 4, herbal medicine displayed significantly greater molecular connectivity than synthetic drugs on most shared targets. Particularly strong herbal associations were observed for *BCL2, TNF, AKT1, PTGS2,* and *ACHE*. In contrast, synthetic drugs exhibited comparatively narrower target connectivity, although *PTGS2, ESR1,* and *AR* showed relatively higher synthetic drug associations than other shared targets.

3.5 Integrated Pharmacological Network Analysis

A network pharmacology-based approach was employed in discovering an intricate molecular network of interactions between TCM herbs and synthetic medications sharing biological targets in pharmacology. The integrated network demonstrates that there are several TCM herbs and synthetic chemicals interacting at common pharmacological targets associated with inflammatory control, apoptosis, metabolic pathways, and neuromodulation. Figure 5 shows the resulting integrated pharmacological network constructed based on highly connected herbs, synthetic chemicals, and molecular targets.

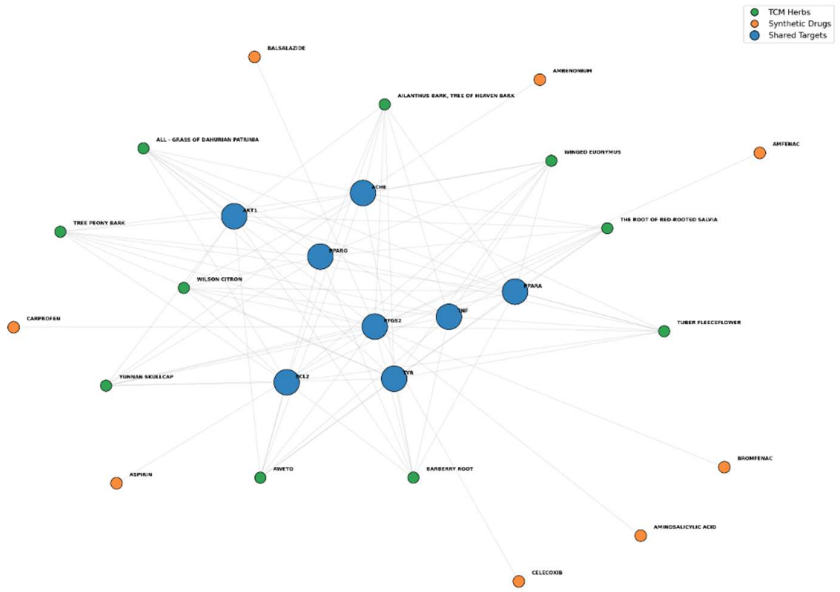

Figure 5. Integrated Pharmacological Network of TCM Herbs, Synthetic Drugs, and Shared Molecular Targets

From the network analysis, it was identified that the targets *PTGS2, TNF, BCL2, ACHE, AKT1*, *PPARG*, and *PPARA* form the core hubs of the pharmacological network. Several synthetic drugs, such as aspirin, celecoxib, bromfenac, carprofen, and amfenac, have shown direct relationships with the common targets. At the same time, many herbal drugs were targeting the same molecular hubs, thereby showing significant pharmacological similarity between herbal drugs and synthetic drugs.

This high degree of connectivity between common targets highlights the multi-target pharmacology nature of TCM. Unlike the selective connectivity seen with synthetic drugs, herbal drugs exhibit more interactions, targeting several pathways.

3.6 Comparative Statistical Analysis of Target Diversity

Statistical comparison of the target diversity showed that there were statistically significant differences in the case of TCM herbs as compared to synthetic drugs. In TCM herbs, the median number of targets per herb was 54, whereas in synthetic drugs, the median number of targets per drug was 1 ($U = 824{,}180$; $p = 4.45 \times 10^{-237}$) (Table 3).

Table 3. Comparative Pharmacological Characteristics of TCM Herbs and Synthetic Drugs

Comparative Metric	Value
Median targets per herb	54
Median targets per synthetic drug	1
Mann–Whitney U statistic	824,180
P-value	4.45×10^{-237}

These results suggest that TCM herbal extracts possess a much greater connectivity between their pharmacological properties when contrasted with artificial drugs. These differences provide evidence for the idea that herb-based medicines rely on the synergistic influence on multiple biological pathways rather than highly specific inhibition of individual targets.

4. Discussion

The obtained data suggest that the field of pharmacology provides many overlaps between TCM herbs and synthetic drugs from the perspective of molecular pharmacology. Identification of 267 molecular targets that TCM and synthetic drugs share shows that herbal and synthetic medicine can act on common biological pathways despite having different origins. Some of the major common molecular targets include *BCL2, PTGS2, TNF, ACHE, AKT1, PPARG, PPARA, ESR1*, and *MAOA*. All of them are directly associated with such biological phenomena as inflammation, apoptosis, metabolism regulation, endocrine functions, cancer development, and neuropharmacology.

One of the most important discoveries is the significant difference in the degree of target diversity between TCM herbs and synthetic medicines. While the median number of targets per herb was 54, synthetic drugs had a median of one molecular target. This difference is statistically significant and suggests that herbal medicines act via more diverse target connections compared to synthetic drugs. The described pattern aligns with the concept of treatment according to the TCM, whereby herbs and their compounds influence multiple biological processes at once instead of acting upon a single target exclusively. This theory is supported by the results of network analysis, which indicate that the genes *PTGS2, TNF, BCL2, ACHE, AKT1, PPARG,*

and *PPARA* contribute substantially to the herbal and synthetic networks. Furthermore, the list of synthetic medications included in the network consists of such notable anti-inflammatory and antitumor medications as aspirin, celecoxib, bromfenac, carprofen, and amfenac.

The importance of common proinflammatory and apoptosis targets identified during the research study is consistent with the current state of scientific knowledge, which implies that novel forms of cellular death, such as ferroptosis, may provide effective therapeutic interventions for inflammation and cancer treatment (Jin et al., 2024). It is noteworthy that the *PTGS2* gene's significant role in common targets is associated with recent studies concerning the influence of the *OXNAD1-PTGS2* pathway on ferroptosis-resistance strategies employed in gastric cancer therapy (Wang et al., 2026). It means that this protein plays an important part in TCM and synthetic networks because of being a common therapeutic pathway. In addition, *PPARG* and *AKT1* common targets correspond to recent scientific findings about the pharmacological activities of various natural products. For example, sanguinarine affects cancer by inducing autophagic apoptosis by acting on the PI3K/AKT pathway mediated by *PPARG* activation (Zhang et al., 2026). Besides, there is sufficient evidence in favor of using network pharmacology and other computational methods to find new mechanisms of neuropharmacological action based on TCM herbs (Wang et al., 2021).

In general, the obtained results correspond to other studies related to the use of network pharmacology and experiments with TCM formulas. For example, Buzhong Yiqi Decoction was recently investigated via network pharmacology, molecular docking, and in vitro experiments to understand its molecular mechanisms in cancer treatment (Zeng et al., 2024). In addition, recent scientific literature contains numerous reports concerning the design of TCM prescriptions based on the concept of a multi-targeted approach (Yu et al., 2025). As a result, the obtained findings confirm the importance of the multi-target strategy for understanding TCM pharmacology. Finally, the high degree of target diversity is supported by another study investigating multi-target anti-inflammatory compounds in TCM using target–effect relationship spectra (Huo et al., 2022). The findings correspond to the general pharmacological principle stating that natural compounds often interact with multiple targets (Bizzarri et al., 2020). In addition, molecular docking approaches are becoming a commonly used tool for exploring the synergistic and additive action of TCM herbs (Rigby, 2024).

The obtained findings are important for modern pharmacology and drug discovery in multiple ways. First of all, the fact of strong overlap between molecular targets of TCM herbs and synthetic drugs suggests that natural compounds included in TCM formulas are pharmaceutically active and target biologically relevant pathways. Secondly, TCM herbs have more targets compared to synthetic medicine, which makes them potentially useful for treating complex diseases characterized by multiple disrupted biological processes, e.g., cancer, inflammation, metabolic disorders, and neurodegenerative diseases. Thirdly, TCM target networks may help identify therapeutic targets, lead compounds, and herb-drug interactions in the future.

There are some limitations that should be noted. First of all, the presented study uses secondary data sets, so it is possible that the findings are determined by the quality of the used database. Second, the focus of this paper is placed on the target diversity and networks but not on the dose-response relationships, efficacy, or other important pharmacological aspects. As a result, further studies should be conducted to confirm the findings experimentally and investigate the biological relevance of common targets. Molecular docking and in vitro experiments should be conducted. Besides, clinical investigation would be helpful for determining the clinical value of the findings.

5. Conclusion

Through its molecular target overlap with conventional therapies, TCM has proved significant from a pharmacological point of view using the modern concepts of molecular pharmacology. There were 267 common molecular targets found among TCM herbs and synthetic drugs. They include key proteins involved in processes of inflammation, apoptosis, metabolism, endocrine function, and neuropharmacology. While herbs were associated with more target proteins than synthetic compounds, the median number of targets was 54 per herb compared with one target per synthetic drug. This confirms the multiplicity of targets typical of herbal medicines in contrast to synthetic drugs. Additionally, the network also showed overlaps between TCM herbs and synthetic drugs in key molecular hubs, including *PTGS2, TNF, BCL2, ACHE, AKT1, PPARG*, and *PPARA*. In conclusion, the above findings indicate that TCM could play a vital role in pharmacology in terms of the provision of biologically relevant multiplicity of interactions in disease studies and drug discovery. However, it is essential to note that the findings should not be viewed from the perspective of therapeutic efficacy but only at the level of molecular pharmacology.

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