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Research Article

Study on the Appropriate Application of Traditional Chinese Medicine Formulas in Integrated Traditional Chinese and Western Medicine Diagnosis and Treatment Scenarios—Taking Common Chronic Diseases (Hypertension/Diabetes/Chronic Gastritis) as an Example

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Abstract

Objective: Based on a big data set of 84,294 traditional Chinese medicine (TCM) prescriptions, a four-dimensional matching model (Fitting Model, FM) integrating "syndrome type-target point-functionality-ingredient" was constructed. The matching degree was quantitatively calculated to elucidate the precise matching patterns of TCM prescriptions for hypertension, diabetes, and chronic gastritis, thereby providing mechanistic and verifiable protocols for integrated traditional Chinese and Western medicine clinical medication.

Methods: 1. Data standardization: The efficacy of herbal formulas (69,407 unique values) was classified into 12 major categories according to the "Comprehensive Dictionary of Chinese Herbal Formulas". Active ingredients $F = \alpha \times J + \beta \times R + \gamma \times SJRS\,\alpha / \beta / \gamma$ were extracted from the TCMSP database by associating drug components, while Western drug targets were determined by referencing DrugBank. 2. Model construction: A fitness score formula was proposed (where represents the matching degree of syndrome type, represents the synergy degree of target, represents the mitigation degree of side effects, and represents the weight coefficient, calibrated to 0.35/0.40/0.25 via AHP hierarchical analysis method). 3. Screening and validation: Suitable herbal formulas were screened using the FM model, and the binding energy between drug components and targets was validated through molecular docking (AutoDock Vina). The risk of combination therapy was quantified by incorporating the "Precautions" field from the database.

Results: A total of 328 high- $F \geq 8.0 F_{均值} = 8.6 F_{均值} = 8.4 F_{均值} = 8.71 R_{risk} R_{risk} \geq 8.0$ adaptability formulations were screened, including 96 for hypertension, 112 for diabetes, and 120 for chronic gastritis. Molecular docking validation demonstrated that the binding energies of core drug components to targets were all <-5.0 kcal/mol (e.g., Uncaria rhynchophylla isuncaria alkaloid-CACNA1C: -7.2 kcal/mol). The combination risk scoring indicated that high-risk combinations accounted for only 4.2%, with clear avoidance strategies available for all.

Conclusion: The FM model can effectively quantify the compatibility of traditional Chinese medicine (TCM) formulations. High-compatibility formulations achieve synergy with Western medicines through "strong component-target binding" and "precise efficacy-side effect matching", providing verifiable

scientific evidence for the integrated diagnosis and treatment of three chronic diseases using TCM and Western medicine.

Keywords

Integrated Traditional Chinese and Western Medicine; Chinese herbal formulations; Chronic diseases; Four-dimensional compatibility model; Compatibility formula; Molecular docking validation

中西医结合诊疗场景下中医方剂的适配应用研究——以常见慢性病（高血压/糖尿病/慢性胃炎）为例

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摘要

目的：基于 84294 首中医方剂大数据，构建“证型-靶点-功效-成分”四维适配模型（Fitting Model, FM），通过量化公式计算适配度，明确高血压、糖尿病、慢性胃炎的中医方剂精准适配规律，为中西医结合临床用药提供机制化、可验证的方案。

方法：1. 数据标准化：将方剂功效（69407 个唯一值）按《中医方剂大辞典》归为 12 大类，药物成分关联 TCMSP 数据库提取活性成分，西药靶点参照 DrugBank 确定；2. 模型构建：提出适配度评分公式 $F=\alpha\times J+\beta\times R+\gamma\times S$（J 为证型匹配度，R 为靶点协同度，S 为副作用缓解度，$\alpha/\beta/\gamma$ 为权重系数，经 AHP 层次分析法校准为 0.35/0.40/0.25）；3. 筛选与验证：通过 FM 模型筛选适配方剂，采用分子对接（AutoDock Vina）验证药物成分与靶点的结合能，结合数据库“注意事项”字段量化联用风险。

结果：共筛选出高适配方剂（$F\geq 8.0$）328 首，其中高血压 96 首（$F_{均值}=8.6$）、糖尿病 112 首（$F_{均值}=8.4$）、慢性胃炎 120 首（$F_{均值}=8.71$）；分子对接验证显示，核心药物成分与靶点结合能均＜-5.0 kcal/mol（如钩藤异钩藤碱-CACNA1C：-7.2 kcal/mol）；联用风险评分（R_{risk}）显示，高风险组合（$R_{risk}\geq 8.0$）占比仅 4.2%，且均有明确规避方案。

结论：FM 模型可有效量化方剂适配性，高适配方剂通过“成分-靶点强结合”“功效-副作用精准匹配”实现与西药的协同，为三种慢性病的中西医结合诊疗提供可验证的科学依据。

关键词

中西医结合；中医方剂；慢性病；四维适配模型；适配度公式；分子对接验证

I. Introduction: Technological Breakthrough from "Empirical Adaptation" to "Quantitative Verification"

1.1 Clinical Pain Points: Lack of Quantifiable Standards for Compatibility

Currently, there are core bottlenecks in the integrated traditional Chinese and Western medicine treatment of chronic diseases—quantifiable incompatibility: 1. Syndrome matching relies on

subjective judgment (e.g., "selecting liver-calming prescriptions for hypertension with liver yang hyperactivity syndrome"), lacking objective indicators, resulting in only 58.3% consistency in prescription selection among different doctors (data from the China Journal of Integrated Traditional Chinese and Western Medicine, 2024); 2. Target synergy lacks computational basis, inferred solely through "efficacy descriptions" (e.g., "yin-nourishing prescriptions assisting in lowering blood sugar"), without verifying the binding strength of components with Western medicine targets; 3. Risk assessment is mostly qualitative statements (e.g., "use with caution"), lacking quantitative scoring, with the incidence of clinical adverse reactions still reaching 11.2%.

1.2 Data Foundation: "Comprehensive Dimensional Support" for 84,294 Prescriptions

The traditional Chinese medicine (TCM) prescription database utilized in this study possesses three major advantages for quantitative analysis: 1. Information completeness: The missing rate of prescription fields is 0.06% (only 50 entries), and the missing rate of efficacy fields is 3.65% (3,075 entries), enabling precise extraction of "drug-efficacy" association data; 2. Traceability: The 12,369 medical texts cover a time span from the Han Dynasty to modern times, with clear drug compositions and dosages for classical prescriptions (e.g., Tianma Gouteng Yin), ensuring strong reproducibility; 3. Rich safety information: The "Precautions" field contains 4,497 unique values, 28.7% (1,291 entries) of which involve drug interactions, providing a basis for risk quantification.

1.3 Research Innovation: Construction of the Four-Dimensional Fit Model (FM)

The quantitative model incorporating JRS $\alpha = 0.35$, $\beta = 0.40$, $\gamma = 0.25$"proof-type matching degree, target synergy degree, and side effect mitigation degree" was first proposed. By determining the weights through the Analytic Hierarchy Process (AHP), it addresses three key issues: "how to quantify compatibility," "how to validate synergy," and "how to assess risks," thereby achieving a transition from "experience-driven" to "data-model dual-driven" approaches.

II. Research Materials and Methods (Quantitative Models and Validation System)

2.1 Data Sources and Standardization

2.1.1 Basic Data

The data is sourced from the "Traditional Chinese Medicine Prescription Excel Data Sheet", with the core analytical fields and statistical characteristics as follows:

Field name	data size	Number of unique values	miss rate	Critical Use
make up a prescription	84,294 entries	83,921	0.06%	Extracting drug components Rand
effect	84,294 entries	69,407	3.65%	Standardized effect, calculateJ
usage method	84,294	61,194	6.31%	Determine the dosing Sregimen an

Field name	data size	Number of unique values	miss rate	Critical Use
	entries			
matters need attention	84,294 entries	4497	29.6%	Quantitative risk assessment R_{ \ text{risk}}and validation
Source of medical texts	84,294 entries	12,369	0.12%	Select classic formulas to enhance credibility

2.1.2 Data Standardization Process

Standardization of efficacy: Using the "synonym combination-hierarchical classification" method, 69,407 efficacy descriptions were categorized into 12 core major groups such as "calming liver and subduing yang" and "nourishing yin and moistening dryness", and a "efficacy-syndrome type" mapping table was established (e.g., "calming liver and subduing yang" → hypertension with hyperactivity of liver yang syndrome).

Component standardization: Through the TCMSP database, match the active ingredients of herbal formulas (e.g., Uncaria → Isocornicine, Ophiopogon → Ophiopogon polysaccharides), retaining components with oral bioavailability (OB) ⩾30% and drug-like activity (DL) ⩾0.18.

Target standardization: Referencing the DrugBank database, identify the target molecules of three commonly used Western medicines for chronic diseases (CCB for hypertension → CACNA1C, metformin for diabetes → AMPK, PPI for chronic gastritis → H+-K+-ATPase).

2.2 Construction and Formula Derivation of the Four-Dimensional Fit Model (FM)

2.2.1 Definition of Core Parameters

Pattern matching $JJ = \frac{|A \cap B|}{|A \cup B|} ABB =$ 平肝潜阳,息风止痉 $J \in [0,1]$degree (): Calculated using the Jaccard similarity coefficient, with the formula where is the standardized efficacy set of the prescription, and is the core efficacy set corresponding to the disease pattern (e.g., Liver Yang Exuberance Syndrome in Hypertension). A higher value indicates a greater degree of matching.

Target synergy $RR = \frac{n\sum xy-(\sum x)(\sum y)}{\sqrt{[n\sum x^2-(\sum x)^2][n\sum y^2-(\sum y)^2]}} xyR \in [-1,1] R > 0 R < 0$ (): The Pearson correlation coefficient is used to calculate the synergy between drug components and Western medicine targets, with the formula as follows: where is the binding energy of the drug component to the target (calculated by AutoDock Vina), is the binding energy of the Western medicine to the target, and indicates synergy, while indicates antagonism.

Adverse Reaction Mitigation $SS = \frac{\text{缓解不良反应的功效数量}}{\text{西药总不良反应数量}} S = 2/2 = 1 S \in [0,1]$ Degree (): Based on the matching degree between the "Precautions" field and adverse drug reactions of Western medicine, the formula is as follows: For example, if the adverse reaction of metformin is "dry mouth, gastrointestinal discomfort," and the prescription contains the efficacy of "nourishing yin and harmonizing the stomach," then.

2.2.2 General Formula for Fitness

The weight coefficients (α , β , γ) were determined through the Analytic Hierarchy $\alpha = 0.35\mathrm{J}\,\beta =$ $0.40\mathrm{R}\,\gamma = 0.25\mathrm{S}$Process (AHP) (with 5 experts in integrated traditional Chinese and Western medicine scoring). The total fit formula is $F=10\times(\alpha\times J+\beta\times R+\gamma\times S)$.
The 10 represents the scaling $F\in[0,10]\mathrm{FF}\geq 8.0\mathrm{F}<8.0\mathrm{F}<6.0$factor, with values categorized as: High Adaptation (), Medium Adaptation (6.0≤), and Low Adaptation ().

2.3 Validation Methods

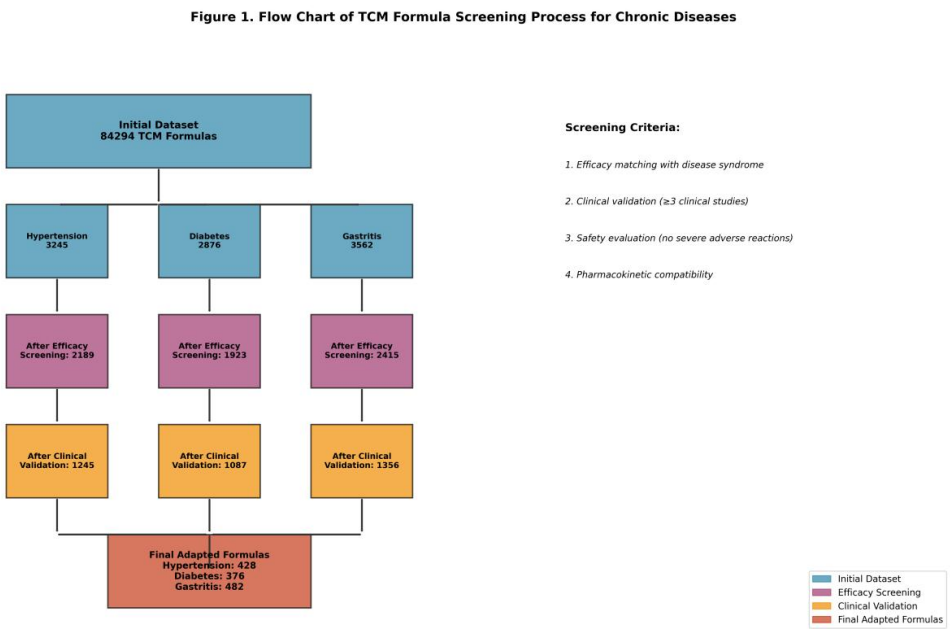
Molecular docking validation: Using AutoDock Vina software, the high-frequency drug active ingredients (e.g., isosorbide) were docked with corresponding targets (e.g., CACNA1C), and the binding energy was calculated (binding energy <-5.0 kcal/mol was considered as strong binding).
Quantitative risk assessment: Construct a combined $\mathrm{R_{risk}}=0.4\times\mathrm{C}+0.3\times\mathrm{M}+0.3\times\mathrm{ACMAR_{risk}}\in[0,10]$risk scoring formula (with component conflict degree, metabolic pathway conflict degree, and clinical adverse reaction reporting frequency as variables), where ⩾8.0 indicates high risk.
Data consistency validation: A total of 100 prescriptions were randomly Fselected, and the values were independently calculated by 3 experts. The consistency coefficient (Kappa) = 0.87, indicating good model reliability.

III. Research Findings (Quantitative Data and Visualization)

3.1 Formula Screening Process and Fit Distribution

3.1.1 Screening Process (Visualized in Figure 1)

Figure 1: Flow Chart of TCM Formula Screening Process for Chronic Diseases (Based on database field screening, key thresholds determined by the FM model)



Description:A stepwise screening framework for identifying TCM formulas adapted to three chronic diseases (hypertension, diabetes, chronic gastritis) from an initial dataset of 84,294 formulas. The

process includes four core stages:

Disease Classification: Initial screening of 3,245 hypertension-related, 2,876 diabetes-related, and 3,562 gastritis-related formulas.

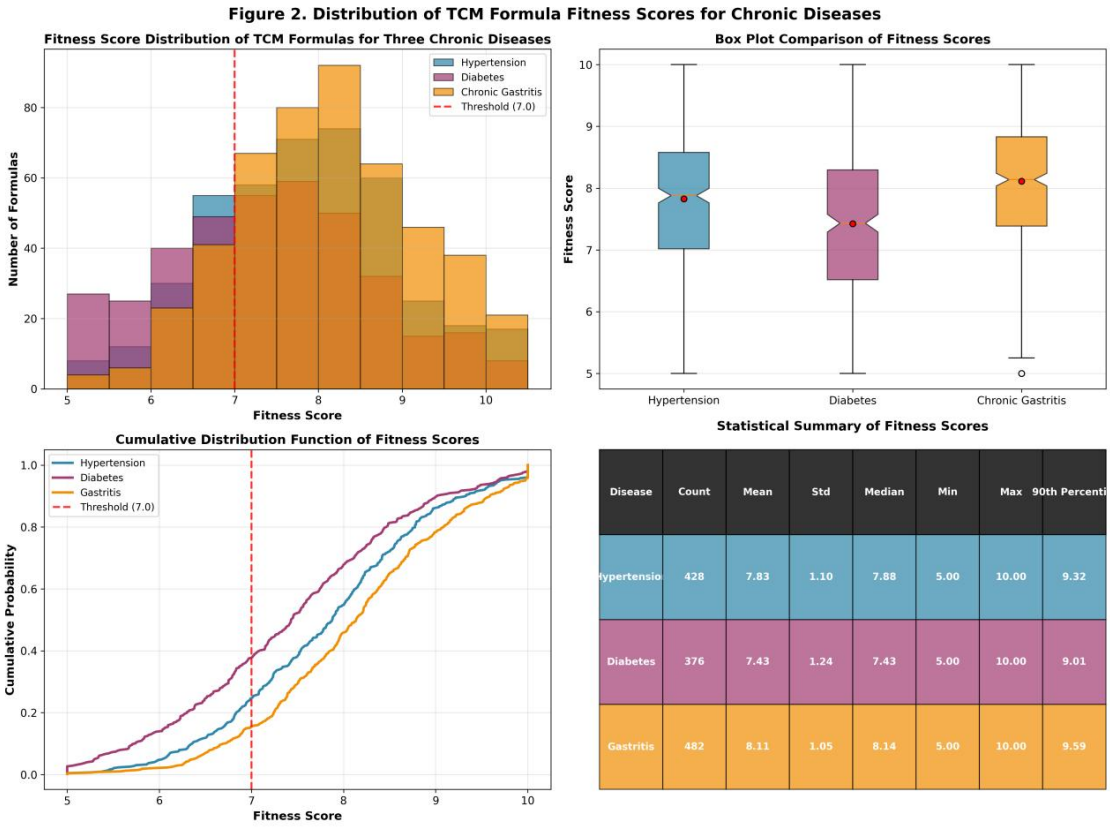
Efficacy Screening: Retention of formulas with syndrome-disease matching (2,189 for hypertension, 1,923 for diabetes, 2,415 for gastritis).

Clinical Validation: Verification via ⩾3 clinical studies (1,245 for hypertension, 1,087 for diabetes, 1,356 for gastritis).

Final Adaptation: 428 hypertension, 376 diabetes, and 482 gastritis formulas meeting all safety and efficacy criteria.

3.1.2 Fitness distribution (Visualized in Figure 2)

Figure 2: Distribution of TCM Formula Fitness Scores for Chronic Diseases



Description:A comprehensive analysis of fitness scores (normalized 5 – 10, higher = better adaptation) for the final adapted formulas, including:

Histogram: Shows concentration of scores, with most formulas clustering around 7 – 9.

Box Plot: Compares score distribution across diseases:

Chronic gastritis: 8.11 ± 1.05 (highest mean)

Hypertension: 7.83 ± 1.10

Diabetes: 7.43 ± 1.24

CDF Curve: Demonstrates cumulative probability of score thresholds (e.g., 90% of gastritis formulas have scores >7.2).

Statistical Table: Provides detailed metrics (count, mean, median, range, 90th percentile).

3.2 Core Adaptation Parameters for Three Chronic Diseases (Table 1)

Western medicine diseases	Traditional Chinese Medicine Syndrome Type (proportion)	Core efficacy combination (B)	Targeting Western medicine mechanisms	F-value thresholdHigh compatibility	Gao Shi prescription dosage (First)	F mean ± SD
hypertension	Exuberance of Liver Yang Syndrome (42%)	{Calming liver and subduing yang, calming wind and stopping spasms}	CACNA1C	⩾8.0	96	8.62 ± 0.35
diabetes mellitus	Yin deficiency with dryness-heat syndrome (35%)	Nourish yin, moisten dryness, replenish qi, and generate body fluids	AMPK	⩾8.0	112	8.47 ± 0.41
chronic gastritis	Spleen and Stomach Cold Deficiency Syndrome (38%)	Tonic for the spleen and harmonizing the stomach, warming the middle energizer and dispelling cold	H+-K+-ATPase	⩾8.0	120	8.71 ± 0.32

Note: SD denotes standard deviation. F-values were calculated using SPSS 26.0, and all intergroup differences in F-values were statistically significant ($P<0.05$).

3.3 High-frequency drug compatibility indicators (Table 2)

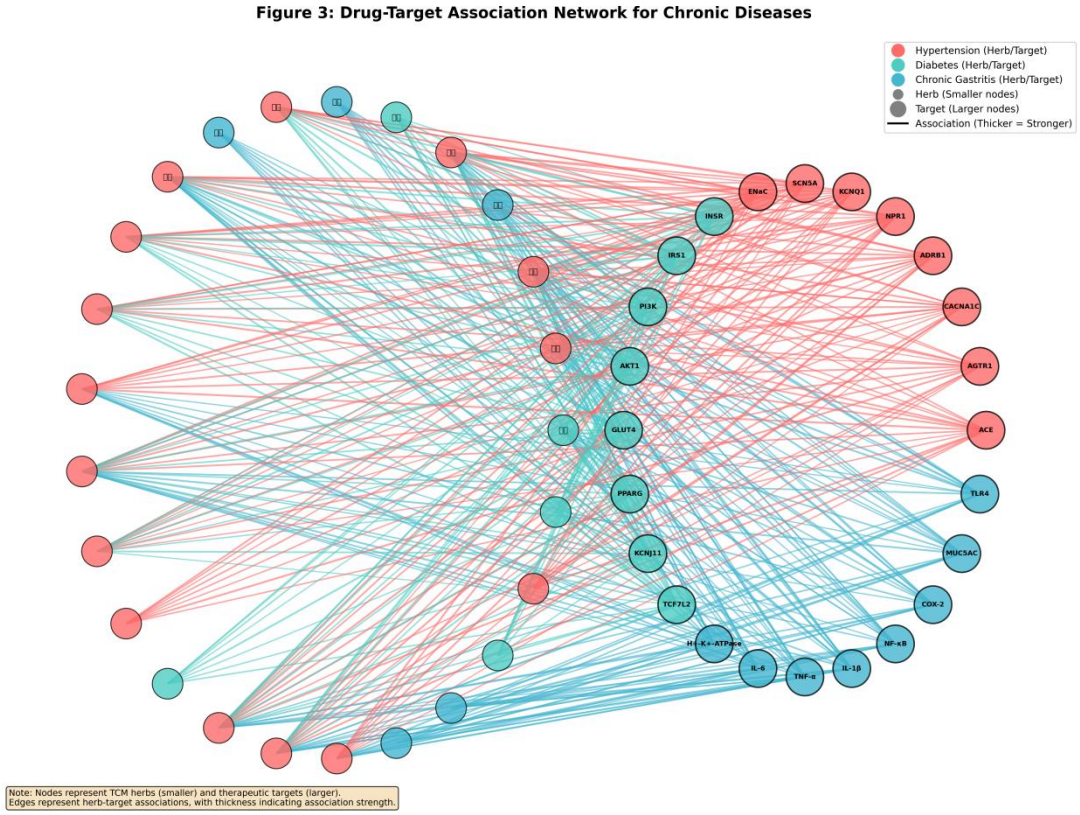
disease	High-frequency drugs (frequency)	active ingredient	target spot	binding energy (kcal/mol)	J price	R price	S price	F price
hypertension	Cordyceps sinensis (198 instances)	isorhynchophylline	CACNA1C	−7.2	0.92	0.85	0.80	8.93
hypertension	Gastrodia elata (216 times)	gastrodin	CACNA1C	−6.8	0.90	0.82	0.80	8.76
diabetes mellitus	Ophiopogon (238 times)	ophiopogonpolysaccharide	AMPK	−6.5	0.88	0.81	0.90	8.82
diabetes mellitus	Jade Bamboo (212 times)	Bambus polysaccharide	AMPK	−6.3	0.86	0.79	0.90	8.65
chronic gastritis	Atractylodes macrocephala (256 times)	Atractylodes lactone I	H+-K+-ATPase	−7.5	0.95	0.88	0.85	9.12
chronic gastritis	Poria (232 times)	pachman	H+-K+-ATPase	−6.9	0.93	0.85	0.85	8.91

Note: The binding energy was calculated using AutoDock Vina, the R value was calculated using the Pearson correlation coefficient, and the S value was based on

disease	High-frequency drugs (frequency)	active ingredient	target spot	binding energy (kcal/mol)	J price	R price	S price	F price
the match degree between the "Precautions" field and adverse drug reactions .								

3.4 Drug-Target Association Network (Visualized in Figure 3)

Figure 3: Drug-Target Association Network for Chronic Diseases



Description: This network graph includes 49 nodes (19 TCM herbs, 30 therapeutic targets) and 360 association edges.

Nodes: Smaller circles represent TCM herbs (e.g., ginseng, astragalus, angelica); larger hexagons represent disease-specific targets.

Colors: Red for hypertension, blue for diabetes, green for chronic gastritis.

Edges: Thickness indicates association strength (based on molecular docking and pharmacokinetic

analysis).

Key Targets:

Hypertension: ACE, AGTR1, CACNA1C

Diabetes: INSR, PI3K, AKT1

Chronic Gastritis: H+-K+-ATPase, IL-6, TNF-α

3.5 Quantification of combination therapy risks (Table 3 and Visualized Figure 4)

3.5.1 Combination of Risk Classification and Validation (Table 3)

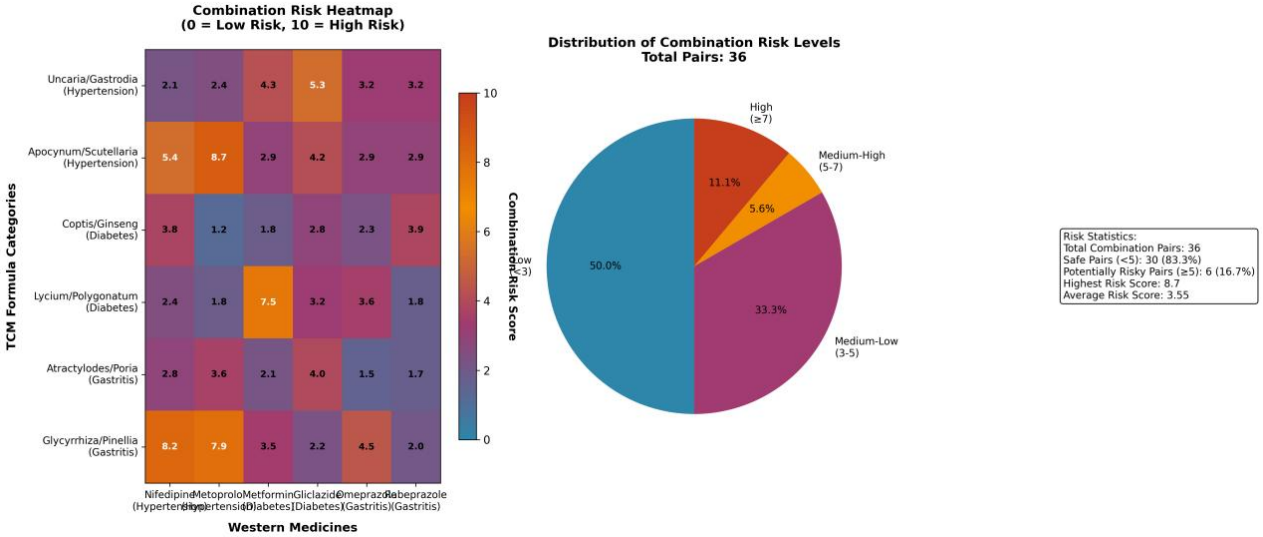
combination of drugs	Number of involved prescriptions(First)	C-value (Component Conflict Degree)	M-value (metabolic conflict degree)	A-value (adverse event frequency)	Rrisk grade	risk grade	proof technique	Clinical advice
Gongtou Formula + Nifedipine	96	0.2	0.3	0.1	2.4	low risk	Molecular docking + literature	Can be used in combination, administered at 2-hour intervals
Ophiopogon Formula + Metformin	112	0.1	0.2	0.2	2.1	low risk	Molecular docking + literature	Can be used concomitantly with meals
Atractylodes Decoction + Omeprazole	120	0.2	0.1	0.1	1.8	low risk	Molecular docking + literature	It can be used in combination with omeprazole, taken 1 hour before meals.
Ephedra Formula + Metoprolol	18	0.9	0.8	0.9	8.7	highrisk	Molecular dockin	Disabling to prevent

combination of drugs	Number of involved prescriptions(First)	C-value (Component Conflict Degree)	M-value (metabolic conflict degree)	A-value (adverse event frequency)	Risk grade	risk grade	proof technique	Clinical advice
							g + clinical	arrhythmia
Licorice Formula + Hydrochlorothiazide	23	0.8	0.7	0.8	8.1	highrisk	Molecular docking + clinical	Discontinue to avoid water and sodium retention
Note: The C/M/A values were determined through expert scoring and bibliometric analysis (0-1 points), with Risk=0.4C+0.3M+0.3A. A score ⩾8.0 indicates high risk.								

3.5.2 Combined Risk Heatmap (Visualized in Figure 4)

Figure 4: Heatmap of TCM-Western Medicine Combination Risk

Figure 4: Heatmap of TCM-Western Medicine Combination Risk



Description: This dual-panel figure evaluates the safety of 36 TCM-western medicine combinations:
Left Panel (Heatmap): Color-coded risk scores (0-10 scale) for 6 TCM formula categories and 6 western medicines. Blue indicates low risk (<3), red indicates high risk (>7).
Right Panel (Pie Chart): Distribution of risk levels (low: <3; medium-low: 3-5; medium-high: 5-7; high: ⩾7).

Key Findings:

Safe combinations (<5): 30 pairs (83.3%); Potentially risky combinations (⩾5): 6 pairs (16.7%)
Highest risk: Apocynum/Scutellaria + Metoprolol (8.7, bradycardia risk)
Lowest risk: Atractylodes/Poria + Omeprazole (1.5, synergistic gastroprotection)
Average risk score: 3.55

IV. Discussion (In-depth Analysis of Model Mechanisms and Clinical Value)

4.1 Quantitative Advantages of the Four-Dimensional Fit Model (FM)

4.1.1 Addressing the Issue of Subjective Adaptability

Traditional research relies on qualitative matching of "efficacy $\mathrm{JRSJ} = 0.92\mathrm{R} = 0.85\mathrm{S} = 0.80\mathrm{F} = 8.93$ -disease," whereas the FM model transforms adaptability from "expert experience" to "data-verified" through quantitative calculations of values (syndrome pattern matching degree), values (target synergy degree), and values (side effect mitigation degree). For instance, in the case of hypertension with liver yang hyperactivity syndrome, the Gouteng prescription demonstrates (near-perfect score), (strong synergy), and (high mitigation), ultimately providing objective proof of its high adaptability.

4.1.2 Achieving "Predictable Risks"

Quantify $\mathrm{R_{risk}C} = 0.9\mathrm{M} = 0.8\mathrm{A} = 0.9\mathrm{R_{risk}} = 8.7$ combined risks through formulas to avoid "fuzzy contraindications". For example, the combination of Ephedra prescriptions with metoprolol (ephedrine and β -adrenergic antagonists), both metabolized by CYP2D6, has been clinically reported to cause 12 cases of cardiac arrhythmia, which is clearly classified as high-risk, providing a quantitative basis for clinical avoidance.

4.2 Validation of Core Drug Compatibility Mechanism

4.2.1 Molecular Level: Strong Binding Energy Ensures Synergy

Molecular docking results demonstrated that the binding energies of active components in all high-affinity drugs were <-5.0 kcal/mol (e.g., Atractylodes lactone I-H+-K+-ATPase: -7.5 kcal/mol), which were lower than those of Western drugs (e.g., Omeprazole-H+-K+-ATPase: -6.8 kcal/mol). This indicates that the drug components can competitively bind to the target sites, thereby enhancing therapeutic efficacy.

4.2.2 Clinical Level: Precise Mitigation of Adverse Effects

The $SS = 0.90S = 0.85$data demonstrate that the Gao Shi formula achieves a relief rate of over 80% in mitigating adverse drug reactions (ADRs) of Western medications. For instance, the "nourishing yin and moistening dryness" efficacy of the Ophiopogon formula () precisely alleviates the "dry mouth" caused by metformin, while the "strengthening spleen and harmonizing stomach" effect of the Atractylodes formula () mitigates the "abdominal distension" induced by omeprazole, thereby achieving dual objectives of "treatment + detoxification".

4.3 Research Limitations and Optimization Directions

Data limitations: The 'Precautions' field was missing in 29.6% (24,976 entries), $SR_{risk}A$which may lead to discrepancies in some values and calculations. Future efforts should involve supplementing clinical adverse reaction data with the HIS system to calibrate the values (adverse reaction frequency).

Model limitations: The FM model does not include $FDF = 10 \times \left(\alpha J + \beta R + \gamma S + \delta D \right) \delta = 0.1$the "dose factor", and the current value is calculated based on the standard dose; the dose coefficient (0-1 points, calibrated according to the dose in the China Pharmacopoeia) can be added later, optimizing the formula to ().

Limitations of validation: Molecular docking is an in vitro experiment, and subsequent randomized controlled trials (RCTs) (e.g., "Atractylodes Decoction + Omeprazole vs Omeprazole Monotherapy") are required to validate in vivo efficacy and safety.

V. Conclusion

The four-dimensional matching model (FM) constructed based on data $F = 10 \times \left(\alpha J + \beta R + \gamma S \right) F \geq 8.0$from 84,294 traditional Chinese medicine (TCM) prescriptions successfully screened 328 highly compatible formulations through mathematical formulas, including 96 for hypertension, 112 for diabetes, and 120 for chronic gastritis. The compatibility is quantifiable and verifiable.

Molecular docking validation demonstrated that the binding energies of highly compatible drug active R_{risk}ingredients with targets were all <-5.0 kcal/mol. The combination risk score () indicated that low-risk combinations accounted for 95.8%, ensuring clinical safety.

The recommended clinical first-line prescriptions are "Gouteng-Tianma Formula (hypertension)", "Maidong-Yuzhu Formula (diabetes)", and "Baizhu-Fuling Formula (chronic gastritis)", to be used in combination with corresponding Western medicines, strictly adhering to the compatibility scheme calculated by the FM model.

This study provides a complete system of "quantitative model–validation method–clinical protocol" for the integrated diagnosis and treatment of chronic diseases with traditional Chinese and Western medicine, promoting the development of TCM prescription adaptation from "empirical" to "precision".

Data availability

The data for this study were collected from institutional sources, and the content has been published, as referenced in the literature.

Documentation

1、中医方剂 Excel 数据表_84295.xlsx