



Artificial intelligence models Traditional Chinese Medicine principles to integrate with biomedicine

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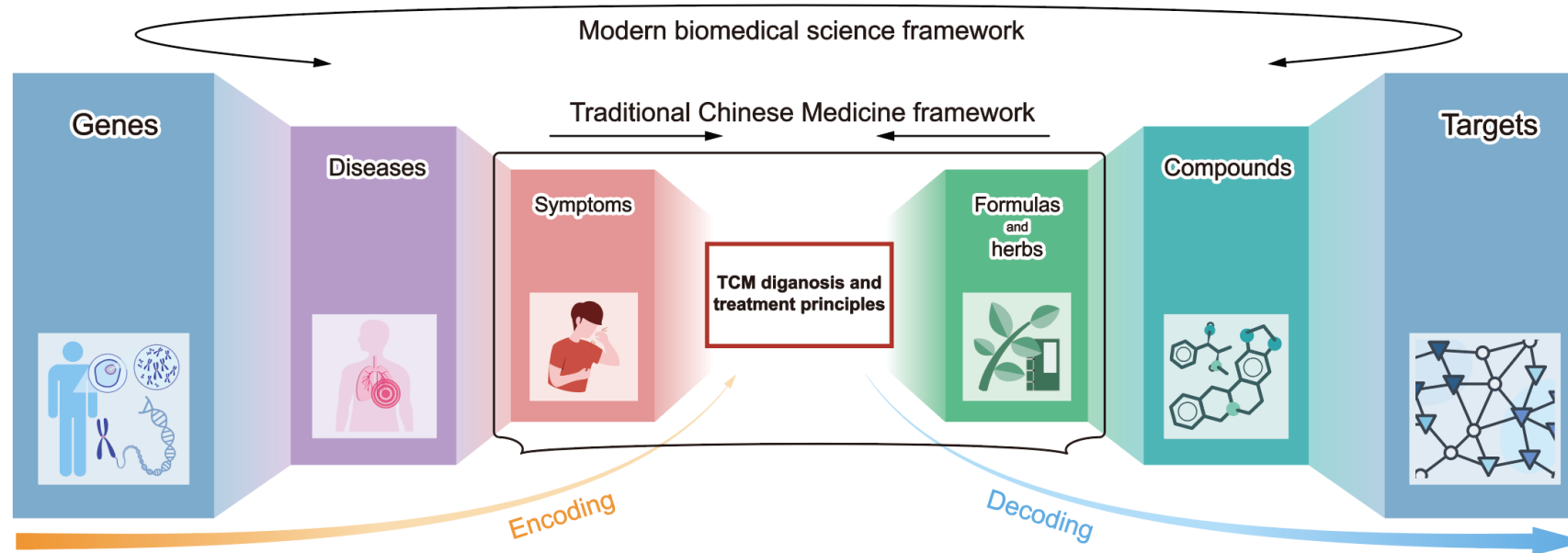
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Background and question

Reductionist / bottom-up: linking clinical manifestations to molecular causes and therapeutic targets



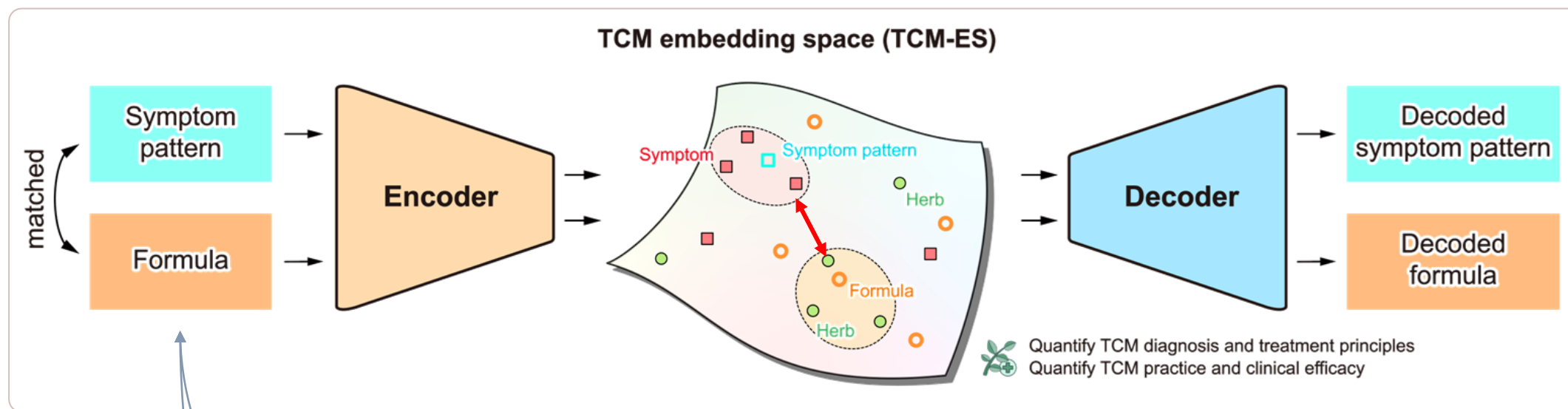
- TCM provides a complementary **holistic** and top-down perspective on complex **patient-specific** symptom-patterns.
- Yet this diagnosis–treatment logic remains largely qualitative, limiting systematic quantitative investigation and integration with modern biomedicine.

Question: Can empirical symptom-pattern–formula relationships be transformed into a **quantitative and interpretable** representation?



A data-driven encoding–decoding framework for quantifying TCM practice

a shared low-dimensional coordinate system for symptoms, herbs, symptom patterns and formulas



Historical TCM formula records

84,491 curated records

↓
26,339 model-eligible records

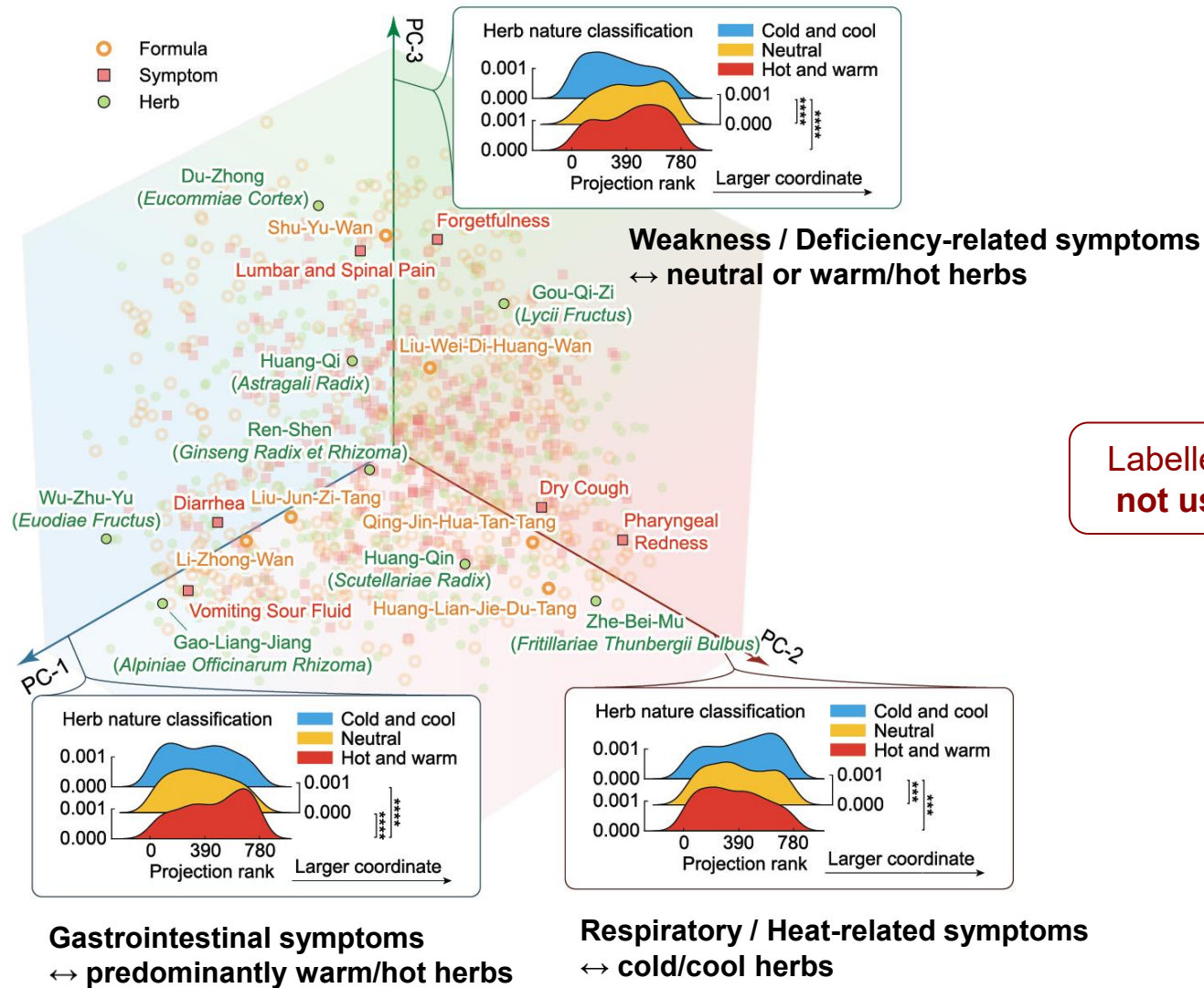
Table 2: Example of TCM Formula Record

Symptom pattern	Loose stools; Decreased appetite; Emaciation; Fatigue of the spirit; Shortness of breath
Syndromes (masked)	Lung-Qi Deficiency (肺气虚证), Spleen-Qi Deficiency (脾气虚证)
Formula	<i>Panax ginseng</i> (Ren-Shen, 人参), <i>Poria cocos</i> (Fu-Ling, 茯苓), <i>Atractylodis Macrocephalae</i> (Bai-Zhu, 白术), <i>Glycyrrhiza uralensis</i> (Gan-Cao, 甘草)

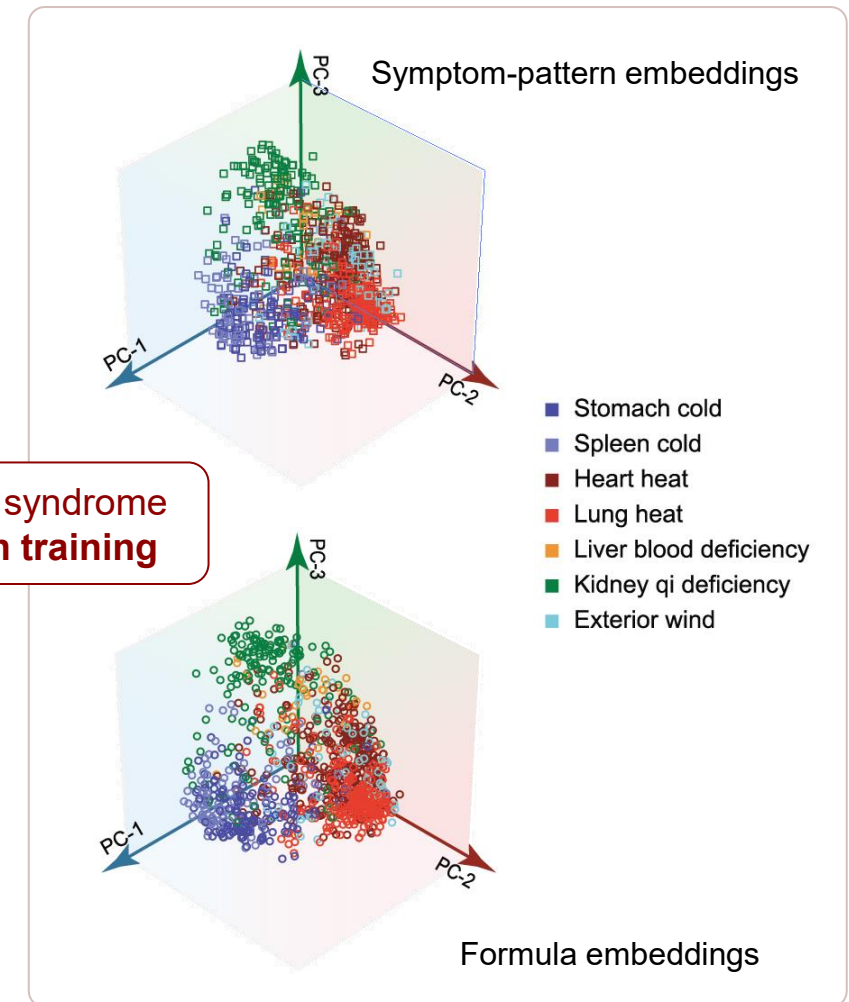
Not used for core model training

- Syndrome labels
- Explicit TCM-principle annotations
- Clinical outcomes
- Biomedical information

The learned TCM-ES aligns with TCM principles not used in training



Labelled by syndrome
not used in training



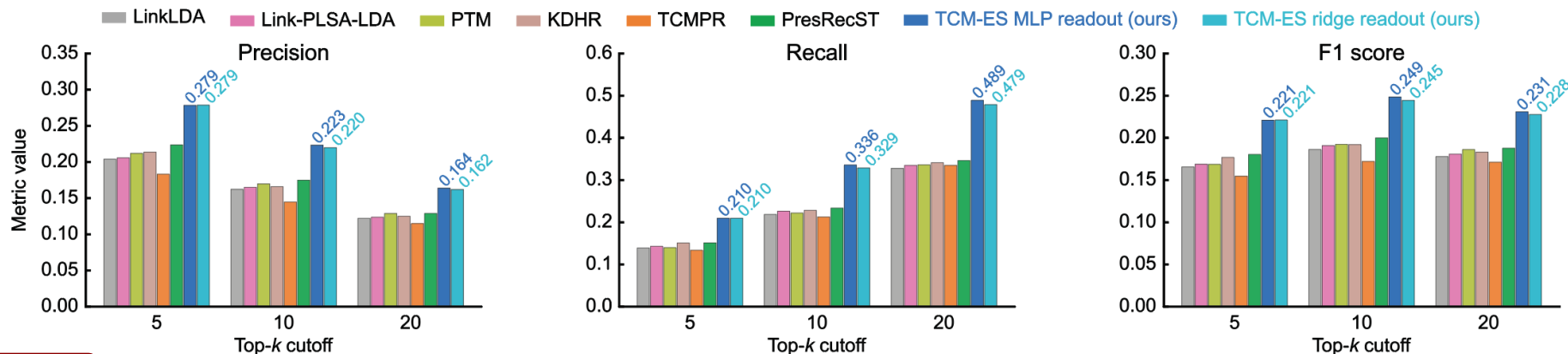
The TCM-ES geometry learned from symptom-pattern–formula mappings is systematically associated with conventional TCM principles.



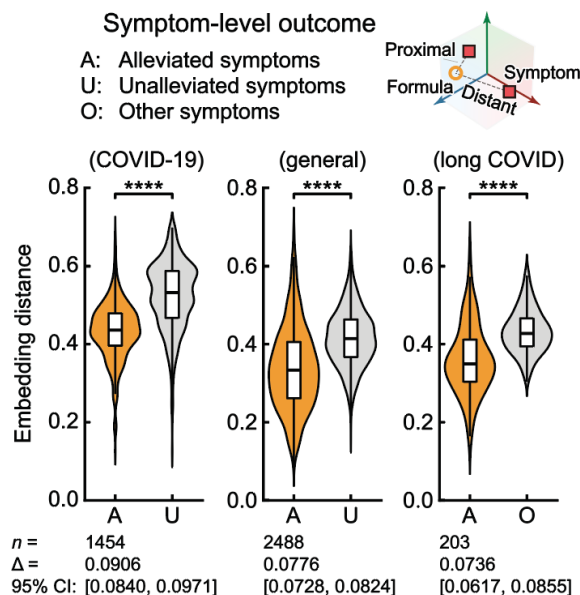
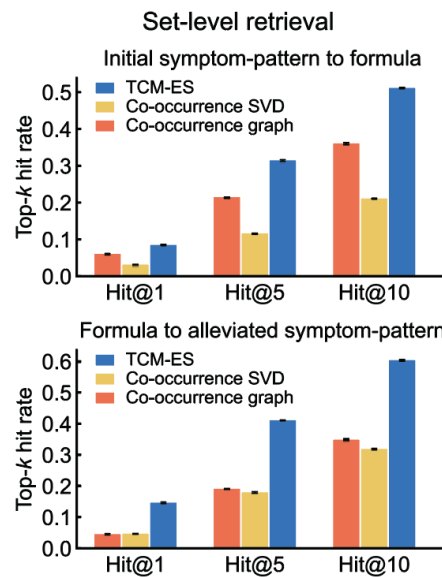
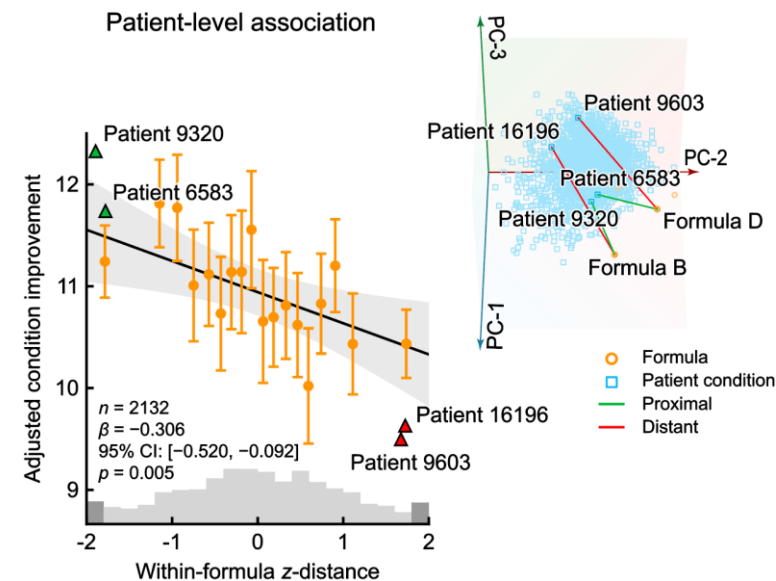
TCM-ES supports downstream prediction and clinical analyses

Formula prediction

Frozen TCM-ES representations were evaluated for formula prediction on the public TCM-PD benchmark.



Quantification of clinical outcomes

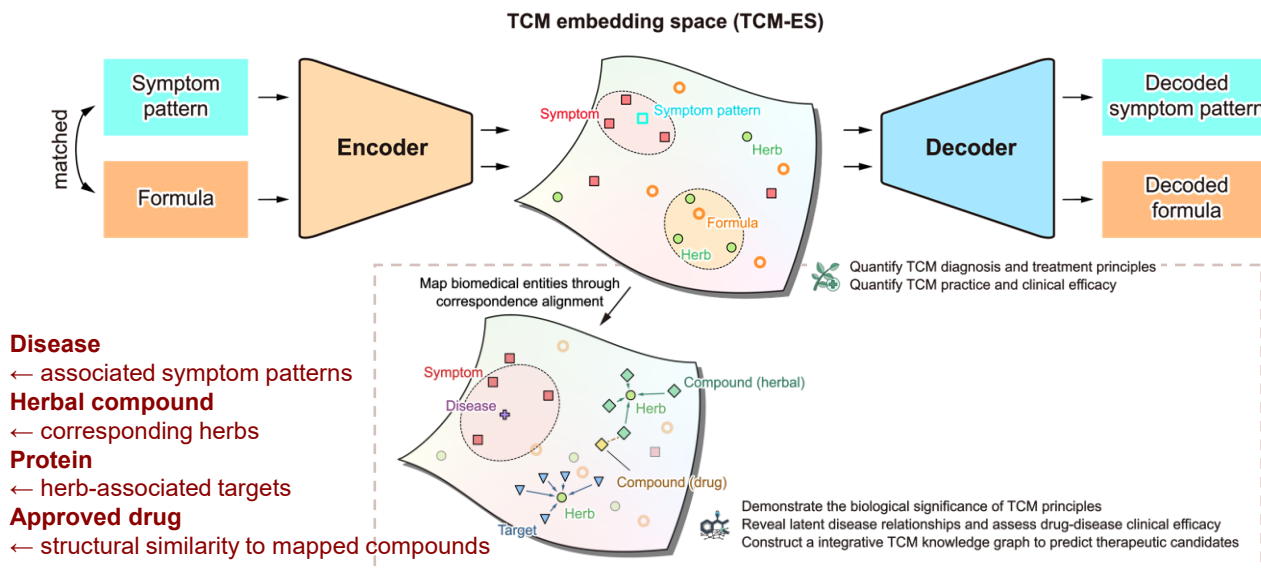


TCM-ES geometry captures information relevant to treatment matching and subsequent clinical outcomes across multiple scales.

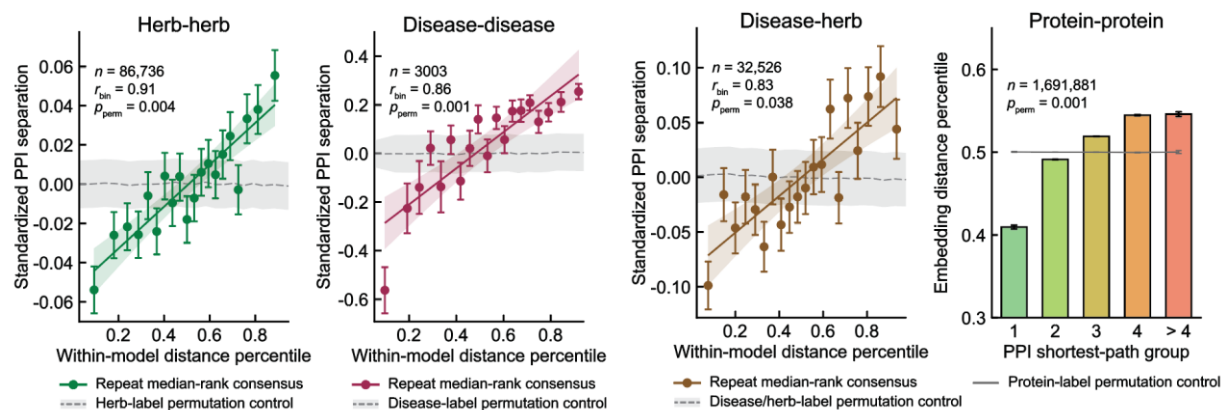


Post-hoc biomedical mapping reveals systematic concordance

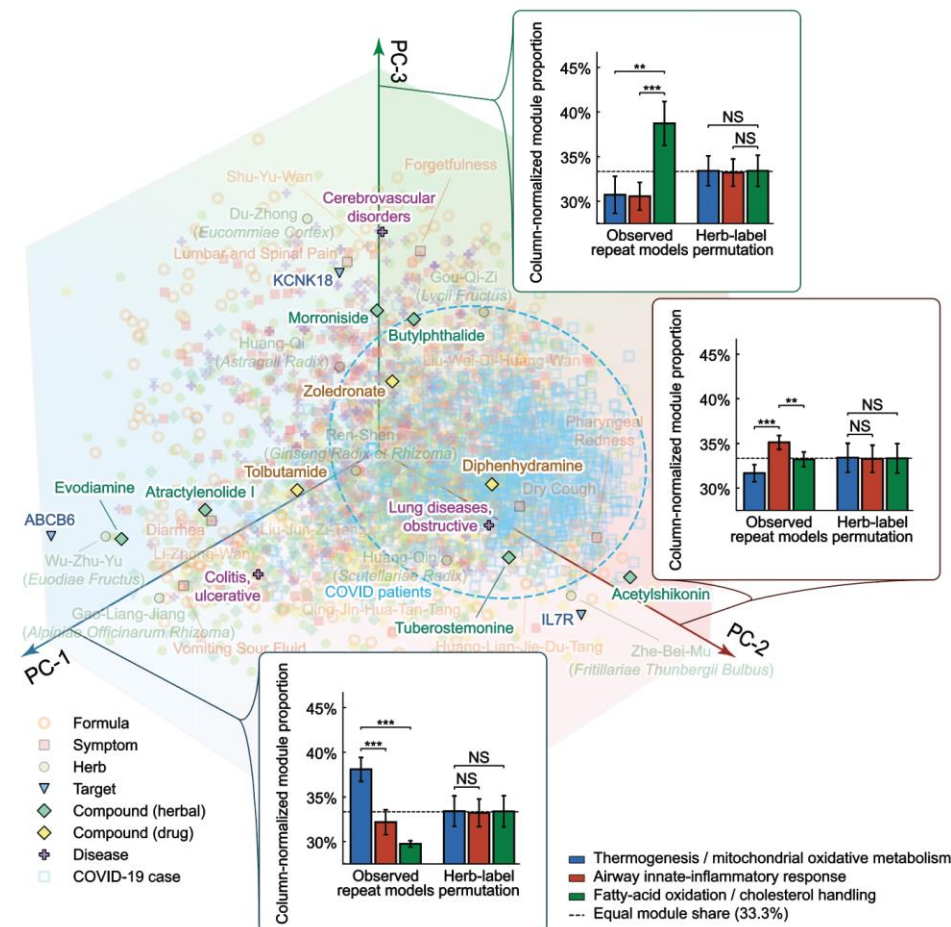
Post-hoc mapping while core TCM-ES fixed



Closer embedding relationships correspond to closer molecular relationships in the human PPI network.



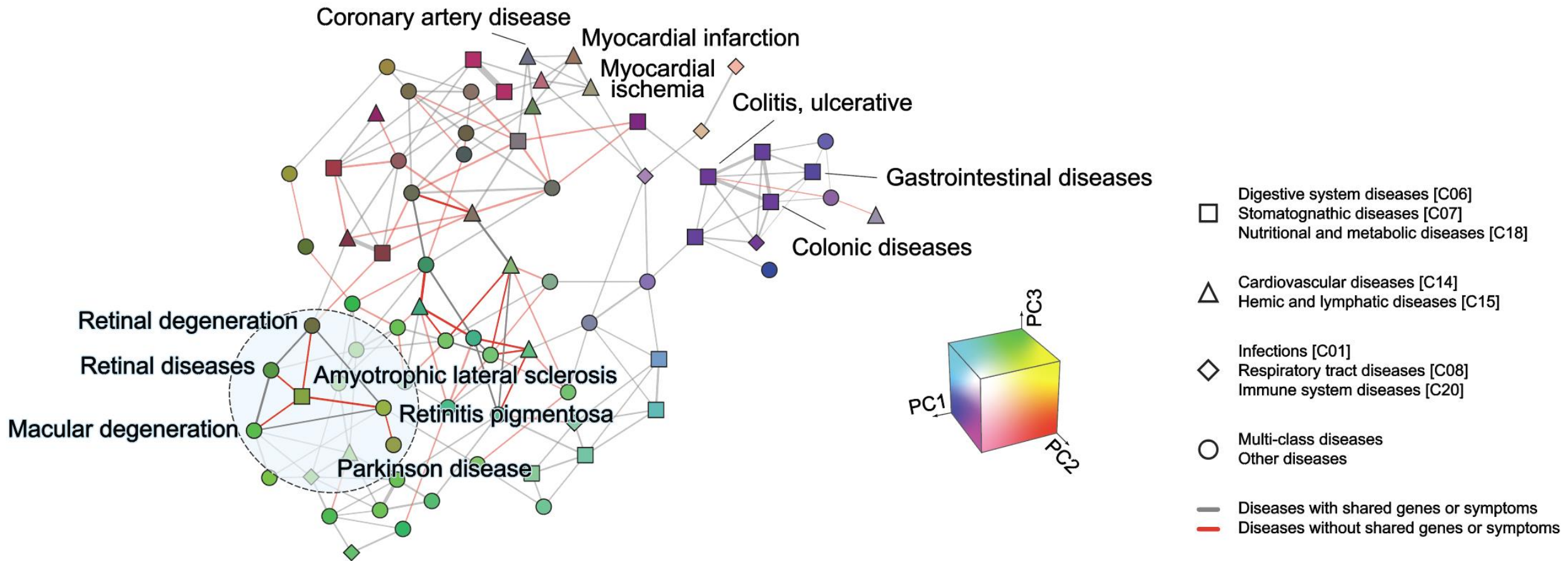
Association with key biological processes



TCM-ES learned without biomedical information nevertheless shows concordance with established biological organization.

TCM-ES provides a symptom-pattern view of disease relationships

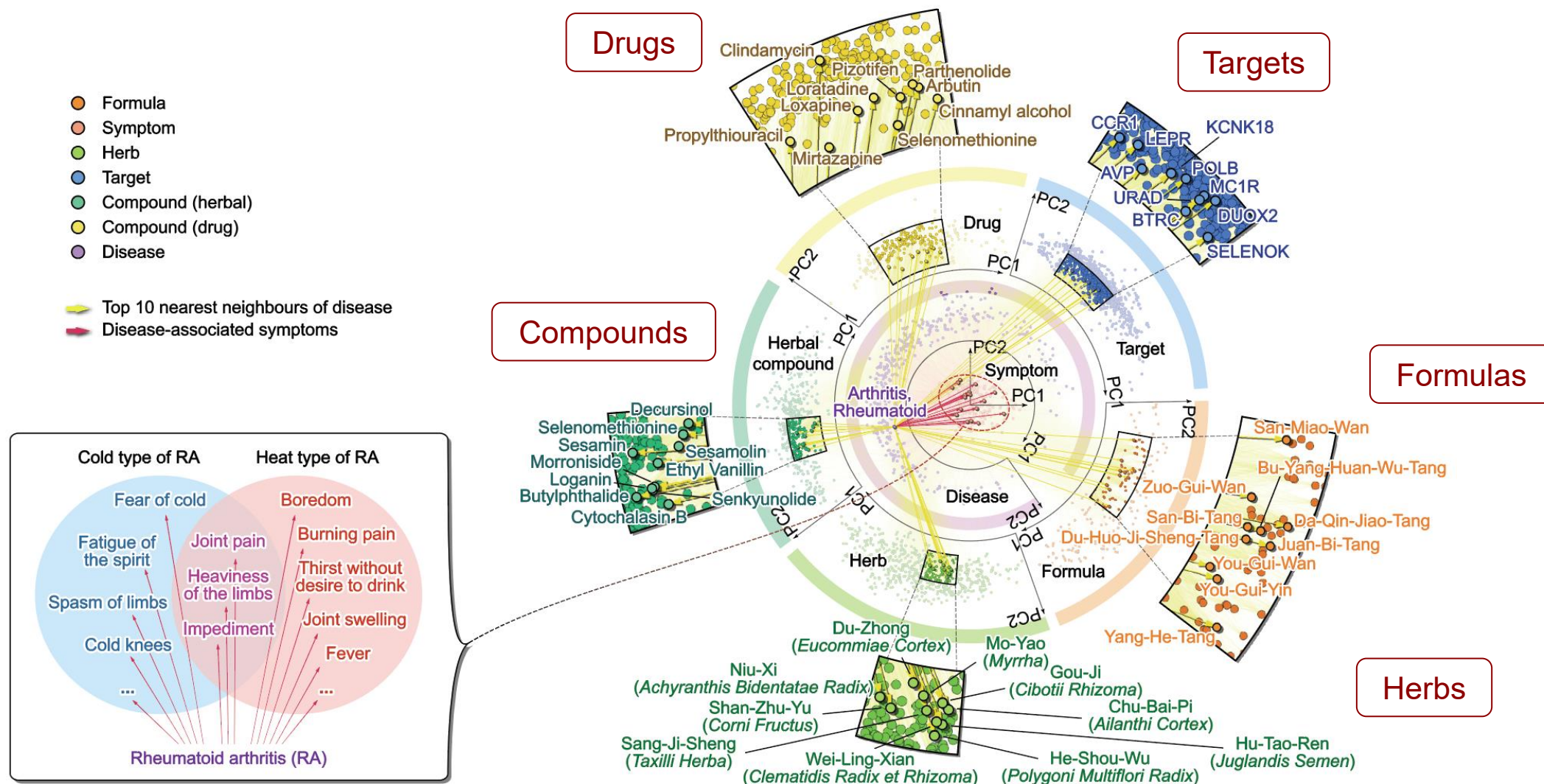
- A disease nearest-neighbour network based on embedding proximity in the integrated TCM-ES.
- Red edges indicate disease pairs **without** shared annotated genes or symptoms





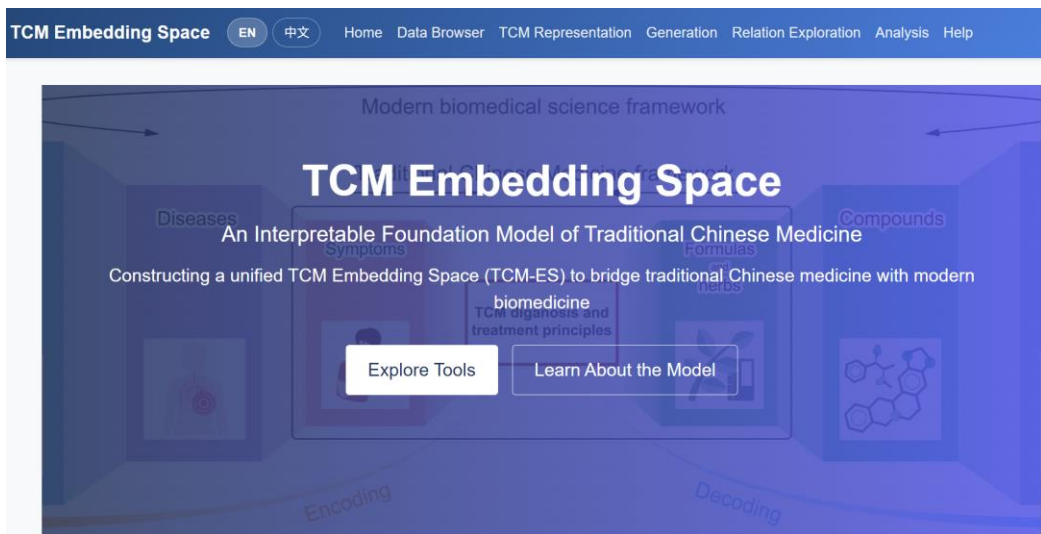
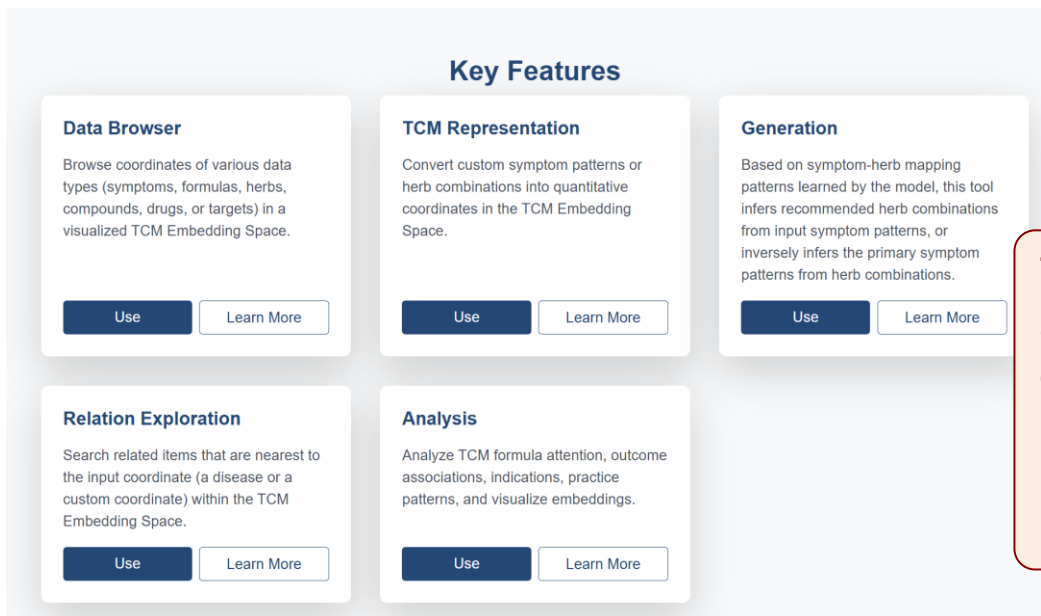
Disease-centred exploration in the integrated TCM-ES

Each disease was connected to nearby proteins, compounds, herbs, formulas, and supported drugs in TCM-ES.





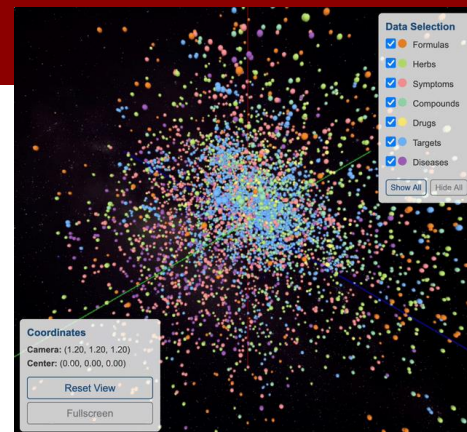
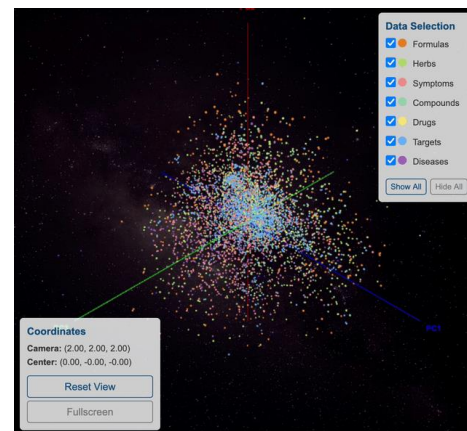
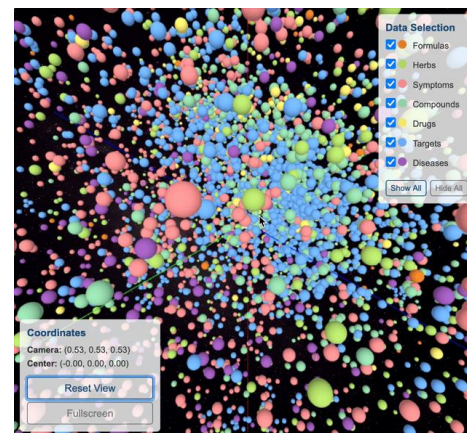
A reusable TCM-ES toolbox



Relation Exploration

Search related items that are nearest to the input coordinate (a disease or a custom coordinate) within the TCM Embedding Space. This helps identify potentially effective formulas, herbs, compounds, drug-repurposing candidates, or disease-target relationships with shared biological mechanisms, enabling new insights from an integrative Chinese-Western medicine perspective. Click entries in the results to open the association view in the visualization space and intuitively inspect distances to the target coordinate.

Visualization



The toolbox makes TCM-ES accessible as a reusable quantitative representation for diverse TCM and integrative biomedical research.

URL: www.tcmes.net



Summary

❑ **A quantitative foundation for TCM practice**

TCM-ES provides a shared quantitative coordinate system linking symptom patterns and herbal treatments.

❑ **An interpretable and clinically relevant representation**

TCM-ES shows quantitative alignment with TCM principles not used in training, and provides a basis for formula prediction and retrospective clinical analyses.

❑ **A bridge to modern biomedicine**

Post-hoc biomedical mapping extends the same coordinate system to biomedical entities, revealing concordance with biological processes and PPI-network organization.

❑ **A platform for disease-centred exploration and broader reuse**

TCM-ES provides a reusable basis for disease relationship analysis, exploratory candidate prioritization, and broader TCM-related and integrative biomedical research.

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