

## Systems Biology of Chinese Herbal Medicine

### 中藥的系統生物學

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Chinese herbal medicine and natural products have always been valuable sources for drug development (Efferth, 2017). Systems biology is a rapidly developing interdisciplinary field that focuses on understanding complex biological systems and their interactions at various levels (cells, tissues, organs). Instead of examining individual genes, proteins, or metabolites, systems biology considers the big picture and how these molecules interact with each other to enable the functioning of entire living systems (Zhou, et al., 2021). Systems biology is primarily based on genome sequencing, omics technologies, and bioinformatic modeling of big data.

Personalised medicine aims to tailor a patient's individual characteristics (genome, lifestyle, exposome) to diagnostics and targeted personalised therapy at increased efficiency and reduced side effects. Artificial intelligence (AI) is used to analyse large datasets and identify patterns relevant to diagnosis and treatment. AI can help further refine personalised medicine by predicting individual treatment approaches more accurately.

We use virtual drug screening, which employs computer-based models and algorithms to predict the interaction of natural products and chemical molecules with target structures (such as proteins, receptors, or enzymes) (Efferth and Barth, 2025). Supported by the Mainz supercomputer "MOGON", we analyse data from chemical databases with over 200,000 substances to identify potentially promising drug candidates (Kadioglu et al., 2021, 2023). Advanced models are applied for the experimental verification of bioinformatic results (Elbadawi and Efferth, 2020; Mahmoud et al., 2022). AI-assisted virtual screening can optimise drug development by identifying potentially toxic compounds or adapting active ingredients to specific cancer cells. We integrate multi-omics data to enable more accurate prediction of drug effects and interactions in the body. Using next-generation sequencing, we have determined the individual profile of clinical tumor biopsies with high precision. We have created personalised predictive models of how a specific patient might respond to a particular therapy.

Genetic diseases also benefit from advances in DNA sequencing and molecular docking for disease prevention. Patients with G6PD deficiency can be genetically tested to prevent severe poisoning by drugs and food (Efferth et al., 2004).

In addition, environmental factors influence human health (exposome). Plastic waste degrades to microplastic compounds, affecting fauna and flora and, thereby, human food. Recently, microplastics have been detected in blood, breast milk, and placenta, underlining their potential effects on human health (Efferth and Paul, 2017).

In conclusion, systems biology complements classical pharmacology but does not replace it. Nevertheless, it is often more suitable for explaining the complex mechanisms of action of Chinese herbal medicine. The scientific explanation of Chinese medicine using modern high-tech methods represents an important step towards its integration into academic medicine.

中藥與天然產物一直是藥物開發的重要來源 (Efferth, 2017)。系統生物學是一個迅速發展的跨學科領域，著重於理解複雜生物系統及其在不同層次（細胞、組織、器官）間的相互作用。系統生物學不同於僅僅檢視單一基因、蛋白質或代謝物，而是思考整體全貌，以及這些分子間的互動如何驅動整個生物體的功能 (Zhou et al., 2021)。此領域主要以基因組測序、組學技術及大數據的生物資訊建模為基礎。

個人化醫學則針對每位患者的個人特徵（基因體、生活型態、外在暴露組）進行診斷，並制定高效率、低副作用的目標個人化治療。人工智能 (AI) 則用於分析大量數據，並辨識與診斷及治療相關的模式。人工智能有助提升個人化醫學，能更精確預測個別患者的治療方案。

我們運用虛擬藥物篩選技術，利用電腦模型與演算法，預測天然產物和化學分子與目標結構（如蛋白質、受體或酶）的相互作用 (Efferth and Barth, 2025)。我們利用德國美因茨約翰內斯-古騰堡大學超級電腦「MOGON」分析化學數據庫中超過20萬種化合物，以篩選具有潛力的候選藥物分子 (Kadioglu et al., 2021, 2023)。先進模型亦被應用於對生物資訊學結果的實驗驗證 (Elbadawi and Efferth, 2020; Mahmoud et al., 2022)。人工智能輔助的虛擬篩選可優化藥物開發流程，能及早辨認可能有毒化合物，或將活性成分調整為特定癌細胞專用。我們結合多組學資料，以期更精確預測藥物在人體內的效應與互動。藉由次世代定序技術，我們能高精度解析臨床腫瘤活檢的個體分子特徵，並建立個人化預測模型，模擬某特定患者對某種療法的反應。

基因疾病亦可受惠於DNA定序與分子對接技術在疾病預防方面的進展。例如，葡萄糖-6-磷酸脫氫酶 (G6PD) 缺乏症患者可接受基因檢測，以預防藥物和食物引致的嚴重中毒 (Efferth et al., 2004)。

此外，環境因素（外在暴露組）亦會影響人類健康。塑膠廢棄物降解為微塑膠，影響動植物，進而進入人類食物鏈。近期在血液、母乳與胎盤中也檢測到微塑膠，顯示其對人體健康的潛在影響 (Efferth and Paul, 2017)。

總結來說，系統生物學能補足傳統藥理學，但無法完全取而代之。儘管如此，對於解釋中藥複雜的藥理機制，系統生物學往往更為適用。運用現代高科技方法對中醫藥進行科學解釋，是中藥融入學術醫學的重要一步。

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