试论中药材全息图谱质量评测人工智能系统构建*

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摘 要:中药材的质量是制约中药现代化与产业化的‘瓶颈”,如何解决这一关键问题?本文基于作者多年来在中药质量控制领域的研究体会,结合国内外该领域的研究进展和发展趋势,从一个新的视角提出了开展中药材全息图谱质量评测人工智能系统构建研究的策略。研究的核心是探讨应用全息图谱(性状图谱、显微特征图谱、基因图谱、化学全成分图谱、主成分含量图谱、血清药化学图谱等)控制中药材质量的研究方法,并在此基础上,利用计算机图像识别技术与专家系统体系,建立一套完整的中药材质量检测人工智能系统,实现中药材的数字化、自动化检测过程。

关键词:中药材 全息图谱 人工智能 质量评测

一、相关领域国内外研究概况

建国以来,国家对中药材的质量控制给予了高度重视,在‘六五”至‘九五”期间均有重点课题资助该方向的研究,中药材质量控制水平有了很大提高。最近化学成分指纹图谱用于控制中药制剂的质量受到多方重视并逐渐达成共识。但是由于中药材质量的特殊性和复杂性,目前中药材质量控制尚存在下列问题:

1. 药材的真伪鉴别主要基于药材的性状和显微特征,主观性较强且需要具有长期实践经验的专业人员方能完成。

2. 药材的优劣评价不够全面。目前主要基于1种或几种成分的含量指标,但中药化学成分复杂、功效多样,常相互协同作用,在目前的技术条件下也不可能将中药所含的化学成分一一搞清楚。

3. 与中药疗效密切相关的化学成分受生长环境、采收季节、生长年限、加工及贮藏方法等随机因素的影响,即使同一种中药也具有多元化情况,造成药材质控处理过程较为繁琐和困难。

4. 多数中药没有合适的疗效评价方法。因而现有的中药质量标准在保证安全、有效、均匀、稳定等各个方面,都缺乏客观化、规范性和标准化,难以达到国际化的要求。

国外对植物药的认识和接受,主要是依据植物药中所含的化学成分,同时进行全面的药理学研究。美国草药典(AHP)已经开始对美国市场上流通的热点植物药五味子、甘草等制订了质量标准,确定了TLC、HPLC的指纹图谱作为该类药

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材的生产和应用的质量依据。美国FDA在植物药制品指导原则（征求意见用草案）中允许申报者提供产品的色谱指纹图谱资料。英国草药典、印度草药典以及加拿大药用及芳香植物学会、德国药用植物学会也都把指纹图谱作为质控标准的内容之一。

在中药材质量评测人工智能系统中运用的人工智能技术是计算机科学最前沿的领域。在过去几十年中，人工智能的研究已经广泛地深入到了各个领域，并都取得了巨大的成绩，已建立了大量的具有人工智能的计算机环境和智能应用系统。这些技术成果与理论研究为中药材质量评价的人工智能系统的建立提供了必要的条件与有力的支持。但是在中药质量人工智能研究领域，国内自1988年首次报道用化学模式识别技术对中药材真伪鉴别和质量评价以来，虽然10余年间该技术日趋成熟并取得可喜进展，已对黄芩等20余味中药开展了模式识别研究；却由于在系统性、与中药材质量因素相关的特征选择方面不够全面、研究没有规范化等各种原因，还难以进入到实际的应用领域。

二、研究目的、意义

如何摆脱中药材质量控制方面的不足呢？作者提出构建中药材质量评测人工智能系统，旨在探讨应用全息图谱（性状图谱、显微特征图谱、基因图谱、化学全成分图谱等）控制中药材质量的研究方法，并在此基础上利用计算机图像识别技术与专家系统体系，建立一套完整的中药材质量检测人工智能系统，实现中药材的数字化、自动化检测。以有利于：

1. 自动化、客观、全面、准确、快捷的控制中药材的质量（真伪、优劣）。

2. 为建立安全有效、可操作、专属性强、技术先进、经济合理的国家质量标准提供坚实的基础，促进中药国际化。

3. 强化药品监督管理的技术依据。

4. 促进外贸，提高中医药产品在国际医药市场的竞争力。

三、研究内容

1. 中药材的全息图谱研究

首期选择常用、质量难以控制且具有很好工作基础的中药开展研究。每一类药材包含不同物种。每一种药材包括不同产地、不同采收期、不同规格、不同加工炮制方法等的样品。

（1）性状、显微图谱的采集：应用配有CCD摄像机的显微镜、或解剖镜等采集。

（2）基因测定：主要测定药材的总基因组DNA的RAPD等指纹图谱；5S－rRNA、18S－rRNA和ITS等间区的基因序列。

（3）全成分定性分析图谱：根据药材中所含的化学成分种类，确定提取方法，建立UV、IR光谱指纹图谱和色谱指纹图谱；对于挥发性成分建立GC或GC/MS色谱指纹图谱，对于非挥发性成分建立HPLC（HPTLC）、LC/MS色谱指纹图谱。

（4）含量图谱：根据化合物的性质建立主成分的HPLC或GC含量测定方法，并对各种样品进行含量测定，获得含量图谱。

（5）血清药化学图谱：中药化学成分是中药药效产生的源泉，但发挥作用的直接物质存在于体内，药物经口服给药后，吸收进入体内发挥作用的可能是原形成分，也可能是其代谢产物。因而，在体外全成分分析方法的基础上，测定药物经口服给药后，血清的化学指纹图谱，与其药效更加贴近。

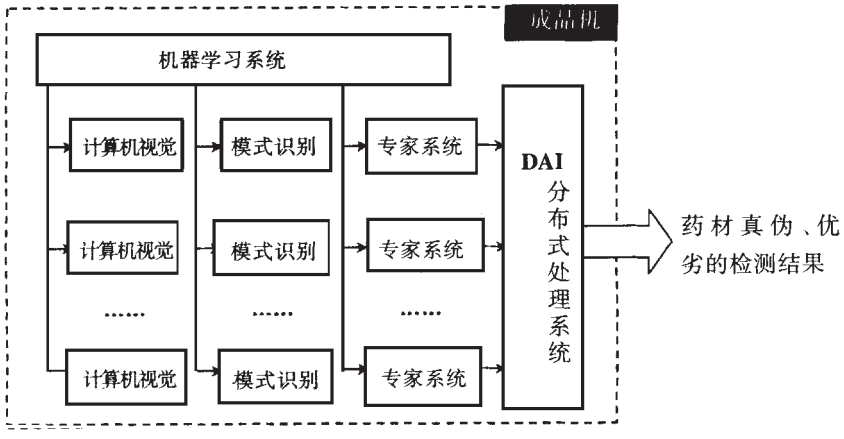
（6）原始模数转换：使用模/数（A/D）转换设备将采集的各种图谱转换为原始的二进数字信息供智能系统进一步分析处理。

2. 人工智能体系构建

为了实现全自动化数字化的高科技中药检验与评价应用目标，我们将中药质量评测人工智能系统的构建分为计算机视觉、中药模式识别、中药评测专家系统、机器学习以及分布式智能处理体系5大组成部分（参见附图）。

（1）计算机视觉：这个部分相当于整个系统的“眼睛”。使用多组立体图像摄影工具仪器、激光测距仪、机械手臂等设备，获取中药材各个角度上不同侧面的立体图像信息，然后将这些数据参数传送至计算机视觉处理器进行数据处理和分析，得到最后的三维图示的符号描述数据，作为实物的图形信息输入到模式识别系统进行处理。

（2）模式识别部分：这一组成部



附图 中药质量评测人工智能系统组成结构示意图

分是整个中药质量评测人工智能系统的基础数据处理模块，将从计算机视觉部分得到的图、影、像等原始数据格式识别转换为中药专家鉴别系统能够处理的有效数据信息，也即把实物识别和图像识别的数据结果与相应的标准图谱做一个对比处理，筛选提取特征数据并进行一些数据预处理工作后交给专家体系下一步的处理分析。

(3) 专家系统：这部分是整个系统的“大脑中枢”。它将模式识别系统部分获得的特征数据相关参数信息，分别送往不同的中药参数分析专家系统（性状、显微、基因、色谱、光谱等）进行处理分析。在这些系统中，计算机处理机根据标准的中药专家系统中的知识库判别系统的专业知识信息对这些参数信息进行推理与逻辑运算，得出各个部分的推理结果，最后将这些结果传送给分布式智能处理系统。

(4) 分布式智能处理系统：这个系统所起到的是一个总处理器的作用。任何一种中药材的鉴别、质量评测都需要对该药材的性状图谱、药材切片组织图谱、粉末图谱、药材基因图谱、药材全成分色谱、光谱指纹图谱、药材主成分含量图谱以及药材生物效价或血清药化学图谱等各项组成参数进行识别与判断计算。分布式处理系统就是这些参数的汇总处理器，它将各个成分的计算结果汇聚到一起，再启动知识库体系对这些参数进行一次总的对比分析处理，得到最后的评测结果进行输出，完成全部的检测工作。

(5)机器学习体系 机器学习体系主要采用基于类比的学习机制，同时综合运用机械学习、基于事例学习机制、概念学习机制、神经网络学习机制以及基于经验的学习机制等多种方式来寻求建立一种最适合中药各种参数鉴别操作的混合型学习方法。在中药材质量评测人工智能系统中运用机器学习体系能够让整个系统具备“自学”的能力，真正产生出“智能”，使质控系统能够在研制阶段甚至实用阶段中不断的从输入的大量测试数据（或称为环境参数）的运算过程中提高系统的“鉴别技能”，增强系统的使用价值。

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ENGLISH ABSTRACTS OF PART OF PAPERS

Study on Functional Genomics of Medicinal Marine Organisms

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In order to catch up with and surpass the world level in the field of genomics, it will undoubtedly be of a breakthrough point to make rapid development of functional genomics of marine organisms which enjoy their advantage in resources in China. In this paper, a new research strategy of functional genomics of medicinal marine organisms is proposed in the fields of modern genomics and the traditional Chinese medicine. The proposal provides new ideas and direction for promoting the modernization of traditional Chinese medicine and for studying active peptides of marine organisms in China.

Key words: marine organisms application of traditional Chinese medicine functional genomics

Current Situation and Prospects on Chinese New Drug Research

This article overviews the different aspects of the China's new drug research through statistic date and analysis, give the general picture of the China's new drug research development and its prospects.

Key words: China New Drug R& D

Promoting Take – off of Medical Industries in China on Basis of Capital Market and by ways of Innovation and Professional Service

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The ten – year development of Chinese securities has showed that capital market has already become a very important channel for financing in the development of medical industries in China. With the driving of capital the integration of TCM, modern pharmaceutical techniques and biotechnology has brought medical industries to a new stage and promoted the extension of new technologies and the further progress of traditional industries, and the development of pharmaceutical companies in their management, capital operation and technical innovations has pushed forward the scale process and the strengthening of competitiveness in key factors of enterprises. They all have become the major driving forces which are advancing the development of medical industries in the country.

This article points out that in the new century, all the medical industries in China will face such problems as the reform of medical system, the readjustment of medical industries and the pressure in intellectual property right when China enters WTO, which will exert great impact on the development of medical industries in the country. It should be noticed however, that there exist quite a lot of chances for Chinese medical industries due to the thriving of herbal drugs and the rapid development of modern biotechnology, and the large – scale development of them undoubtedly needs the support of capital market. With the setting – up of paterns of founding undertakings and the establishment of stimulation mechanisms the initiative of scientific and technologic personnel will be brought to a full play and Chinese medical industries will step into springtime in which technical innovations will play a major role.

Key words: Capital market traditional Chinese medicine(TCM) internationalization

A Tentative Remark on Establishment of Artificial intelligence system for quality evaluation of Chinese medicinal materials via characteristic fingerprinting of multi – data

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The quality of Chinese medicinal materials is a key problem which obstructs the modernization and industrialization of Traditional Chinese medicine. Based on the practice of many years in the research of traditional Chinese medicine and in

combination with the development in this field, the authors suggest to establish an artificial intelligence system for quality evaluation of Chinese medicinal materials. This system uses the characteristic fingerprinting of multi – data (macroscopoc, microscopic, and genetic fingerprinting as well as qualitaticve fingerprinting for the analysis of chemical components of Chinese medicinal material plus computer image recognition technology and expert system to achieve digital and automatic control of their quality.

Key words: Chinese medicinal materials Characteristic fingerprinting of multi – data Artificial intelligence quality evaluation

Analysis of TCM Injection Fingerprinting

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Starting from the four aspects of the significance, stage and details as well as the promotion of TCM industry of TCM injection fingerprinting, this article expounds the role of fingerprinting in the improvement of TCM quality as well as the feasibility and operability of the establishment of fingerprinting and therefore, it is an inevitable trend to establish fingerprinting in TCM modernization, as indicated above.

Key words: TCM fingerprinting HPLC

Opinion on the Innovation of the Theory of TCM — To Analyze the Critical Problem of the Research on the Basic Theory of TCM

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At present, how to give the play to the advantages and characteristics of TCM, and explore a new situation of the research with the features of Chinese culture and scientific ideology on the basic theory of TCM are the critical problem of TCM basic theory research. For this cause, we should clarify the following questions in the process of studying the basic theory of TCM, i. e. the guiding idea of TCM, the distinction between the modern medicine and TCM, the special ways of diagnosis and treatment of TCM, and the status of TCM in the medical and healthy care in the future. By analyzing and thinking over these questions, we can revise the unreasonable research direction and supply some new idea for the innovation of the research on the basic theory of TCM.

Key words: the basic theory of TCM modern research academic exploration clue and method comparison between the modern medicine and TCM

The International Standardization of the Writing in the prescription of the Traditional Chinese Clinical Soupy Medicaments in Common Use

Liao Jun Liu Hui

To solve the long – term suspecting problem – different names for the same medicinal plant in TCM and one name shared by different herbs, we worked at the way of an international standard for the TCM prescriptions for its popularity in the world. Method: The key research lies in the international standard of the herb' s names as the standardization of the dosage has been achieved, which combined with the herb' s names makes the clinical prescription in TCM. Our modal proves practical that is made up of two parts – "Latin word of the medicinal part of the plant " + "Latin word of the plant' s source". Solution: The prescriptions written by Latin modal should be added to the " China Pharmacopoeia" and the national textbook "TCM Formula"(the 6th publication). Conclusion: Latin modal for TCM prescription in clinic proves necessary and feasible as well.

Application of Molecular Biological Technology in Identification of Traditional Chinese Medicine

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We summarized the application of molecular biological technology in identification of TCM in recent years, including the identification of animal and plant medicine. We also described in brief the principles and methods of the molecular biological techniques. These techniques applied are divided into three parts, Electrophoresis, Immunity and DNA Molecular Genetic Marker. The third one includes 1) techinques based on Polymerase Chain Reaction, which includes