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中英科技桥

Science Bridges China Research Profile

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SUMMARY OF MY RELEVANT RESEARCH AREAS:

My research focuses on the development of data mining strategies using artificial intelligence technologies for a range of pharmaceutical applications including formulation design, process optimisation, dealing with fractured data, in vitro in vivo correlation, and metabonomic data mining for biomarker discovery.

我的研究重点是通过人工智能技术开发数据挖掘战略在药剂学上的应用，包括剂型制定，工艺优化，处理断裂的数据，体外体内外相关性，及用于生物标志物的发现的代谢组学数 据的挖掘。

Primary Research interests:

The development of pharmaceutical product formulation is challenging due to the complex non-linear relationships between the formulation composition, process conditions and product properties. In most cases, a formulation consists of a drug, a number of formulation ingredients and process conditions that affect interactively the quality of the final product. Thus, the successful design of a formulation is highly dependent on the level of knowledge regarding the application domain. With advantages over traditional statistical techniques in dealing with the complex non-linear relationships involved in product formulation, artificial intelligence technologies have gained increasing interest in modelling and knowledge generation for formulation with the aim of obtaining an improved understanding of the behaviour of the formulation during the manufacturing process in recent years.

My primary research interests are: Knowledge engineering and artificial intelligence as applied to pharmaceutical applications and traditional Chinese Medicine (TCM) modernisation.

- Investigation and establishment of appropriate strategies for modelling and data-mining pharmaceutical data with various characteristics from wide application domains (e.g. formulation design and process optimisation, in-vitro in-vivo correlation, Biomarker discovery) using artificial intelligence tools.
- Development of data mining methodologies and tools based on AI technologies for the application to the modernisation of traditional Chinese Mecdicine.
- Evaluation of broad range of knowledge engineering and AI technologies as applied to pharmaceutical applications.

Topics in which you would like to develop collaborative research:

- **Product formulation design and process optimization**
- **Data mining for product scale up process**
- **Metabonomic, protenomic and genomic data mining**

Relevant existing collaborations (academic/clinical/commercial) inside or outside China.

Prof. Guo An Luo, Tsinghua University

Prof. Jiwen Zhang, Shanghai Institute of Materia Medica

Prof.Jingkai Gu, Jilin University

Publications and other outputs relevant to your interest in this programme (up to 5)

Shao, Q., Xia, J.F.,York, P., Luo, G.A. (2011), Identification of potential biomarkers associated with Type 2 Diabetes using artificial intelligence technologies. Presented at AAPS annual meeting, Washington DC, US.

Shao Q., Rowe R. C., York P. (2010) Comparison of two data mining strategies in generating knowledge from an effervescent tablet formulation database with limited data using artificial intelligence technologies. Presented at 7th World Meeting on Pharmaceutics, Biopharmaceutics and Pharmaceutical Technology, Malta.

Matas, M. De., Shao, Q., Richardson, C.H. and Chrystyn, H. (2008). Evaluation of in-vitro in-vivo correlations for dry powder inhaler delivery using artificial neural networks
Eur. J. Pharm. Sci. 33(1): 80-90.

Shao, Q., Rowe, R.C. and York, P. (2007). Data mining of fractured experimental data using neurofuzzy logic – discovering and integrating knowledge hidden in multiple formulation databases for a fluid-bed granulation process. J. Pharm. Sci., 97(6): 2091-2101.

Shao, Q., Rowe, R.C. and York, P. (2007). Comparison of decision trees and neurofuzzy logic in discovering knowledge from experimental data of an immediate release tablet formulation. Eur. J. Pharm. Sci., Vol. 31, 129-136.