



Innovation China UK  
中英科技创新计划

**KING'S**  
*College*  
**LONDON**

University of London

# ICUK Launch Event

**22 November 2007**

*Phytochemical informatics applied to  
Traditional Chinese Medicine*

**Peter Hylands**  
**King's College London**  
**[peter.2.hylands@kcl.ac.uk](mailto:peter.2.hylands@kcl.ac.uk)**

# UK perspective

Huge increase in use of alternative medicines

Many conventional drugs derived from natural sources

Traditional Chinese Medicine, TCM, is an important part of the sector

# Chinese perspective

High priority given to unique cultural heritage of TCM

Desire for internationalisation via commercialisation

Growing sector estimated at - @\$18billion

New companies emerging

## Not as easy as all that !!

Major barrier in the TCM sector  
regulatory issues  
safety and efficacy

Only way is by good, controlled trials

Huge need for improved standardisation

# Centre for Natural Medicines

## Research Aims

Working with Chinese academic partners on application of innovative approaches to:

Improve **standardisation**, leading to clinical trials

Undertake drug **discovery**

Introduce effective, safe and licensed **medicinal products to market**

# Collaborators in China

**Institute of Medicinal Plant Research, Beijing**

Professor Xiao Peigen

**Dalian Institute of Chemical Physics**

Professor Liang Xinmiao

**Zhejiang University, Hangzhou**

**Shanghai Institute of Materia Medica**

Professor Hualiang Jiang

**Heilongjiang University of TCM, Harbin**

Professor Kwang

# Current projects

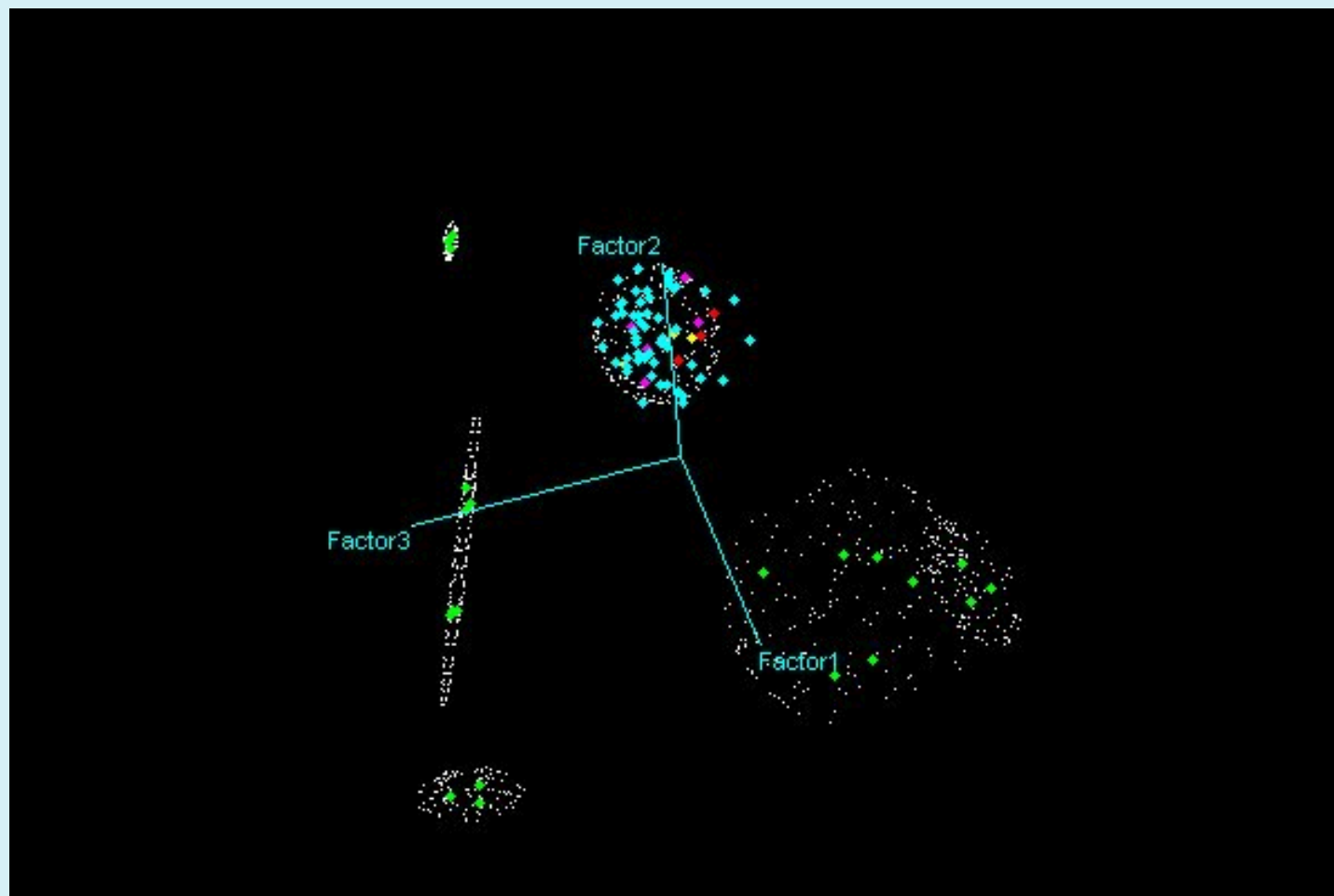
Innovative methods of standardisation

Metabonomics

Acupuncture

Informatics and drug discovery

# Metabonomic standardisation





# Acupuncture and PET scanning

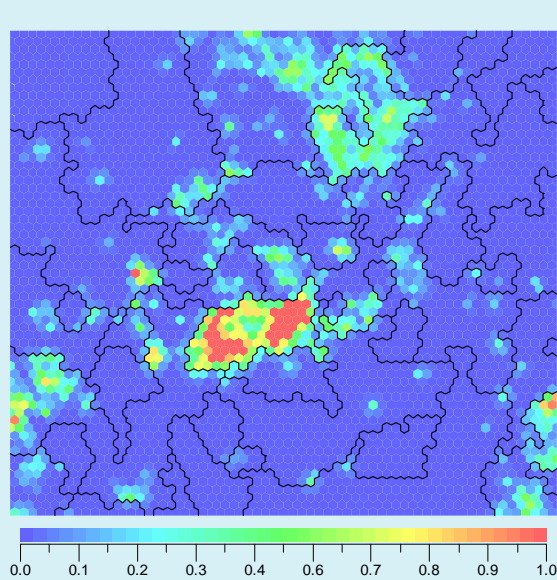


# Informatics and drug discovery

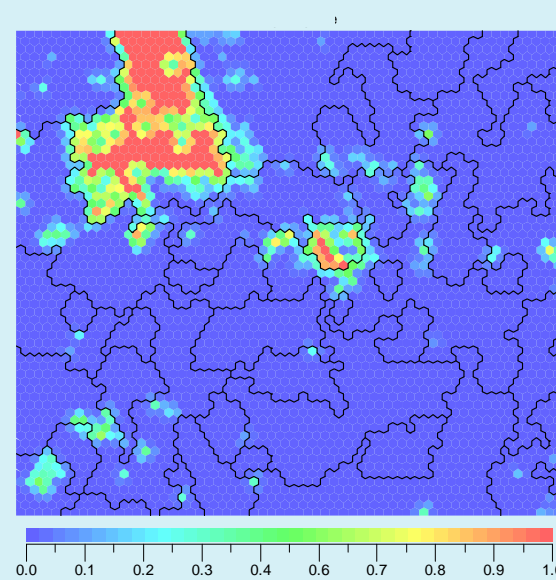
## Self-Organising Maps

Distribution of compounds among the 40 classes visualised separately to show the proportion of compounds of that type found in each category

**Alkaloids**



**Sesquiterpenes**



**Compounds with similar TCM profiles tend to belong to the same phytochemical class**

# Current sources of funding

## **Commercial**

International consumer company

TCM companies

## **Charity**

Kidney Research UK

## **Government / Learned Society**

Chinese Academy of Sciences

The Royal Society

# Most recent achievements

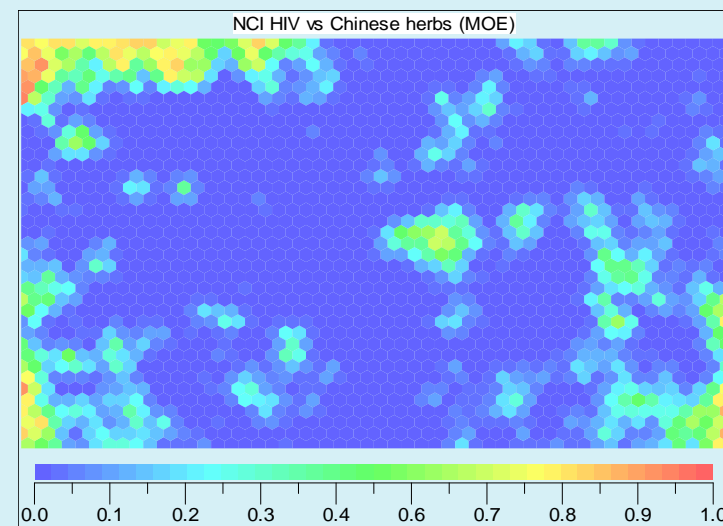
A series of studies on the applications of a different type of informatics

Database

Virtual screening

Prioritisation of putative actives

`for development



**Virtual screening of traditional Chinese herbs** established that a relatively large number of herbs were predicted to inhibit multiple targets, as well as a number which appeared to contain inhibitors of the same target from different phytochemical classes.

# Significant commercial interest

Consumer healthcare product companies

Natural product companies (including TCM companies)

Pharmaceutical companies

# Benefits that ICUK will bring:

**Access to Proof of Concept Fund to develop applications to address barriers in the TCM market**

**eg, potential projects with Shanghai Institute of Materia Medica include:**

**Opportunity to develop** the database for commercial use

**Opportunity to combine and develop** docking studies with analytical technologies and services for commercial use

**Access to Partnership Grant** for staff exchanges and new collaborations will drive innovation

**Thank you for your attention**

**peter.2.hylands@kcl.ac.uk**