



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

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

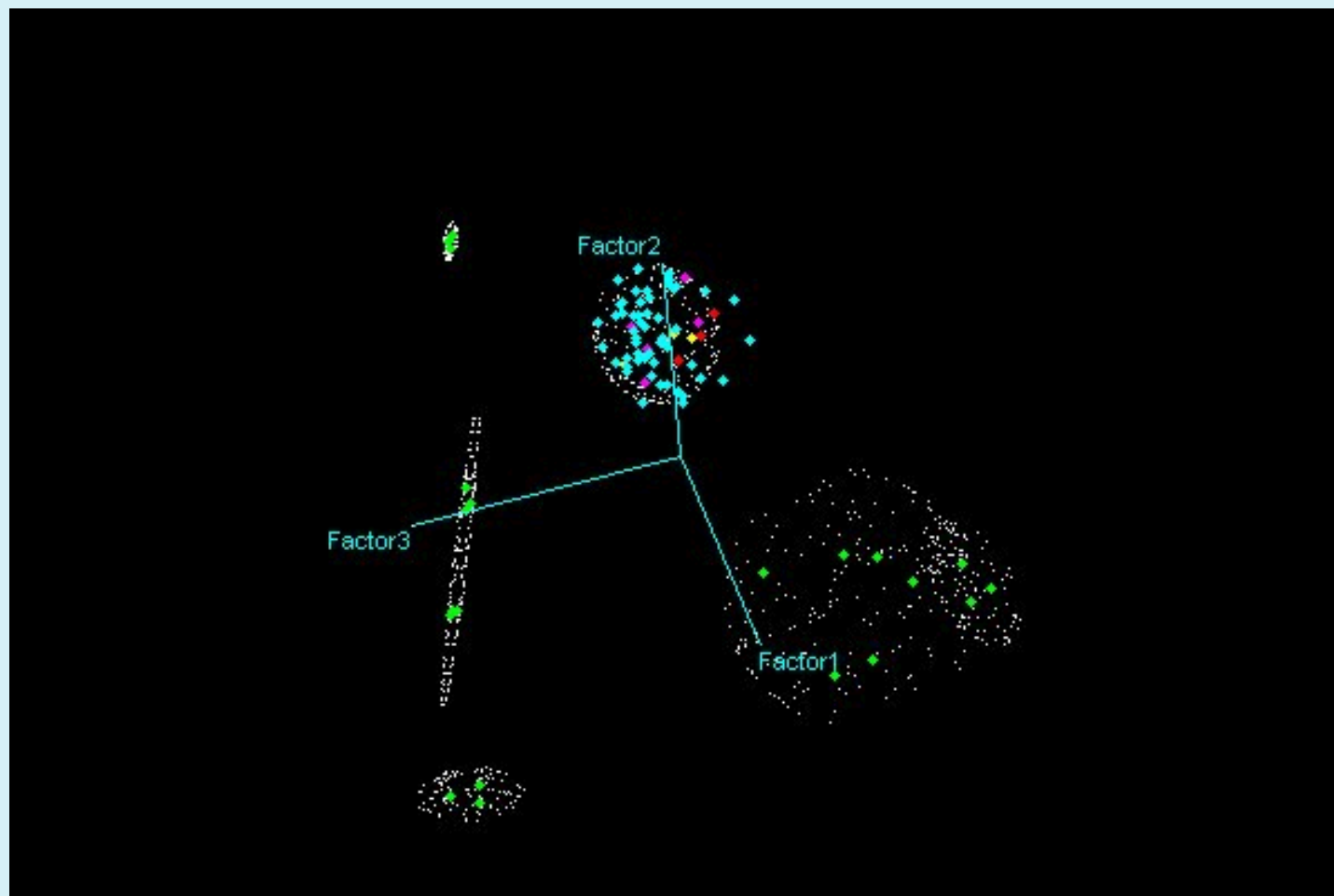
Innovative methods of standardisation

Metabonomics

Acupuncture

Informatics and drug discovery

Metabonomic standardisation



Acupuncture and PET scanning

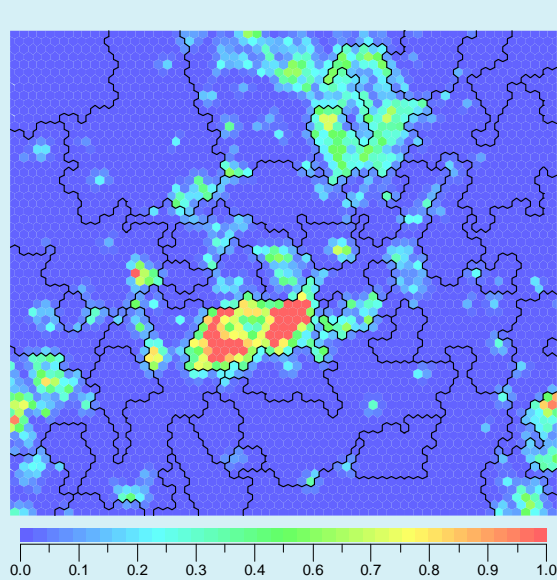


Informatics and drug discovery

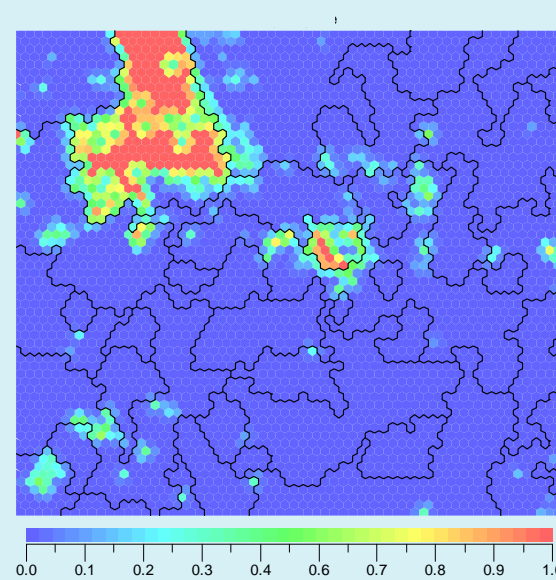
Self-Organising Maps

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

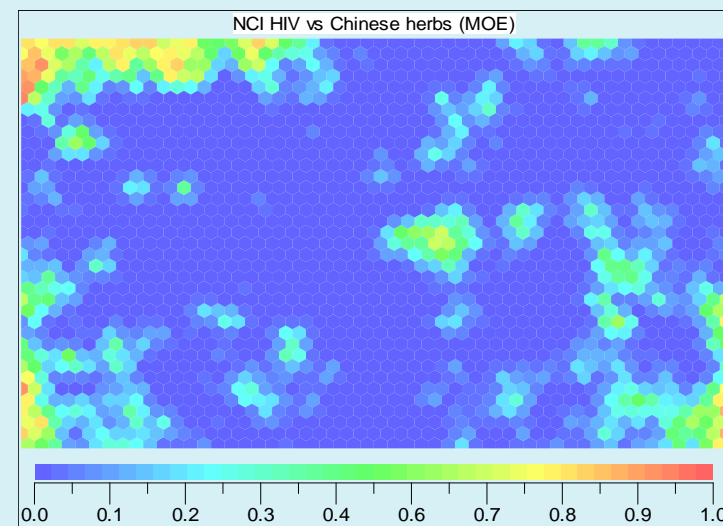
A series of studies on the applications of a different type of informatics

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