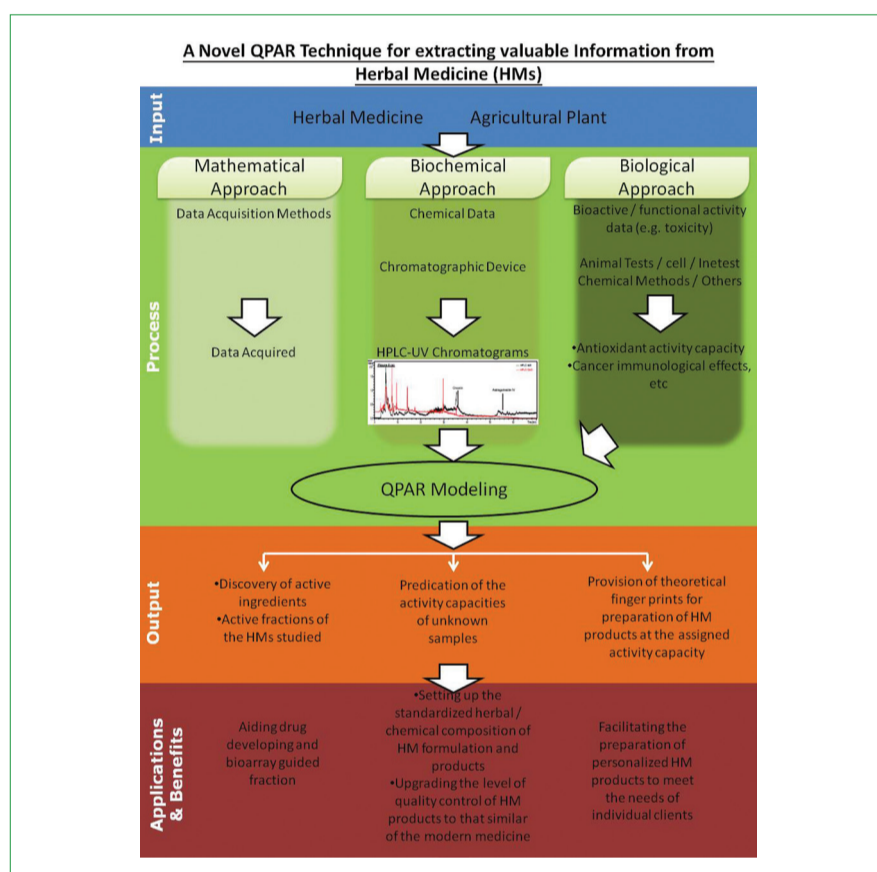# QPAR：一個提取中藥內隱藏珍貴訊息的創新技術
A Novel QPAR Technique for Extracting Valuable Information from Herbal Medicines

這創新QPAR技術只需輸入中藥產品的化學指紋圖譜和相關生物活性數據，便能有效及精準地提供有關產品內藏的生物活性指標

A novel QPAR technique provides effective and accurate bioactivity indicators of herbal products by merely inputting chemical fingerprints and related bioactivity data

在分析混合物（如中藥）生物活性特性時，這創新QPAR技術，量化地結合了'化學組份'和'生物活性'的關係，因而能突破性地解答了兩個現存重大難題：(1)能否只透過分析混合物（如中藥）的色譜圖資料，就能準確地預測未知物的生物活性指標？(2)能否指出活性化合物在色譜圖中的位置？在研究中西草藥時，清楚地証明這創新技術能有效和精準地解決這些難題。在第一個難題方面，它能準確地預測一種樣本對抗癌症免疫方面指標的能力高達92％。

另一突破，就是無需在實驗室內進行任何分餾來分離樣本內與活性關連的化合物組份，它也能成功地預測到另一樣本中那些組份含抗氧化的能力和水平。

特色與優點

這創新QPAR技術將兩組關於含生物活性的混合物的內藏不同資訊併合起來，因而大大減低了提取有用訊息所需的時間，成本及勞工資源。在併合中引出了一個模型，透過它，便可利用混合物的化學色譜圖找出其活性指標，同時也可以發現在色譜圖中那些化學部份能與生物活性連上關係。

應用

QPAR適用於中藥、食品、農產品、環境保護等方面，透過數據分析出來的結果，更快更容易地找出在功能上、活性上，或有毒的成份。此外，從品質管理的角度來看，這技術能提昇檢測相關產品水平高至與現代化醫藥的水平看齊。

獎項

- 第40屆瑞士日內瓦國際發明展 ─金獎 (2012年4月)
- 第五屆國際功能食品座談會：促進身體健康及發展一個可持續發展的環境 - 最佳科學演繹獎（海報組）（2011年3月10及11日）

系統圖
System Diagram

中草藥樣本
Herbal Medicines

This novel quantitative-pattern-activity-relationship (QPAR) technique brings the breakthrough to answer two significant existing problems in the studying of complex active mixtures: (1) Can we predict accurately the total functional activities of unknown sample based on only the chromatographic profile? and (2) Can we identify those features in the chromatographic fingerprint responsible for such activities? In studying two herbal medicines, the results obtained clearly demonstrated the ability of the technique in solving these two problems. Its prediction capability is better than 92% in the total immunological enhancement bioactivity of one of them. Another breakthrough is successful prediction of the antioxidant active fractions of the other one without the need of separating individual fractions through experimentation.

Special Features and Advantages

The novel QPAR technique greatly reduces the time, cost and labor to data-mine the two pieces of important information about complex active mixtures like herbal medicines. It provides a model for predicting total functional activity from the chromatographic profile, and the features in the chromatographic fingerprint responsible for the activity.

Application

QPAR can be applied to study samples in herbal medicines, foods, agricultural plants, environmental protection, etc. Through these investigations, the bioactive, functional and toxic ingredients can be obtained much easier. Also the quality of related products can be evaluated quantitatively based on their functional activities, like that of western medicines.

Awards

- Gold Medal - 40th International Exhibition of Inventions of Geneva, Switzerland (April 2012)
- Award in recognition of the Best Submitted Scientific Presentation (Poster Session). The 5th International Functional Food Symposium, Promoting Good health & developing a sustainable environment (March 2011)

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