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研究快报

超高效液相色谱/飞行时间质谱法分析尿液中的代谢物用于区分人类性别的研究卢果

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摘要 尿中的代谢产物可以反映生命个体的生理状态。为了考察在非严格控制条件下(即对志愿者的饮食、生活方式以及样品采集时间等诸多条件不加以控制)基于尿中代谢物的指纹图谱对男女性别进行区分的可行性，采用超高效液相色谱/飞行时间质谱(UPLC/TOF-MS)联用技术分析了31个随机尿样，并用主成分分析法（PCA）和偏最小二乘法判别分析（PLS-DA）两种数据处理方法对数据进行处理,与PCA法比较，PLS-DA法能提高分类效果，并筛选出4种可能的与性别相关的生物标记物。研究结果表明,UPLC/MS联用技术通量高,数据量丰富；模式识别数据处理方法适合于从大量数据中提取信息,两者的结合有利于代谢组学的研究。

关键词 代谢组学 超高效液相色谱 质谱 尿液 性别差异 偏最小二乘法判别分析

分类号

Study on Gender Difference Based on Metabolites in Urine by Ultra High Performance Liquid Chromatography/ Time of Flight Mass Spectrometry

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Abstract

Metabolites in urine can illustrate the physical condition of an individual as a whole. Ultra high performance liquid chromatography/time of flight mass spectrometry (UPLC/TOF-MS) is a relative new technique for the separation of complex samples. The aim of this study is to assess the feasibility of metabonomics in gender difference in unrestricted conditions, i.e. for healthy volunteers there are no strict controls such as food, life style and the collection of urine samples. In this work, 31 spontaneous urine samples were collected and analyzed by using UPLC/TOF-MS. Principal components analysis (PCA) and partial least squares discriminant analysis (PLS-DA) models were tested and compared in samples classification. The gender discrimination was highly improved and some gender related biomarkers were found by PLS-DA. These preliminary results suggested that UPLC/MS-based approaches coupled with pattern recognition show promise for metabonomics.

Key words metabonomics ultra high performance liquid chromatography (UPLC) mass spectrometry (MS) urine gender difference partial least squares discriminant analysis (PLS-DA)

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