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硕士学位论文

基于NMR技术的啤酒白酒成分分析与分类判别

Components Analysis and Classification of  
Beer and White Spirit Based on NMR Approach

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## 摘要

食品是人类生活中一类重要的必需品，各种食品具有不同的特性和成分，直接关系到人体的健康。近年来，我国食品安全问题受到社会公众群体的广泛关注。核磁共振（NMR）技术相比于其他传统的检测方法，具有对样品的制备要求低、预处理简单，无损检测和高灵敏度等特点，在食品科学研究中得到广泛应用。

酒精类饮料属液态食品，啤酒更是继水、茶之后世界第三大饮用品，白酒则是中国特有酒种。目前基于NMR技术对啤酒的研究多停留在定性分析，化学成分的描述一般只针对某类化合物，对总体化学成分的全面研究较少。而基于NMR的白酒研究集中在国内，多是根据乙醇峰信号的基本波谱参数探究目标因素的影响，鲜少关注其他微量成分。本文利用NMR技术对几种常见啤酒及白酒的成分进行检测，结合模式识别分析不同品牌或香型酒的主要成分差异，并进行定性与定量分析，构建基于Fisher的酒类判别模型。文章主要内容如下：

一、简要介绍核磁共振技术、模式识别方法及其在食品研究中的应用。概述酒类研究现状，提出本研究的意义和内容。

二、应用高分辨 $^1\text{H}$  NMR谱学技术对福建产青岛、雪花、雪津麦之初和惠泉一麦等品牌啤酒进行成分检测。结合多元统计方法分析不同啤酒的差异成分，获得麦芽糖、葡萄糖、丙氨酸、乙酸等26种主要差异成分，并结合2种重要风味物质甘氨酸、丙酮酸，定量分析这28种主要成分，并分析其对啤酒风味的影响。进而建立啤酒的Fisher判别模型，对不同品牌啤酒进行分类判别。

三、在啤酒研究方法的基础上，设计实验方案，优化实验方法与参数，排除多重强峰（水峰、乙醇峰）干扰，获得高酒精含量的白酒的微量成分信息。利用多元统计分析结合半定量分析三种品牌浓香型白酒及五粮液三种香型白酒之间微量差异成分。最后建立Fisher判别模型，验证该模型对白酒分类的可行性。

NMR技术结合多元统计方法及Fisher判别模型可为酒类及液态食品的检测、鉴别与分析提供良好的技术平台。随着NMR技术的进一步完善，NMR在食品科学研究中将会有更为广阔的应用前景。

**关键词：**核磁共振；酒；成分分析

## Abstract

Food is indispensable necessities in human life, different food has different characteristics and ingredient, all of these have a significant influence on human health. In recent years, the problems of food safety draw widespread public attention in China. Food analysis is complex due to the great variety and multiple ingredients. High resolution Nuclear Magnetic Resonance (NMR) technology combined with pattern recognition methods is widely used in the food research. Compare with the traditional detection method, NMR has some advantages on simple sample preparation, non-destructive and high-sensitivity, and has widely used and developed in the research of food science.

Alcoholic drink is a kind of liquid food, which has many complex components, and suitable for researching by using NMR technique. Recently, the study on beer using NMR mainly focused on the qualitative analysis. While, there are no global studies on all the compounds in beer. White spirit is a kind of special wine in China. In general, white spirit is mainly composed of ethanol and water, and the trace elements in white spirit determine the taste and flavor of the liquor. For these decades, many researches have been developed in this area, chemical analysis and gas chromatography analysis were employed to determine the main chemical standards (including the content range of the trace elements). However, there are less interesting on trace elements analysis between different kinds of white spirit using NMR.

In this thesis, NMR combined with multivariate pattern recognition method including principal components analysis (PCA) and Fisher discriminant, were employed to analyze the different composition in order to qualitative or quantitative analysis of trace composition and brand identification in beer and white spirit. The main works were summarized as follows:

Firstly, NMR technology, pattern recognition method and their application in food

field are briefly introduced in this thesis. The contents and methods of liquor research are summarized, and the significance and content of this study are presented.

Secondly, the chemical components in Tsingtao, Snow, Xuejin and Huiquang beer samples from Fujian were quantitatively analyzed by using  $^1\text{H}$  NMR spectroscopy, and their differential components were identified by multivariate statistical analysis with a consequence of the variations in 26 chemical components including sugar, amino acids and organic acids. Quantitative analysis of 28 principal components which include maltose, glucose, alanine, acetic acid, glycine and pyruvate were carried out to confirm the compositional differences between these four kinds of beer and understand their influence on the special flavor of beer. Furthermore, the Fisher classification discriminant model was successfully established the classification method of different brands of beer.

Thirdly, based on the previous study methods of the beer, new experiment design, methods and parameters were optimized in order to suppress the strong multiple solvent peak (i.e. peak of water and ethanol), and obtain the high resolution NMR profiling of trace components in Chinese white spirits with high alcohol content. Further study was carried out to qualitatively analyzed the trace differential components between different white spirits by using multivariate statistical methods (PCA). Then, the Fisher discriminant model was also developed for the classificatory analysis between different brand Chinese white spirits, and validated the feasible of this model in white spirits analysis.

NMR techniques combined with multivariate statistical methods and Fisher discriminant model provided a new method for comprehensive analysis of complex liquid food samples, which can not only clarify the chemical compositions in different samples, but also identify characteristic components quickly. With the development of NMR techniques, it will be widely used in food science in the future.

**Keywords:** NMR; liquor; components analysis

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