IFT BASIC SYMPOSIUM SERIES

# Flavor Measurement

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Marcel Dekker, Inc. New York • Basel • Hong Kong

**Library of Congress Cataloging-in-Publication Data**

Flavor measurement / edited by Chi-Tang Ho, Charles H. Manley.
p. cm. -- (IFT basic symposium series)
Includes bibliographical references and index.
ISBN 0-8247-9056-1
1. Flavor--Measurement--Congresses. I. Ho, Chi-Tang.
II. Manley, Charles H. (Charles Howland). III. Series.
TX541.F54 1993
664'.07--dc20 93-19305
CIP

The publisher offers discounts on this book when ordered in bulk quantities. For more information, write to Special Sales/Professional Marketing at the address below.

This book is printed on acid-free paper.



MARCEL DEKKER, INC.
270 Madison Avenue, New York, New York 10016

Current printing (last digit):
10 9 8 7 6 5 4 3 2 1

PRINTED IN THE UNITED STATES OF AMERICA

# Flavor Measurement

# ift Basic Symposium Series

Edited by
INSTITUTE OF FOOD TECHNOLOGISTS
221 N. LaSalle St.
Chicago, Illinois

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# Preface

Each year the Institute of Food Technologists (IFT) and the International Union of Food Science and Technology (IUFoST) sponsor a two-day Basic Symposium held in conjunction with the IFT annual meeting. The symposium is designed to cover new, basic developments in a major field of interest to the food scientist. Flavor Measurement, the 16th annual symposium, took place June 19-20, 1992, in New Orleans before the IFT's 52nd Annual Meeting and was designed to help the food scientist and flavor researcher to understand the methods available in measuring flavor. The chapters in this book deal with the major topics covered during that symposium.

Flavor is always of major interest to food scientists and technologists. It represents a major attribute of food and a deciding factor in the public's measurement of the quality of food. A major factor in a food technologist's ability to measure the quality of food is the ability to measure flavor. Although many texts have focused on the sensory properties of food flavor, few have delved into the numerous methods that science has developed to measure flavor. Typically symposia have selected such topics as the chemical aspects of flavor or the organoleptic/sensory measurement techniques used to describe a flavor. This volume

covers several broad topics, which allow for a total understanding of the measurement of flavor. Flavor science is a complex study of not only the flavor itself, but also the way in which the observer reacts to it. Understanding only one aspect of the measurement of flavor leaves one with a very small understanding of what a flavor is.

Five major areas are covered in this book: chemical and physical measurement, sensory methods, measurement at the molecular level, measurement of sweetness, and authentication and safety measurements.

Although there have ben many publications on the chemical and physical methods of measuring flavor, the research has expanded greatly; this book reflects the current state of the science. Chapters 1-4 consider the use of statistical methods to understand and interpret gas chromatographic data of complex flavor systems (Chapter 1) and uses of direct adsorbent trapping and thermal desorption for gas chromatographic-mass spectrometer analysis (Chapter 2), contain detailed discussions of the biases in analytical flavor profiles introduced by isolation methods (Chapter 3), and put forth the latest advances in the use of gas chromatography as an olfactometry in flavor analysis (Chapter 4).

The second major area of consideration is the sensory methods used in measuring flavor. Chapters 5-8 review the descriptive methods of flavor evaluations (Chapter 6), cover the basic concepts and computer programs for multidimensional scaling (Chapter 7), and discuss the use of the technique in characterization of odor quality (Chapter 8). The final decision of quality in the measurement of flavor is the consumer, and Chapter 5 covers the methods used to measure consumer acceptance of flavor.

The third area covered is the measurement of the flavor or odorant at the molecular level and the interaction of the flavor molecule with the human olfactory system. Chapter 9 focuses on the interaction of the odorant at the cellular level and the chemical messengers which the odorant can stimulate. Chapter 10 discusses the brain activity response to odorant stimulation.

The two remaining areas deal with measurement of sweetness and the topic of authentication and safety measurements. Chapter 11 begins with the sensory methods for sweetener evaluation and the mechanism of human sweet taste. Chapter 12 probes the various methods to establish the authenticity of the flavor and risks involved in the use of ingredients to make flavors. Chapter 13 considers the methods for analysis of essential oils as components of flavors and their differentiation. In Chapter 14 various methods are explored which allow for the establishment of the origin of flavors and flavor ingredients. A review of the current status of risk or safety assessment and the means of making those evaluations concludes the volume.

We acknowledge the help provided by the present and former Basic Symposium Committee members and their chairman, Henry G. Schwartzberg, University of Massachusetts; past-chairman, Barbara P. Klein, University of Illinois; and

chairman-elect, Nevam Hettiararchchy, North Dakota State University. The symposium organizers also thank John H. Litchfield, 1991-1992 IFT President; Daniel E. Weber, IFT Executive Director; John B. Klis, Director of Publications; and Anna May Schenck, Associate Scientific Editor, for their support of this symposium. We are also indebted to Ms. Deanna Mann, Secretary to Dr. Manley, for helping us keep track of all the paperwork for the symposium.

Most of all, we would like to thank the authors for their worthy contributions. Without their dedication, expertise, and hard work, timely publication of these proceedings would not have been possible. We now invite you to enjoy the quality and excitement of their work.

Chi-Tang Ho
Charles H. Manley

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# Flavor Measurement

# Contents

# 1

# Use of Statistical Methods to Better Understand Gas Chromatographic Data Obtained from Complex Flavor Systems

**Mingjien Chien and Terry Peppard**

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## INTRODUCTION

Capillary gas chromatography is one of the most commonly used analytical techniques currently available for the investigation of complex food and flavor systems. Great improvements in both resolution and sensitivity for GC have, in recent years, resulted in very large data sets for these types of system. Unfortunately, a problem frequently encountered is that more data do not always lead to more information. It is often difficult to distinguish between meaningful information and random variation in data. To resolve this problem by traditional univariate methods based on simple algorithms is extremely difficult, because important information is often contained within combinations of variables. Multivariate methods, on the other hand, examine many variables simultaneously, seeking a reduced number of factors (combinations of the original variables) that contain maximal information. In essence, they seek to reduce the dimensionality of the data set, enabling classification of the individual samples that make up the data set

according to their degree of similarity/dissimilarity. Further, multivariate methods allow investigation of the underlying relationships existing between variables and consequently the interpretation of sample classification on the basis of these variables.

In the field of food and flavor chemistry, methods of correlating sensory and analytical data represent a very useful application of multivariate methods. In applying these statistical procedures, we hope to establish meaningful correlations between subjective sensory data and objective instrumental data. The ultimate aim is to understand how differences in organoleptic properties among a range of samples are caused by variations in chemical composition. One may wish to know this in order to be able to alter organoleptic properties in a predictable manner by, for example, changing one or more variables in a manufacturing process. Alternatively, one may simply want the ability to make reliable forecasts of the organoleptic properties of certain products based on GC analysis.

A minority of organoleptic materials are characterized by well-defined sensory attributes originating from specific odor impact compounds; in such cases correlation of sensory and instrumental data is relatively straightfor-

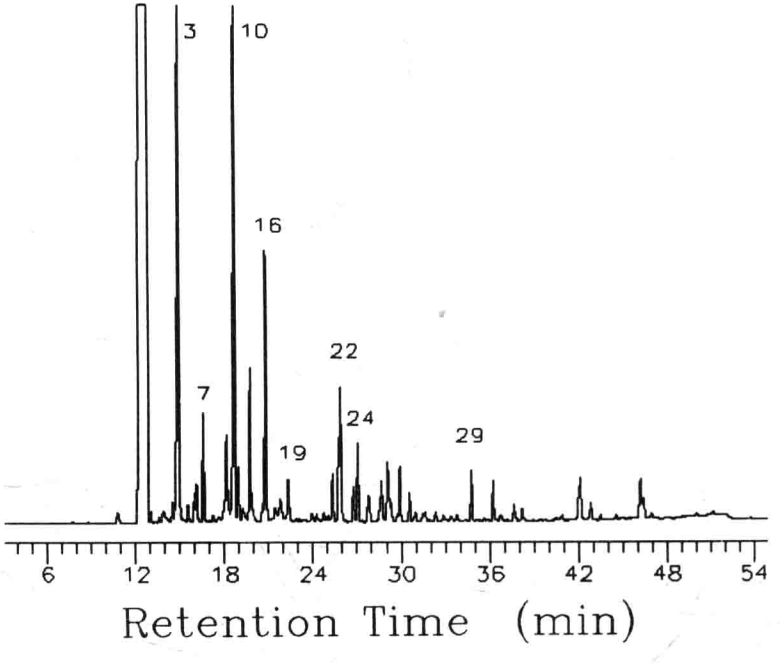


**FIG. 1.1** Gas chromatogram of orange oil using a J&W DB-1 column, programmed from 50 to 230°C at 4°C/min.

ward. For most products, however the situation is vastly more complicated because perceived sensory characteristics generally result from a multitude of chemical constituents acting in concert. Organoleptic properties are truly a multivariate phenomenon, so the task of characterizing them realistically requires multivariate methods of solution.

In this paper we will outline a number of different strategies, each relying on multivariate statistics, which enable us to achieve a better understanding of the organoleptic properties of complex food and flavor systems based on GC data. Various examples, drawn both from the literature and from work carried out in our own laboratories, will be presented to illustrate how sensory/instrumental correlations may be elucidated.

## THE NATURE OF MULTIVARIATE DATA

We will begin by briefly discussing the nature of multivariate data sets. When n samples are analyzed by GC and m peaks are measured in each sample, the data are expressed by an n × m data matrix:

Variables (GC peaks)

$$D = \begin{vmatrix} x_{11} & x_{12} & \cdot & \cdot & x_{1j} & \cdot & \cdot & x_{1m} \\ x_{21} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & x_{ij} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ x_{n1} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & x_{nm} \end{vmatrix} \text{ Samples}$$

where $x_{ij}$ is the normalized GC peak area of component j in sample i. In such a configuration, the m variables constitute an m-dimensional space and sample i is represented by a vector $X_i = (x_{i1}, x_{i2}, \ldots, x_{im})$ which can be considered a point in the m-dimensional space.

To ensure the best chance of obtaining meaningful results from a statistical study, it is always good practice to investigate the nature of the data sets before choosing a particular statistical analysis method. Using a standard statistical technique with an inappropriate data set will always be of questionable value, and, in some cases, it may even lead to false conclusions. Some common properties of multivariate data sets are discussed below.

To illustrate the concepts discussed in the following sections, we will use a set of orange oil data obtained from one of the Givaudan-Roure Quality Control Departments. Forty orange oil samples were analyzed by GC, and 30 peaks from each sample were measured. Figure 1.1 shows a typical gas