

Third Edition

Fats *and* Oils

Formulating and
Processing for
Applications

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CRC Press
Taylor & Francis Group
Boca Raton London New York

CRC Press is an imprint of the
Taylor & Francis Group, an Informa business

CRC Press
Taylor & Francis Group
6000 Broken Sound Parkway NW, Suite 300
Boca Raton, FL 33487-2742

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Printed in the United States of America on acid-free paper
10 9 8 7 6 5 4 3 2 1

International Standard Book Number-13: 978-1-4200-6166-6 (Hardcover)

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Library of Congress Cataloging-in-Publication Data

O'Brien, Richard D.
Fat and oils : formulating and processing for applications / Richard D. O'Brien.
-- 3rd ed.
p. cm.
Includes bibliographical references and index.
ISBN-13: 978-1-4200-6166-6
ISBN-10: 1-4200-6166-6
1. Oils and fats, Edible. I. Title.

TP670.O27 2009
664'.3--dc22

2008020476

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The U.S. Nutritional Labeling and Education Act define total fat content as the sum of all fatty acids, calculated as triglycerides per 100 grams of product. This requirement necessitates the use of an internal standard. Evaluation of a number of fatty acids prepared as internal standards indicated that C-13:0 was preferred because it showed the least interactions with the sample fatty acid profile.²⁴ Both the AOAC method 996.06, appropriate for determination of fat in food products and AOCS Ce 1f-96, applicable to the determination of *cis* and *trans* fatty acids in fats and oils recommend glycerotride-canoate (C-13:0) as an internal standard.²³

Fourier transform-near infrared spectroscopy (FT-NIR) methods for *trans* fatty acid composition determinations are also approved by AOCS and AOAC International. Analytical laboratories have preferred the GLC methods because they provide a profile of all the fatty acids including *trans* isomers. The FT-NIR method only provides the total *trans* fatty acids. However, a technique has been developed that reportedly combines the speed of FT-NIR with the specificity and accuracy of GLC determinations to obtain a complete fat or oil fatty acid profile. U.S. Patent Application No. 10/840277 was submitted in May 2004 for the FT-NIR technology.²⁵

3.4.5 Calculated Iodine Value

Iodine value measures unsaturates or the average number of double bonds in a fat; therefore, it is logical that an iodine value can be easily calculated from a fatty acid composition analysis. The constants for the most common unsaturated fatty acids required for calculation of a triglyceride iodine value are shown below.²⁶

Unsaturated Fatty Acid Constants

Fatty Acid	Constant	Fatty Acid	Constant
C-10:1 Decenoic	1.388	C-16:3 Hexadecatrienoic	2.895
C-12:1 Lauroleic	1.203	C-18:3 Linolenic	2.616
C-14:1 Myristoleic	1.062	C-20:3 Dihomo- γ -linolenic	2.386
C-15:1 Pentadecanoic	1.002	C-22:3	2.194
C-16:1 Palmitoleic	0.950		
C-17:1 Margaroleic	0.903	C-16:4 Hexadecatetraenoic	3.888
C-18:1 Oleic	0.860	C-18:4 Stearidonic	3.512
C-20:1 Gadoleic	0.785	C-20:4 Arachidonic	3.202
C-22:1 Erucic	0.723	C-22:4 Docosatetraenoic	2.943
C-24:1 Nervonic	0.669	C-20:5 EPA	4.028
C-12:2	2.427	C-21:5 Henicosapentaenoic	3.855
C-14:2	2.141	C-22:5 Clupanodonic	3.699
C-16:2 Hexadecadienoic	1.915	C-24:5 Tetracosapentaenoic	3.419
C-17:2	1.756		
C-18:2 Linoleic	1.732	C-20:6	4.864
C-20:2 Eicosadienoic	1.581	C-22:6 DHA	4.464
C-22:2 Docosadienoic	1.454	C-24:6 Tetracosahexaenoic	4.125

The calculated iodine value is determined simply by multiplying the percentage of each unsaturated fatty acid by its constant and addition of the results. This procedure has not replaced the regular iodine value. It can be utilized as an audit for the chemical iodine value and does provide the capability of obtaining two results from one analysis.

3.4.6 Glyceride Structure

The chemical, physical, and biological properties of fats and oils depend not only on the kind and quantity of participating fatty acids, but also on the positions of these fatty acids in the triglyceride molecule. In general, fats and oils are composed of mixed glycerides rather than mixtures of simple glycerides. When all three fatty acids are identical, the product is a simple triglyceride. A mixed triglyceride has two or three different fatty acids joined to the glycerol. The characteristics of a triglyceride depend on the position that each fatty acid occupies on the glycerin molecule. As a general rule, fats with uniform triglyceride molecules have β -crystals in the most stable state. Fats that are stable in the β' -crystal form contain mixtures of types of triglycerides that prevent large growth. For example, fully hydrogenated soybean, corn, canola, and peanut oils are essentially all tristearin due to a low level of palmitic fatty acid and form stable β -crystals. Cottonseed and palm oils with high palmitic fatty acid levels have mixtures of stearic and palmitic fatty acids when fully hydrogenated, which form β' -crystals. Lard and cocoa butter have high palmitic fatty acid levels, but crystallize in the β form due to the uniform triglyceride structure. For lard, palmitic fatty acid is always found in the *sn*-2 position of the glycerin molecule, and cocoa butter always has oleic fatty acid in the *sn*-2 position.²⁷

Analysis of the complex mixtures of triglycerides present in natural fats has been carried out by many methods. Early analytical techniques employing crystallization and counter-current distribution were not reproducible and required large samples and long analysis times. Extensive evaluations of chromatography techniques have led to high-performance liquid chromatography (HPLC), which partially fulfills the ideal requirements of an accurate, quick, and easy analytical procedure. HPLC procedures have provided rapid methods for the determination of relative amounts of glycerides present in a fat. HPLC can be used to monitor the modification of a fat, as well as to detect adulteration, and as a developmental tool for specialty fats and oils. It appears that triglyceride structure analyses can be very useful research and development tools, but are not practical for quality control purposes.

3.4.7 Emulsifier Analysis

A rapid, precise, and easily reproducible method for the determination of monoglyceride in fats became an essential requirement from a quality control standpoint when the use of monoglyceride in shortening and margarine blends became widespread. Hydroxyl number determinations, interfacial tension measurement, and alcohol extractions, among other procedures, were investigated and found not specific and sensitive enough or suitable for quality control purposes. The most satisfactory