

THEORETICAL AND EXPERIMENTAL STUDIES
ON THE EFFECTS OF FATTY ACIDS ON THE
PERFORMANCE OF NATURAL AND SYNTHETIC
ANTIOXIDANTS IN INHIBITING THE OXIDATION
OF PALM OLEIN AND CORN OIL

RADIAH BINTI ALI

MASTER OF SCIENCE

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Thesis Submitted in Fulfillment of the Requirement for the
Degree of Master of Science in the School of Fundamental Science
Universiti Malaysia Terengganu

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DEDICATION

I lovingly dedicate this thesis to my family; a special feeling of gratitude to my loving parents whose words of encouragement;

My siblings for supporting me all the way,

To Ayahku, Balqis and Rose for giving this golden opportunity and believed in me.

Abstract of thesis presented to the Senate of Universiti Malaysia Terengganu in fulfillment of the requirements for the degree of Master of Science

THEORETICAL AND EXPERIMENTAL STUDIES ON THE EFFECTS OF FATTY ACIDS ON THE PERFORMANCE OF NATURAL AND SYNTHETIC ANTIOXIDANTS IN INHIBITING THE OXIDATION OF PALM OLEIN AND CORN OIL

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Main Supervisor : Ku Halim Ku Bulat, Ph.D
Co-Supervisor : Juriffah Ariffin, Ph.D
School : School of Fundamental Science

The aim of this research project was to study the effects of adding saturated and polyunsaturated fatty acids on the performance of synthetic antioxidant, *tert*-butylhydroquinone and natural antioxidant, α -tocopherol in inhibiting the autoxidation of selected vegetable oils. Two types of vegetable oils have been used in this study: palm olein and corn oil. Palm olein was chosen because it contains high level of saturated fatty acid of palmitic (C16:0), approximately 46% while corn oil shows high content of polyunsaturated fatty acid of linoleic (C18:2), 54%, respectively. In this research, two types of fatty acids, palmitic and linoleic acid were utilized to test their effectiveness on antioxidants performance both, experimentally and theoretically. For the experimental studies, the vegetable oils were mixed with fatty acids at four different concentrations: 0.25, 0.5, 1.0 and 3.0 % in the presence or in the absence of antioxidants. The mixture was heated in the oven at 60 °C for 15 days. Samples were taken after 0, 1, 3, 6, 10, and 15 days for analyses such as

peroxide value and acid value. In the theoretical studies, a quantum mechanical software package of Gaussian09 at the theoretical level of DFT B3LYP/ 6-31G (d,p) were employed in optimizing hydroperoxyl radicals, antioxidants, fatty acids single species structure as well as their complexes. The chosen physical parameters were dipole moment, stabilization energy and bond indexes. *Tert*-butylhydroquinone is the best antioxidant in reducing the peroxide formation and decomposition of triacylglycerides compared to α -tocopherol. Results indicate that, in the presence of fatty acids, the effect of fatty acids depends on the type of oils, triacylglyceride's fatty acids composition and concentration of fatty acids added. The addition of fatty acid which is the main component of triacylglycerides decreased the oxidation and gave less effect to the degradation of triacylglycerides. It is supported by theoretical calculations by Gaussian09 software package. Overall results show that, for both vegetable oils, the addition of fatty acids either palmitic (saturated) or linoleic (polyunsaturated) will promote decomposition of triacylglycerides but at the same time it may reduce the peroxide formation. In the presence of TBHQ and α -tocopherol, for both vegetable oils, synergistic behavior was found between fatty acid and antioxidants. These experimental observations were supported by theoretical studies, where complexes with TBHQ were more stable than complexes with α -tocopherol. Results showed that the interaction energy is the major contributor to the performance of the antioxidants.

Abstrak tesis yang dikemukakan kepada Senat Universiti Malaysia Terengganu sebagai memenuhi keperluan untuk Ijazah Sarjana Sains

KAJIAN SECARA TEORI DAN EKSPERIMEN KE ATAS KESAN ASID LEMAK TERHADAP PRESTASI ANTIOKSIDA SEMULAJADI DAN SINTETIK DALAM MENGHALANG PENGOKSIDAAN MINYAK SAWIT OLEIN DAN MINYAK JAGUNG

RADIAH BINTI ALI

September 2014

Penyelia Utama : Ku Halim Ku Bulat, Ph.D
Penyelia Bersama : Juriffah Ariffin, Ph.D
Pusat Pengajian : Pusat Pengajian Sains Asas

Tujuan penyelidikan ini adalah untuk mengkaji kesan penambahan asid lemak tepu dan tak tepu terhadap prestasi antioksidasi sintetik butylhydroquinone tertiar dan antioksidasi semulajadi α -tokoferol dalam menghalang pengoksidaan minyak sayuran yang dipilih. Dua jenis minyak sayuran telah digunakan di dalam kajian ini iaitu minyak sawit olein dan minyak jagung. Minyak sawit olein dipilih kerana ia kaya dengan kandungan asid lemak tepu, asid palmitik (C16:0), sekurang-kurangnya 46% manakala minyak jagung mempunyai kandungan asid lemak tak tepu yang tinggi, asid linoleik (C18:2), 54%. Dalam penyelidikan ini, dua jenis asid lemak iaitu asid palmitik dan linoleik digunakan untuk menguji kesannya terhadap prestasi antioksidasi secara eksperimen dan teori. Bagi kajian secara eksperimen, minyak sayuran dicampur dengan asid lemak pada empat kepekatan yang berbeza: 0.25, 0.5, 1.0 dan 3.0 % dengan kehadiran atau ketidakhadiran antioksidasi. Campuran ini dipanaskan di

dalam ketuhar pada suhu 60 °C selama 15 hari. Sampel diambil selepas 0, 1, 3, 6, 10 dan 15 hari untuk dianalisa seperti nilai peroksida dan nilai asid. Dalam kajian secara teori, pakej perisian Gaussian09 pada aras teori DFT B3LYP/ 6-31G (d,p) digunakan untuk pengoptimuman struktur spesies tunggal bagi radikal hidroperoksil, antioksidan, asid lemak dan kompleksnya. Parameter fizikal yang dipilih ialah seperti momen dwikutub, tenaga kestabilan dan indeks ikatan. Butylhydroquinone tertiar merupakan antioksidan terbaik bagi mengurangkan pembentukan peroksida dan penguraian triasilgliserida berbanding α -tokoferol bagi kedua-dua minyak yang diuji, minyak sawit olein dan minyak jagung. Keputusan menunjukkan dalam kehadiran asid lemak, kesan penambahan asid lemak terhadap minyak didapati berubah-ubah mengikut jenis minyak, komposisi asid lemak dan kepekatan asid lemak yang ditambahkan. Penambahan asid lemak yang merupakan komposisi utama triasilgliserida mengurangkan pengoksidaan dan memberi kesan yang sedikit kepada penguraian triasilgliserida. Secara keseluruhannya, bagi kedua-dua jenis minyak, didapati penambahan asid lemak sama ada asid palmitik (tepu) atau asid linoleik (tak tepu) akan menggalakkan proses penguraian triasilgliserida minyak tetapi pada masa yang sama dapat mengurangkan pembentukan peroksida. Bagi kedua-dua minyak, dalam kehadiran butylhydroquinone tertiar dan α -tokoferol, wujudnya sifat sinergistik di antara asid lemak dan antioksidan. Keputusan eksperimen ini disokong oleh kajian secara teori dimana kompleks bersama butylhydroquinone tertiar adalah lebih stabil berbanding dengan kompleks bersama α -tokoferol. Keputusan menunjukkan tenaga interaksi merupakan penyumbang utama kepada prestasi antioksidan.