

UNIVERSITI PUTRA MALAYSIA

LIQUID CHROMATOGRAPHY-MASS SPECTROMETRYBASED METABOLOMICS OF OIL PALM (Elaeis guineensis Jacq.) LEAF

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By

NOOR IDAYU MHD TAHIR

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Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the degree of Master of Science

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Chair : Prof. Khozirah Shaari, PhD

Faculty : Institute of Bioscience

The profiling and characterization of plant metabolome provide depiction of its metabolic events and permit the harnessing of valuable chemicals. However, the effort is often hindered by their structural complexity. The oil palm leaves are the most abundant by-product of the oil palm sector but the usage of the waste is marginal. Researches that facilitate its efficient utilization are necessary to sustain the industry. As phenotypes of organisms are not direct representations of their genotypes and are largely influenced by their environment, ecological metabolomics is required to capture metabolite shifts in response to external factors. An immediate chemical description of the oil palm leaves metabolome was achieved using liquid chromatography (LC) combined with mass spectrometry (MS). Commercial standards were unavailable for most of the chemicals, thus, mass spectrometry with data mining techniques such as neutral loss analysis aided

the identification of compounds. The metabolome of oil palm spear leaf was compared to that of mature oil palm frond using both positive and negative ion mode. The spear leaf contains seven apigenin glycosides-hydroxymethylglutaric acid complexes and an O-glycosylated apigenin that were not present in the frond tissue. Conversely, four luteolin glycosides and two isomers of apigenin diglycosides were absent in the spear leaf sample. A total of 53 compounds including metal salt complexes, amino acids, amines, organic acids, catechins, phenolic acid glycosides, flavonoid glycosides and a stilbenoid glycoside in the oil palm leaves were identified in this work. The oil palm leaves extracts exhibited good antioxidant activities with the frond tissue demonstrated the highest DPPH radical scavenging activity value per g of leaf tissue dry weight, followed by the hydrolyzed fraction of frond extract, hydrolyzed spear leaf extract and spear leaf extract. The metabolome of oil palm clones were influenced by their planting conditions regardless of their genotypes. Organic acids, amino acid and dihydroxyphenethylamine isomers discriminated the clones grown under different planting conditions. LC-MS proved to be an effective, sensitive and rapid technique in acquiring information that to-date has been scarce for this important species. The profiling of oil palm leaves provided essential information on the chemical properties of the tissue that will in turn promote utilization of the waste. Principal component analysis (PCA) aided the assessment of oil palm status and paved ways to more ecological investigations in oil palm researches.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Sarjana Sains

KAJIAN METABOLOM DAUN SAWIT (*Elaeis guineensis* Jacq.) MENGGUNAKAN KROMATOGRAFI CECAIR-SPEKTROMETER JISIM

Oleh
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Pemprofilan dan pencirian metabolom yakni kandungan metabolit tumbuhan dapat memberikan gambaran terperinci keadaan metabolik tumbuhan tersebut dan membenarkan penemuan bahan kimia berharga. Walau bagaimanapun, struktur bahan kimia yang kompleks menyukarkan usaha ini. Daun sawit adalah bahan sisa terbesar daripada aktiviti perladangan sawit di mana penggunaan semula bahan ini adalah tidak meluas dan memerlukan penyelidikan untuk meningkatkan potensinya. Memandangkan fenotip sesuatu organisma adalah bukan terjemahan sepenuhnya daripada genotip dan dipengaruhi pula oleh faktor persekitaran, kaedah metabolomik diperlukan untuk mengkaji perubahan metabolik organisma tersebut. Metabolom daun sawit diprofil menggunakan kromatografi cecair (LC) dan spektrometer jisim (MS). Analisis data spektrometer jisim berganda (MS/MS) seperti analisis kehilangan fragmen neutral membantu dalam pengenalpastian bahan kimia. Metabolom daun pucuk dibandingkan

dengan daun pelepah matang menggunakan kedua-dua mod ion positif dan negatif spektrometer jisim. Daun pucuk mengandungi tujuh jenis kompleks glikosida apigeninasid glutarik metilhidroksi dan satu apigenin glikosida-O yang tidak terdapat di dalam daun pelepah. Empat jenis glikosida luteolin dan dua isomer glikosida apigenin pula tidak terdapat di dalam daun pucuk. Sejumlah 53 bahan kimia termasuk kompleks garam, asid-asid amino, amina, asid-asid organik, katechin, glikosida asid fenolik, glikosida stilbenoid dan glikosida flavonoid dikenal pasti dalam penyelidikan ini. Tisu daun sawit merekodkan aktiviti antioksidan yang baik dengan daun pelepah menunjukkan aktiviti tertinggi penurunan radikal DPPH per g berat tisu kering, diikuti dengan ekstrak hidrolisis daun pelepah, ekstrak hidrolisis daun pucuk dan ekstrak daun pucuk. Metabolom daun sawit dipengaruhi oleh persekitaran walaupun klon sawit yang digunakan adalah daripada genotip yang sama. Asid organik, asid amino dan isomer amina fenetildwihidkroksi membezakan antara klon sawit yang ditanam di dalam rumah pemerhatian, di ladang dan di tanah gambut dan mineral. LC-MS terbukti merupakan kaedah berkesan, sensitif dan pantas dalam mendapatkan maklumat metabolom daun sawit yang sebelumnya tiada bagi spesies penting ini. Maklumat ini juga akan meningkatkan potensi penggunaan sisa daun sawit demi industri yang lebih lestari. Penggabungan kaedah LC-MS dan analisis komponen prinsipal (PCA) pula membantu dalam penyelidikan ekologi sawit.

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"O Allah Lord of the worlds, Owner of knowledge, splendor and generosity, make best our affairs, our acts and our deeds, grant us good beginning and good ending, and bless us with Your bountiful mercy..." I certify that a Thesis Examination Committee has met on (date of viva voce) to conduct the final examination of Noor Idayu Mhd Tahir on her thesis entitled "Liquid Chromatography-Mass Spectrometry-Based Metabolomics of Oil Palm (*Elaeis guineensis* Jacq.) Leaf" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the Master of Science.

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DECLARATION

I declare that the thesis is my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously, and is not concurrently, submitted for any other degree at Universiti Putra Malaysia or at any other institution.



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