

**EXTRACTION OF BIOCHEMICAL COMPOUNDS IN DATES
USING THREE MIXTURE DESIGN AND IDENTIFICATION BY
GC-MS AND LC-TOF-MS WITH PRINCIPAL COMPONENTS
ANALYSIS**

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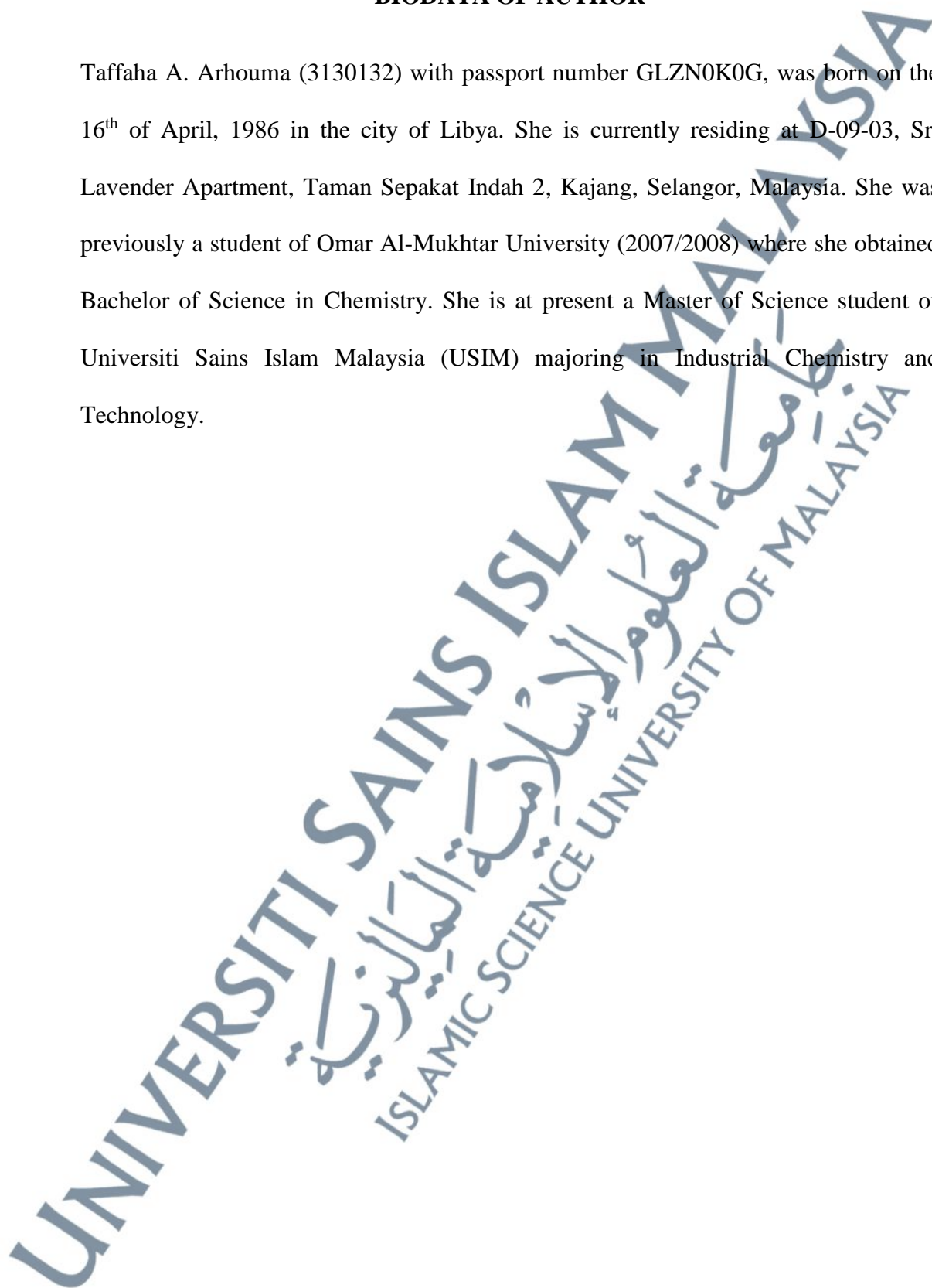
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ABSTRAK

Dalam kajian ini, pengekstrakan menggunakan pelarut berbeza (kloroform, metanol dan heksana) dengan reagen N, O-bis (trimethylsilyl) trifluoroacetamide (BSTFA) dan 1% trimethylchlorosilane (TMCS) dan kombinasi campuran tersebut telah digunakan untuk mengekstrak sebatian biokimia dalam tiga jenis kurma (Kheseab (Tamar), Segae (Rutab) and Khalas (Tamar). Sebatian tersebut telah ditentukan menggunakan gas kromatografi-spektrometri jisim (GS-MS) dan kromatografi cecair masa penerbangan jisim spectrometer (LC-TOF-MS). Keputusan GC-MS menunjukkan bahawa pengekstrakan menggunakan campuran metanol dan kloroform (50 % : 50 %) telah mengekstrekan 16 sebatian diikuti oleh metanol dengan heksana (50%: 50%) yang mengekstrekan 15 sebatian, dan campuran tiga pelarut (33.3 % : 33.3 % : 33.3 %) 14 sebatian. Sementara itu, campuran pelarut yang lain memberikan jumlah sebatian diekstrak yang kurang berbanding dengan campuran sebelumnya. Keputusan LC-TOF-MS menunjukkan bahawa pengekstrakan menggunakan metanol dan kloroform (50 % : 50 %) dalam Khalas (Tamar) dapat diekstrak 27 sebatian diikuti oleh Segae (Rutab) dengan 17 sebatian manakala dalam Khalas (Tamar) hanya 10 sebatian telah diekstrakkan. Analisis Komponen Utama (PCA) telah dilakukan ke atas data "multivariates" GC-MS untuk mengkaji hubungan di antara sebatian yang diekstrak dengan kepolaran campuran pelarut dari plot skor dan loading.

Kata Kunci: Kurma, reka bentuk campuran, BSTFA, TMCs, GC-MS, LC-TOF-MS, Sebatian Biokimia dan Analisis Komponen Utama (PCA).

ABSTRACT

In this study, the extraction using different solvents (chloroform, methanol and hexane) with reagent N,O-bis(trimethylsilyl)trifluoroacetamide (BSTFA) and 1 % trimethylchlorosilane` (TMCS) and their mixtures were used to extract biochemical compounds in three types of dates Kheseab (Tamar), Segae (Rutab) and Khalas (Tamar). The compounds were determined using Gas chromatography–mass spectrometry (GS-MS) and Liquid chromatography time-of-flight mass spectrometer (LC-TOF-MS). The results of GC-MS showed that the extraction using the mixture of methanol and chloroform (50 % : 50 %) extracted 16 compounds followed by methanol with hexane (50 % : 50 %) which extracted 15 compounds, and mixture of three solvents (33.3 % : 33.3 % : 33.3 %) 14 compounds. While the other mixture of solvents, less number of compounds were extracted as compared with the previous mixtures. The results of LC-TOF-MS showed that the extraction using methanol and chloroform (50 % : 50 %) in Khalas (Tamar) was able to extract 27 compounds followed by Segae (Rutab) with 17 compounds while in Kheseab (Tamar) only 10 compounds were extracted. Principal Components Analysis (PCA) was performed on multivariate data of GC-MS results to study the relationship between compounds extracted with polarity of solvents mixture from the scores and loadings plots.

Keywords: Dates, Mixture design, BSTFA, TMCS, GC-MS, LC-TOF-MS, Biochemical Compounds and Principal Components Analysis (PCA).

ملخص البحث

في هذه الدراسة، نقوم بعملية الاستخلاص مستخدمين في ذلك ثلاث انواع من المذيبات المختلفة (كلوروفورم، والميثانول والهكسان) مع الكواشف N,O-bis(trimethylsilyl)trifluoroacetamide (BSTFA) and trimethylchlorosilane (TMCS) 1% با استخدام ثلاث انواع من التمر (خلاص و تمر و رطب) بحيث تتم عملية الاستخلاص باستخدام كل مذيب علي انفراد ثم نقوم بمزج كل محلولين مع بعضهما ومن ثم نقوم بمزج المحاليل مع بعضها البعض وذلك لرؤية مدي فاعلية كل محلول في استخلاص اكبر قدر ممكن من المركبات البيوكيميائية يتم استعمال تقنية الفصل الكروماتوغرافي بالغاز (GC-MS) وتقنية (LC-TOF-MS) وذلك للتعرف علي المركبات اللتي تم استخلاصها . أظهرت نتائج الفصل الكروماتوغرافي الغاز (GC-MS). أن مزيج من الميثانول والكلوروفورم (50% : 50%) استخلص 16 مركب تليها الميثانول مع الهكسان (50% : 50%) التي استخلص منها 15 مركب ايضاً، ومزيج من ثلاثة المذيبات (33.3% : 33.3% : 33.3%) هو ايضاً استخلص 14 مركب في حين أن مجموعات أخرى من المذيبات كان عددها أقل من المركبات بالمقارنة مع مجموعات السابقة . نتائج LC-TOF-MS أظهرت أن الاستخراج باستخدام الميثانول والكلوروفورم (50% : 50%) في الخلاص (التمر) قادر هو ايضاً على استخلاص 27 مركبات تليها ساقى (الرطب) 17 مركب في حين ان الخصيب (التمر) تم استخلاص 10 مركب فقط. تم إجراء تحليل المكونات الرئيسية (PCA) على متغيرات مختلفة من بيانات النتائج GC-MS اللتي تدرس العلاقة بين المركبات المستخرجة مع قطبية المذيبات القطبية scores و loadings plots .

الكلمات المفتاحية : التمر، مزج المذيبات، استخلاص المركبات البيوكيميائية، BSTFA، TMCS، GC-MS و LC-TOF-MS وتحليل المكونات الرئيسية (PCA).

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ABBREVIATIONS

PCA	Principal Components Analysis
PC(s)	Principal Component(s)
GC-MS	Gas Chromatography - Mass Spectrophotometry
LC-TOF-MS	Liquid Chromatography -Time of Flight -Mass Spectrophotometry
BSTFA	N,O-bis(trimethylsilyl)trifluoroacetamide
TMCS	Trimethylchlorosilane

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