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STRUCTURAL ELUCIDATION OF JOJOBA PLANT *(Simmondsia Chinensis)* OIL FROM SAUDI ARABIA

SUUDİ ARABISTANDA YETİŞEN **JOJOBA** *(Simmondsia Chinensis)* BİTKİSİNDEN ELDE EDİLEN YAĞIN YAPISININ AYDINLATMASI

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ÖZET

Simmondsia chinensis'in tohumlarından bir yağ izole edildi. Elde edilen yağın yapısı spektroskopik yöntemlerle [UV, FTIR, ^{1}H NMR, ^{13}C NMR, DEPT, COSY, HETCOR, EIMS] aydınlatıldı ***1.***

Anahtar Kelimeler: Jojoba oil, jojoba, simmondsia chinensis

ABSTRACT

An oil has been isolated from the seeds of Simmondsia chinensis. Structure of the oil, ***1,*** *was elucidated by spectral methods [UV, FTIR, ^{1}HNMR, ^{13}C NMR, DEPT, COSY, HETCOR, EIMS].*

Key Words: Jojoba oil, jojoba, simmondsia chinensis

INTRODUCTION

Jojoba *[Simmondsia Chinensis or Simmondsia californica* Nutt] is a plant that can grow in semi-arid areas. This evergreen dessert shrub is native to arid hills of Arizona, southern California and adjacent parts of Mexico. The leaves and young twigs are much browsed by sheep, cattle and goats. The seeds are edible for man and are used extensively by American Indians for food (1)

Jojoba yields a crop of seeds that contain mean 40-50 % oil (2,3), that is unique in nature. No other plant on earth produces an oil like jojoba's (4). It is used in the cosmetic (as a highly effective cleanser, conditioner, moisturizer and softener for the skin and hair) (4-10), pharmaceutical (as an anti-foaming agent in the production of penicillin; as a treatment for minor rashes, cuts, acne, psoriasis , neurodermatitis and to prevent anal leakage) (4,11), food product (as a diet aid) (4), manufacturing[as a non-contaminating lubricant for food machinery, a leather softening agent, a replacement for petrochemicals such as linoleum products, adhesive and for heat-resistant materials, detergents, emulsifiers and multifunctional lubricating oil additive] (4,12) and automotive industrie (as a superior lubricant in high speed machinery, tool work and metal cutting) (4). It is also a renewable energy resource (4,13). This work was aimed to structural identify the oil from jojoba grown in Saudi Arabia. This paper deals with the isolation of jojoba oil from seeds and elucidated by spectral methods (UV, FTIR, 1H NMR, ^{13}C NMR, DEPT, COSY, HETCOR, EIMS).

EXPERIMENTAL SECTION

1H NMR and COSY(2-D) spectra were recorded using a Bruker GmbH DPX-400, 400 MHz High Performance Digital FT-NMR. ^{13}C NMR(100 MHz), DEPT, HETCOR spectra were also recorded at same spectrometer with $CDCl_3$ as solvent. Chemical shifts were referenced to tetrametylsilane. FTIR and UV spectra were observed on MATSON 1000 spectrometer and BECKMAN DU-600 spectrometer, respectively. Electron impact mass spectrometry at an ionization potential of 70 eV was performed with a Micro MASS UK Platform LC-MS.

Plant Material

Seeds of *Simmondsia chinensis* were collected from Saudi Arabia, close to Yutama in August 1997.

Extraction of ***Jojoba oil***

Jojoba seeds were ground to a size of approximately 1 mm. A soxhlet extractor with a thimble volume of 50 mL was used for extraction with hexane as the extracting solvent. After extraction, the solvent was recovered using a rotavapor. The oil was further heated in an oven and kept at 120 °C for another half an hour to assure the complete evolution of hexane.

RESULT AND DISCUSSION

The purity of oil was checked by TLC. Structure of the isolated oil was characterized by spectroscopic methods such as ^{1}H NMR, ^{13}C NMR, DEPT, COSY, HETCOR, FT-IR, UV, EIMS. The ^{1}H NMR and ^{13}C NMR spectra and also other analyses of compound 1 showed that its olefinic chain parts are symmetric.

$$CH_3(CH_2)\text{„}CH_2CH{=}CHCH_2(CH_2)_mCH_2COOCH_2(CH_2)_{m+1}CH_2CH{=}CHCH_2(CH_2)_nCH_3$$

1 *(n+m=14)*

bp:289 °C; UV λ_{max} (MeOH) 222

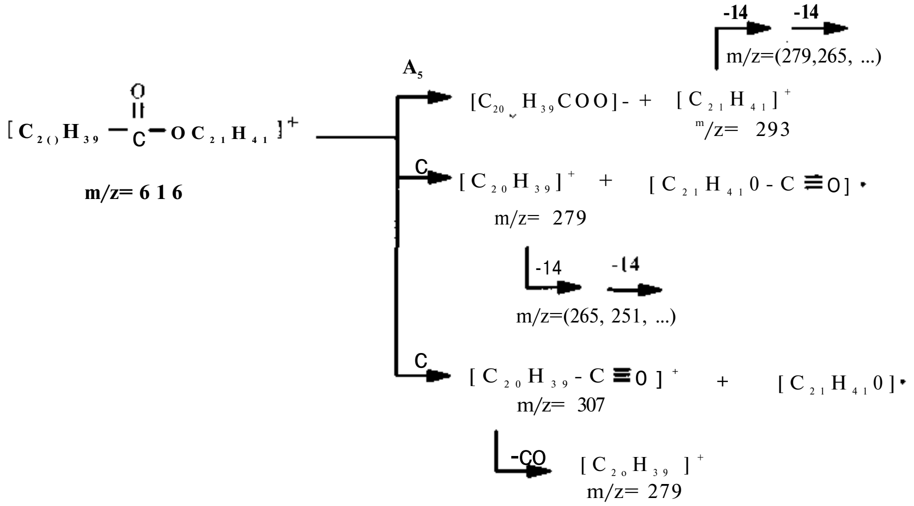
Data of IR spectrum (KBr,cm^{-1}) indicate that compound is an ester (1741 cm^{-1}, carbonyl stretching; 1170 cm$^{''1}$, C-O-C asymmetric stretching) which has olefinic chain (3020 cm^{-1}, vinylic C-H stretching; 2957 cm^{-1}, aliphatic C-H stretching; 1464 cm^{-1} C-H in-plane bending) and also the double bond (at 1650 cm^{-1}) is not conjugate with the carbonyl group.

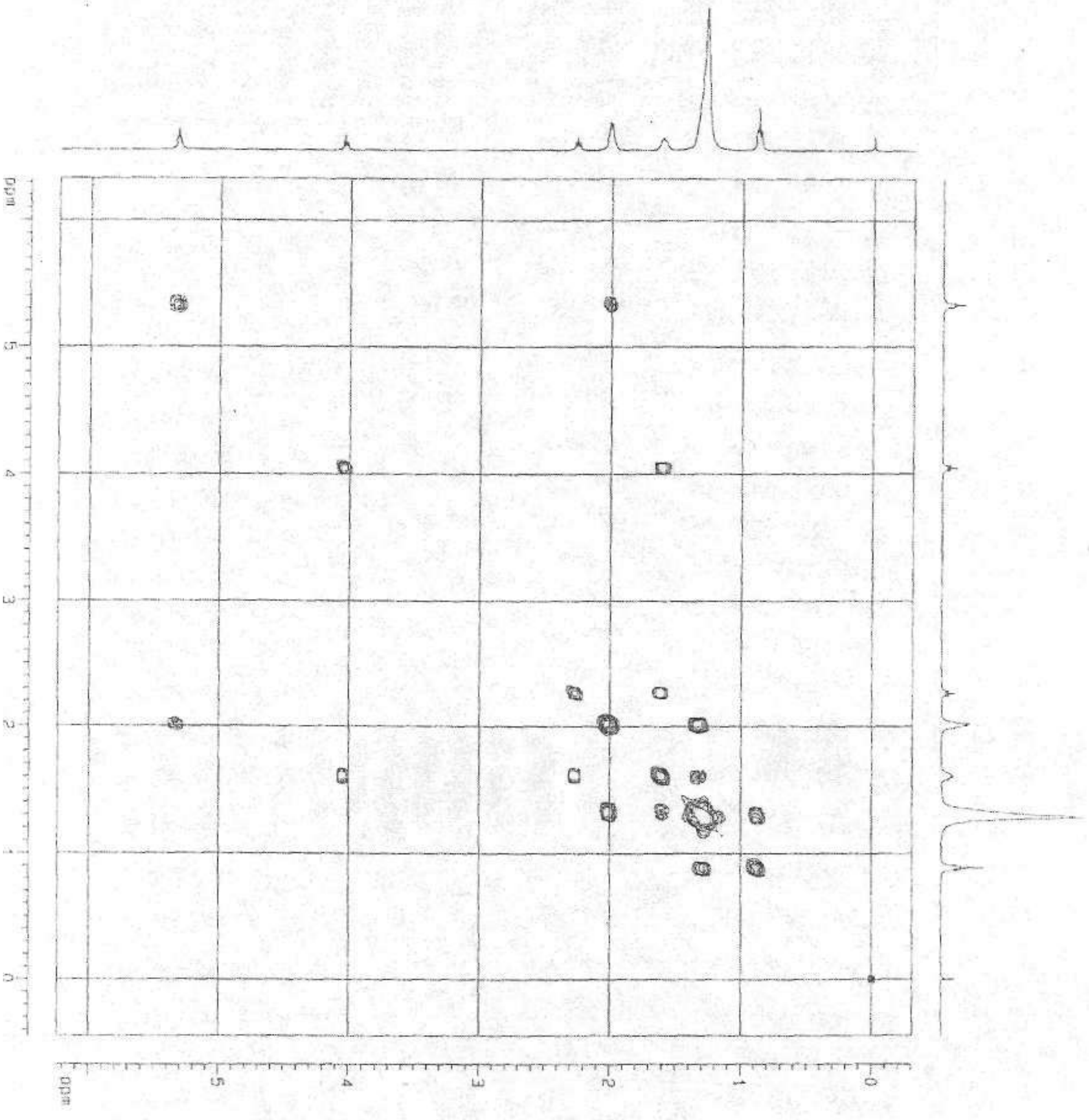
The relative integration ratios indicate that compound is nearly symmetric (2:1:1:4:2:27:3). It has been determined that the number of proton in the compound is eighty ($C_{20}H_{39}COOC_{21}H_{41}$) and this number is compatible with relative integration ratio (4H:2H:2H:8H:4H:54H:6H). The four vinylic proton at δ 5.43 as triplet; two proton of methylene attached to the oxygen at δ 4.05 as triplet; two protons of methylene attached to the carbonyl group at δ 2,27 as triplet; eight allylic protons at 2,01 as broad quartet; four protons of methylenes adjacent to carbonyl bonding methylene and oxygen bonding methylene at δ 1.61 as broad multiplet; fifty-four protons of other methylenes at δ 1.27 as broad and six protons belong to two methyl groups at 0,88 as triplet are in accord with the proposed compound. And also COSY data (Figure 1), ^{13}C and DEPT data (they are given below) and HETCOR data (Figure 2) verify the proposed compound.

^{13}C NMR data: (100 MHz, $CDC1_3$, δ ppm): 173.5(C=0); 130.30, 130.27, 130.25, 130.22 (C=C and C=C); 64.58(-C(O)-OCH_2-); 34.76(-CH_2-C(O)-); 32.59, 30.42, 30.33, 30.25, 30,21. 30.17, 30.13, 30.01, 29.97, 29.92, 2 2, 29.39, 27.81, 26.62, 25.59, 23.31(-CH_2-); 14.61 (CH_3- of acid root and -CH_3 of alcohol **root)**

DEPT ***data:*** (100 MHz, $CDC1_3$, δ ppm): *DEPT 90* (<u>CH)</u> ; 130.30; 130.27; 130.25; 130.22; *DEPT 135* (-<u>CH_2</u>) ; 64.58, 34.76, 32.59, 30.42, 30.33, 30.25, 30,21, 30.17, 30.13, 30.01, 29.97, 29.92, 29.82, 29.39, 27.81, 26.62, 25.59, 23.31

Mass Spectrometry. **m/z, (M+H)$^+$** 617. Other fragmentation products and procedures are given below:





Figurel

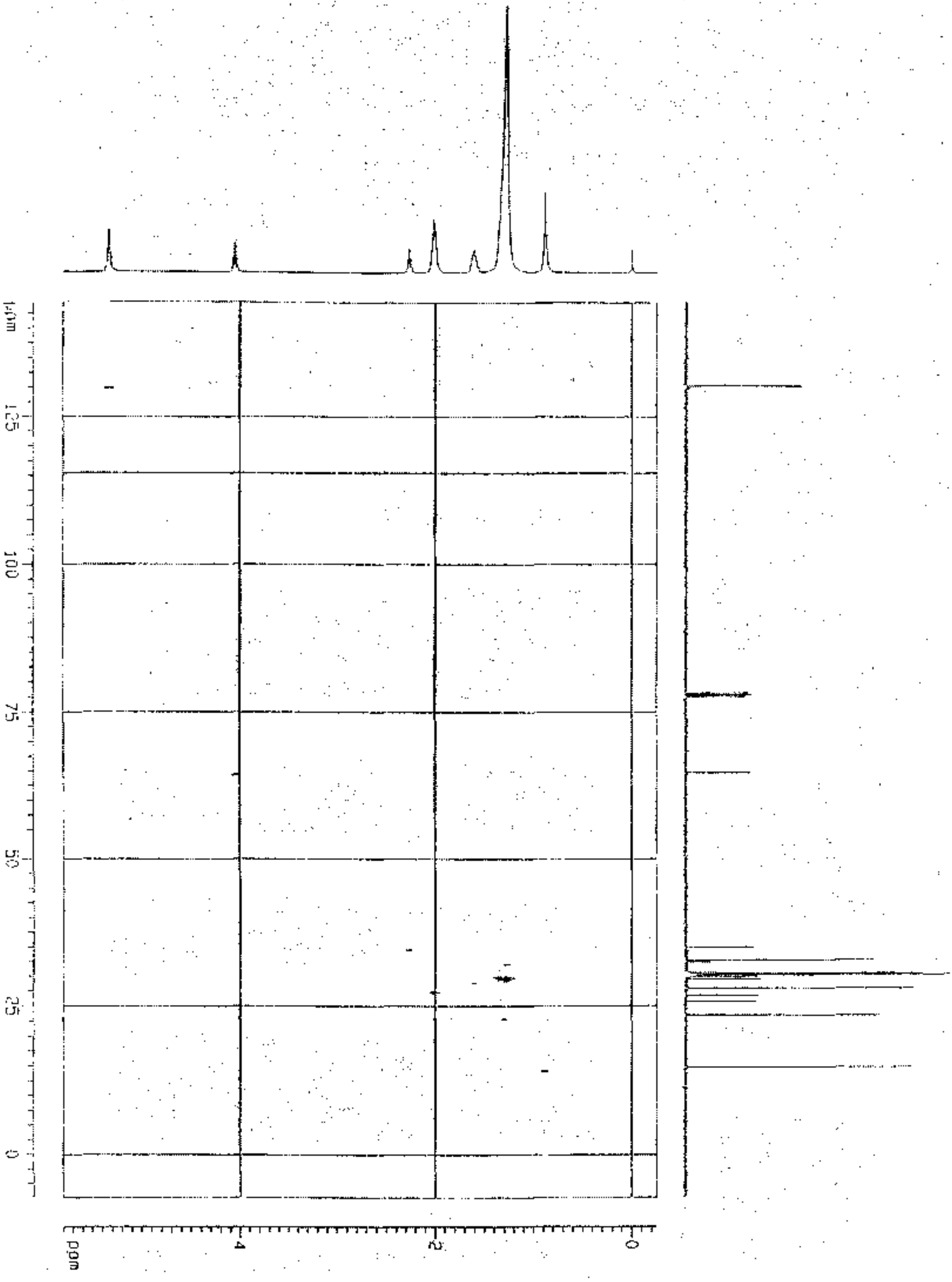


Figure2

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