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Phytochemical investigation of *Mesua ferrea* L. (Seeds)

***1 Faizan Danish Khaleel, 2 BK Mehta**
[1] Department of Chemistry, Govt. Degree College Shopian, Jammu Kashmir, India
[2] S.S. in Chemistry Vikram University, Ujjain, Madhya Pradesh, India

Abstract

Phytochemical compound was isolated from the *Mesua ferrea* L. (seeds) by using hexane. The new compound Henicosanyl-3-hydroxyoctanoate was identified by spectral (IR, ^{1}H NMR, Mass spectrum, elemental analysis) and chemical analysis. The compound being novel is first time reported by us.

Keywords: *Mesua ferrea* L, *calophyllaceae*, aliphatic

1. Introduction

Mesua ferrea L. commonly known as Nagkesar belongs to family Calophyllaceae. The plant is used medicinally in various ailments (Ambasta SP, 1994). The decoction of seeds of *M. ferrea* is given for the treatment of gastritis, bronchitis and to cure snake bite. Leaves of *M. ferrea* are antidote for snake bites and scorpion sting (Garg S, 2009). The different extracts of plants have shown anti- ulcer, anti-venom, anti protozoal, anti-cancer, anti-oxidant activities (Sahni KC, 1998). The present study reports the isolation and structural elucidation of novel compound isolated from the seeds of *Mesua ferrea* L.

2. Experimental

2.1 General procedures

Melting points (mp) are uncorrected. ^{1}H NMR was recorded on 400 MHz Varian XL spectrometer, ^{13}C NMR spectrum (100 Hz), IR spectra were recorded in KBr disk on Perkin Elmer-377 spectrometer, EIMS on Jeol-JMS D 300 mass spectrometer. All chemical shifts (d) are given in ppm and Me_4Si was used as internal standard.

The carbon type (CH_3, CH_2, CH) was determined by DEPT experiments. Chemicals are of analytical-reagent grade and column chromatography was carried out on alumina grade III and TLC on silica gel G (CDH/Glaxo laboratories). Spots were visualized by exposure to iodine vapor or by spraying with H_2SO_4-vanillin solution followed by heating at 105 _C for 5 min.

2.2 Plant material

The seeds (10 kg) of *M. ferrea L.* were collected from the market of Ujjain city and were identified by the authorities of the Institute of Environment Management and Plant Science, Vikram University, Ujjain. A voucher specimen was deposited in the herbarium of the School of Studies in Botany, Vikram University, Ujjain, India.

2.3 Extraction and isolation

The seeds (10kg) were shade dried, cleaned, coarsely powdered and extracted with hexane in soxhlet-extractor for 72 h. The extract was concentrated by rotary evaporator to afford solid mass (50mg). The hexane extract was separated by repeated column chromatography on alumina grade III. The column was eluted by gradient elution in increasing order of polarity like hexane, benzene, EtOAc and methanol. The fractions were collected in bulk and monitored by TLC. The residue (5 g) of hexane fraction was chromatographed on alumina on the basis of increasing order of polarity of eluents. A well-stirred suspension of alumina III (100–150 g in petroleum ether 60–80) was poured into the column (150 cm long and 50 mm in diameter). When the absorbent was well settled, the excess of hexane was allowed to pass through the column. With silica gel in hexane, the mass was made into a slurry and digested in a well stirred column. The column was successively eluted with the hexane, benzene, EtOAc and methanol and their mixtures of increasing polarity. Fraction (c) hexane: ether (3:1, v/v) fraction was purified and identified as Henicosanyl-3-hydroxyoctanoate.

Compound Designation: Henicosanyl-3-hydroxyoctanoate, State: Solid**,** Molecular formula: $C_{29}H_{58}O_3$**,** Molecular ion peak: M^+ 454 [M^+-4H]**,** TLC system: Hexane (pure)**,** Recrystallization: Methanol**,** M.P. 160ºC**,** Solubility: $CDCl_3$, I.R. (KBr, cm^{-1}): 2921, 1737, 1179, 730- 720 cm^{-1}. ^{1}H NMR spectrum (400MHz, $CDCl_3$, TMS, δ), δ 0.71 (s, 6H, 2×CH_3, J= 7.5 Hz), δ 2.3 (t, 2H,-CH_2-COO-, J= 7.0 Hz), δ 4.11 (t, 2H, -OCH_2), δ1.23 (brs, 23CH_2- 46H).^{13}C NMR spectrum (100 Hz, $CDCl_3$, ppm), 174.25, 64.6, 33.9, 29.9- 26.9, 23.40, 14.07 ppm. ESI-MS Spectrum (m/z, rel. inte.): M^+ 452 [M^+-2H], 437, 419, 411, 393, 381.

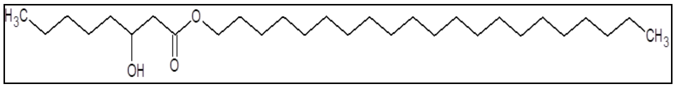

Fig 1: Henicosanyl-3-hydroxyoctanoate

3. Results and Discussions

The compound was identified mainly by its IR, ^{1}H NMR, ^{13}C

NMR and Mass spectrometry analysis. Compound. IR Spectrum (ʎmax, KBr, cm^{-1}), It showed absorption bands at 2921, 2850 and 1439 cm^{-1} due to C-H stretching and bending vibrations. An absorption band at 1737.1 cm^{-1} was assigned to ester group. Bands at 1179 and 730-720 cm^{-1} were due to long chain aliphatic nature of molecule (Dyer, 1984). ^1H NMR spectrum (400MHz, $CDCl_3$, TMS, δ), in ^1H NMR spectrum the terminal methyl groups were resonated at δ 0.71 (J= 7.5 Hz) for six protons. Peaks at δ 2.3 and δ 4.1 as triplet were due to $–CH_2$-CO- and $–OCH_2$ groups, present in the molecule respectively. Rest of the methylene protons were resonated at δ 1.23 as singlet. The hydroxyl proton was resonated at δ 1.59 and carbinolic proton at δ 3.6. Hence the compound was proposed to be a long chain aliphatic ester (Silverstein *et al*., 1981). ^{13}C NMR spectrum (100 Hz, $CDCl_3$, ppm). It showed a peak at 174.2 ppm due to carbonyl ester ($-OCH_2$). The peaks at 64.6 and 33.9 ppm were due to methylenoxy and α-methylene ($-CH_2$-CO-) carbon atoms of ester respectively. The peak at 13.80 ppm was due to terminal methyl carbon atoms. A bunch of peaks at 29.71 ppm corresponds to the remaining methylene carbons (Yamguchi, 1970).In ESI-MS spectrum, molecular ion peak was absent and quasimolecular ion peak was present at m/z 450 which correlated molecular ion at m/z 454, corresponding to molecular formula $C_{29}H_{58}O_3$ [M^+-4H] suggesting long chain aliphatic ester. The abundant fragments at m/z 411 were formed by Mc- Lafferty rearrangement, indicating the position of ester group. Other abundant fragments at m/z 437, 393, 381 and 321 were also in agreement with the proposed structure (James; 1976). Thus the compound identified as long chain aliphatic ester and on the basis of above spectral data the compound was designated as Henicosanyl-3-hydroxyoctanoate.

4. Conclusion

To the best of our knowledge the compound was novel and being reported first time by us from seeds of *M. ferrea* L.

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