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Identification of novel phytochemical constituent from Mesua ferrea L. (Seeds)s

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ABSTRACT

Novel phytochemical compound was isolated from the hexane extract of Mesua ferrea L. (seeds) by using n-hexane. The new compound 13-hexadecanol-11-ene octacosanoate was identified by spectral (IR, ^{1}H NMR, ^{13}C NMR, Mass spectrum, elemental analysis) and chemical analysis. The compound being novel is first time reported by us.

Key words: Mesua ferrea L.,Calophyllaceae, Aliphatic.

I.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.

II.EXPERIMENTAL

2.1 General procedures

Melting points (mp) are uncorrected. ^{1}H NMR was recorded on 300 MHz Varian XL spectrometer, ^{13}C NMR spectra were recorded on Varian XL 75 MHz spectrometer, 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.

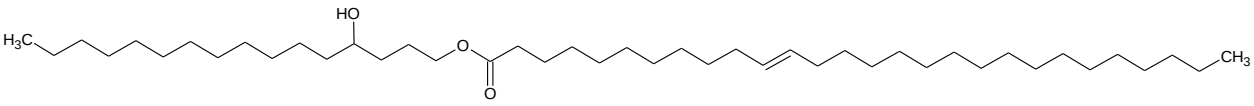
2.2 Plant material

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 oil (265 mL). The oil was saponified by the alcoholic potash method (Mohan, 2003). Usual work up yielded (32g) an unsaponifiable matter which 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 (6.8 g) of hexane fraction was rechromatographed 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 (a) hexane: benzene (8:2, v/v) fraction was purified and identified as 13-hexadecanol-11-ene octacosanoate.

Compound. 13-hexadecanol-11-ene octacosanoate, State: White Solid, Molecular formula: $C_{44}H_{86}O_3$, Molecular ion peak: M^+ 662, TLC system: Benzene: MeOH: Acetic acid (8:2: 1v/v), Recrystallization: Chloroform: Methanol, M.P. 86 ^{0}C, Solubility: $CDCl_3$**,** I.R. (KBr, cm^{-1}): 3447, 2919, 2850, 1731, 1635, 1173, 719 cm^{-1}. ^{1}H NMR spectrum (300MHz, $CDCl_3$, TMS, δ) δ 0.89 (t, 6H, 2×-CH_3), δ 4.03 (t, 2H, -CH_2OCO), δ 2.38 (t, 2H, CH_2COO), δ 5.40 (s, 2H, CH=CH), δ 3.18 (t, 2H, -CHOH), δ 1.61 (s, 1H, -OH), δ 1.28 (brs, 76H, 38×-CH_2). ^{13}C NMR spectrum (100 Hz, $CDCl_3$, ppm). 174.0, 66.4, 131.1, 134.2, 34.2, 34.4, 31.9, 31.43, 30.78, 26.63, 25.3, 14.7 ppm. Mass spectrum. 662 [M^+], 634, 533, 413, 301, 225, 193, 166, 124, 57.



13-hexadecanol-11-ene octacosanoate

III. RESULTS AND DISCUSSIONS

The novel compound was identified mainly by its IR, ^{1}H NMR, ^{13}C NMR and Mass spectrometry analysis. **Compound. IR Spectrum (ʎ max, KBr, cm^{-1}),** A broad and strong absorption band at 3447 cm^{-1} and 1731 cm^{-1} were due to hydroxyl and carbonyl group of ester. Bands at 2919 and 2850 cm^{-1} were due to –CH stretching vibration and bands at 1471 cm^{-1} were due to –CH bending vibration. A peak at 1635 cm^{-1} was due to the presence of unsaturation in the molecule. All the data leads into long chain aliphatic nature of the molecule (Dyer, 1984). **^{1}H NMR spectrum (300MHz, $CDCl_3$, TMS, δ),** The ^{1}HNMR spectrum showed a triplet at δ 0.89 for terminal methyl groups. The hydroxyl proton resonated at δ 1.61. A multiplet at δ 3.18 was due to carbinolic proton and triplet at δ 5.40 was attributed to double bond present in the molecule. Triplets at δ 4.03 and δ 2.38 (J=6.8 Hz) were due to methylene adjacent to ester group. Rest of the methylene protons were resonated at δ 1.28 as a singlet (Silverstein et al., 1981). **^{13}C NMR spectrum (100 Hz, $CDCl_3$, ppm),** It showed the carbinolic carbon resonated at 64.4 ppm. A peak at 174.0 ppm was attributed to carbonyl group of ester. The olefinic carbon gave a peak at 131.1 and 134.2 ppm. The end methylene carbons were resonated at 14.7 and 15.4 ppm (Yamguchi., 1970). **Mass spectrum,** The mass spectrum established molecular formula of the compound as $C_{44}H_{86}O_3$ and molecular ion peak at m/z 662. The peak at m/z 193, 301 and 435 resulted from α- cleavage to hydroxyl, carbonyl group of ester and unsaturation respectively. Major fragments were obtained at m/z 634, 533, 413, 225, 166, 158, 124, 57. Thus on the basis of above spectral evidences, compound was identified and characterized as 13-hexadecanol-11-ene octacosanoate.

IV.CONCLUSION

From the survey of the literature to the best of our knowledge the compound was novel and being reported first time by us from seeds of *M. ferrea* L. and further examination of the constituents of this plant is currently in progress.

V.ACKNOWLEDGEMENT

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