Isolation and spectroscopic characterization of a long chain 22C fatty acid erucic acid 1 is reported from the pseudobulb of Crepidium acuminatum (Jeevak). The molecule constitute a long chain hydrocarbon with one carboxyl group attached at one end of the molecule and a double bond at the C13 position. Energy minimized structure revealed that the molecule is 2.42 nm long having a polar ‘COOH’ group attached at the end of lipophilic hydrocarbon chain making it useful as an amphiphile for nanoscience and nanotechnology.

Keywords: Astavarga, Crepidium acuminatum (Jeevak), Erucic acid, Chyawanprash

Chyawanprash, an ayurvedic health tonic, is well known for its anti-ageing activities since the ancient period. Jeevak (Crepodium acuminatum) is one of the ‘set of eight ingredients’ called ‘Astavarga’ present in Chyawanprash.’ The eight Astavarga plants namely Kakoli, Kshrikakoli, Jeevak, Rishvok, Meda, Mahameda, Riddhi and Vrddhi grow naturally in small patches in particular ecological environments in the Himalaya especially in the North-Western Himalaya at an elevation of 1200 – 4000 m above the sea level. Recent attempts by a group scientists and sages have enabled the proper identification of the eight Astavarga plants. In continuation of our studies on the chemical investigation of the phytochemicals present in the Astavarga plants, we have reported the first isolation of stigmasterol from the medicinal plant Roscoea purpurea Sm. (Kakoli). Antioxidant activities of various parts of Crepidium acuminatum (Jeevak), Roscoea purpurea Sm. (Kakoli), Polygonatum cinctilolium (Mahameda), Habenaria Edgeworthii (Vrddhi) and Habenaria intermedia (Rddhi) and their use in the green syntheses of metal nanoparticles have also been reported by us. Tremendous medicinal activities of Jeevak (Crepodium acuminatum) have been reported. Thorough literature search by us have revealed that there is no report of the active chemical constituents of most of the Astavarga plants. Herein we report the first isolation of erucic acid from the medicinal plant Crepidium acuminatum (Figure 1).

The Crepidium acuminatum sample used in this study was collected from Barlow Ganj, Mussoorie, Uttarakhand, India, in July 2016. Powdered pseudobulb of Crepidium acuminatum (10 g) were extracted with ethyl acetate (250 mL) during 24 h at room temperature. The volatiles were removed under reduced pressure to afford a brownish solid material (0.636 g). The crude extract was purified by successive column chromatography (thrice, Si-gel, 100–200 mesh) using 10-20% ethyl acetate/petroleum ether as the eluent to yield compound 1 as a brownish solid 0.17 % isolated yield (unoptimized). Characterization of compound 1 was carried out by NMR, FTIR and HRMS.

High resolution mass spectrum (Figure 3) of the sample showed a molecular ion peak (M+) at 338.3284 corresponding to a molecular formula C_{22}H_{42}O_2 (calc. 338.3184). The stretching frequency at 3009 cm^{-1} in FTIR spectrum (Figure 4) is assigned to C-H str. vibration of cis-double bond (C=C-H) and 2921-2849 cm^{-1} shows C-H asymmetric and symmetric stretching vibrations of the CH_{2}/CH_{3} aliphatic bond. The band 1707 cm^{-1} showed the stretching vibrations of carbonyl group (C=O) of ‘COOH’ of free fatty acid. The ^{13}C NMR spectrum (Figure 5b) showed 22 carbon signals supporting the molecular formula C_{22}H_{42}O_{2}. The peak at 179.87 indicates

Figure 1: Photograph of Jeevak (Crepodium acuminatum) taken in the month of July, 2016 at Barlowganj, India.
the C1 carbon and the peaks at 129.73 and 130.02 indicating the C13 and C14 groups respectively. The $^1$H NMR spectrum (Figure 5a) exhibited one multiplet for two olefinic protons at $\delta$ 5.36 ppm, and two-proton triplet for H-2 at $\delta$ 2.36 ppm ($J$ = 7.3 Hz), four protons multiplets for H-12,15 at $\delta$ 2.02 ppm, two-protons multiplet at $\delta$ 1.63 ppm probably due to H-3 and three protons triplets at $\delta$ 0.90 ppm due to H-22 and the multiplets ranging from $\delta$ 1.5-1.1 ppm most probably due to the rest fourteen methylene protons (28H, m, 14×CH$_2$). The NMR data obtained for the compound 1 matched with the data reported previously in the literature. Erucic acid is present in several other plants. But to our knowledge, erucic acid is the first compound isolated from the *Crepidium acuminatum*.

Energy minimization carried out with PCModel program revealed that the molecule is 2.42 nm long making it useful in nanoscience and nanotechnology.

In conclusion, isolation and characterization erucic acid is reported from the pseudobulb of *Crepidium acuminatum*. According to our knowledge, this is the first report of the isolation of erucic acid from *Crepidium acuminatum*. Molecular modeling studies have revealed that erucic acid can act as a functional nano-entity with tremendous potential application in supramolecular chemistry and nano-science.

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References and notes


3. A. C. Barai, B. G. Bag, First isolation of stigmasterol from the Indian medicinal plant Roscoea purpurea Sm. (Kakoli), Prayogik Rasayan. 2019, 3 (2), 5-6.


15. Characterization data of compound 1:

HRMS: m/z calculated for C_{22}H_{42}O_{2} (M^+) is 338.3184 found 338.3284. m/z calculated for C_{22}H_{42}O_{3}NH_{4} [M+NH_{4}]^+ is 356.3527; found 356.3513.

$^1$H NMR (400 MHz, CDCl$_3$): δ = 5.36 (2H, m, H-13,14), 2.36 (2H, t, J = 7.3 Hz, H-2), 2.02 (4H, m, H-12,15), 1.63 (2H, m, H-3), 1.5-1.1 (28H, m, 14×CH$_2$), 0.90 (3H, t, J = 6.0 Hz, H-22) ppm.

$^{13}$CNMR (100 MHz, CDCl$_3$): δ = 179.87 (C-1), 34.02 (C-2), 129.73 (C-13), 130.02 (C-14), 23.0-34.0 (17×CH$_2$), 14.3 (C-22,CH$_3$) ppm.

FTIR: (ATR Neat) ν = 3009 (w), 2921 (s), 2849 (s), 1707 (s), 1446 (m), 1415 (w), 1287 (m), 1232 (w), 1106 (w), 940 (m), 721 (m) cm$^{-1}$.

MP = 32 – 34°C.


