Isolation and characterization of aliphatic constituents of *Tephrosia purpurea*

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n-Hentriacontanol has been isolated from pod husk as well as seeds whereas trans-2-trideceno-1,13-dioic acid, a new compound isolated from pod husk of *Tephrosia purpurea*. The compounds have been characterized on the basis of spectral data analysis and chemical reactions.

The compounds *Tephrosia purpurea* (Linn.) Pers. commonly known as “Sarphonkha” is a polymorphic, perennial herb found throughout India. The plant is known for its medicinal importance, therefore, it was selected for systematic analysis. A large number of compounds belonging to steroids, rutin and rotenoids, flavones and their glycosides, flavanones, isoflavones, alkaloids, oils and fatty acids and other compounds like quercetin were isolated from *Tephrosia purpurea* and other species of *Tephrosia*.

The present communication reports the isolation and structure determination of n-hentriacontanol (A) from pod husk as well as seeds and trans-2-trideceno-1,13-dioic acid (B) from pod husk.

### Results and Discussion

**Compound A**: mp 87-87.5 °C, analyzed as C_{31}H_{64}O on the basis of molecular peak, M’ at 452, IR, NMR and oxidation to hentriacontanoic acid. The compound A is thus identified as n-hentriacontanol.

**Compound B**: Elemental analysis and molecular ion peak M’ at 242 in the mass spectrum of B indicated its molecular formula to be C_{13}H_{22}O_4. It gave effervescence with sodium bicarbonate indicating the presence of carboxyl group and carboxyl group determination indicated it to be a dibasic acid. Thus, all the four oxygen atoms of B were accounted for. The compound also decolourised bromine water indicating unsaturation. As was clear from its molecular formula, there was a possibility of only one double bond, which was further confirmed by reducing B with hydrogen and platinum oxide. The reduction product was identified as brassyllic acid having a molecular formula C_{13}H_{22}O_4. Thus, formation of brassyllic acid (tridecane 1,13-dioic acid) from B clearly indicated it to be tridecane 1,13-dioic acid. The position of the double bond was confirmed by oxidising B with potassium permanganate. The oxidation product was identified as undecane dioic acid, thus clearly confirming the position of double bond between second and third carbon atoms of B. As the melting point of B was much higher than the m.p. reported for 6-tri-decenedioic acid (m.p. 72°C) and was very close to the melting point for trans-2-dodecenedioic acid (m.p. 165-66°C), it appeared to have a trans structure.

The proposed structure is further supported by its IR absorption band at 3300-3100 (COOH), 1720 (keto group) and 1695 cm\(^{-1}\) (COOH) which showed the molecular ion peak at M’ 242. Further fragmentation showed the presence of peaks at m/z 225 due to M-OH, 224 due to M-H_2O, 198 due to M-CO_2, and at m/z 170 due to M-acrylic acid. The base peak at m/z 72 indicated the formation of acrylic acid due to rearrangement thus confirming the presence of a double bond conjugated to a carboxyl group. The intense peaks at m/z 28 due to CO, m/z 44 due to CO_2, m/z 60 due to C_8H_16O_2, m/z 43, 57 and 71 due to alkyl groups were also present in its mass spectrum. The presence of an intense peak at m/z 60 clearly indicated McLafferty re-arrangement during fragmentation. Thus, the mass spectrum also confirmed B to be 2-trideceno-1,13-dioic acid.

**Experimental Section**

The powdered pod husk and seeds were extracted with pet. ether (PE), benzene and ethanol successively. The pet. ether extract of pod husk was passed through silica gel column after concentration. The concentrated fraction was absorbed on silica gel (25 g) and dried in air. The dried material was chromatographed over silica gel column. The column
was eluted successively with pet. ether and benzene mixtures v/v. The pet. extract of seeds was concentrated and washed with ethanol, the oily layer was not worked out. The ethanol washings on concentration and recrystallisation gave a compound similar to A.

**Compound A**: Fractions eluted with pet. ether-benzene (3:1) gave a compound which on recrystallisation with acetone and methanol yielded n-hentriacontanol, mp 87-87.5°C, acetyl derivative, mp 75-76°C and oxidized derivative 1-hentriacontanoic acid, mp 93°C. Anal. Found: C, 82.45; H, 13.95; OH, 3.90, Calcd for C₃₁H₆₃O₈: C, 82.30; H, 14.15; OH, 3.76%, IR (KBr). 3400-3350, 2920, 2850, 1470, 1385, 1300, 1050, 720 cm⁻¹.

**Compound B**: The compound B was crystallised from pet. ether-benzene (2:1) and (1:1) fractions obtained from silica gel column of pod husk extract. Recrystallisation from ethanol yielded compound B, mp 166-68°C. Anal. Found: C, 64.20; H, 9.18; M⁺, 242. Caled for C₂³H₄₄O₂: C, 64.46; H, 9.09%, Mol. wt. 242, IR (KBr and CHCl₃): 3300-3100, 2910, 2845, 1720, 1695, 1460, 1340, 1250, 1020, 980, 965 and 720 cm⁻¹.

The hydrogenation of compound B gave colourless needles, m.p. 113°C (114°C for brassyllic acid). Oxidation of compound B with potassium permanganate yielded colourless needles, m.p. 110°C (111-12°C for undecane dioic acid). Carboxyl group estimation was done by dissolving the compound in formanide and titrating it with sodium methoxide. Found: COOH % = 36.88 (Caled = 37.19%).

**References**