Compound **4**. 82.3/82.6 (G-5), 79.3 (G-3), 73.3–75 (G-1, 2 × A), 71.2 (G-2, A), 70.5 (G-4), 69.9 (A), 68.8 (A), 61.1/61.7 (G-6), 57.4/56.5 (OMe) ppm.

Compound **8**. 75.1 (2 × A), 74.5 (2 × A), 70.6–71.3 (2 × A), 69.2 (4 × A) ppm.

Compound **9**. 74.3–75.3 (4 × A), 70.6/70.8 (2 × A), 69.1 (4 × A), 60.3 (4′-OMe), 56.3 (3′-OMe) ppm.

Acknowledgements—The authors are grateful to Dr. R. Newman of the Chemistry Division, D.S.I.R., for running the ^{13}C NMR spectra.

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Phytochemistry, Vol. 20, No. 6, pp. 1458–1459, 1981.
Printed in Great Britain.

0031-9422/81/061458-02 $02.00/0

AN OCTAMETHOXYFLAVONE FROM *POGOSTEMON PURPURASCENS**

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(*Received* 3 *October* 1980)

Key Word Index *Pogostemon purpurascens*; Labiatae; purpurascenin; 3,5,6,7,8,2′,4′,5′-octamethoxyflavone.

Abstract—3,5,6,7,8,2′,4′,5′-Octamethoxyflavone has been isolated from the whole plant of *Pogostemon purpurascens*.

Pogostemon purpurascens (Labiatae) is a herb found growing in the Deccan Peninsula [1]. Fresh leaves of this plant are used to clean wounds and the root extract is reportedly used as antidote to scorpion and snake bites [2]. Here we report the isolation and characterization of a new flavone, purpurascenin (**1**), from the acetone extract of the whole plant collected from the Bhimashanker area of Maharashtra. This is the first report of an octamethoxyflavone from the Labiatae. Exoticin [3] (3,5,6,7,8,3′,4′,5′-octamethoxyflavone, the dimethyl ether of digicitrin [4] is the only other octamethoxyflavone isolated so far from natural sources.

The UV and ^1H NMR spectra of **1** indicated it to be a flavonoid. The ^1H NMR spectrum displayed five sharp singlets between 3.8 and 4.08 ppm comprising eight methoxyls and two singlets (1 H each) at 6.66 and 6.88 ppm. There was no indication of any hydroxyl in the spectrum. In the mass spectrum, the peak at *m/z* 241 ($C_{11}H_{13}O_6$) indicated that all four positions in ring A were substituted by methoxyls. The fragment at *m/z* 419 corresponding to the loss of acetyl radical from the molecular ion clearly showed the presence of methoxyl at C_3 [5]. It was obvious that the two free positions were in ring B; this was also supported by fragments at *m/z* 195 ($C_{10}H_{11}O_4$) and 192 ($C_{11}H_{12}O_3$). As the ring B protons exhibited two sharp singlets, these could either be at C3′, C6′ or C4′, C6′. The decision in favour of the former was made by degradation. On treatment with alkali, purpurascenin gave an acidic and a neutral product. The acidic fraction yielded a crystalline compound, mp 143–144°, identified as asaronic acid [6] (2,4,5-trimethoxybenzoic acid, mp, mmp). The neutral fraction, after chromatographic purification, was a gum whose spectral properties were in accord to its being formulated as 2-hydroxy-3,4,5,6,ω-pentamethoxyacetophenone. On the basis of the above data, the structure of purpurascenin can be assigned as 3,5,6,7,8,2′,4′,5′-octamethoxyflavone (**1**).

EXPERIMENTAL

The reported mps are uncorr. TMS was used as internal standard in the ^1H NMR spectra.

The whole plant, *Pogostemon purpurascens* (roots, stem, leaves and flowers) was dried in the shade and powdered material (1 kg) was extracted with Me_2CO (4 l. × 3). Solvent from the filtered extract was removed at 40°/40 mm to give a dark viscous mass (30 g, 3%). This (19 g) was chromatographed over Si gel (1 kg). The C_6H_6–Me_2CO (9:1) eluate yielded pale greenish yellow solid, **1**, purpurascenin (2.4 g; 17.9%), mp 132–133°. An analytical sample was prepared by passing the solid through a

* NCL communication No. 2577.

short column of activated magnesium oxide and recrystallizing from C_6H_6–petrol; fine needles, mp 140–142°. UV λ (MeOH): 253, 337 nm (log ε 4.39, 4.08). ^{1}H NMR ($CDCl_3$, ppm): δ 3.80 (3H, *s*), 3.88 (6H, *s*), 3.95 (6H, *s*), 4.0 (6H, *s*), 4.08 (3H, *s*) (8 × OMe); 6.66 (1H, *s*, C3′), 6.88 (1H, *s*, C6′). MS *m/z* (rel. int.): 462 (M^+, 40) 461 (6), 447 (100), 431 (41), 419 (3), 417 (6), 373 (6), 241 (8), 225 (9), 197 (27), 195 (15), 192 (4), 179 (11), 151 (17), 121 (9). Found: C, 59.20; H 5.79. $C_{23}H_{26}O_{10}$ requires: C, 59.74; H, 5.67%.

Degradation of purpurascenin. **1** (200 mg) was refluxed with KOH (6g) and 50% aq. EtOH (20 ml) for 15 hr. EtOH was removed under red. pres. and the aq. layer was extracted with $CHCl_3$. The $CHCl_3$ extract was washed with water, dried and the solvent removed. The yellow viscous liquid obtained was purified by prep. TLC (C_6H_6–Me_2CO, 97:3) to give a single spot material, 30 mg, 2-hydroxy-3,4,5,6,ω-pentamethoxyacetophenone. ^{1}H NMR (CCl_4, ppm): δ 3.38 (*s*, $-CH_2-O-\underline{CH_3}$), 3.7 (*s*), 3.76 (*s*), 3.91 (*s*), 3.96 (*s*), (4 × $O\underline{CH_3}$); 4.46 (2H, *s*, $-\underline{CH_2}-OMe$) 10.27 (1H, *s*, OH). MS *m/z* (rel. int.): 287 (69), 286 (M^+ 79, $C_{13}H_{18}O_7$), 255 (50), 241 (100), 240 (70), 225 (69), 211 (67), 197 (44), 167 (29), 153 (31).

The aq. layer was acidified with dil HCl and extracted with $CHCl_3$. The $CHCl_3$ extract was washed with H_2O and dried. The solid residue, after removal of solvent, was crystallised from C_6H_6–petrol to give asaronic acid, 2,4,5-trimethoxybenzoic acid (50 mg), mp 143°, mmp 143–144°. ^{1}H NMR ($CDCl_3$, ppm): δ 3.86 (*s*), 3.93 (*s*), 4.03 (*s*) (9H, 3 × OMe), 6.53 (1H, *s*, C3), 7.56 (1H, *s*, C6). Authentic asaronic acid was synthesized from quinone in four steps according to known procedures [7, 8].

Acknowledgement—Dr. V. D. Vartak kindly identified the plant and helped in its collection.

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