

## 3-Substituted-furanyl Compounds of *Perilla ocimoides*

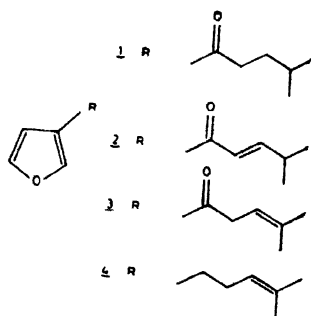
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The *Perilla ocimoides* L., possesses perilla ketone, isoegomaketone, egomaketone and perillene besides other compounds in its aerial parts. The presence of furanyl ketones, perilla ketone in particular, a pulmonary edemagenic agent, suggests possible hazard to grazing cattle and human health.

*PERILLA ocimoides* Linn. (syn. *P. frutescens* L.) an annual herb of Lamiaceae is commonly cultivated in the Northern hill region of India. Several genetically stable chemotypes of *P. frutescens* have been reported with perillaldehyde, elsholtziaketone, perillaketone, citral and phenyl propanoids as the markers of these varieties<sup>1,2</sup>. In a recent communication<sup>3</sup>, rosefuran, perillaketone and  $\beta$ -caryophyllene have been reported from the essential oil from the inflorescence of *P. ocimoides*, cultivated in Lucknow and its perfumery potential has been suggested because of rosefuran. Peterson<sup>4</sup> reported *P. frutescens* as a causative agent of a lethal respiratory disease of cattle, known as acute bovine pulmonary emphysema (ABPE). In the present communication we report the identification of 3-substituted-furanyl compounds (1-4) from the inflorescence of cultivated *P. ocimoides*.



### Experimental

The plant material (2 kg) consisting of dry inflorescence of *P. ocimoides* (after the growers had removed the seeds) was collected from Balwari (Pithoragarh, India) where it is commonly cultivated with other crops in October. The volatile oil (5 ml) obtained with hexane from the steam distillate was dried over anhydrous  $\text{Na}_2\text{SO}_4$ .

The GC analysis was performed on a Varian Vista 6000 instrument controlled by a DS 604 data processor using a fused silica capillary column (DB-Wax, 60 m  $\times$  0.25 mm). GC-MS (70 eV under

EI condition) was done in a Hewlett-Packard 5840A instrument interfaced with a Hewlett-Packard 5985 mass spectrometer using DB-5 column (fused silica 30  $\times$  0.25 mm) with He as carrier gas.

The oil from *P. ocimoides* (4.0 ml) was chromatographed on a column of Si-gel, elution being effected by n-hexane followed by 2-10% diethyl ether in n-hexane. The hexane-ether fractions containing 1 and 2 were concentrated separately and purified by hplc using n-hexane-ether (9:1) on a  $\mu$ -porasil column (7.8  $\times$  300 mm). The  $^1\text{H}$  nmr spectra were recorded on a QE 300 spectrometer.

**Compound 1:** It was liquid with sharp odour,  $\text{C}_{10}\text{H}_{14}\text{O}_2$ ;  $m/z$  (%) 166  $M^+$  (5), 110 (80), 95 (100) besides small intensities of 151, 137, 123, 81, 67 and 55;  $\nu_{\text{max}}$  (neat) 3 125, 1 670, 1 560, 1 150, 867 and 740  $\text{cm}^{-1}$ ;  $\delta$  ( $\text{CDCl}_3$ ) 0.91 (6H, d,  $J$  6 Hz), 1.51-1.63 (3H), 2.71 (2H, t,  $J$  7.5 Hz), 6.75 (1H, dd), 7.42 (1H, m) and 8.01 (1H, m).

**Compound 2:** It was liquid with sharp odour,  $\text{C}_{10}\text{H}_{14}\text{O}_2$ ;  $m/z$  (%) 164  $M^+$  (13), 149 (9), 135 (31), 95 (100) besides small intensities of 121, 107, 91, 77, 67 and 53;  $\nu_{\text{max}}$  (neat) 3 130, 1 670, 1 625 and 980  $\text{cm}^{-1}$ ;  $\delta$  ( $\text{CDCl}_3$ ) 1.08 (6H, d,  $J$  7 Hz), 2.52 (1H, m,  $J$  7 Hz), 6.48 (1H, d,  $J$  15 Hz), 6.81 (1H, dd), 7.02 (1H, dd,  $J$  15 Hz), 7.42 (1H, m) and 8.01 (1H, m).

### Results and Discussion

From the GC of the steam volatile oil of *P. ocimoides* it was found that 1 ( $\text{C}_{10}\text{H}_{14}\text{O}_2$ ; 42.1%) and 2 ( $\text{C}_{10}\text{H}_{14}\text{O}_2$ ; 17.0%) are the main components of the sample. The  $^1\text{H}$  nmr, mass and ir spectral data identify compounds as 1-(3'-furanyl)-4-methylpentan-1-one (perillaketone) (1)<sup>5</sup> and 1-(3'-furanyl)-4-methyl-2-penten-1-one (isoegomaketone) (2)<sup>6</sup>.

The GC-MS results further identify egomaketone (3; 3.5%) and perillene (4; 4.5%)<sup>7</sup> as the two other 3-substituted-furan present in the sample. It is interesting to note that the 3-substituted-furanoids constitute about 68% of the oil. Citral, perillaldehyde, elsholtziaketone, rosefuran and phenylpropanoids reported in other genotypes of *P. frutescens*<sup>8</sup> were

not detected in this plant. Wilson *et al.*<sup>8</sup> reported that the perillaketone possesses lung toxic properties. The presence of perillaketone as the major compound in *P. octmoides* justifies its restricted or carefully controlled cultivation near the fodder grasses. Furthermore, considering the structural relationship of egomaketone and isoegomaketone with perillaketone it is highly possible that those would also be toxic for animal and human beings. It is, therefore, proposed that due care in utilisation of this species for its essential oil or its cultivation near the house or grass-fields be taken. The co-occurrence of 1-4 in the same species suggests involvement of common biogenetic precursor and their interrelationship.

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#### References

1. Y. KORZUKA, G. HONDA and M. TABATA, *Yoshakugaku Zasshi*, 1984, 30, 238.
2. Y. KORZUKA, G. HONDA and M. TABATA, *Phytochemistry*, 1986, 25, 859.
3. L. N. MISHRA and A. HUSSAIN, *Planta Med.*, 1987, 379.
4. D. T. PETERSON, "Proceedings of the Symposium on Acute Bovine Pulmonary Emphysema", University of Wyoming, Laramie, 1965, p. R1-R13.
5. K. INOMATA, M. SUMITA and H. KOTAKE, *Chem. Lett.*, 1979, 709.
6. R. A. MASSY-WESTROFF and G. D. REYNOLD, *Aust. J. Chem.*, 1966, 19, 891.
7. S. DEV, "CRC Handbook of Terpenoids", CRC Press, Florida, Vol. I, 1982, p. 129.
8. B. J. WILSON, J. E. GARST, R. D. LINNABARY and R. B. CHANNEL, *Science*, 1977, 197, 573.