



## Note

### Phytochemical investigation of *Pelargonium graveolens* and isolation of flavonol derivative

Laxmi Chaitanya Neeladri<sup>a,c</sup>, Sridhar Balasubramanian<sup>b</sup> & China Raju Bhimapaka<sup>\*a,c</sup>

<sup>a</sup> Department of Natural Products and Medicinal Chemistry  
and

<sup>b</sup> Department of Analytical and Structural Chemistry,  
CSIR-Indian Institute of Chemical Technology,  
Hyderabad 500 007, Telangana, India

<sup>c</sup> Academy of Scientific and Innovative Research (AcSIR)  
CSIR-HRDC Campus, Postal Staff College Area  
Sector 19, Kamla Nehru Nagar, Ghaziabad 201 002  
Uttar Pradesh, India

E-mail: chinaraju@iict.res.in, chinaraju@gmail.com

Received 12 September 2024; accepted (revised) 24 December 2024

The compound 5-hydroxy-3,7-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one (flavonol derivative) has been isolated from *Pelargonium graveolens* for the first time. The isolated bio-active compound has been obtained from the chloroform extract of the *Pelargonium*. The compound has been analysed by spectral data and its structure confirmed by X-ray crystallography analysis.

**Keywords:** 4H-Chromenone, *Pelargonium graveolens*,  
New source

*Pelargonium graveolens* (PG) belongs to the family of *Geraniaceae* and genus of the *Pelargonium*<sup>1</sup>. The oil of the PG has huge demand due to the presence of value added chemicals including flavonoids, terpenoids and alkaloids<sup>2</sup>. PG leaves are widely used in traditional medicine to address the disorders such as cardiovascular, gastrointestinal and respiratory systems<sup>3</sup>. Further, *Pelargonium* species are used for the treatment of fever, cold, sore throat, wounds, nephritis, hemorrhoids, and gonorrhoea<sup>4</sup>. The marker compounds isolated from this plant has been used as cytotoxic, anti-oxidant, anti-microbial, metabolic and cyclooxygenase (COX) enzymes inhibitory activity<sup>5</sup>.

The compound 5-hydroxy-3,7-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one is an important flavonol derivative has been previously extracted from the plants<sup>6</sup> such as *Cheilanthes farinosa*, *Piper philippinum*, *Kaemferia parviflora*, *Zingiber*

*zerumbet*, *Croton muscicarpa*, *Gynandropsis gyrendra*, *Hedychium thyriforme* and *Lippie rugose*. The compound has been known for its biological properties such as anti-hypertensive, anti-microbial, anti-oxidant, anti-viral and Alzheimer<sup>7</sup>. Therefore, the molecule has immense importance and scope to develop the molecule either by isolation or synthesis.

As part of our research work on isolation, identification of natural products<sup>8</sup> and synthesis of bio-active heterocyclic compounds<sup>9</sup>, we have isolated the compound 5-hydroxy-3,7-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one from plant material *Pelargonium graveolens* (CSIR-CIMAP, Hyderabad/Lucknow) for the first time. The research results are discussed below.

### Results and Discussion

Initially, the plant material *Pelargonium graveolens* (500g) was subjected to the steam distillation and the extracted essential oil was separated. The left over material (3×50g) was subjected for Soxhlet extraction using hexane, chloroform, acetone (each 500 mL) to find out the compounds. After, the extraction, the material was decanted/filtered using sintered funnel and the solvent was removed under reduced pressure below 40°C. The obtained extracts were analyzed by LC-Mass and Ultra-performance liquid chromatography (UPLC) analysis. LC-MASS analysis of the hexane extract was shown the compounds namely Agaro furan, Butanoic acid,  $\alpha$ -Pinene, Carene and Ocimene. The chloroform extract was shown the compounds propionic acid, butanoic acid, 2-butanoic acid, Linalool and Agaro furan. The acetone extract was shown the compounds propionic acid,  $\alpha$ -Pinene, Carene, Ocimene, Citral, Linalool, Butanoic acid respectively.

The Ultra-performance liquid chromatography (UPLC) analysis has been performed for the individual extracts and the hexane extract provided following compounds such as  $\alpha$ -Pinene, Carene, Ocimene, Linalool, Isomenthone, L-Menthone, Geraniol,  $\alpha$ -Terpineol and compared with the literature reports. Compounds Aromadendrene, Ledol, Eudesmol and Cadinol are obtained from chloroform extract. Acetone extract did not show any compounds.

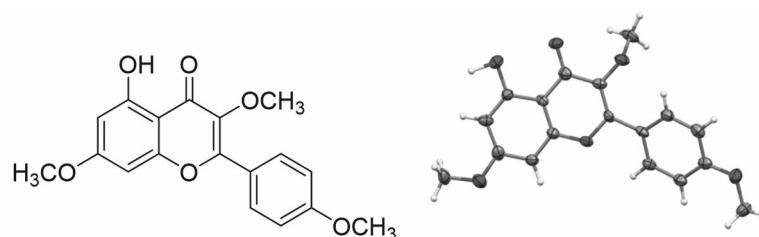


Fig. 1 — Structure of 5-Hydroxy-3,7-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one

The crude material obtained from hexane extract (3.88g) was subjected for column chromatography using silica-gel (100-200 mesh). The compounds such as Agarofuran, Butanoic acid,  $\alpha$ -Pinene, Carene, Ocimene were obtained (Hexane is the eluted solvent). The extract of chloroform and acetone (2.85 g and 4.50 g) were combined and subjected for column chromatography purification using silica-gel (100:200). Total 5 fractions were separated and the major 5<sup>th</sup> fraction (0.040g) was again subjected for column purification (using hexane as solvent) was provided 5-hydroxy-3,7-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one (0.07g) as colorless solid<sup>10</sup>. The compound was well characterized by spectral data (NMR, Mass, HRMS) and compared with the literature report<sup>11</sup>. Further, the compound was subjected for crystallization using methanol as solvent and grown the crystal was analyzed and structure was confirmed by its single crystal X-ray diffraction analysis (Fig. 1)<sup>11</sup>. It is interesting to note that this compound is obtained for the first time from this plant. Further, we are working on the fractions of the extract and will report if any of the new compounds obtain in due course.

### Experimental Section

*Pelargonium graveolens* was supplied by CSIR-CIMAP, Hyderabad/Lucknow. Solvents and silica-gel were procured from local suppliers. Extractions were monitored by thin layer chromatography (TLC) on pre-coated silica gel 60 F<sub>254</sub> (mesh); spots were visualized under UV light. Column chromatographic separations were carried out by using silica gel (100-200 mesh). Melting point was determined on a *Mettler-Temp* apparatus and are uncorrected. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on an Avance 400 MHz spectrometer. Chemical shifts ( $\delta$ ) are quoted in parts per million and are referenced to tetramethylsilane (TMS) as internal standard. ESI-MS were obtained on quato micro spectrometer. HRMS were measured on Agilent Technologies 6510, Q-TOFLC/MS ESI-Technique. X-ray analysis was

carried out by using Bruker Smart Apex CCD diffractometer instrument.

### Extraction procedure for the plant *Pelargonium graveolens*

*Pelargonium graveolens* plant material (50 g) was soaked in hexane (500 mL) and transferred to a Soxhlet extraction apparatus. The contents were refluxed for 36 h and monitored by TLC. Similarly, the plant material was extracted with solvents such as chloroform and acetone using Soxhlet extraction. The contents were filtered using sintered funnel and the decant was subjected to rotary evaporation to remove the solvent under reduced pressure below 40°C. The crude material was purified by column chromatography using hexane as the solvent and the obtained compounds have been described in the manuscript. The 5<sup>th</sup> fraction of chloroform extract provided the compound 5-hydroxy-3,7-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one (0.07 g) as a colourless solid. The compound has been well characterized by spectral data and its structure confirmed by single crystal X-ray crystallography. All the data have been depicted in the Supplementary Information.

### Conclusion

In conclusion, *Pelargonium graveolens* was extracted with hexane and chloroform solvents. The compound 5-hydroxy-3,7-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one was obtained by column chromatography from chloroform extract using hexane as solvent. This compound is being reported for the first time from *Pelargonium graveolens* and has been confirmed from spectral characterization data and single crystal X-ray crystallographic analysis.

### Supplementary Information

Supplementary information is available in the website <http://nopr.niscpr.res.in/handle/123456789/58776>.

### Acknowledgements

The authors thank the Director, CSIR-ICT for providing the research facilities. Neeladri thanks

Dr. Sandip B. Bharate, Head, DNPMC and Dr. Sreepriya Vedantam, Principal Scientist, CSIR-IICT for constant support to carry out the Aroma Mission Project. Neeladri thanks Director, CSIR-IICT for financial support (Aroma Mission Phase-III, HCP-0007). CSIR-IICT manuscript communication no. IICT/Pubs./2024/327.

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