



# Structure elucidation of a flavonoid glycoside from the roots of *Clerodendrum serratum* (L.) Moon, Lamiaceae

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**RESUMO:** Apigenin-7-glucosídeo, C<sub>21</sub>H<sub>20</sub>O<sub>10</sub> (7-(β-D-glucopiranosiloxi)-5-hidroxi-2-(4-hidroxifenil)-4H-1-benzopiran-4-ona), foi isolado pela primeira vez das raízes de *Clerodendrum serratum* (L.) Moon, Lamiaceae. A elucidação estrutural da substância foi feita através de estudos de <sup>1</sup>H NMR e FAB-MS.

## Unitermos:

**ABSTRACT:** Apigenin-7-glucoside, C<sub>21</sub>H<sub>20</sub>O<sub>10</sub> (7-(β-D-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one), was first time isolated from the roots of *Clerodendrum serratum* (L.) Moon, Lamiaceae. Structure elucidation of the compound was carried out by <sup>1</sup>H NMR and FAB-MS studies.

**Keywords:** Apigenin, *Clerodendrum serratum*, FAB-mass spectroscopy.

## INTRODUCTION

*Clerodendrum serratum* (L.) Moon, Lamiaceae, is a deciduous shrub distributed in the forests of Western Ghats of India (Manjunatha et al., 2004). In Indian system of medicine, the plant is well known as Bharangi (Sanskrit) and commonly known as Blue glory (English). As per the traditional claims roots are potential source of drugs for ailments such as asthma, cholera, and rheumatism (Keshavamurthy, 1994). Phytochemically the root bark extract contain D-mannitol, stigmaterols and three triterpenoids - oleanolic acid, queretic acid and cerratagenic acid (Banarjee, 1969). This communication reports the structure elucidation of apigenin-7-glucoside (1), a new flavonoid glycoside from the roots of the plant.

## MATERIALS AND METHODS

### General

Melting points were measured on Buchi 545 B, UV Spectra was recorded on Shimadzu 1801, IR spectrum was recorded on Parkin Elmer FT-IR spectrophotometer, FAB-MS was recorded on a Jeol SX 102/Da-600 mass spectrophotometer and <sup>1</sup>H-NMR spectra was recorded on Varian Mercury YH-300 MHz.

### Plant material

Roots of *Clerodendrum serratum* (L.) Moon, Lamiaceae, were collected from foothills of Sinhagad Pune (India), and authenticated by Botanical Survey of India, Pune with voucher specimen no. SSBC1. A herbarium was also deposited for future reference.

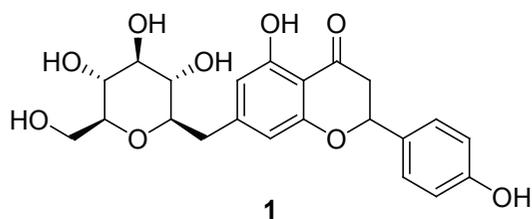
### Extraction and isolation

Roots were shade dried for a week and powdered. Powdered material (500 g) was extracted using Soxhlet apparatus with 95% ethanol for about 36 h. The extract was filtered and concentrated *in vacuo* under reduced pressure using rotary flash evaporator. A dark brown colored viscous mass weighing 50 g (10.0% w/w) was obtained. The extract (10 g) was treated with lead acetate, resulting an yellow precipitate which was then suspended in methanol, treated with hydrogen sulphide to remove the lead and then filtered. After evaporating the filtrate, the residue was treated with boiling water and extracted with ether. The concentrated ether fraction was extracted with sodium hydrogen carbonate solution and acidified with hydrochloric acid. Recrystallization from alcohol-water resulted a yellowish brown amorphous solid (30 mg) which was further subjected to spectral analysis.

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## RESULTS

Apigenin-7-glucoside (**1**) was obtained as yellowish brown amorphous solid having the melting point 178-180 °C. The compound also gave positive color reactions for a hydroxyl flavone with several reagents (Kaneta, 1971). Spectral data for apigenin-7-glucoside as UV-Vis: (ethanol)  $\lambda_{\text{max}}$ : 247, 352. FT-IR: (KBR) ( $\text{cm}^{-1}$ ); 3402, 2920, 2850, 1631, 597.  $^1\text{H-NMR}$  (300 MHz, TMS,  $\text{DMSO } d_6$ ):  $\delta$  (ppm); 3.5 (t,  $J=3.6$ , H-3, CH), 3.8 (t,  $J=1.8$ , 2-H,  $\text{CH}_2\text{OH}$ ), 4.0 (q,  $J=31.5$ , 1-H, CH-O), 4.7 (t,  $J=19.5$ , 1-H,  $\text{CH}_2\text{OH}$ ), 4.9 (d,  $J=22.5$ , 3-H, OH), 6.0 (d,  $J=18.3$ , 1-H, CH-O), 6.7 (s, 3-H, Ar C-H), 7.1 (d,  $J=6.9$  4-H, Ar C-H), 8.5 (s, 2-H, Ar-OH). FAB-MS:  $m/z$ : 433  $[\text{M}+\text{H}]^+$ , 432 $[\text{M}^+]$ , 271(glucose residue). Molecular formula:  $\text{C}_{21}\text{H}_{20}\text{O}_{10}$ ; Cal. C-58.282%, H-4.662% found; C-58.10%, H-4.59%. From these spectral studies the compound isolated thus confirms of apigenin-7-glucoside.



## DISCUSSION

Flavonoids are benzo-pyrone derivatives, which resemble coumarin and are ubiquitous in photosynthesizing cells. Their occurrence is therefore widespread in the plant kingdom and about 500 varieties of flavonoids are known (Hausteen, 1983). Previous studies suggests that apigenin-7-glucoside (**1**) has demonstrated anti-inflammatory (Fuchs & Milbradt, 1993), antimicrobial (Pereira et al., 2007), hepatoprotective (Barbenko & Shakhova, 2003) and antidiarrheal properties (Meite et al., 2009). The compound also showed significant protection against Alzheimer's disease in mice (Patil et al., 2003). The above literature review describes its importance and therapeutic significance. This communication highlights a new potential source of its occurrence in the roots of *Clerodendrum serratum* (L.) Moon, Lamiaceae that are widely available throughout the western ghats of India and also explores an opportunity for further research on the biological activity of this group of compounds. As a result, the chances of discovering new plant constituents that may be biologically active are promising.

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