Supplementary Information

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

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Experimental Section

1. General Information

Pelargonium graveolens was procured from 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_{254} (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. ^{1}H NMR and ^{13}C NMR spectra were recorded on a *Avance 400* MHz spectrometers. Chemical shifts (δ) are quoted in parts per million and are referenced to *tetramethylsilane* (TMS) as internal standard. ESI-MS obtained on quarto 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.

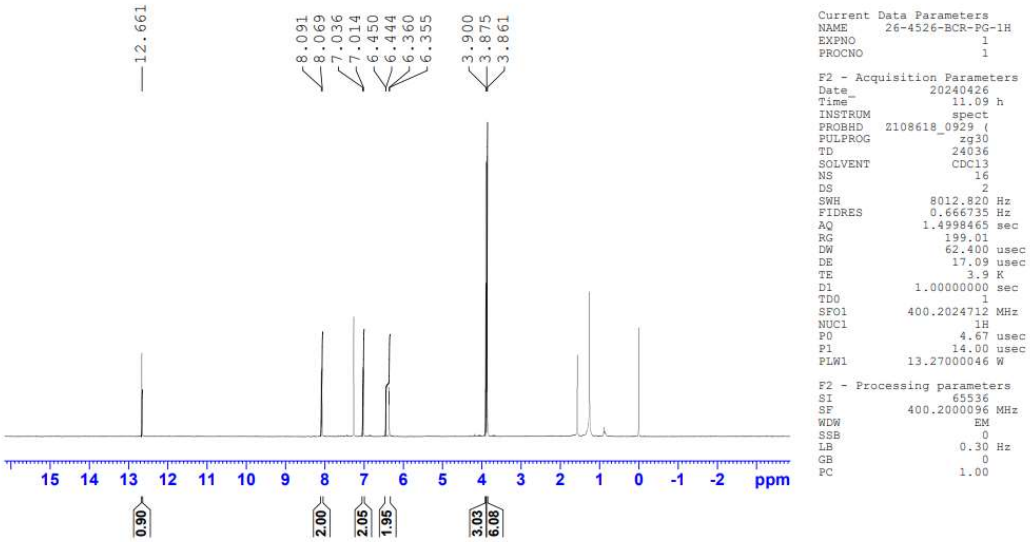
Extraction procedure for the plant *Pelargonium graveolens*: *Pelargonium graveolens* plant material (50g) was soaked in hexane (500 mL) and transferred to the *Soxhlet* extraction apparatus. The contents were refluxed for 36 hours and monitored by TLC. Similarly, the plant material was extracted with the solvents such as chloroform and acetone using *Soxhlet* extraction. The contents were filtered using sintered funnel and the decant was subjected for rotavapor to remove the solvent under reduced pressure below 40 ^{o}C. The crude material was purified by column chromatography using hexane as the solvent and the obtained compounds were discussed in the manuscript. The 5^{th} fraction of chloroform extract was provided the compound 5-hydroxy-3,7-dimethoxy-2-(4-methoxyphenyl)-4*H*-chromen-4-one (0.07g) as

colourless solid. The compound was well characterized by spectral data and confirmed by single X-ray crystallography. All the data were depicted in the supporting information.

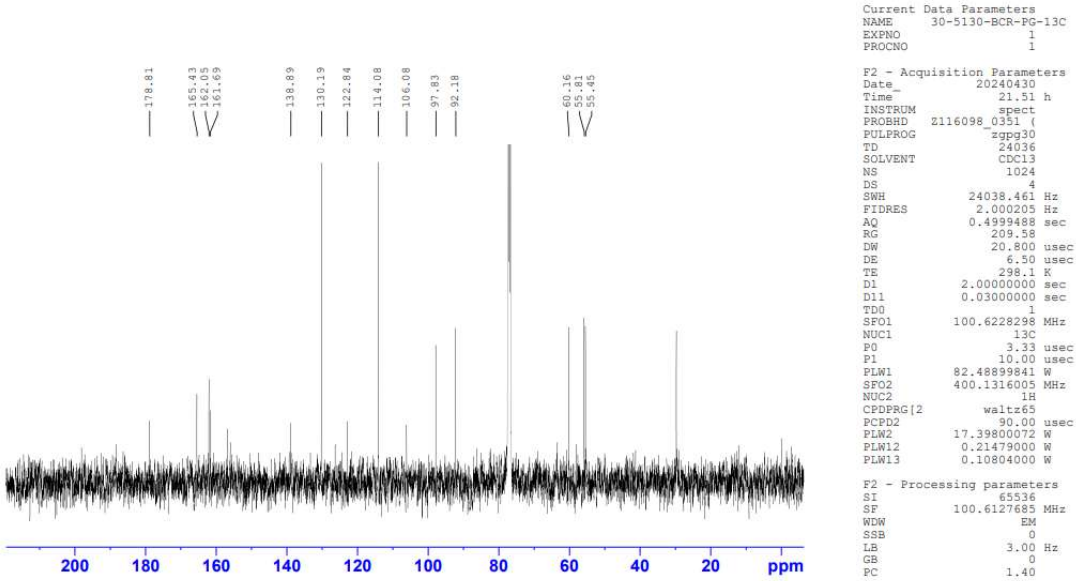
2. Spectral data

5-Hydroxy-3,7-dimethoxy-2-(4-methoxyphenyl)-4*H*-chromen-4-one: Colourless solid; M.P: 138-140 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.66 (s, 1H, OH D_2O exchangeable), 8.07-8.09 (d, J = 12.4 Hz, 2H, aromatic), 6.44-6.45 (d, J = 12.4 Hz, 2H, aromatic), 6.35-6.36 (d, J = 8.2 Hz, 2H, aromatic), 3.90 (s, 3H, OCH_3), 3.86 (s, 6H, $2OCH_3$ ppm. ^{13}C NMR (101 MHz, $CDCl_3$): δ 178.81, 165.43, 162.05, 161.69, 138.89, 130.19, 122.84, 114.08, 106.08, 97.83, 92.18, 60.16, 55.81, 55.45 ppm. MS-ESI: (*m/z*) 329 $[M+H]^+$; HRMS-ESI: Calcd for $C_{18}H_{17}O_6$ $[M+H]^+$ 329.1025; found 329.1023.

3. Spectra of compounds



H-NMR Spectum of Compound Flavonol



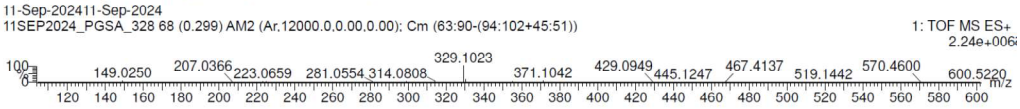
^{13}C-NMR Spectrum of Flavonol

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

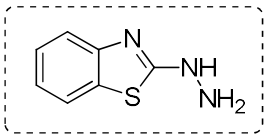
Monoisotopic Mass, Even Electron Ions
84 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-18 H: 0-18 N: 0-2 O: 0-6 F: 0-1 S: 0-1

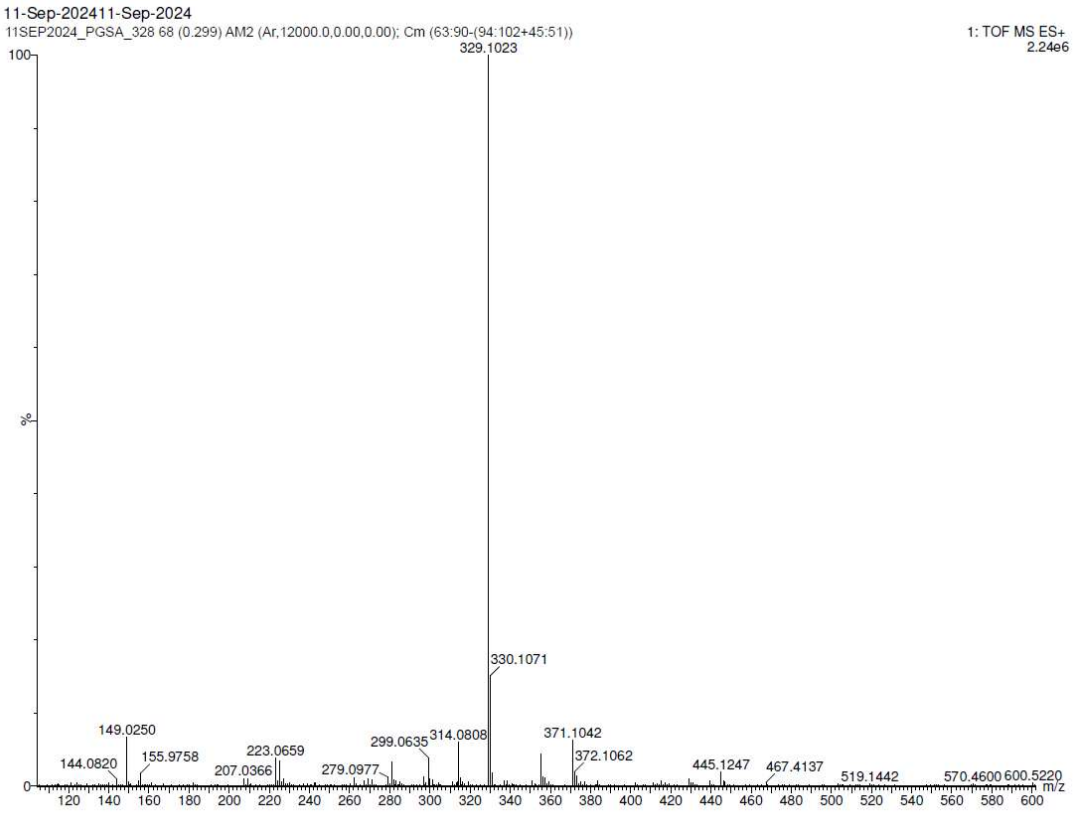
11-Sep-202411-Sep-2024
11SEP2024_PGSA_328 68 (0.299) AM2 (Ar,12000.0,0.00,0.00); Cm (63:90-(94:102+45:51))



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
329.1023	329.1025	-0.2	-0.6	10.5	472.6	n/a	n/a	C18 H17 O6

HRMS Specturm of Flavonol





Mass Spectrum of Flavonol

4. X-ray Crystallography

The isolated compound was dissolved in methanol solvent and allowed to form the crystal. X-ray data was collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromated MoKα radiation (λ=0.71073Å) with ω-scan method [1, 2]. Preliminary lattice parameters and orientation matrices were obtained from 180 frames.

Crystal structure of the Compound Flavonol was recorded and compared with the reported literature structure [3].

1. Bruker (2001). SAINT (Version 6.28a) & SMART (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA.
2. Sheldrick, G. M. *Acta Cryst*, 3 (2015) C71.
3. Nakao K, Murata K, Deguchi T, Itoh K, Fujita T, Higashino M, Yoshioka Y, Matsumura S, Tanaka R, Shinada T, Ohfune Y & Matsuda H, *Biol. Pharm. Bull*. 34 (2011) 1143.