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A new glycopyranoside from *Scutellaria scandens* Bark

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Abstract

From bark of *Scutellaria scandens* yielded a new α -D-Glucopyranoside whose structure was assigned as 4-methoxycarbonyl-3-methyl phenyl-6'-O-4''-methoxy sinapoyl- α -D-glucopyranoside. The structure of Fig. 1 was determined through FABMS and ^1H and ^{13}C NMR studies.

Keywords: *Scutellaria scandens*, Glucopyranoside, structure, methoxycarbonyl

1. Introduction

Scutellaria scandens belonging to the family Lamiaceae, is perennial erect shrub widely distributed in north western Himalayas in India. *Scutellaria* species have been used as antimicrobial medicine for a variety of purposes [1]. The chemical examination of *Scutellaria* species [2] has been reviewed. The present study has led to the isolation of a new α -D-Glucopyranoside from an ethanolic extract of the bark of *Scutellaria scandens*. The structure of compound has been elucidated through extensive mass, ^1H & ^{13}C NMR studies.

2. Result and Discussion

It is as colourless amorphous compound. Molecular weight of 548 as deduced by the presence of the $[\text{M}+\text{H}^+]$ at $m/z = 549$ and fragment peaks 535, 429, 397, 391, 369, 307 etc. in the positive ion FAB-MS. Elemental analysis of compound corresponded to the molecular formulae $\text{C}_{27}\text{H}_{32}\text{O}_{12}$. The ^1H Spectrum (Table-1) showed characteristic signals for anomeric proton (H-1') at $\delta 3.8$ (s) indicate the presence of α -linkage. Acidic hydrolysis (7% MeOH-HCl, 10ml, 60 to 80 $^\circ\text{C}$, 8hr) furnished aglycone (4-methoxycarbonyl-3-methyl phenol) identified by comparing its spectral data with that of literature (2) and D-glucose by co-TLC.

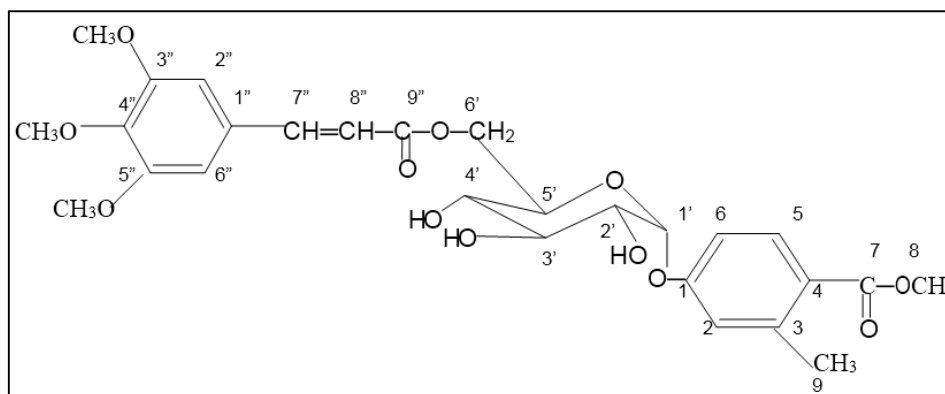
^1H -NMR of the compound showed singlet at $\delta 5.3$ for tetra substituted benzene and two sharp singlets at $\delta 3.6$ & $\delta 3.4$ for two type methoxy groups respectively. The signals for two α, β -methine was reported at $\delta 6.6$ (d, 6.8Hz) and $\delta 6.25$ (d, 4.4Hz) for sinapic acid (6'-O-4''-methoxy-sinapoyl). Two singlet signal at $\delta 5.6$ and 5.15 for tri substituted benzene and sharp singlet at $\delta 3.1$ & 1.2 for one methoxy of ester group and one methyl group respectively assigned for aglycone (4-methoxy carbonyl-3-methyl phenyl). For sugar moiety, six peaks were observed at $\delta 3.8$ (s), $\delta 4.75$ (d, 4.4Hz), $\delta 4.85$ (t, 5.2Hz), $\delta 4.9$ (t, 4.8Hz), $\delta 4.0$ (dd, 7.2Hz and 10.4 Hz) and three singlet peak at $\delta 4.6$ (s), 4.45 (s), 4.50 (s) for hydroxyl groups (2).

^{13}C -spectrum NMR of the compound showed chemical shifts of the carbon singles at $\delta 100.4$ (C-1'), 73.2(C-2'), 76.4(C-3'), 69.8(C-4'), 73.8(C-5'), 63.3 (C-6') which corresponding with analogous data of the glucose (1). The signals for aglycone part $\delta 156.2$ (C-1) aromatic carbons, 116.2, 135.3, 128.6, 130.3, 116.2 for C-2, 3, 4, 5, 6 respectively. The signals at $\delta 171.25$ (C-7) for -CO-O group $\delta 51.6$ for methoxy carbon, $\delta 21.3$ for methyl group. The signals for sinapic acid were reported at $\delta 124.4$ (C-1''), 106.2 (C-2''), 148.2 (C-3''), 149.2 (C-4''), 148.0 (C-5''), 116.2 (C-6'') were reported for aromatic carbons and the signal for -CH=CH- were reported at $\delta 145.5$ & 114.7 and $\delta 166.5$ (C-9'' -CO-O). Two signals were observed at $\delta 57.1$ (C-10'') and 56.5 (C-11'') for methoxy groups. These data correlate with the reported data of sinapic acid (2).

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Table 1: ^1H NMR (400MHz, DMSO) and ^{13}C NMR (75MHz, DMSO) Data of Compound

Position	δ_{H}	J (Hz)	δ_{C}		
1'	3.8 (s)		100.4	CH	Glucose
2'	4.75 (d)	(5.2 Hz)	73.2	CH	
3'	4.85 (t)	(5.2 Hz)	76.4	CH	
4'	4.90 (t)	(4.8 Hz)	69.8	CH	
5'	4.25 (t)	(6.8 Hz)	73.8	CH	
6'	4.0 (dd)	(4.4Hz, 4.0 Hz)	63.8	CH ₂	
	4.6 (s)		-	-OH	
	4.45 (s)			-OH	
	4.50 (s)			-OH	
1	-		156.2	C	Aglycone
2	5.15 (s)		116.2	CH	
3	-		135.3	C	
4	-		128.6	C	
5	5.60 (s)		130.3	CH	
6	5.15 (s)		116.2	CH	
7	-		171.25	-CO-O	
8	3.1(s)		51.6	-OCH ₃	
9	1.2 (s)		21.3	-CH ₃	
1''	-		124.4	C	Sinapic acid
2''	5.3 (s)		106.2	CH	
3''	-		148.2	C	
4''	-		149.0	C	
5''	-		148.0	C	
6''	5.3 (s)		116.2	CH	
7''	6.6 (d)	(6.8 Hz)	145.5	CH	
8''	6.25(d)	(4.4 Hz)	114.7	CH	
9''	-		166.5	-COO-	
10''	3.6 (s)		57.1	-OCH ₃	
11''	3.4 (s)		56.5	-OCH ₃	

**Fig 1**

2.1 Experimental

The bark of *Scutellaria scandens* were collected from Gogalgaon, District Chamoli Uttarakhand in the month of October and identified from Department of Botany, P.G. College Gopeshwar where Baucher specimen deposited. The air dried bark (2.0 Kg) were crushed into powder and was exhaustively extracted with 90% EtOH and concentrated under reduced pressure. The extract was fractionated by successive partition with CHCl_3 and EtOAc. The EtOAc fraction was purified by repeated column chromatography on silica gel with CHCl_3 , CHCl_3 – MeOH with increasing MeOH content afforded compound (Fig. 1).

The FABMS was recorded on JEOL DX-300 instrument. ^1H NMR (400 MHz, DMSO), ^{13}C NMR (75 MHz, DMSO) spectra were recorded on a JEOL GSX-400 spectrophotometer, using TMS as internal standard. The

chemical shifts are reported in parts per million, and the coupling constants are in Hertz.

3. Acknowledgement

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4. References

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