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A New Chromone Glycoside from *Cassia siamea* Lam.

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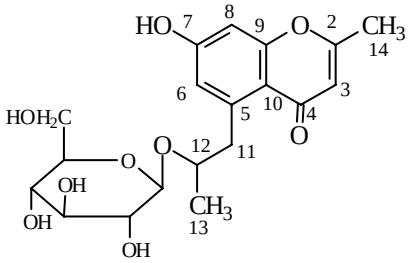
Abstract: 2-methyl-5-propyl-7, 12-dihydroxy chromone-12-O-β-D-glucopyranoside was isolated from the stem of *Cassia siamea*. The structure was elucidated by chemical and spectral evidences.

Keywords: *Cassia siamea*, 2-methyl-5-propyl-7, 12-dihydroxy-chromone-12-O-β-D-glucopyrano -side.

Cassia siamea Lam. (CSL) is a common tree in the southern part of China. It has been used as folk medicine for aperient, antiarthritic and swellings[1]. We report here the isolation and structural elucidation of a new chromone glucoside, 2-methyl-5-propyl-7, 12-dihydroxy chromone-12-O-β-D-glucopyranoside (**1**), from the *n*-butanol-soluble fraction of CSL extract .



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The 80% ethanolic extract of CSL was dissolved in water and partitioned with petroleum ether, dichloromethane and *n*-butanol. The *n*-butanol fraction was further separated by silica gel column chromatography eluting with CH_2Cl_2 : CH_3OH (5:1), and purified by sephadex LH-20 to obtain **1**.

The compound **1** was pale powder, mp 232~233°C, FAB-MS *m/z*: 396(M^+). According to the NMR, DEPT spectra and FAB-MS, the chemical formula was suggested to be $C_{19}H_{24}O_9$. The spectral data of ^1H and ^{13}C-NMR are listed in **Table.**

Compared with NMR spectrum of 2-methyl-5-acetonyl-7-hydroxychromone[2], it was found that **1** was a 2, 5, 7 substitutive chromone. ^{1}HNMR spectrum suggested the presence of the structural fraction CH_3CHCH_2 [δ 1.05 (d, 3H, J=6.3 Hz), 2.98 (m, 1H), 3.69 (m, 1H,), 3.97 (m, 1H)], confirmed by DEPT spectrum [δ 20.8 (CH_3), 41.0 (CH_2), 74.6 (CH)]. The correlation between δ_H 3.69, 2.98 and δ_C 142.0 in HMBC indicated

that this structural fraction was connected to C-5 position.

When the methyl singlet (δ 2.29) was irradiated , the signal of H-3 (δ 6.01) was sharpened in the NOE spectrum. So the methyl group should be attached to C-2. A signal at δ 10.57 in ^{1}HNMR spectrum indicated the presence of a hydroxyl group which attached to a benzene ring, and two aromatic protons [δ 6.68 (d, 1H, J=2.0 Hz), 6.7 (d, 1H, J=2.0 Hz)] should be suggested in a *meta*-position on the benzene ring. Thus the hydroxyl group was at C-7.

Six signals ranging from δ 61.1 to 101.4 in DEPT spectrum suggested the presence of a glucose moiety. The signal of an anomeric proton (d, δ 4.42, J=7.8 Hz) revealed that the glucose moiety should be β-D-glucose, which was identified by TLC after the compound was hydrolyzed by concentrated HCl. According to a correlation δ_H 4.42 (d, J=7.8 Hz) with δ_C 74.6 (C-12) in HMBC spectrum, it could be concluded that β-D-glucose was connected at C-12.

Table ^{1}H and ^{13}C-NMR spectral data in DMSO-d_6 (300 MHz)

H	δ_H (ppm)	J (Hz)	C	δ_C (ppm)
3	6.01 (s)		2	163.8
6	6.70 (d)	2	3	110.7
8	6.68 (d)	2	4	178.0
11a	3.69 (m)		5	142.0
11b	2.98 (m)		6	117.9
12	3.97 (m)		7	160.7
13	1.05 (d)	6.3	8	101.2
14	2.29 (s)		9	159.2
glc-1′	4.42 (d)	7.8	10	113.9
2′	2.92 (m)		11	41.0
3′	3.13 (m)		12	74.6
4′	3.06 (m)		13	20.8
5′	3.13 (m)		14	19.3
6′a	3.65 (m)			101.4
6′b	3.42 (m)		gl	73.6
			c-	76.8
			1′	70.1
			2′	76.6
			3′	61.1
			4′	
			5′	
			6′	

In order to confirm the ascription of all NMR signals and the location of every substituent, HMQC, HMBC and NOESY were introduced. And all the evidences supported the proposed structure of the new compound.

From these chemical and spectral evidences, the compound was identified as 2-methyl-5-propyl-7, 12-dihydroxy chromone-12-O-β-D-glucopyranoside.

References

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