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A New 10-Hydroxyl Anthrone Glycoside from *Cassia siamea* Lam.

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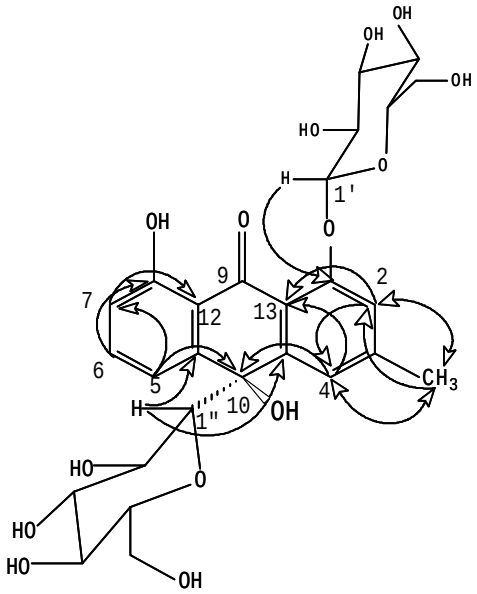
Abstract: A new 10-hydroxyl anthrone glycoside, 1, 8, 10 - trihydroxyl-1–O–β–D–glucopyranosyl-3-methyl-10- C (S) – β – D- glucopyranosyl-anthrone-9 **1** was isolated from the stem of *Cassia siamea* Lam. The structure was elucidated by spectral evidences, especially by 2 D techniques.

Keywords: *Cassia siamea*, anthrone, 1, 8, 10 -trihydroxyl-1-O-β-D-glucopyranosyl-3-methyl–10-C (S) -β-D- glucopyranosyl-anthrone-9 **1**.

Formerly we have reported the isolation of a chromone glycoside[1]. Here we report the isolation and structural elucidation of a 10-hydroxyl anthrone glycoside, which was the new natural product, 1, 8, 10 - trihydroxyl-1 – O –β – D –glucopyranosyl -3-methyl -10-C (S) –β – D- glucopyranosyl-anthrone-9 **1** from the stem of *Cassia siamea* Lam.

Figure 1 HMBC and NOESY correlations of compound **1**



Compound **1**, yellow solid, mp 138-139°C, the UV λ_{max}nm (MeOH) (log∈): 207(5.26), 268(3.76), 301(4.09), 360(4.03); IR KBr νcm^{-1} : 3408，2924，1632，1606，1572，1485，1452，1294; revealed strong resemblance to those of 10-hydroxyaloin B[2]. ^{1}H and ^{13}CNMR data of **1** are listed in **Table 1**. FAB-MS: 580[M^{+}]; thus the molecular formula of **1** was suggested to be $C_{27}H_{32}O_{14}$. Based on the above[2, 3] evidences, **1** was a typical anthrone.

Table 1 ^{1}H-NMR (300 MHz) and ^{13}C-NMR (75 MHz) spectral data of **1** in CD_3OD-d_4

C	δ_C (ppm)	H	δ_H (ppm)	J (Hz)
1	158.8			
2	120.1	2	7.30(brs)	
3	147.8			
4	121.8	4	7.62(brs)	
5	118.0	5	7.35(d)	7.6
6	135.3	6	7.52(t)	7.6, 8.3
7	117.9	7	6.92(d)	8.3
8	161.5			
9	191.5			
10	76.9			
11	144.8			
12	119.8			
13	121.4			
14	149.4			
15	22.3	15	2.45(s)	
O-Glu-1′	105.2	1′	4.92(d)	7.5
2′	75.0	2′	3.58(m)	
3′	77.2	3′	3.55(m)	
4′	71.4	4′	3.50(m)	
5′	78.6	5′	3.52(m)	
6′	62.6	6′a	3.91(m)	
		6′b	3.73(m)	
C-Glu-1″	83.8	1″	3.18(d)	9.4
2″	71.6	2″	2.80(m)	
3″	79.4	3″	3.29(m)	
4″	73.1	4″	2.98(m)	
5″	81.5	5″	2.90(m)	
6″	63.3	6″a	3.32(m)	
		6″b	3.52(m)	

In its ^{1}HNMR spectrum, the signal at δ 2.45(s, 3H) suggested the presence of methyl group connected with a benzene ring. The aromatic proton signals at δ_H 7.30 (brs), 7.62 (brs) indicated the presence of a *m*-substitued benzene ring. In its HMBC, the correlation between δ_H 2.45(s, 3H) and δ_C 120.1(C-2), δ_H 2.45(s, 3H) and δ_C 121.8 (C-4) indicated that the methyl group was connected to C-3 position, and it was confirmed by its NOESY spectrum. And the signals at δ_H 6.92 (d, 1H, J=8.3), 7.35 (d, 1H, J=7.6), 7.52 (dd, 1H, J=7.6, 8.3) were due to H-7, H-5 and H-6 of the anthrone respectively.

Twelve signals in DEPT spectrum ranged from δ_C 105.2 to 62.7, together with the signals of anomeric proton δ_H 3.18 (d, J=9.5) and δ_H 4.92 (d, J=7.5) in ^{1}HNMR suggested the presence of two β-D-glucoses. And from the chemical shift of the anomeric carbon

of the glucoses (δ_C 83.8, δ_C 105.2), it could be concluded that one glucose formed O-glucoside and the other formed C-glucoside.

A quaternary carbon at δ_C 76.9 (10-C) was observed in DEPT, according to the reference[2,3], it could be confirmed that one of the β-D-glucose and a hydroxyl group all attached at the C-10 position and formed C-glucoside. The correlation of δ_H 3.18 (H-1″) and δ_C 144.8 (C-11) and 149.4 (C-14) in HMBC is the further evidence for the formation of C-glucoside. The other anomeric proton at δ_H 4.92 (H-1′) exhibited the correlation with δ_C 158.8 (C-1) suggesting the connection of O-glucoside at C-1.

The absolute configuration of C-10 for **1** was *S*, as 10-hydroxyaloin B, comparing the CD spectrum of compound **1** with that of 10-hydroxyaloin B[4, 5].

So, the structure of compound **1** was elucidated as 1, 8, 10 - trihydroxyl-1-O-β -D–glucopyranosyl -3-methyl-10- C (S) – β – D- glucopyranosyl-anthrone-9 **1**.

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