Chinese Chemical Letters Vol. 13, No. 1, pp 59 – 60, 2002
http://www.imm.ac.cn/journal/ccl.html

A New Flavonol Oligosaccharide from the Seeds of *Aesculus chinensis*

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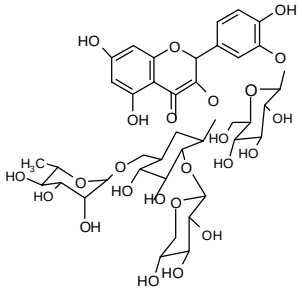
Abstract: A new flavonol oligosaccharide, quercetin-3-O-[β-D-xylopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside-3′-O-β-D-glucopyranoside, named aescuflavoside was isolated from *Aesculus chinensis*. It′s structure was elucidated by spectra FAB-MS, 1D NMR and 2D NMR including ^{1}H NMR, ^{13}C NMR, HMQC and HMBC techniques.

Keywords: *Aesculus chinensis*, flavonol oligosaccharide, aescuflavoside, antivirus activity.

Aesculus chinensis is a traditional chinese medicinal plant widely distributed in China, which has been used to treat stomach disease. From recent research its seeds contain many flavonoids and proanthocyanidin A_2, which have potential venotonic and vasoprotective action and powerful antioxidant activity. In this paper, we report the isolation and the structure elucidation of a new flavonol oligosacchride. Bioassay results showed that the compound exhibited an antivirus activity.



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Compound **1** was isolated as a yellow powder from the EtOH extract of the seeds of this plant. UVmax (MeOH) 268, 352nm, and positive results of Molish and Mg/HCl reactions suggested that **1** was a flavonoid type compound. The FAB-MS of **1** displayed quasi-molecular ions $[M+H]^+$ and $[M+Na]^+$ at *m/z* 905 and 927 respectively, consistentwith a molecular formula of $C_{38}H_{48}O_{25}$. Complete acid hydrolysis of **1** afforded quercetin, which was identified by comparison of its NMR and IR data with

those reported in the literatures[1-2], and glucose, xylose and rhamnose identified by TLC. The FAB-MS data 905 $[M+H]^+$, 773 $[M-Xyl+H]^+$, 627 $[M-xyl-rha+H]^+$, 302 $[M-xyl-rha-glc-glc]^+$ confirmed above conclusion. The four sugar residues were clearly indicated by the signals at δ_C 98.05, 102.03, 104.32, 100.26 in ^{13}C NMR spectrum, signals at δ_H 5.61 (d, J = 7 Hz), 4.86 (d, J = 7 Hz), 4.58 (d, J = 7 Hz), 4.36 (s) in ^1H NMR spectrum[3]. Above data together with the results in 2D NMR indicated that the saccharide part was composed of two β-glucose, one β-xylose and one α-rhamnose residues. The absolute configurations of β-glucose and β-xylose were assumed to be D, and α-rhamnose be L.

Table 1 ^{13}C NMR data for compound **1** in DMSO-d6 (δ ppm)

No.	δ_C	No.	δ_C	No	δ_C	No.	δ_C
2	155.22	2'	116.49	6''	60.69	4''''	69.62
3	133.00	3'	145.11	C3-glc1'''	98.05	5''''	65.99
4	177.23	4'	149.75	2'''	81.55	Rha 1'''''	100.26
5	161.06	5'	116.49	3'''	75.84	2'''''	70.30
6	98.67	6'	125.57	4'''	68.17	3'''''	71.81
7	164.25	C-3'-Glc 1''	102.03	5'''	76.03	4'''''	73.36
8	93.88	2''	73.76	6'''	65.69	5'''''	69.64
9	156.35	3''	76.95	Xyl 1''''	104.32	6'''''	17.64
10	103.74	4''	69.62	2''''	73.36		
1'	121.19	5''	76.71	3''''	76.03		

Table 2 the data of HMBC of compound **1** (δ ppm)

No.	δ_H	Correlation of C	No.	δ_H	Correlation of C
1'''	5.61	C-3 (133.00), C-2''' (81.55), C-5''' (76.03)	1'''''	4.36	C-6''' (65.61)
1'''''	4.58	C2''' (81.55)	5'''	3.25	C-6''' (65.61)
1''	4.86	C3' (145.11)			

Hence, the structure of **1** was established to be quercetin-3-O-[β-D-xylopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→6)]-β-D-gluc-opyranoside-3′-O-β-D-glucopyrano-side, named aescuflavoside.

References and Notes

1. D. Q. YU, J. S.YANG, *Fenxi Huaxue Shouce* (*Hand book of Anal. Chem.*), Chemical Industry Press, Beijing, **1999**, p.820.
2. D. C. CHEN, *The Application of ^{13}C NMR in Natural Products Chemistry*, People's Health Press, Beijing, **1993**, p.360.
3. ^1H NMR (δ ppm) of **1,** 6.17 (d, 1H, 2, H-6), 6.46 (d, 1H, 2, H-8), 7.78 (d, 1H, 2, H-2′), 6.89 (d, 1H, 8.5, H-5′), 7.95 (dd, 1H, 2, 8.5 H-6′), 4.86 (d, 1H, 7, H-1''), 5.61 (d, 1H, 7, H-1'''), 4.36 (bs, 1H, H-1'''').

Received 12 March, 2001
Revised 20 September, 2001