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A New Limonoid from the seed of *Aphanamixis polystachya*

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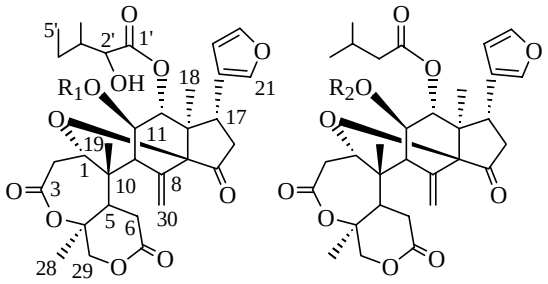
Abstract: A new limonoid named rohituka-15 **1**, with a known limonoid dregeana-1 **2**, was isolated from the seed of *Aphanamixis polystachya* (Meliaceae). The ^{13}C NMR data assignment of dregeana-1 **2** and the structural elucidation of the new compound **1** were based on spectral analysis including ^{1}H-^{1}H COSY, HMQC and HMBC experiments.

Keywords: *Aphanamixis polystachya*, Meliaceae, limonoid, rohituka-15, dregeana-1.

Figure 1 Structures of Compounds **1**, **2**, **3**, and **4**



1 R_1=H Rohituka-15 **2** R_1=HCO Dregeana-1 **3** R_2=H Rohituka-12 **4** R_2=HCO Polystachin

The seed of *Aphanamixis polystachya* J. N. Parker (Syn: *Amoora rohituka* Weight. & Arn.), Meliaceae, is a rich source of limonoids[1, 2]. As part of our interest in the chemistry of the family Meliaceae, we herein report the ^{13}C NMR data assignment of a known limonoid dregenan-1 **2** and structural elucidation of a new limonoid **1** designated as rohituka-15, isolated from the EtOH extract of the seeds of *Aphanamixis polystachya* collected in Yunnan province, the People's Republic of China.

Compound **1**, amorphous, mp 122-124°C, $[\alpha]_D^{27}$ –105.7 (*c* 0.29, $CHCl_3$). In ^{13}C NMR spectrum of **1** (**Table 1**), 32 carbon signals were observed. The multiplicities of the carbons determined by DEPT led to the attribution: 5 CH_3, 6 CH_2, 11 CH, 10 C, including one keto group (C-15), one oxymethylene group (C-29), four oxymethine groups (C-1, 11, 12, 2') and two oxyquaternary carbons (C-4, 14). According to ^{13}C NMR and ^{1}H NMR data (**Table 2**) and IR spectrum (absorption at ν 3484, 3400, 1750, 1510, 874 cm^{-1}), one β-substituted furanyl ring and two hydroxyl and three ester groups

(δ_C 168.2, 174.0, 175.3) should exist. EI mass spectrum of **1** exhibited a molecular ion peak at *m/z* 600 $[M]^+$, thus the molecular formula of **1** was deduced to be $C_{32}H_{40}O_{11}$. The NMR spectra of **1** were similar to those for **2** (**Figure 1**)[3] but lacked the resonances due to formate group at C-11 β presented in the NMR spectra of **2**. ^1H-^1H COSY and HMQC spectra indicated that H-11 α resonated at δ 4.01 (m) and C-11 at δ 74.4. Thus one hydroxyl group was placed at C-11 β instead of the formate. These results were substantiated by comparing the NMR data to those of rohituka-12 **3** and polystachin **4** [2] isolated from the seeds of the same plant and confirmed by ^1H-^1H COSY, HMQC and HMBC experiments. So structure **1** was assigned to rohituka-15.

Table 1 ^{13}C NMR data of compound **1** and **2** (in $CDCl_3$, 125 MHz, δ in ppm)

C	1	2	C	1	2	C	1	2	C	1	2	C	1	2
1	74.2	74.2	8	135.8	134.2	15	205.6	205.0	22	110.4	110.3	3′	38.6	38.1
2	38.6	38.4	9	56.4	55.3	16	41.1	41.1	23	143.5	143.3	4′	24.0	23.1
3	168.2	167.5	10	50.7	50.0	17	37.1	36.8	28	28.1	29.1	5′	11.7	11.4
4	79.4	78.6	11	74.4	72.1	18	12.5	12.3	29	74.1	74.3	3′-CH_3	15.0	15.1
5	41.0	40.7	12	79.2	74.4	19	22.6	22.2	30	117.8	119.3	formate		160.3
6	32.5	32.8	13	48.8	49.2	20	122.2	121.8	1′	175.3	174.9			
7	174.0	172.3	14	87.3	87.3	21	140.5	140.6	2′	75.1	75.1			

Table 2 ^1H NMR data of compound **1** (in $CDCl_3$, 500 MHz, δ in ppm, J in Hz)

Pos.		Pos.		Pos.	
H-1	3.68 (dd, 10.7, 7.2)	H-17	3.85 (dd, 10.1, 9.3)	H-30	5.36 (s), 5.33 (s)
H-2	3.12 (m), 2.88 (m)	H-18	0.80 (s)	H-2′	3.52 (d, 4.1)
H-5	3.14 (m)	H-19	1.08 (s)	H-3′	1.60 (m)
H-6	3.12 (m), 2.67 (m)	H-21	7.22 (s)	H-4′	1.20 (m), 0.92 (m)
H-9	2.69 (d, 6.2)	H-22	6.19 (s)	H-5′	0.78 (t, 7.3)
H-11	4.01 (m)	H-23	7.35 (s)	3′-CH_3	0.82 (d, 5.2)
H-12	5.84 (d, 9.8)	H-28	1.83 (s)		
H-16	2.82 (m), 2.33 (m)	H-29	4.22 (d, 11.7), 4.00 (d, 11.7)		

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