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A New Caffeoylquiniclactone, Neochlorgeniclatone from the Leaves of *Betula platyphylla* Suk.

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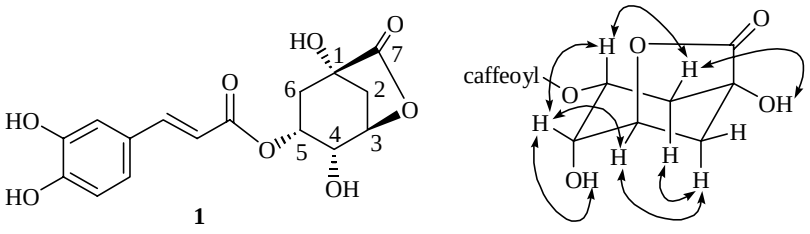
Abstract: A new caffeoylquiniclactone, named neochlorgeniclatone, was isolated from the leaves of *Betula platyphylla* Suk. The structure was established by spectroscopic data.

Key words: Neochlorgeniclatone, *Betula platyphylla* Suk., leaves.

Betula platyphylla Suk., whose bark and juice are used as anti-inflammatory and cough relieving agent[1], is widespread in China. Previous investigations of this plant have led to the isolation of various compounds[2,3]. We herein report structural elucidation of a new caffeoylquiniclactone, named neochlorgeniclatone (**1**) isolated from the leaves of *Betula platyphylla* Suk..

Compound **1** was obtained as white powder (EtOAc). The EI-MS gave ion fragments at *m/z* 336 $[M]^+$, 163 $[caffeoyl]^+$, which indicated the formula of compound **1** as $C_{16}H_{16}O_8$ and was further confirmed by ^1H and ^{13}C NMR spectroscopic data. The ^1H NMR spectra showed a series of proton signals between δ 6.20 and 9.70, which was similar with the caffeoyl. The protons signals from δ 1.82 to 6.20 were assigned to the skeleton of quiniclactone according to the ^1H-^1HCOSY and NOESY (**Figure 1**) experiments. The ^{13}C NMR spectra showed seven quiniclactone carbon signals and nine caffeoyl ones. In HMBC experiment, H-3 (δ 4.68) showed cross-peaks with C-7(δ 177.4), by which the presence of lactone could be deduced. H-5 (δ 4.72) showed correlation to C-9′(δ 165.7), by which it could be inferred that the caffeoyl was combined with 5-OH. The structure and ^1H, ^{13}C NMR data assignments (**Table 1**) were confirmed by ^1H-^1H

Figure 1 The structure and main NOESY correlation of compound **1**



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COSY, HMQC, HMBC experiments. The relative configure was determined by NOESY experiment, the results of which were shown in **Figure 1**.

Table 1 The ^{1}H, ^{13}C NMR data and HMBC, NOESY correlation of compound **1**†

position	^{13}C	^{1}H	HMBC correlations	NOESY correlations
1(OH)	71.5	6.14 s	C-2, C-6, C-1, C-7	H-2
2 e	36.5	2.21 m	C-1, C-3, C-4, C-6	H-3, 1-OH, H-2a
2 a		2.37 d (11.4) ‡	C-1, C-6, C-7	H-3, H-2e, H-6a
3	75.7	4.68 brt (5.0)	C-1, C-5, C-7	H-4, H-2
4	62.8	4.14 (m)	C-2, C-3, C-6	4-OH, H-5, H-3
4 (OH)		5.68 d (5.0)	C-3, C-4	H-4, H-3
5	68.5	4.72 m	C-1, C-9′	H-4, H-6
6 e	35.7	2.02 m	C-4	H-5, 1-OH, H-6a
6 a		1.93 t (11.7)	C-1, C-2, C-3, C-7	H-5, H-2a,H-6e
7	177.4			
1′	125.5			
2′	114.7	7.03 s	C-3′, C-4′, C-6′, C-7′	3′-OH
3′ (OH)	145.6	9.17 s	C-2′, C-3′, C-4′	2′OH
4′ (OH)	148.5	9.61 s	C-3′, C-4′, C-5′	H-5′
5′	115.8	6.75 d (7.5)	C-1′, C-3′, C-4′, C-6′	4′-OH, H-6′
6′	121.5	7.01 d (7.5)	C-2′, C-4′	H-5′
7′	145.6	7.52 d (15.8)	C-1′, C-2′, C-6′, C-8′, C-9′	H-8′
8′	113.9	6.24 d (15.8)	C-1′, C-9′	H-7′
9′	165.7			

† ^{1}H &^{13}C NMR recorded on 300 &75 MHz at 25°C in DMSO-d_6 with chemical shifts (δ) in ppm from TMS.
‡ Coupling constants (J) in parentheses (Hz).

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