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A Novel Prenylchalcone from *Humulus lupulus*

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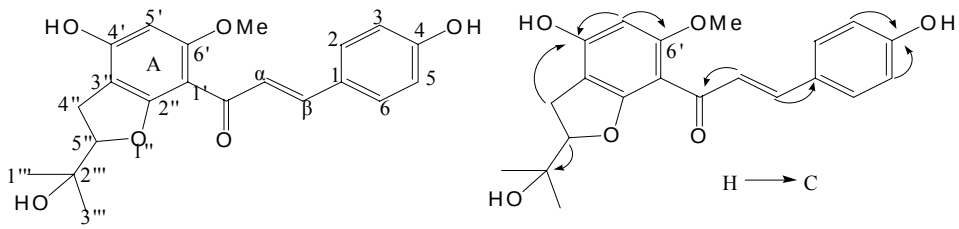
Abstracts: From hops of *Humulus lupulus*, a novel prenylchalcone was isolated, which showed inhibition against BGC-823 cells. The structure was elucidated as 5"-(2"'-hydroxyisopropyl-)-dihydrofurano-[2", 3"-B]-4, 4'-dihydroxy-6'-methoxychalcone**,** by HRFABMS and NMR spectra.

Keywords: *Cannabinaceae*, *Humulus lupulus*, prenylchalcone.

Hops (the inflorescences) of *H. lupulus L.* (*Cannabinaceae*) are added into beers to give its flavor and bitterness, and are also used as stomachics, diuretic and tranquilizer in China[1]. We report here a novel prenylchalcone isolated from 80% ethanol extracts of hops collected in Xinjiang Province, which showed inhibition activity against human stomach carcinoma cells BGC-823 (IC_{50}: 1.87 μmol/mL).

1 was obtained as yellow oil. There are 21 carbon signals in its ^{13}C NMR and DEPT spectra, including 9 x C, 8 x CH, 1 x CH_2 and 3 x CH_3. HRFABMS gave a $[M+H]^+$ peak at *m/z* =371.149334 (Calcd. for $C_{21}H_{23}O_6$ 371.149464). The molecule formula was then determined as $C_{21}H_{22}O_6$, U=11. ^1H and ^{13}C NMR spectrum showed a xanthohumol skeleton[2] (**Table 1**). However, in the ^{13}C NMR, a quatenary carbon at δ 70.1 and an oxygenated CH at δ 90.1 appeared without two double bonds in prenyl of xanthohumol. ^1H NMR indicated an oxygenated proton at δ4.52 (t, 1H, J=9.0Hz). Furthermore, due to the unsaturated degree, a furan structure should exist between the phenyl and **A** ring of this chalcone[3]. In fact, HMBC spectrum of **1** indicated cross peaks between H-5' δ 5.95(s)

Figure 1 Structure of new prenylchalcone **1** and the key correlations in HMBC



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and two carbons δ 160.3 (C-4') and δ 158.8 (C-6'), which could only be observed in the structure stated in **Figure 1**. Therefore, compound **1** was identified as 5"-(2"'-hydroxyisopropyl) dihydrofurano-[2", 3"-B]-4, 4'-dihydroxy-6'- methoxychalcone.

Table 1 ^{1}H and ^{13}C NMR data of **1**[a] (d_6-DMSO, 400MHz for proton and 100MHz for carbon)

Protons	δ_H (*J*)	Carbons	δ_C	Carbons	δ_C
α	6.97 (d, 16.0)	α	125.4	4'	160.3
β	7.26 (d, 16.0)	β	141.9	5'	92.1
2, 6	7.45 (d, 8.8)	C=O	189.2	6'	158.8
3, 5	6.75 (d, 8.8)	1	125.6	4"	26.2
5'	5.95 (s)	2, 6	130.1	5"	90.1
4"	2.90 (dd, 16.0, 9.0) / 2.93 (dd, 16.0, 9.0)	3, 5	115.9	1"'	26.2
5"	4.52 (t, 9.0)	4	160.0	2"'	70.1
1"'	1.07 (s)	1'	105.2	3"'	24.5
3"'	1.06 (s)	2'	156.2	6"-OMe	55.7
6'-OMe	3.62 (s)	3'	105.2		

The assignments were based on DEPT and 2D NMR (^{1}H-^{1}H COSY, HMQC, HMBC) spectra.

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