

## HETEROPHYLLOL, a PHENOLIC COMPOUND WITH NOVEL SKELETON FROM *ARTOCARPUS HETEROPHYLLUS*

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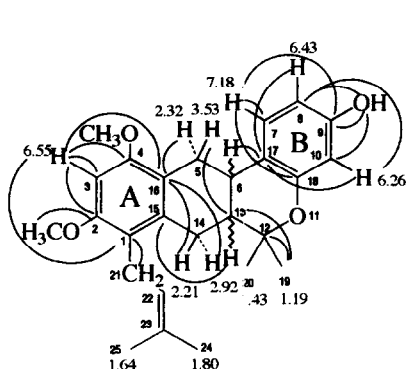
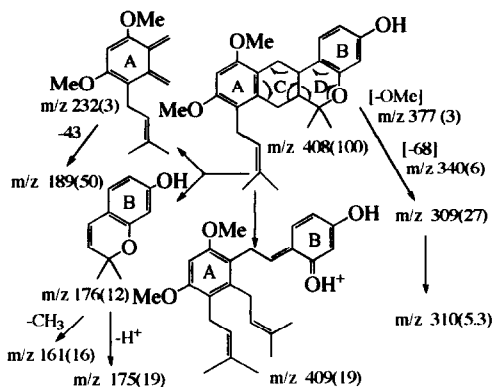
**Abstract:** From the root bark of *Artocarpus Heterophyllus*, a novel phenolic compound, heterophyllol, was isolated and determined by spectroscopic methods.

In previous papers,<sup>1-5</sup> we reported a series of prenylflavonoids from the root bark of *A. communis* and *A. heterophyllus*. In continuation of this work, we describe herein the structure elucidation of a novel phenolic compound, heterophyllol(1), obtained from the root bark of *A. heterophyllus*.

The root bark of *A. heterophyllus* was collected at Ping-Tung Hsien, Taiwan, R.O.C. during July, 1992. The acetone extract was chromatographed over silica gel. Elution with cyclohexane-CHCl<sub>3</sub> yielded 1 in addition to two 2',4',6'-trioxygenated flavanones, heteroflavanone A and heteroflavanone B.<sup>5</sup>

Compound 1, colorless needles, mp 217-218°C, [ $\alpha$ ]<sub>D</sub><sup>24</sup>-3° (c 0.1, acetone), exhibits IR bands at 3420, 1620 and 1600 cm<sup>-1</sup>. High resolution MS revealed a [M]<sup>+</sup> at m/z 408.2318 which corresponded to the molecular formula C<sub>26</sub>H<sub>32</sub>O<sub>4</sub>. The UV spectrum showed absorption maxima at 204 (4.82), 228 (sh)(4.29) and 284 nm (3.94), which indicated an unconjugated aromatic system.<sup>6-7</sup> Its <sup>1</sup>H NMR (1D and 2D) spectra defined the following substructures: a pentasubstituted and a trisubstituted benzene rings (A and B), a  $\gamma,\gamma$ -dimethylallyl group located at an aromatic ring, two methines connected to each other between two methylenes and 2 methyl groups attached to a quaternary carbon. The <sup>13</sup>C NMR and <sup>13</sup>C-<sup>1</sup>H COSY spectrum of 1 showed signals of all the 26 carbons and their corresponding protons in the molecule including the signals of the structures mentioned above, two methoxyl and the quaternary carbon of [(Me)<sub>2</sub>C<O] (Table 1).

In addition to the above results, information from long range <sup>13</sup>C-<sup>1</sup>H COSY spectrum of 1 (Fig. 1) and by comparing the <sup>13</sup>C NMR data of A ring with those of tetrahydronaphthalene<sup>8</sup> established its substitution pattern. The long range <sup>13</sup>C-<sup>1</sup>H COSY spectrum (Fig. 1) data of 1 also confirmed the substitution pattern of the B ring and established the connectivity of the 4 aliphatic carbons and the moiety of [(Me)<sub>2</sub>C<O] as shown in Fig. 1. This structure was supported by the fragmentation pattern (scheme 1) in EI-MS of 1.<sup>9,10</sup> The stereochemistry of H-6 and H-13 was reasonably assigned to be diaxial for J<sub>6,13</sub> = 12 Hz.

Fig. 1  $^1\text{H}$ - $^{13}\text{C}$  long range coupling of **1**Scheme 1. MS of **1** (major fragmentation)Table 1.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **1**\*(Acetone- $\text{D}_6$ )

No C	$\delta^{13}\text{C}$ ppm	$\delta^1\text{H}$ ppm	mult(J,Hz)	No C	$\delta^{13}\text{C}$ ppm	$\delta^1\text{H}$ ppm	mult(J,Hz)
1	119.2			14	25.2	2.21; 2.92	dd(12,16); (5,16)
2	155.9 <sup>a</sup>			15	129.7		
3	93.1	6.55	s	16	116.0		
4	156.1 <sup>a</sup>			17	116.7		
5	33.6	2.32;3.53	dd(12,16);dd(5,16)	18	154.1		
6	31.9	2.61	dt(5,12)	19	18.4	1.16	s
7	127.4	7.18	d(8.5)	20	27.0	1.43	s
8	107.8	6.43	dd(2.5,8.5)	21	23.5	3.34	d(6.9)
9	156.7	8.15	s	22	123.5	5.03	m
10	103.4	6.26	d(2.5)	23	135.6		
12	76.5			24	17.0	1.80	s
13	43.2	1.65	dt(5,12)	25	24.9	1.64	s
OMe	54.6; 55.2	3.83; 3.84	s				

\*The number of directly attached protons to each individual carbons was verified with DEPT pulse sequence; <sup>a</sup>Values may be reversed

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