

# Studies on Chemical Constituents of *Caesalpinia bonduc* L. Roxb

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**Abstract:** A new compound caesanol **1** and a known diterpene  $6\beta$ ,  $7\beta$ -dibenzoyloxyvouacapen- $5\alpha$ -ol **2** is isolated for the first time from ethanolic extract of aerial part of this plant. Structures of both were elucidated on the basis of spectroscopic analysis.

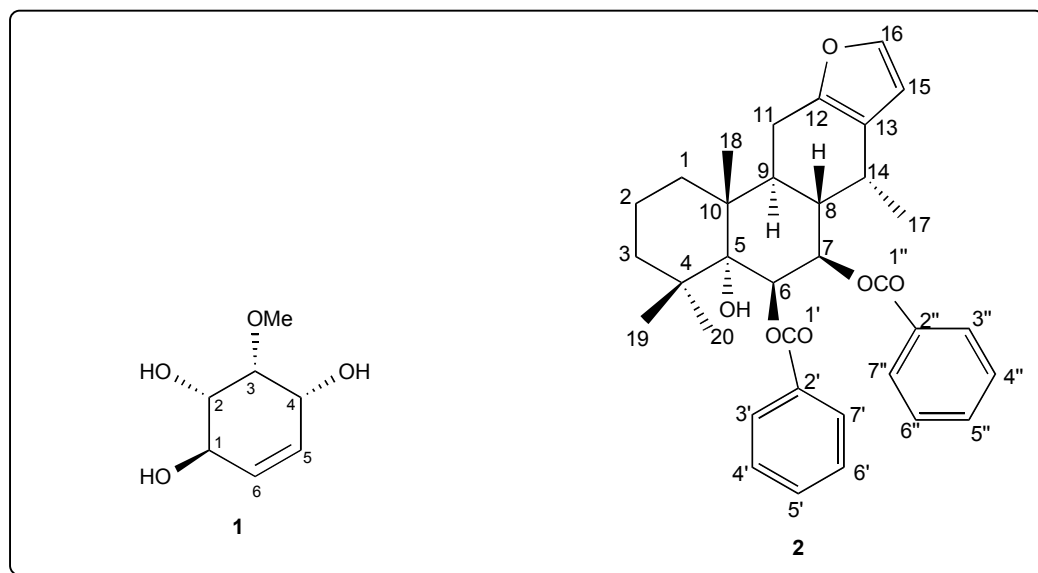
**Keywords:** *Caesalpinia bonduc*, *Caesalpinia pulcherrina*, caesanol,  $6\beta$ ,  $7\beta$ -dibenzoyloxyvouacapen- $5\alpha$ -ol, isolation.

## 1. INTRODUCTION

This plant grows throughout India and Bengal [1-2]. In Peninsular Malaysia, it is common in thickets as well as along seashores [3]. Previously cassane type diterpens have been isolated from seeds [4] and roots [5]. Caesalpins [6-9] and steroids [10] were reported from this specie. We have investigated and reported extraction and isolation of two compounds, caesanol **1** and  $6\beta$ ,  $7\beta$ -dibenzoyloxyvouacapen- $5\alpha$ -ol **2** isolated from aerial part and fruit of plant respectively. **2** is previously isolated from *C. pulcherrina* [11].

( $C_6H_9O_4^{++}$ ). The IR spectrum shows characteristic absorptions of free hydroxyl groups ( $3400\text{ cm}^{-1}$ ) and of methoxy at ( $1730\text{ cm}^{-1}$ ). Resonance assigned by  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectrum are shown in Table 1, shows the presence of six methine carbons C-1 to C-6 and one methoxy moiety at C-3 ( $\delta$  3.30, m). HMBC 2D NMR showed interaction of C-1 to H-4 and C-2 to H-3 COSY showed correlations for H-1 to H-6, H-5 to H-6.

$6\beta$ ,  $7\beta$ -dibenzoyloxyvouacapen- $5\alpha$ -ol **2** was obtained as a white solid. Its molecular formula was determined to be  $C_{34}H_{38}O$  ( $m/z$  462.200) from



## 2. RESULT AND DISCUSSION

Caesanol (3-methoxycyclohex-5-ene-1,2,4-triol) **1** is isolated as white solid crystals. The EI-MS exhibited ion at  $m/z=160$  (calculated 160.07 for  $C_7H_{12}O_4$ ).  $m/z=158$  ( $C_7H_{10}O_4^{++}$ )  $m/z=116$  ( $C_5H_8O_6^{++}$ )  $m/z=101$

HREIMS.  $^{13}\text{C}$  NMR spectra indicated the presence of four methylenes, two carbonyl carbons, seven quaternary carbons, seventeen methines and four methyls. Their signals suggested that its structure consist of two benzoyloxy groups at C-6 and C-7 position. The HMBC spectrum revealed that H-6 ( $\delta$  3.84, d,  $J=7.2$  Hz) was related to the carbonyl group ( $\delta$  166.1) of a benzoyloxy moiety while H-7 ( $\delta$  4.1, dd,  $J=7.2$  Hz) to another carbonyl group of the second benzoyloxy moiety ( $\delta$  171.1). The  $^1\text{H}$  NMR established

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doublet of doublets at  $\delta$  7.89 ( $J=8.0, 2.0$ ),  $\delta$  7.80 ( $J=8.0, 2.0$ ) and  $\delta$  4.1 ( $J=7.2$ ), triplets at  $\delta$  7.49 ( $J=8.0$ ) and  $\delta$  7.42 ( $J=8.0$ ) and doublets at  $\delta$  7.13 ( $J=7.4$ ) and  $\delta$  6.15 ( $J=7.3$ ). The presence of methylene was showed by the multiplets at  $\delta$  1.16-1.76 and  $\delta$  2.4-2.5.

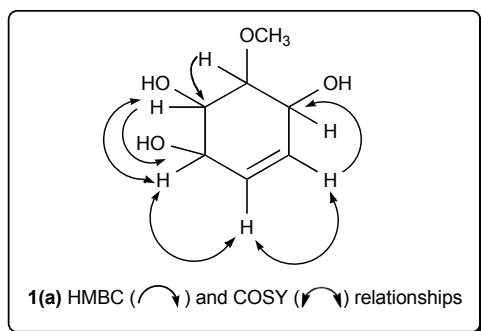


Table 1:  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR Spectral Data of Caesanol

Position	$^1\text{H}$ NMR	$^{13}\text{C}$ NMR
1	4.47 (dd, $J=3.5, 3.3$ )	70.9
2	4.67 (d, $J=3.6$ )	72.0
3	3.15 (s)	83.8
4	4.35(d, $J=3.4$ )	70.1
5	3.61 (s)	118.8
6	3.61 (s)	118.8

The structure of this compound was established from its  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectral data which indicated it to be  $6\beta, 7\beta$ -dibenzoyloxyvouacapen-5-ol previously isolated from *C. pulcherrina* [11].

### 3. EXPERIMENTAL

#### 3.1. General Experimental Procedures

Low resolution electron impact mass spectra were recorded on Finnigan-MAT-312A mass spectrometer, coupled with PDP 11/34 computer system.

High-resolution mass measurement and Gas chromatographic mass measurements were carried out on Jeol-JMS-HX 110 mass spectrometer.

$^1\text{H}$  NMR spectra were recorded at 600 MHz and  $^{13}\text{C}$  NMR at 75 MHz on Bruker AM-400 nuclear magnetic resonance spectrometers using  $\text{SiMe}_4$  as an internal standard. Solvents used for NMR spectrometry was DMSO and  $\text{CDCl}_3$

Vacuum liquid chromatography was performed on silica gel (Si 60, 70-230 mesh, E. Merk). The ethanolic fraction was subjected to VLC over silica gel. It was eluted with *n*-hexane, *n*-hexane/ethylacetate, ethyl acetate, ethyl acetate/methanol, methanol. The ethyl acetate fraction is further subjected for column chromatography.

Pre-coated silica gel GF254 preparative plates (20x20, 0.5 mm thick; E. Merk) were used for preparative thick layer chromatography. Purity of samples was also checked on the same pre-coated plates.

#### 3.2. Plant Material

The aerial parts and fruit of *C. bonduc* were collected from Malir Karachi in February 2012. It is identified by the taxonomist of department of Botany, University of Karachi. Where a voucher specimen has been deposited in the herbarium (voucher No. 86443)

#### 3.3. Extraction and Isolation

The aerial parts (10 kg) of *C. bonduc* were soaked in ethanol for the period of 4 weeks and fruit (2 kg) were soaked in ethanol for the period of 6 weeks.

Vacuum liquid chromatography was performed on silica gel (Si 60, 70-230 mesh, E.Merk). The ethanolic fraction was subjected to VLC over silica gel. It was eluted with *n*-hexane, *n*-hexane/ethylacetate, ethyl acetate, ethyl acetate/methanol, methanol. The ethyl acetate fraction is further subjected for column chromatography.

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