



Structure Characterization of Alkaloid Scorodocarpienes Derivative from Fruits of *Scorodocarpus borneensis* Becc (Olacaceae)

RUDI KARTIKA^{1,*}, TONEL BARUS², RIBU SURBAKTI² and PARTOMUAN SIMANJUNTAK^{3,4}

¹Faculty of Mathematics and Natural Sciences, Mulawarman University, Samarinda, Indonesia

²Faculty of Mathematics and Natural Sciences, Sumatra Utara University, Jalan Padang Bulan, Medan, Indonesia

³Research Centre for Biotechnology, Indonesian Institute of Science, Cibinong 16911, Indonesia

⁴Faculty of Pharmacy, Pancasila University, Srengseng Sawah Jagakarsa, Jakarta, Indonesia

*Corresponding author: E-mail: rudi_biokimia@yahoo.com; ddy_iwn@yahoo.com

Received: 22 October 2013;

Accepted: 16 January 2014;

Published online: 1 September 2014;

AJC-15851

Two tryptamine-type alkaloids dehydroxyl scorodocarpine, a new compound **1** and scorodocarpine B (**2**) were isolated from *n*-hexane extract of the fruits of *Scorodocarpus borneensis* Becc by chromatographic methods. Their structures were established based on spectroscopic analysis (UV, IR, NMR, MS) and comparison with those related compounds.

Keywords: *Scorodocarpus borneensis*, Olacaceae, Anticancer, Indonesian medicinal plant.

INTRODUCTION

Bawang hutan (wood garlic), *Scorodocarpus borneensis* Becc. which belongs to the family Olacaceae, is a tall tree which attain a height c.a 20 metres and easily recognized by its onion smell like a garlic. Garlic of the *Allium* genus, one of the most widely known spices, is noted for the enzymatic formation of large amount of organic sulphur compounds when it is crushed. The powerful flavor and possible medical application of the decomposed sulphur products have attracted the attention of chemist for more than a century, as many reviews have been published. In contrast, chemical studies on "wood garlic" have not been done because the trees are grown only in very limited area as Sumatra, Borneo and the Malay peninsula. Since its smell and utility for cooking are very similar to garlic, the volatile flavor components and antimicrobial activity were investigated¹⁻³.

The leaves and barks of the plants were reported to contain sesquiterpene, scorodocarpine alkaloid (scorodocarpine A-C) and sulphur containing compounds⁴⁻⁶. In the course of our research for bioactive metabolites from the plants used in traditional medicine, therefore it's interested in characterizing the chemical constituents. In this report, the structure characterization of isolated compounds **1** and **2** (Fig. 1) from the fruit of *S. borneensis* will be discussed.

EXPERIMENTAL

¹H and ¹³C NMR spectra were recorded at 500 MHz (¹H) and 125 MHz (¹³C) on Jeol Spectrometer using Deuterium

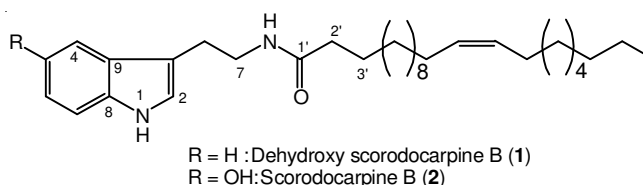


Fig. 1. Chemical structure of scorodocarpine alkaloids

solvent for calibration of the spectra. IR spectra were recorded on Shimadzu FTIR 8500 Spectrophotometer in KBr disc. The UV-visible spectrum was obtained on a Shimadzu UV-visible spectrophotometer (UV 160 PC). Column chromatography (CC) were performed on silica gel Merck 9385 (230-400 mesh).

Scorodocarpus borneensis was collected in Samarinda, East Kalimantan Indonesia. A voucher specimen was identified and deposited at Herbarium Bogoriensis Research Center for Biology, Indonesian Institute of Sciences (LIPI) Cibinong Indonesia.

Extraction and isolation: Small slices of fruit (500 g) were macerated with *n*-hexane and then the residue was macerated with aethylacetate and ethanol respectively. *n*-Hexane extract then was evaporated under reduced pressure to give a greenish yellow mass (16.93 g). A portion of this extract (10 g) was preabsorbed on silica gel and chromatographed over a column of silica with increasing amount of aethylacetate in *n*-hexane. Fractions which gave similar pattern on TLC were combined and tested for antioxidant activity (DPPH test)⁷. The most active fraction was chromatographed in same way to give dehydroxy scorodocarpine B (**1**) and scorodocarpine B (**2**).

RESULTS AND DISCUSSION

The MS spectrum (LC-MS) of dehydroxy scorodocarpine B (**1**) showed a molecular ion peak at m/z 480 (M)⁺ that corresponded to a molecular formula $C_{32}H_{52}ON_2$. The ^{13}C NMR spectrum of this compound (Table-1) supported the molecular formula and application of the DEPT techniques revealed that there were 1 methyl, 1 carbonyl, 18 methylenes and 8 carbons for tryptamine (5 methines and 3 quaternary carbons) and 2 methynes for olephenic. One carbonyl (δ_C 173.34 ppm) were assigned to amide carbonyl group, as well as confirmed by the presence of carbonyl bond at IR spectrum.

TABEL-1
 1H NMR DATA FOR DEHYDROXY
SCORODOCARPINE B (1) AND SCORODOCARPINE B (2)

No	1 (500 MHz, CDCl ₃)	2 (500 MHz, CDCl ₃)	Scorodocarpine B (According to Wiart <i>et al.</i> ⁶ , (500 MHz, CDCl ₃ + CD ₃ OD)
1.	8.14 (br,s)	8.00 (br,s)	8.40 (br, s)
2.	7.03 (s)	6.97 (s)	6.93 (s)
3.	-	-	-
4.	7.37 (d, $J=7.8$)	7.03 (d, $J=2.0$)	6.99 (d, $J=2$)
5.	7.21 (t, $J=6.0;1.2$)	-	-
6.	7.13 (t, $J=7.8$)	7.120 (d, $J=8.5;2.0$)	6.75 (dd, $J=8.5;2$)
7.	7.61 (d, $J=8.5$)	6.81 (d, $J=8.5$)	7.17 (d, $J=8.5$)
8.	-	-	-
9.	-	-	-
10.	2.98 (t, $J=7.0$)	2.88 (t, $J=7.0$)	2.85 (t, $J=7$)
11.	3.60 (t, $J=7.0$)	3.55 (t, $J=7.0$)	3.48 (t, $J=7$)
1'	-	-	-
2'	2.09 (t, $J=7.5$)	2.11 (t, $J=7.5$)	2.08 (t, $J=7$)
3'	1.58 (m)	1.57 (m)	1.53 (m)
4'	1.27 (m)	1.28 (m)	1.23 (br,s)
5'	1.27 (m)	1.28(m)	1.23 (m)
6'	1.27 (m)	1.28 (m)	1.23 (m)
7'	1.27 (m)	1.28 (m)	1.23 (m)
8'	1.27 (m)	1.28 (m)	1.23 (m)
9'	1.27 (m)	1.28 (m)	1.23 (m)
10'	1.27 (m)	1.28 (m)	1.23 (m)
11'	1.27 (m)	1.28 (m)	1.23 (m)
12'	2.02 (m)	2.00 (m)	1.98 (m)
13'	5.35 (t, $J=4.5$)	5.35 (t, $J=4.5$)	5.32 (dd, $J=5.5$)
14'	5.35 (t, $J=4.5$)	5.35 (t, $J=4.5$)	5.32 (dd, $J=5.5$)
15'	2.08 (m)	2.00 (m)	1.98 (m)
16'	1.27 (m)	1.28 (m)	1.23 (m)
17'	1.27 (m)	1.28 (m)	1.23 (m)
18'	1.27 (m)	1.28 (m)	1.23 (m)
19'	1.27 (m)	1.28 (m)	1.23 (m)
20'	1.27 (m)	1.28 (m)	1.23 (m)
21'	1.27 (m)	1.28 (m)	1.23 (m)
22'	0.88 (t, $J=7.0$)	0.88 t, $J=7.0$)	0.55 (t, $J=7$)

Further examination of the 1H and ^{13}C NMR spectra of these molecules were interpreted by the assistance of two dimensional (2-D) NMR techniques. The 1H and ^{13}C correlation spectroscopy (HMQC) of **1** revealed the connection between respective protons and carbons (Table-1). The plane structure of **1** was constructed on the basis of 1H - 1H COSY correlation spectroscopy (1H - 1H COSY) and correlation spectroscopy carried out through the Hetero *Multiple bond connectivity* (HMBC) NMR experiments. Thus, the 1H - 1H COSY of **1** indicated the presence of 3 partial structure: from C-4 to C-7;

C-10 to C-11 and C-2' to C-22' (Fig. 2). The HMBC spectrum of **1** displayed long range correlations between methine proton at δ_H 7.37 (H-4) with carbons at δ_C 122.16 (C-5); 118.93 (C-6) and 119.68 (C-7) and between methine proton at δ_H 7.61 (H-7) with carbons with at δ_C 122.16 (C-5); 118.93 (C-6) and 136.57 (C-8) and between methine proton at δ_H 7.03 (H-2) with carbons at δ_C 136.57 (C-8); 113.29 (C-3); 127.53 (C-9) of tryptamine ring.

Methylene proton at δ_H 3.60 (H-11) with carbons at δ_C 25.55 (C-10); 113.29 (C-3) and 173.34 (C-1'), methine proton at δ_H 5.35 (H-13') with carbon at δ_C 27.39 (C-12') and methyl proton at δ_H 0.88 (H-22') with carbons at δ_C 22.87 (C-21') and 32.09 (C-20') of ring mono-unsaturated with 20 carbons.

The 1H - 1H correlation spectroscopy COSY and the HMBC experiments showed the compound **1** has a *N*-acyl-5-hydroxy-tryptamine type structure which the acyl residue as unsaturated (20 carbons) for compound **1** (Table-1).

Confirmation for chemical structure of compound **1** was carried out by comparing scorodocarpine B compound isolated by Wiart *et al.*⁶ showed that compound **2** gave proton signal at C-5 (δ_H 7.21 ppm; δ_C 122.6 ppm), indicated that a hydroxyl group from scorodocarpine compound was missing [δ_C 150.2 (s) (Table-2)]. Thus, chemical structure of **1** is dehydroxy-scorodocarpine B as a new compound.

TABEL-2
 ^{13}C NMR DATA FOR DEHYDROXY
SCORODOCARPINE B (1) AND SCORODOCARPINE B (2)

No	1 (500 MHz, CDCl ₃)	2 (500 MHz, CDCl ₃)	Scorodocarpine B (According to Wiart <i>et al.</i> ⁶ , (500 MHz, CDCl ₃ + CD ₃ OD)
1.	-	-	-
2.	122.40 (d)	123.15 (d)	123.2 (d)
3.	113.29 (s)	112.44 (s)	123.2 (d)
4.	111.41 (d)	113.40 (d)	112.4 (d)
5.	122.16 (d)	150.20 (s)	150.2 (s)
6.	118.93 (d)	112.86 (d)	112.6 (d)
7.	119.68 (d)	112.44 (d)	112.1 (d)
8.	136.57 (t)	131.69 (t)	131.7 (s)
9.	127.53 (s)	128.25 (s)	128.3 (s)
10.	25.55 (t)	25.64(t)	25.7 (t)
11.	39.80 (t)	39.87 (t)	40.0 (t)
1'	173.34 (s)	173.86 (s)	173.8 (s)
2'	37.11 (t)	37.08 (t)	37.2 (t)
3'	25.93 (t)	25.95 (t)	26.0 (t)
4'	27.39 (t)	32.10 (t)	29.8 (t)
5'	27.39 (t)	32.10 (t)	29.8 (t)
6'	27.39 (t)	32.10 (t)	29.8 (t)
7'	27.39 (t)	32.10 (t)	29.8 (t)
8'	27.39 (t)	32.10 (t)	29.8 (t)
9'	27.39 (t)	32.10 (t)	29.8 (t)
10'	27.39 (t)	32.10 (t)	29.8 (t)
11'	27.39 (t)	32.10 (t)	29.8 (t)
12'	27.39 (t)	27.41 (t)	27.4 (t)
13'	130.09 (d)	130.08 (d)	130.1 (d)
14'	130.09 (d)	130.08 (d)	130.1 (d)
15'	27.39 (t)	27.41 (t)	29.8 (t)
16'	27.39 (t)	32.10 (t)	29.8 (t)
17'	27.39 (t)	32.10 (t)	29.8 (t)
18'	27.39 (t)	32.10 (t)	29.8 (t)
19'	27.39 (t)	32.10 (t)	29.8 (t)
20'	32.09 (t)	32.10 (t)	32.1 (t)
21'	22.87 (t)	22.87 (t)	22.9 (t)
22'	14.31 (q)	14.31 (q)	14.3 (q)

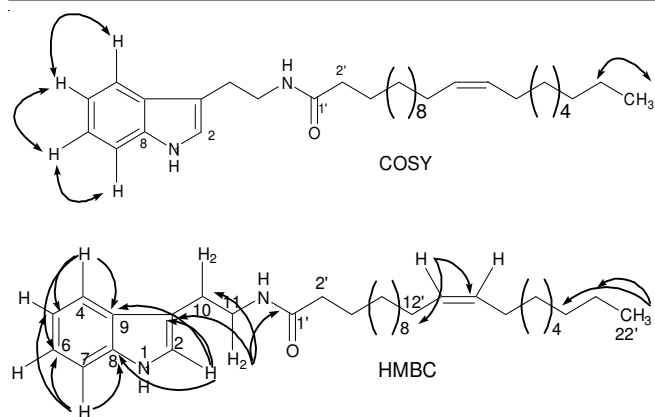


Fig. 2. Significant COSY and HMBC correlation of compound 1

The MS spectrum of compound 2 showed a molecular ion peak at m/z 496, corresponding to a molecular formula of $C_{32}H_{52}O_2N_2$. The ^{13}C NMR spectrum of this compound (Table-2) supported the molecular formula and application of the DEPT techniques revealed that there were 1 methyl, 20

methylenes, 6 methines and 5 quaternary carbon including carbonyl group. Confirmation for chemical structure of compound 2 with 2-D NMR (HMQC, COSY, HMBC) and compared with scorodocarpin B data (Tables 1 and 2), compound 2 identified as scorodocarpin B.

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