

# ISOLATION AND IDENTIFICATION OF SIMIARENOL FROM THE LEAVES OF *FICUS AURANTIACEA* GRIFF (MORACEAE)

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## ABSTRACT

*Ficus aurantiacea* Griff (Moraceae) collected from Bukit Kaba forest park, Bengkulu, was studied for the isolation and identification of its bioactive constituents. This plant is a climbing tree, having large colored fruits, orange to red marbled with white spots. The methanol-soluble extract of the leaves was eluted to silica-gel column chromatography several times using mixtures of chloroform-methanol as the elution solvent, leading to the isolation of a known compound, simiarenol. The structure of simiarenol was judged by its data comparison to published values, and based on the evaluation results of its physical and spectroscopic data, such as UV, IR, MS, one- and two-dimensional NMR, HMQC and HMBC.

## INTISARI

*Ficus aurantiacea* Griff (Moraceae) yang dikoleksi dari hutan lindung Bukit Kaba, Bengkulu, diteliti untuk isolasi dan identifikasi kandungan senyawa bioaktifnya. Tumbuhan ini merambat, dan mempunyai buah yang berwarna-warni, warna jingga ke merah dengan bercak-bercak putih. Ekstrak yang larut dalam metanol dari daun, dielusikan ke kolom khromatografi silika gel beberapa kali, dengan elusi campuran kloroform dan metanol, terisolasi sebuah senyawa yang telah diketahui, simiarenol. Struktur senyawa ini ditentukan berdasarkan perbandingan data yang telah dipublikasi, dan didasarkan pada hasil analisa data fisika dan spektroskopi, seperti UV, IR, MS, satu-dan dua-dimensi NMR, HMQC dan HMBC.

## INTRODUCTION

Historically, plants have played an important role as sources of prescription drugs in Western medicine. Their active principles also serve as templates for synthetic drug optimization and provide intermediates used in the production of semi-synthetic drugs. World wide, hundreds of higher plants species are collected from the forests for substances useful in medicine and pharmacy. Indonesian rain forest community is known to be rich of its species biodiversity in the world. Every plant species in Indonesian rain forest has individual characteristic in nature. The richer of its biodiversity, the more its genetic variety. Any plant species is potential in term of its

bioprospecting, that may give benefit for human being welfare for the future<sup>(1)</sup>.

The forest plant species that have been used by the local people in Bengkulu have been studied<sup>(2)</sup>. The plant species used as traditional medicines in Bengkulu, consist of 71 species belong to 39 families. Among these plant species, 54 % are wild collection from Bengkulu rain forest. Some of the plant species are considered rare need special attention for their conservation. The most frequent used as medicines are the leaves<sup>(3)</sup>.

One of known medicinal plants in Bengkulu forests is *Ficus aurantiacea* Griff (Moraceae), is synonymous to *F. callicarpa* Miq; *F. pomifera* Kurz; *F. megacarpa* Merr and has a local name *beringin jeruk*<sup>(4)</sup>. This climbing plant was found in Bukit Kaba, Bengkulu natural forest park. The colorful fruits are reported to be poisonous and having the same size of tangerines (citrus). Traditionally, leaf shoots are heated slowly over a fire and applied as a poultice on skin itches. The leaves are also used to treat fever and toothache. Since the leaves of this plant are used as medicine traditionally, the chemical components need to be studied, especially the active constituents. The use of traditional medicine are usually passed on from older generation, without scientific knowledge, so this study aims to elaborate phytochemically the leaves of this rare plant *Ficus aurantiacea* Griff.

## MATERIALS AND METHODS

*Plant Materials:* The leaves of *Ficus aurantiacea* Griff was collected in Bukit Kaba forest park (1500 m above sea level), and identified by Dr. S. Riswan, Bogor Herbarium. The voucher specimens were deposited at Herbarium Bogoriensis, Bogor, Indonesia.

*General Procedures:* Melting point was measured at Kofler hotstage and uncorrected. UV spectra was recorded on Hitachi U-2000 spectrometer. IR spectra was obtained on Perkin Elmer FT-IR-6PC (KBr) interferometer. <sup>1</sup>H- and <sup>13</sup>C-NMR spectra were recorded on a Varian XL-300, Bruker DPX 300 and 400 MHz NMR instruments. Low-resolution mass spectra were obtained with a Varian MA 112S and Finnigan MAT L521.

**Extraction and Isolation Procedures:** The pulverized dried leaves of *Ficus aurantiacea* (800 g) were 95% ethanol extracted to get 47 grams of EtOH extract. The EtOH extract was further defatted (extraction with n-hexane), and the residue was subjected to chloroform and water (1:1) for further partition. The water part was extracted with n-butanol; all of the extracts were rotary evaporator dried to get the n-hexane (10 g), chloroform (19 g), n-butanol (9 g) and water (9 g) extracts. The chloroform extract was selected for the isolation of the active constituents. The chloroform extract (18 g) was subjected to silica gel column chromatography (400 g silica gel in 6 cm glass column diameter) using solvent system of chloroform-hexane 9:1, led to the isolation of a white crystal compound as compound 1.

## RESULTS AND DISCUSSION

Compound 1 has similar <sup>1</sup>H-NMR similar to that of β-amyrin or of β-sitosterol. However, this compound has a molecular ion at *m/z* [M<sup>+</sup>] 426.3864 in the high resolution-EIMS, which is suitable for C<sub>30</sub>H<sub>50</sub>O (requires 426.3861).

Figure 1 and 2 shows the <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 1. Figures 3 and 4 shows the HMQC and HMBC to elaborate the direct and long-range correlations between the <sup>1</sup>H- and <sup>13</sup>C-NMR, respectively. As shown in Figure 4, the long-range <sup>1</sup>H-<sup>13</sup>C connectivity is in accordance to the connectivity of the simiarenol structure attached in Figure 4. The assignments of <sup>13</sup>C-NMR resonans follow those of published values<sup>(6)</sup>. The total amount of carbon atom found was 30, with chemical shifts as shown below. Compound 1, is hopane type triterpene that previously was isolated from *Rhododendron brachycarpum*<sup>(6)</sup>, from *Euphorbia piscatoria*<sup>(7)</sup>, from *Dorstenia asaroides*<sup>(8)</sup>, and from *Strychnos nux-vomica*<sup>(9)</sup>.

The mass fragmentations of compound 1 as shown at Fig. 5, was in accordance to those of pentacyclic triterpenoids<sup>(10)</sup>.

The spectroscopic datas indicated the presence of hydroxyl group, shown by vibration at 3400 cm<sup>-1</sup> in IR spectrum, confirm by absorption at 3.46-3.48 ppm in <sup>1</sup>H NMR spectrum and absorption at 76.35 ppm in <sup>13</sup>C NMR spectrum. Besides that, the presence of olefinic structure was indicated by vibration at 1650 cm<sup>-1</sup> in IR spectrum,

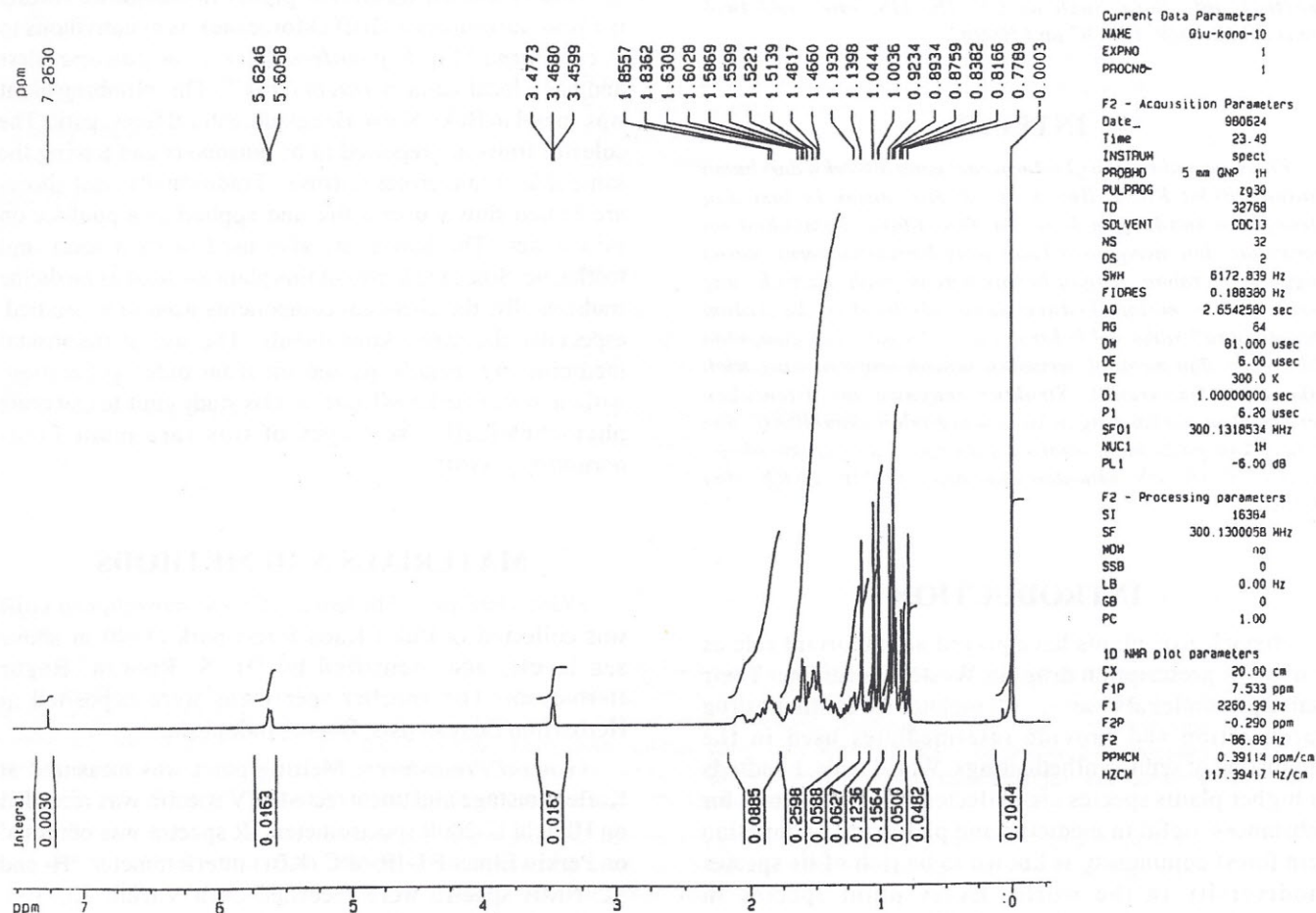


Figure 1. <sup>1</sup>H-NMR of compound 1

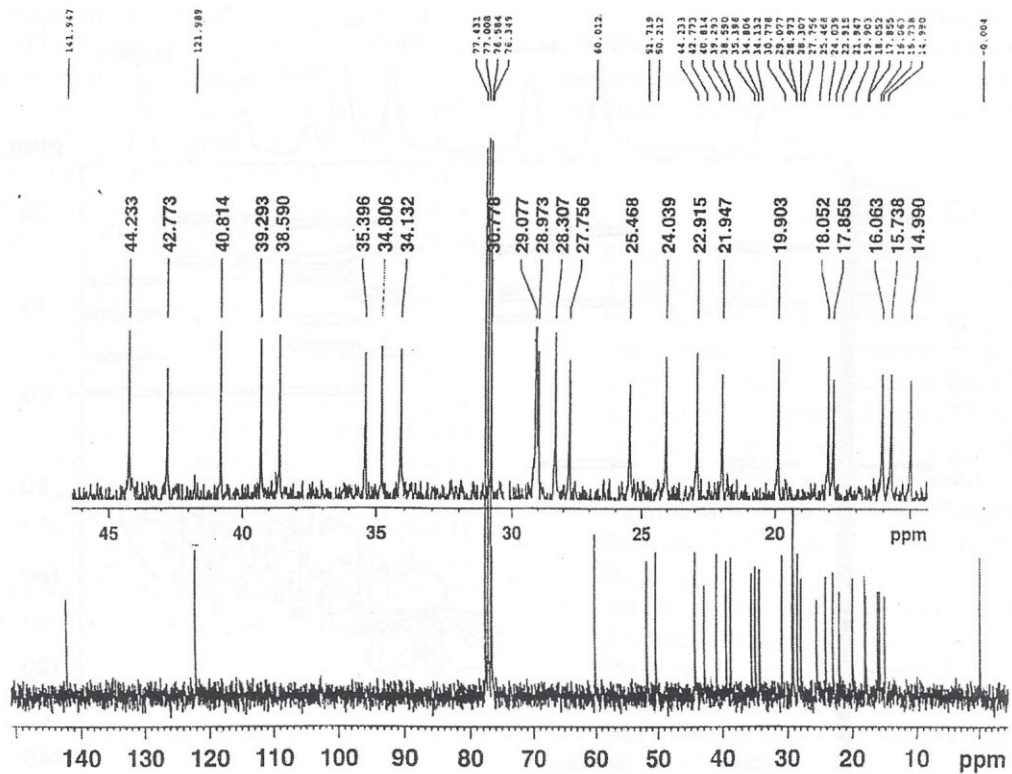


Figure 2.  $^{13}\text{C}$ -NMR of compound 1

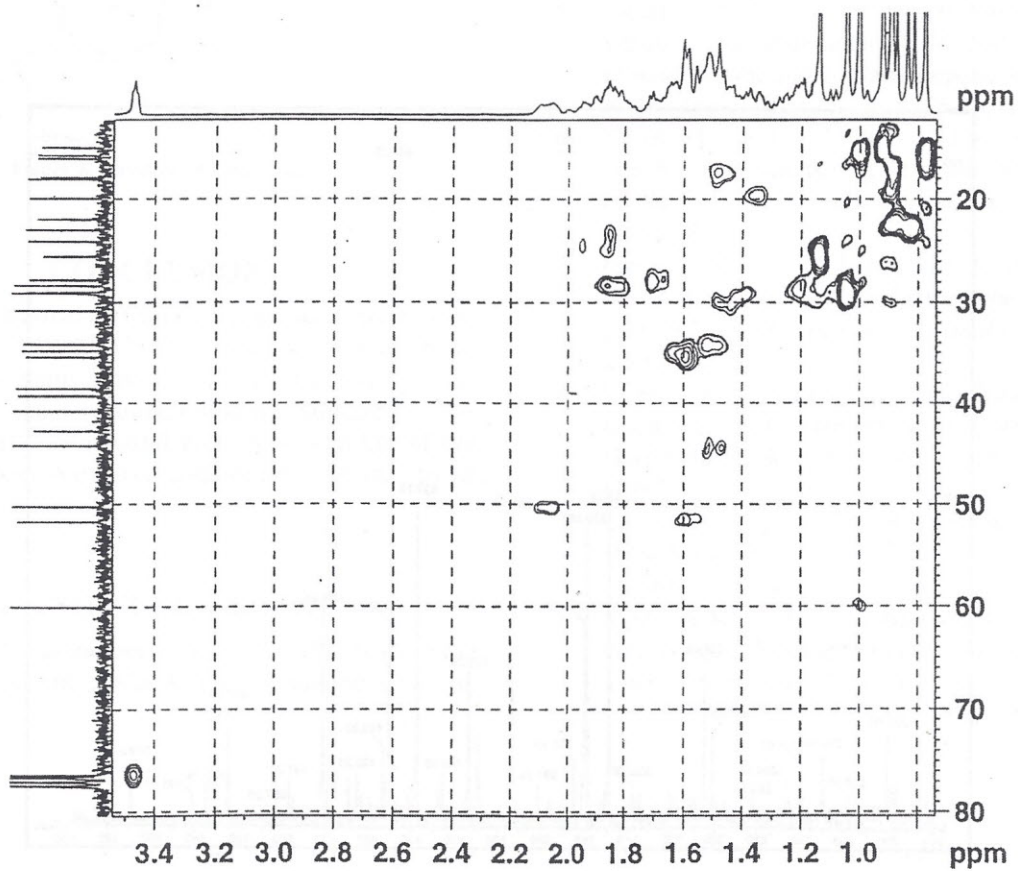


Figure 3. HMQC of compound 1

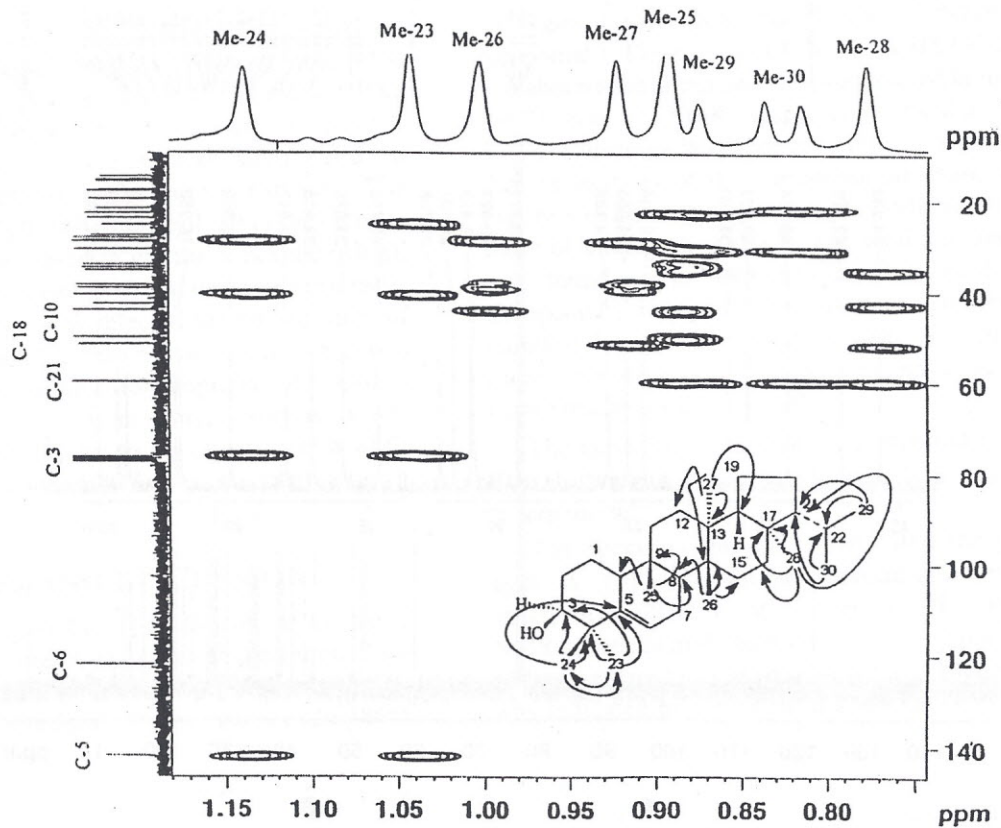


Figure 4. HMBC of compound 1

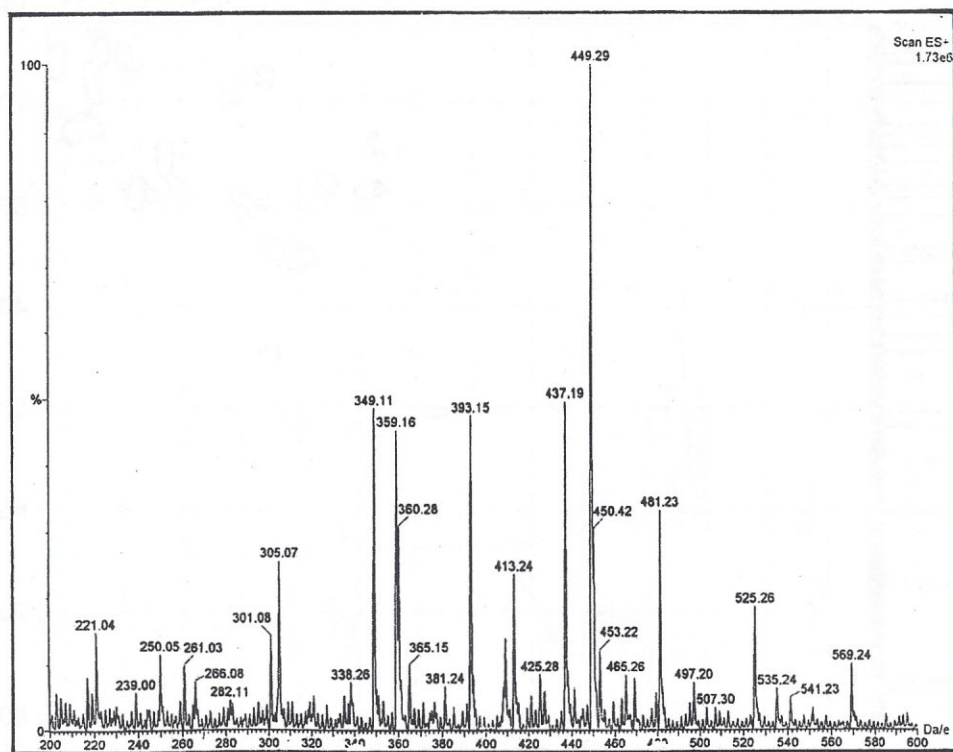


Figure 5. Mass spectra of compound 1

absorption at 5.6 ppm in  $^1\text{H}$  NMR spectrum and absorption at 121.99 and 141.95 ppm in  $^{13}\text{C}$  NMR spectrum. The complete absorption data is indicated below:

*Compound 1 (simiarenol)* : white needle crystals, mp. 182-184°C; UV  $\lambda_{\text{max}}$  ( $\text{CHCl}_3$ ) 254 nm,  $\log \epsilon$  (3.2); IR  $\nu$  3400, 2992, 1650, 1555, 1020  $\text{cm}^{-1}$ ;  $^1\text{H}$ -NMR ( $\text{CDCl}_3$ , 300 MHz.)  $\delta$ : 1.04 (3H, s,  $\text{CH}_3$ -23), 1.14 (3H, s,  $\text{CH}_3$ -24), 0.82 (3H, d,  $J=6.5$  Hz.,  $\text{CH}_3$ -29), 0.88 (3H, d,  $J=5.2$  Hz.,  $\text{CH}_3$ -30), 0.78 (3H, s,  $\text{CH}_3$ -25), 0.89 (3H, s,  $\text{CH}_3$ -26), 0.92 (3H, s,  $\text{CH}_3$ -27), 1.00 (3H, s,  $\text{CH}_3$ -28), 3.47 (1H, t,  $J=3.0$  Hz, H-3), 5.60 (1H, dt,  $J=6.0, 2.0$  Hz, H-6);  $^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 300 MHz.)  $\delta$ : 18.05 (C-1), 27.76 (C-2), 76.35 (C-3), 40.81 (C-4), 141.95 (C-5), 121.99 (C-6), 24.04 (C-7), 44.23 (C-8), 34.81 (C-9), 50.21 (C-10), 34.13 (C-11), 28.97 (C-12), 38.59 (C-13), 39.29 (C-14), 29.08 (C-15), 35.39 (C-16), 42.77 (C-17), 51.72 (C-18), 19.90 (C-19), 28.31 (C-20), 60.01 (C-21), 30.78 (C-22), 29.08 (C-23), 25.47 (C-24), 17.86 (C-25), 15.74 (C-26), 14.99 (C-27), 16.06 (C-28), 21.95 (C-29), 22.92 (C-30); Electrospray MS  $m/z$  449  $[\text{M}+\text{Na}]^+$  (100). HEIRM  $m/z$  426.3864 ( $\text{C}_{30}\text{H}_{50}\text{O}$ , requires 426.3861).

Structure of simiarenol is shown in Figure 6.

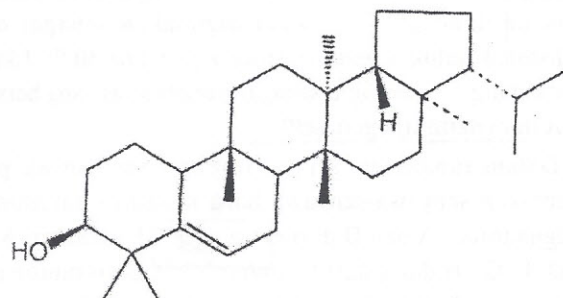


Figure 6. Structure of Simiarenol

## CONCLUSION

Based on physical and spectroscopic data, such as IR, MS,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, HMQC, HMBC and comparison of those spectroscopic data with published values, it was concluded that the compound found was simiarenol. The bioactivity of this compound and the possibility of the presence of other bioactive compounds has still to be studied.

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