Indonesian Medicinal Plants. XVIII.[1] Kompasinol A, a New Stilbeno-Phenylpropanoid from the Bark of *Koompassia malaccensis* (Fabaceae)

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A new stilbeno-phenylpropanoid named kompasinol A (1), together with four known compounds, was isolated from the bark of *Koompassia malaccensis* (Fabaceae), an Indonesian medicinal plant collected in Sumatra Island, Indonesia. The chemical structure of kompasinol A (1) has been elucidated on the bases of its chemical and physicochemical properties.

Key words Indonesian medicinal plant; *Koompassia malaccensis*; Fabaceae; kompasinol A; stilbeno-phenylpropanoid

Koompassia malaccensis (Fabaceae) is a large tree reaching up to 80 m in height, widely distributed in the southern parts of Thailand and Malaysia, and in Sumatra and Borneo.[3] This tree is important economically because of its use for construction, poles for carrying cables, railway sleepers, and pulp production.[3,4] During our expedition in 1990, searching for Indonesian traditional medicinal plants, we became aware that people around the Indragiri Hulu area of Sumatra use the decoction of the bark of *Koompassia malaccensis*, called "kompas" in that area, for the treatment of dysentery.[5]

As a part of our chemical characterization studies of Indonesian medicinal plants,[1,5] we have been investigating the chemical constituents of the bark of *Koompassia malaccensis*, collected in the above-mentioned area. We have so far isolated a new stilbeno-phenylpropanoid named kompasinol A (**1**),[6] together with betulinic acid (**5**, a triterpene),[7] 4-hydroxy-2′,4′-dimethoxychalcone (**6**, a phenylpropanoid),[8] vincoside lactam (**7**, an indole alkaloid glycoside),[9] and (+)-cathechin 3-*O*-α-L-rhamnopyranoside (**8**, a phenolic glycoside).[10] In the present paper, we describe the structure elucidation of the new stilbeno-phenylpropanoid kompasinol A (**1**), which was isolated from the ethyl acetate-soluble portion of the bark.

The methanol extract of the bark was partitioned into a mixture of ethyl acetate and water. The water-soluble portion was further partitioned with *n*-butanol to give an *n*-butanol-soluble portion and a water-soluble portion. Separation and purification of the ethyl acetate-soluble portion by repeated silica gel column and subsequent Sephadex LH-20 column chromatographies provided kompasinol A (**1**, 0.002% from the air-dried bark), betulinic acid (**5**, 0.02%), and 4-hydroxy-2′,4′-dimethoxychalcone (**6**, 0.001%). On the other hand, separation and purification of the *n*-butanol-soluble portion (*n*-BuOH extract) by silica gel and Sephadex LH-20 column

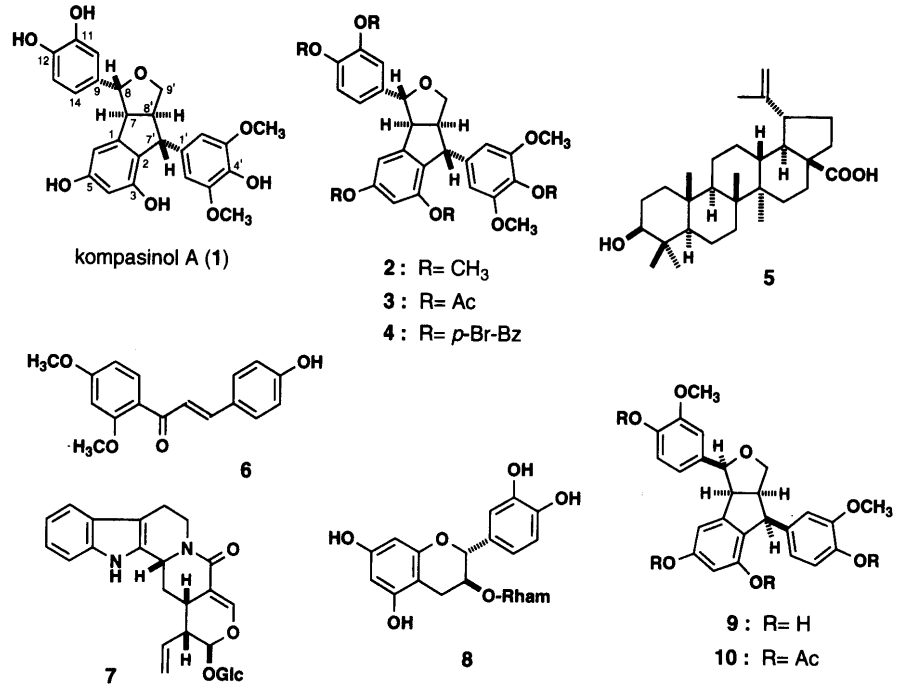

Fig. 1

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chromatographies and subsequent HPLC using reversed-phase adsorbent octadecyl silica (ODS) afforded vincoside lactam (**7**, 0.0007%) and (+)-catechin 3-*O*-α-L-rhamnopyranoside (**8**, 0.006%) (Fig. 1).

Kompasinol A (**1**) was obtained as a pale-yellow amorphous solid, which colored blue with ferric chloride reagent on TLC. In its fast atom bombardment mass spectrum (FAB-MS), **1** gave a *quasi*-molecular ion (M^+) peak at *m/z* 452, the composition of which was defined as $C_{25}H_{24}O_8$ from the high-resolution MS analysis. The IR spectrum of **1** showed absorption bands due to hydroxyl groups (3304 cm^{-1}) and aromatic rings (1606 cm^{-1}), whereas the UV spectrum of **1** showed absorption maxima at 283 nm ($\log\varepsilon = 3.93$) and 325 nm ($\log\varepsilon = 3.42$) which are also suggestive of the presence of aromatic rings.

The ^{1}H-NMR spectrum of kompasinol A (**1**), including a ^{1}H–^{1}H correlation spectroscopy (COSY) experiment, showed the presence of one 1,3,4-trisubstituted phenyl group [signals at δ 6.74 (1H, dd, J=8.6, 1.7 Hz), 6.78 (1H, d, J=8.6 Hz), 6.87 (1H, d, J=1.7 Hz)], one asymmetrical 1,2,3,5-tetrasubstituted phenyl group [δ 6.21 (1H, d, J=1.7 Hz), 6.26 (1H, d, J=1.7 Hz)], one symmetrical 1,3,4,5-tetrasubstituted phenyl group [δ 6.33 (2H, s)], and two methoxyl residues (Table 1). Characteristic signals, assignable to an oxymethine proton [δ 4.66 (1H, d, J=5.1 Hz, 8-H)] and oxymethylene protons [δ 4.46 (1H, dd, J=8.6, 7.7 Hz, 9′-Hα), 3.54 (1H, t, J=8.6 Hz, 9′-Hβ)], were also observed, together with the signals due to three methine protons [δ 4.14 (1H, br s, 7′-H), 3.77 (1H, m, 7-H), 3.03 (1H, ddd, J=8.6, 7.7, 1.7 Hz, 8′-H)]. Connectivities of these protons were defined by the following COSY correlations: i) between 8-H and 7-H; ii) between 7-H and 8′-H; and iii) between 8′-H and 9′-Hα, 9′-Hβ. These findings led us to presume that **1** has a 3-oxabicyclo[3.3.0]octane ring system. Treatment of **1** with diazomethane furnished a pentamethylated derivative (**2**), which showed no absorption band due to hydroxyl groups in its IR spectrum.

The ^{13}C-NMR spectrum of kompasinol A (**1**) showed signals attributable to eighteen aromatic carbons, two methoxyl carbons, one oxymethylene carbon, one oxymethine carbon, and three methine carbons. Based on the ^{1}H–^{13}C COSY and heteronuclear multiple bond correlation (HMBC) experiments, all carbon signals of **1** were assigned as shown in Table 2. The plane structure of kompasinol A (**1**) has been constructed on the basis of many HMBC correlations (*e.g.* between aromatic protons and methine carbons: 6-H and C-7, 10-H, 14-H and C-8; 6′-H and C-7′ and between methine protons and aromatic carbons: 7-H and C-1, C-2, C-9; 8-H and C-9, C-10; 7′-H and C-1, C-2, C-1′, C-2′; 8′-H and C-1, C-2, C-1′), as depicted in Fig. 2.

Next, the relative stereostructure of kompasinol A (**1**) was inferred on the basis of two dimensional (2D) nuclear Overhauser effect (NOE) correlations (2D-NOESY), as shown in Fig. 3. Thus, the following NOE correlations were observed: i) between 8′-H and 9′-Hα, 7-H, 6′-H; ii) between 9′-Hβ and 7′-H; iii) between 7-H and 10-H; iv) between 8-H and 10-H, 14-H. These observations indicated that the 3,4-dihydroxyphenyl group is attached to C-8 and the 3,5-dimethoxy-4-hydroxyphenyl group at C-7′ is

Table 1. ^{1}H-NMR Data for Kompasinol A (**1**), Kompasinol A Pentamethylether (**2**), and Kompasinol A Pentaacetate (**3**)[a]

Proton(s)	**1**[b]	**2**[c]	**3**[c,d]
4	6.21 (d, 1.7)	6.36 (d, 1.7)	6.78 (d, 2.0)
6	6.26 (d, 1.7)	6.42 (d, 1.7)	6.90 (d, 2.0)
7	3.77 (m)	3.89 (m)	3.84 (dd, 8.6, 6.3)
8	4.66 (d, 5.1)	4.80 (d, 4.3)	4.84 (d, 6.3)
10	6.87 (d, 1.7)	6.98 (d, 1.7)	7.23 (d, 2.0)
13	6.78 (d, 8.6)	6.89 (d, 8.6)	7.22 (d, 8.2)
14	6.74 (dd, 8.6, 1.7)	6.99 (dd, 8.6, 1.7)	7.30 (dd, 8.2, 2.0)
2′	6.33 (s)	6.24 (s)	6.31 (s)
6′	6.33 (s)	6.24 (s)	6.31 (s)
7′	4.14 (br s)	4.17 (br s)	4.27 (d, 5.9)
8′	3.03 (ddd, 8.6, 7.7, 1.7)	3.14 (m)	3.33 (m)
9′-α	4.46 (dd, 8.6, 7.7)	4.54 (dd, 8.6, 8.3)	4.38 (dd, 9.2, 6.9)
9′-β	3.54 (t, 8.6)	3.60 (dd, 8.9, 8.6)	3.97 (dd, 9.2, 4.6)
3′-OCH_3	3.72 (s)	3.76 (s)	3.75 (s)
4′-OCH_3		3.81 (s)	
5′-OCH_3	3.72 (s)	3.76 (s)	3.75 (s)
3-OCH_3		3.68 (s)	
5-OCH_3		3.83 (s)	
11-OCH_3		3.92 (s)	
12-OCH_3		3.90 (s)	

a) The δ values are in ppm and J values in Hz. *b*) Measured at 270 MHz in CD_3OD. *c*) Measured at 270 MHz in $CDCl_3$. *d*) Signals for acetyl groups were observed at 1.77 (3H, s), 2.29 (3H, s), 2.30 (6H, s), and 2.32 (3H, s) ppm.

Table 2. ^{13}C-NMR Data for Kompasinol A (**1**), Kompasinol A Pentamethyl ether (**2**), and Kompasinol A Pentaacetate (**3**)[a]

Carbon	**1**[b]	**2**[c]	**3**[c,d]
1	148.6	146.8	146.0
2	123.0	124.1	133.5
3	156.3	157.5	147.5
4	102.9	97.7	115.8
5	160.0	161.7	151.1
6	103.3	100.3	115.8
7	59.8	58.9	59.3
8	89.3	87.4	85.4
9	135.2	134.9	140.6
10	114.6	109.2	121.0
11	146.0	149.2	142.2
12	146.5	148.5	141.5[e]
13	116.3	111.0	123.6
14	119.1	118.5	123.8
1′	137.9	141.1	141.4[e]
2′	105.4	104.0	104.0
3′	149.1	153.0	152.3
4′	134.6	136.4	127.4
5′	149.1	153.0	152.3
6′	105.4	104.0	104.0
7′	52.1	51.1	55.0
8′	56.5	54.7	57.5
9′	75.0	74.0	73.4
3′-OCH_3	56.7	56.0	56.2
4′-OCH_3		60.8	
5′-OCH_3	56.7	56.0	56.2
3-OCH_3		55.3	
5-OCH_3		55.5	
11-OCH_3		55.9	
12-OCH_3		55.9	

a) The δ values are in ppm and J values in Hz. *b*) Measured at 67.8 MHz in CD_3OD. *c*) Measured at 67.8 MHz in $CDCl_3$. *d*) Signals for acetyl groups were observed at 20.1, 20.5, 20.7, (2C), 21.2, 168.2 (2C), 168.4, 168.8, and 169.1 ppm. *e*) The assignments may be interchangeable.

cis-oriented to 7-H and 8′-H. Among the NOE correlations shown in Fig. 3, the interactions observed between 7-H(α) and 8-H(β) and between 7′-H(β) and 8′-H(α) appeared rather unusual, although, in the previous study, such interactions were reported to occur in *cis*-oriented bicyclo[3.3.0]octane-type structures.[11] The decisive NOE correlation that confirmed the relative stereostructure of kompasinol A (**1**) was observed between 7-H and 6′-H. This correlation would only be possible in the case that the phenyl group at C-7′ and 7-H are in the *cis* orientation.

In 1991, Lin *et al.*[12] isolated a similar type of phenylpropanoid–stilbene condensate, gnetifolin F (**9**), from the lianas of *Gnetum parvifolium* (Gnetaceae) and reported its relative stereostructure. Based on the ^{1}H-NMR data ($J_{7,8}=6.5$ Hz; $J_{7',8'}=5.5$ Hz) and NOE examinations of the tetraacetyl derivative **10**, they proposed that 7-H and 8-H, 7-H and 8′-H, and 7′-H and 8′-H are all in *cis*-orientation, and this was finally confirmed by the X-ray crystallographic analysis of **9**.

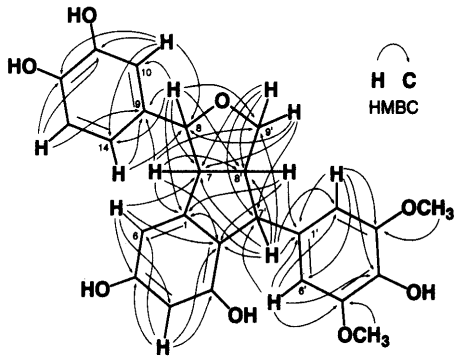

Fig. 2. HMBC Correlations Found for Kompasinol A (**1**)

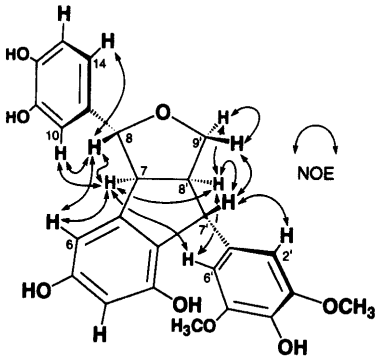

Fig. 3. NOESY Correlations Observed for Kompasinol A (**1**)

We then prepared a pentaacetyl derivative **3** by treatment of kompasinol A (**1**) with acetic anhydride in pyridine and compared in detail the ^{1}H-NMR data for **3** with those for **10**. Instead of the broad singlet ($J_{7',8'}=ca.$ 0 Hz) of 7′-H[13] observed in kompasinol A (**1**), the 7′-H signal of pentaacetylkompasinol (**3**) was observed as a doublet ($J_{7',8'}=5.9$ Hz), the change of this signal pattern being similar to that observed between gnetifolin F (**9**) and tetraacetylgnetifolin F (**10**).[12,14] The NOESY spectrum of **3** showed the presence of similar correlations to those observed in the case of **1**. Moreover, acidic hydrolysis of the pentaacetate **3** resulted in recovery of the parent kompasinol A (**1**), thus guaranteeing that no isomerization had occurred during the acetylation of **1** to **3**. It is presumed therefore that the dihedral angle (*ca.* 90°) between 7′-H and 8′-H in kompasinol A (**1**) is changed to *ca.* 120° in the pentaacetate **3**.

The elucidated structure of kompasinol A (**1**) should be chiral, but the optical rotatory values of kompasinol A (**1**) and its derivatives **2** and **3** were zero. To shed light on this matter, we prepared the penta-*p*-bromobenzoylated derivative **4** and examined its optical properties by measuring the $[\alpha]_D$ value and CD spectrum. Compound **4** was also found to be optically inactive, thus leading us to presume that kompasinol A (**1**) is a racemic compound. In order to confirm this presumption, the penta-*p*-bromobenzoylated derivative **4** was subjected to HPLC analysis using a chiral column (Ceramosphere, elution with MeOH), and it was found that **4** gave two peaks with 1 : 1 ratio.

Kompasinol A (**1**) is a stilbeno-phenylpropanoid derivative with a rare carbon skeleton. A possible route for the biosynthesis of **1** is shown in Fig. 4. This involves 1)

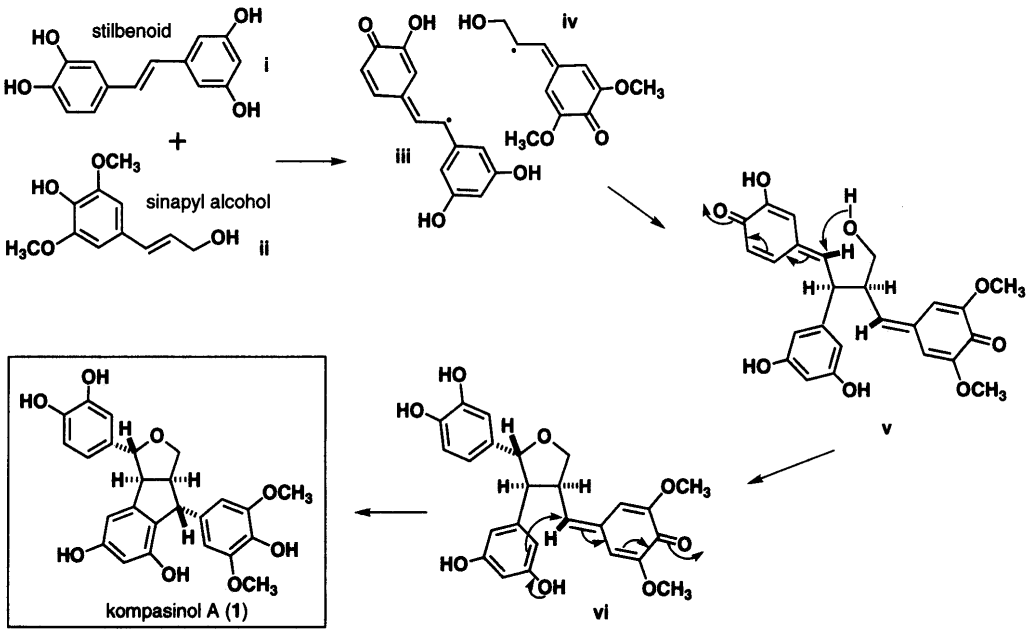

Fig. 4. Possible Biogenetic Pathway for Kompasinol A (**1**)

initial phenol-oxidative coupling of a stilbenoid **i** with a sinapyl alcohol (**ii**), 2) formation of the 3-oxabicyclo[3.3.0]octane system in **1** through **v** and **vi**. The biological activity of kompasinol A (**1**) will be the subject of future investigation.

Experimental

The UV spectra were obtained with a Hitachi 330 spectrophotometer, and the IR spectra were taken with a JASCO FT/IR-5300 spectrometer (by a diffusion–reflection method on KBr powder). The EI-MS were taken on a JEOL JMS-D300 spectrometer, while the FAB-MS were taken on a JEOL SX-102 double-focused high-resolution mass spectrometer with a JMA DA-6000 data system by a direct inlet method. The ^{1}H-NMR and ^{13}C-NMR spectra were measured with a JEOL JNM EX-270 spectrometer and a JEOL GX-500 spectrometer. Optical rotations were measured in a 0.5 dm length cell with a JASCO DIP-370 digital polarimeter. The CD spectra were obtained with a JASCO J-500A spectropolarimeter equipped with a 501N data processor. For HPLC, a JASCO 887-PU Intelligent Pump was used with a JASCO 875-UV Intelligent UV/VIS detector, and a Cosmosil 5C_{18}-AR 10 × 250 mm (Nacalai Tesque) column and a Ceramosphere Chiral RU-1 4.6 × 250 mm (Shiseido) column were used for semi-preparative and analytical separations, respectively. Column chromatography was carried out using Kieselgel 60 (70—230 mesh, Merck) or Sephadex LH-20. TLC was conducted on precoated Kieselgel 60 F_{254} plates (0.25 mm, Merck) and detection of the spots was carried out by spraying 1% $Ce(SO_4)_2$/10% H_2SO_4 on the TLC plates followed by heating or by spraying a ferric chloride reagent.

Plant Material The bark of *Koompassia malaccensis* (Fabaceae) was collected in the Indragiri Hulu area, Riau Province, Sumatra island, Indonesia, in August 1990. The plant was identified at Herbarium Bogoriense, Research and Development Centre for Biology-LIPI, Indonesia. Voucher specimens have been deposited at the Herbarium Bogoriense and the Faculty of Pharmaceutical Sciences, Osaka University.

Isolation of Kompasinol A (1) and Other Known Constituents The air-dried bark (2 kg) of *Koompassia malaccensis* (Fabaceae) was extracted with hot methanol under reflux. The combined solvent was evaporated off under reduced pressure from the extract to give the MeOH extract (126 g, 6.3% from the bark). The MeOH extract was partitioned into ethyl acetate–water (1 : 1) and the upper layer (AcOEt phase) was taken and concentrated under reduced pressure to give the AcOEt extract (58.4 g, 2.9%). The lower layer (aqueous phase) was further partitioned with *n*-BuOH to give the *n*-BuOH phase and the aqueous phase, which were each concentrated under reduced pressure to afford the *n*-BuOH extract (29 g, 1.5%) and the aqueous extract (38 g, 1.9%).

The AcOEt extract (54 g) was subjected to silica gel column chromatography (SiO_2 350 g, gradient elution with $CHCl_3$: MeOH = 100 : 1 → 10 : 1 → MeOH) to give fr. EA-1 (0.7 g), fr. EA-2 (12.9 g), fr. EA-3 (8.4 g), fr. EA-4 (6.8 g), and fr. EA-5 (24.5 g). Fr. EA-2 was again chromatographed on silica gel (SiO_2 200 g, *n*-hexane : AcOEt = 10 : 1 → 5 : 1) and Sephadex LH-20 (Sephadex LH-20 50 g, $CHCl_3$: MeOH = 1 : 1) to afford betulinic acid (**5**, 0.38 g, 0.02%) and 4-hydroxy-2′,4′-dimethoxychalcone (**6**, 26 mg, 0.001%), which were identified by comparing their spectral data (NMR, IR) with those reported.[7,8] Separation and purification of fr. EA-4 with Sephadex LH-20 (Sephadex LH-20 200 g, $CHCl_3$: MeOH = 1 : 1) and silica gel [SiO_2 25 g, $CHCl_3$: MeOH : H_2O = 15 : 3 : 1 (lower phase)] column chromatographies afforded kompasinol A (**1**, 40 mg, 0.002%).

The *n*-BuOH extract (28 g) was subjected to silica gel column chromatography [SiO_2 300 g, $CHCl_3$: MeOH : H_2O = 10 : 3 : 1 (lower phase) → MeOH] to give fr. Bu-1 (0.8 g), fr. Bu-2 (1.2 g), fr. Bu-3 (2.6 g), fr. Bu-4 (3.6 g), fr. Bu-5 (3.3 g), fr. Bu-6 (5.4 g) and fr. Bu-7 (5.9 g). Fr. Bu.3 (2.5 g) was then subjected to Sephadex LH-20 column chromatography (Sephadex LH-20 100 g, developed with MeOH) to afford fr. Bu-3.1 (0.6 g), fr. Bu-3.2 (1.7 g), and fr. Bu-3.3 (0.07 g). Separation and purification of fr. Bu-3.2 with silica gel column chromatography (SiO_2 50 g, $CHCl_3$: MeOH = 5 : 1) and HPLC (Cosmosil 5C_{18}-AR ODS 10 × 250 mm, MeOH : H_2O = 60 : 40) provided vincoside lactam (**7**, 14 mg, 0.0007%), which was identified by comparing its spectral data (NMR, IR, UV, $[\alpha]_D$) with those reported.[9] Separation and purification of fr. Bu-5 with Sephadex LH-20 (Sephadex LH-20 100 g, MeOH) and silica gel [SiO_2 20 g, $CHCl_3$: MeOH : H_2O = 7 : 3 : 1 (lower phase)] column chromatographies, and subsequent HPLC (Cosmosil 5C_{18}-AR ODS 10 × 250 mm, MeOH : H_2O = 20 : 80) gave (+)-catechin 3-*O*-α-L-rhamnopyranoside (**8**, 124 mg, 0.006%), which was identified on the basis of its physicochemical properties (NMR, IR, acidic hydrolysis and $[\alpha]_D$), and by comparing the NMR spectrum of its heptaacetyl derivative with that reported.[10]

Kompasinol A (**1**): A pale-yellow amorphous solid, $[\alpha]_D$ 0° (c = 0.38, MeOH, 25 °C). IR (KBr) cm^{-1}: 3304, 2924, 1606, 1516, 1462, 1115. UV λ_{max} (MeOH) nm (log ε): 283 (3.93), 325 (3.42). ^{1}H-NMR (270 MHz, CD_3OD, δ): as given in Table 1. ^{13}C-NMR (67.8 MHz, CD_3OD, δ_C): as given in Table. 2. FAB-MS m/z: 452 (M^+). High-resolution FAB-MS m/z: Calcd for $C_{25}H_{24}O_8$: 452.1471. Found : 452.1466.

Methylation of Kompasinol A (1) Giving the Pentamethylated Derivative (2) A methanolic solution (1 ml) of **1** (3 mg) was treated with ethereal diazomethane at 25 °C for 12 h. The reaction mixture was evaporated under reduced pressure to give the pentamethylated derivative (**2**, 3.6 mg)

2: A pale-yellow amorphous solid. $[\alpha]_D$ 0° (c = 0.20, MeOH, 20 °C). IR (KBr) cm^{-1}: 2934, 1593, 1514, 1462, 1126. ^{1}H-NMR (270 MHz, $CDCl_3$, δ): as given in Table 1. ^{13}C-NMR (67.8 MHz, $CDCl_3$, δ_C) : as given in Table 2. FAB-MS m/z: 522 (M^+). High-resolution FAB-MS m/z: Calcd for $C_{30}H_{34}O_8$: 522.2254. Found : 522.2259.

Acetylation of Kompasinol A (1) Giving the Pentaacetyl Derivative (3) A solution of **1** (7 mg) in pyridine (0.35 ml) was treated with acetic anhydride (0.175 ml), and the mixture was stirred at 25 °C for 30 min, then poured into ice-water, and the whole was extracted with $CHCl_3$. Work-up of the $CHCl_3$ extract in a usual manner gave **3** (9 mg).

3: A pale-yellow amorphous solid. $[\alpha]_D$ 0° (c = 0.35, MeOH, 20 °C). IR (KBr) cm^{-1}: 2937, 1767, 1604, 1506, 1209, 1115. ^{1}H-NMR (270 MHz, $CDCl_3$, δ): as given in Table 1, and NOESY correlations: i) between 8′-H and 9′-Hα, 7-H, 6′-H; ii) between 9′-Hβ and 7′-H, 8-H; iii) between 7-H and 10-H, 6′-H. ^{13}C-NMR (67.8 MHz, $CDCl_3$, δ_C): as given in Table 2. EI-MS m/z: 662 (M^+). High-resolution EI-MS m/z: Calcd for $C_{35}H_{34}O_{13}$: 662.1997. Found : 662.1997.

Acidic Hydrolysis of the Pentaacetyl Derivative (3) Affording Kompasinol A (1) A solution of **3** (2 mg) in acetone (0.5 ml) and 5% aqueous HCl (0.5 ml) was heated under reflux for 3 h. The reaction mixture was then poured into water and extracted with AcOEt. Work-up of the AcOEt soluble portion in a usual manner gave **1** (1 mg) (identified by HPLC and ^{1}H-NMR comparisons).

Esterification of Kompasinol A (1) with *p*-Bromobenzoyl Chloride Giving the Penta-*p*-bromobenzoylated Derivative (4) A solution of **1** (2 mg) in pyridine (0.5 ml) was treated with *p*-bromobenzoyl chloride (30 mg), and the mixture was stirred at 70 °C for 8 h, then poured into ice-water and extracted with AcOEt. Work-up of the AcOEt extract in a usual manner gave **4** (3.1 mg).

4: A white amorphous solid. $[\alpha]_D$ 0° (c = 0.25, MeOH, 20 °C). IR (KBr) cm^{-1}: 2924, 1741, 1589, 1261. ^{1}H-NMR (270 MHz, $CDCl_3$, δ): 3.51 (1H, m, 8′-H), 3.53 (6H, s, 3′, 5′-OMe), 4.00 (2H, m, 7- and 9′-Hβ), 4.30 (1H, d, J = 5.5 Hz, 7′-H), 4.48 (1H, dd-like, J = *ca.* 8, 7.5 Hz, 9′-Hα), 4.94 (1H, d, J = 6.2 Hz, 8-H), 6.25 (2H, s, 2′- and 6′-H), 7.05 (1H, d, J = 2.3 Hz, 4-H), 7.18 (1H, d, J = 2.3 Hz, 6-H), 7.58 (1H, d, J = 2.1 Hz, 10-H), 7.40—8.09 (22H, m, 13-, 14-H, and the *p*-bromobenzoyl moiety protons). FAB-MS m/z: 1367. High-resolution FAB-MS m/z: Calcd for $C_{60}H_{39}O_{13}{}^{79}Br_5$: 1362.8367. Found: 1362.8315. CD (c = 4.39 × 10^{-4}, MeOH): no maximum.

Acknowledgement The authors are grateful to Drs. Tahan Uji, Herbarium Bogoriense, Research and Development Centre for Biology-LIPI, Indonesia for collection and identification of the plant material. This work was supported by a Grant-in-Aid for Scientific Research in the International Scientific Research Program from the Ministry of Education, Science, Sports, and Culture of Japan.

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