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**Secondary metabolites of *Bagassa guianensis* Aubl. wood, a study of the chemotaxonomy of the Moraceae family.**

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23

24 **Abstract**

25

26 In effort to explain wood durability of Moraceae plants family, a phytochemical study was  
27 undertaken on *Bagassa guianensis*. The phytochemical investigation of the ethyl acetate  
28 extract obtained from the heartwood led to the isolation of 18 secondary metabolites,  
29 including 6 moracins [the new 6-*O*-methyl-moracin M (**3**), 6- *O*-methyl-moracin N (**4**) and  
30 moracin Z (**5**); the known moracin M (**1**), moracin N (**2**) and moracin P (**6**)], 8 phenolic  
31 derivatives [the new (-)-epialboctalol (**12**), arachidin 4 (**10**) and the known alboctalol (**11**),  
32 *trans*-resveratrol (**7**), arachidin 2 (**9**), *trans*-oxyresveratrol (**8**) and artogomezianol (**13**)], the 3  
33 known flavonoids steppogenin (**14**), katuranin (**15**), dihydromorin (**16**), the  $\beta$ -sitosterol (**17**)  
34 and the resorcinol (**18**). Comparison with literature data indicates that stilbenoids are  
35 presumably responsible for the natural durability of the wood. In addition, chemical  
36 composition points out that *B. guianensis* is closely related to *Morus* sp. in the phylogeny and  
37 should be placed within the Moreae s. s. tribe in the Moraceae family.

38

39 **Keywords:** *Bagassa guianensis*, Moraceae, secondary metabolites, stilbenes, moracins,  
40 flavonoids, natural durability

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42

43

## 44 **1. Introduction**

45 Wood as a material is used extensively in construction and other applications where it can be  
46 degraded by many different organisms, mainly fungi and insects. However, some trees have  
47 specialized considerably long-lasting heartwoods. It has been demonstrated in the past that  
48 wood natural durability can be ascribed to the presence of extractives (Smith et al., 1989;  
49 Wang et al., 2005; Hsu et al., 2007), although structural components of the cell wall may also  
50 contribute to its resistance to biodegradation (Silva et al., 2007). Heartwood natural durability  
51 can also result from synergetic or additive effects of compounds with various modes of action  
52 (toxic, hydrophobic, free radical scavengers and so on) (Suttie and Orsler, 1996; Okitani et al.,  
53 1999; Schultz and Nicholas, 2000; Schultz et al. 2007; Binbuga et al., 2008). Future processes  
54 to preserve wood constructions may involve returning to mankind's historical use of naturally  
55 durable heartwood as well as discovering eco-friendly wood protection agents inspired from  
56 long-lasting woods (Schultz et al., 2007).

57

58 *Bagassa guianensis* Aubl. (Moraceae) commercially known as tatajuba is a large rather  
59 infrequent unbuttressed canopy tree naturally occurring in French Guiana. *Bagassa guianensis*  
60 is a member of Moraceae family, which is divided in 5 unequal tribes when comparing the  
61 number of species in these tribes (Mabberley, 2002). *Bagassa guianensis* (the only member of  
62 its genus) was originally classified in the Artocarpeae tribe, but Weiblen genoma-based  
63 classifications have suggested recently that this species would better be included in Moreae  
64 tribe (Datweyler and Weiblen, 2004; Zerega et al, 2005).

65

66 Species in the Moraceae family have important economic and medicinal value. They are  
67 widely acknowledged as a rich source of bioactive secondary metabolites such as flavonoids,

68 stilbenes, triterpenoids and xanthenes (Lee et al., 2009; Ngadjui et al., 2005; Han et al., 2006;  
69 Jayasinghe et al., 2008). Also, some of them like *Maclura pomifera* and *B. guianensis* are  
70 capable of specializing very long-lasting woods (Scheffer and Morrell, 1998; Schultz et al.,  
71 1995), although in the latter case, the substances responsible for this high durability were  
72 unknown. We therefore embarked upon identifying secondary metabolites of tatajuba wood  
73 that may responsible for its natural durability. In addition, our secondary goal here was to  
74 confirm (or refute) botanical classification of the *Bagassa* genus by chemotaxonomy.

75

## 76 2. Results and Discussion

77 The dried heartwood of *Bagassa guianensis* was extracted with ethyl acetate. This extract was  
78 fractionated by silicagel column chromatography to give 9 fractions. Subsequent preparative  
79 HPLC purifications of these fractions allowed us to isolate compounds **1-18** (figure 1).

80

81 **Figure 1** Compounds **1-18** isolated from *Bagassa guianensis* (Moraceae). (a) New  
82 compounds; (b) New names.

83

84 Compounds **1** to **6** shared several common spectral characteristics. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR  
85 spectral data (Table 1) indicate the presence of two independent aromatic systems with a 3,5-  
86 dihydroxyphenyl and a substituted benzofuran. For example, **3** exhibited the 3,5-  
87 dihydroxyphenyl with characteristic  $^1\text{H}$  spectrum composed of one doublet at  $\delta$  6.78 for H-  
88 2'/H-6' and a triplet at  $\delta$  6.25 for H-4'. These protons are coupled to each other with a  $^4J$   
89 coupling of 2.1 Hz. In addition,  $^{13}\text{C}$  spectrum indicates the presence of two equivalent aryl  
90 hydroxyl groups at  $\delta$  159.7. The 3,5-dihydroxyphenyl moiety was linked to C-2 by the  
91 observation of a long range  $^1\text{H}$ - $^{13}\text{C}$  correlation between H-2'/H-6' and C-2 at  $\delta$  156.5. The  
92 second aromatic system appeared characteristic of a 6-monosubstituted benzofuran with

93 signals of protons H-4, H-5 and H-7 being a broad doublet at  $\delta$  7.43 ( $J = 8.5$  Hz), a doublet of  
94 doublet at  $\delta$  6.85 ( $J = 8.5$  and 2.0 Hz) and a doublet at  $\delta$  7.09 ( $J = 2.0$  Hz), respectively. On  
95 the furan ring H-3 gives a doublet at  $\delta$  6.95 ( $J = 0.6$  Hz) due to a long range  $^5J$  coupling with  
96 H-7 (confirmed by the presence of crosspeak between H-3 and H-7 on COSY NMR  
97 spectrum). When compared to moracin M (**1**), it became obvious from signal at  $\delta$  3.85 (3H, s)  
98 and the presence of crosspeak at  $\delta$  56.2 in the  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectra that compound **3** was a  
99 moracin M methyl ether. The  $^1\text{H}$ - $^{13}\text{C}$  long-range HMBC spectra gave a crosspeak with C-6 at  
100  $\delta$  159.6 unambiguously placing the methoxy group on C-6. HREIMS of **3** allowed us to  
101 ascertain molecular formula  $\text{C}_{15}\text{H}_{12}\text{O}_4$  further confirming that we had isolated the new 6-*O*-  
102 methyl-moracin M (**3**).

103

104 **Table 1**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopic data for moracins **3-5** in  $\text{CD}_3\text{OD}$

105

106 Compound **4** was isolated as yellowish amorphous powder. The HREIMS indicated a  
107 molecular formula  $\text{C}_{20}\text{H}_{20}\text{O}_4$  deduced from the ion peak at  $m/z$  325.1437 [ $\text{M} + \text{H}$ ] $^+$  (calcd  
108 325.1434). The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectral data of **4** were closely related to those of moracin N  
109 (**2**) (Lee et al., 2001) except for the replacement of hydroxyl group by a methoxy group as  
110 described for the above compound **3**. Indeed, the  $^1\text{H}$  NMR data of **4** (Table 1) demonstrated  
111 the presence a methoxy group on C-6 in the benzofuran ring, with a signal at  $\delta$  3.88 (3H, s), a  
112 crosspeak at  $\delta$  56.2 in the  $^1\text{H}$ - $^{13}\text{C}$  HSQC experiment and a crosspeak with C-6 at  $\delta$  157.4 in  
113 the  $^1\text{H}$ - $^{13}\text{C}$  long-range HMBC spectra. This novel molecule was named 6-*O*-methyl-moracin  
114 N.

115

116 Compound **5** was isolated as an amorphous brown powder. The molecular formula  $C_{20}H_{22}O_5$   
117 was deduced from the HREIMS at  $m/z$  343.1542  $[M + H]^+$  (calcd 343.1540). The  $^1H$ - and  $^{13}C$ -  
118 NMR spectral data of **5** were closely related to those of 6-*O*-methyl-moracin N (**4**) (Table 1).  
119 The main difference was observed in the prenyl moiety at C-5. The double bond is absent in **5**  
120 and it was unambiguously established that side chain at C-5 is hydrated and is therefore a 3-  
121 hydroxy-3-methylbutyl group, with the upfield shifts of methylene group H-1'' from  $\delta$  3.34 to  
122  $\delta$  2.73 and the apparition of a methylene H-2'' at  $\delta$  1.74 in place of the vinyl proton at  $\delta$  5.52;  
123 in addition, the two methyl groups H-4'' and H-5'' became equivalent at  $\delta$  1.27 (Table 1).  
124 The  $^1H$ - $^{13}C$  long-range HMBC spectra exhibited a crosspeak between the methylene group H-  
125 1'' and H-2'' with C-5 at  $\delta$  128.6 proving the linkage C-1''/C-5 between the 3-hydroxy-3-  
126 methylbutyl moiety and the benzofuran ring. This molecule is a hydrate of 6-*O*-methyl-  
127 moracin N and was named moracin Z.

128  
129 Spectral data along with HREIMS of **1**, **2** and **6** allowed us to determine and ascertain by  
130 comparison with literature data that we had also isolated moracin M (**1**) (Basnet et al. 1993,  
131 Zhou et al., 1999), moracin N (**2**) (Lee et al. 2001) and moracin P (**6**) (Dat et al., 2009).

132  
133 Stilbenoids *trans*-resveratrol (**7**) (Lee et al. 2001; Su et al., 2002), *trans*-oxyresveratrol (**8**)  
134 (Likhitwitayawuid and Sritularak, 2001; Lee et al., 2001; Su et al., 2002; Li et al., 2007),  
135 arachidin 2 (**9**) (Orsini et al., 2004) and artogomezianol (**13**) (Likhitwitayawuid and  
136 Sritularak, 2001) were identified by comparison of the respective spectral and chemical data  
137 with those described in the literature (Figure 1).

138  
139 Compound **10** was a colorless syrup with molecular formula  $C_{19}H_{22}O_4$  as deduced from the  
140 HREIMS at  $m/z$  315.1592  $[M + H]^+$  (calcd 315.1591). The  $^1H$  spectral data of **10** were closely

141 related to those of arachidin 2 (**9**) (Table 2) and suggested a stilbenoid compound with a *para*-  
142 disubstituted aromatic ring A, a *trans* double bond between the aromatic rings, and a  
143 1',3',4',5'-tetrasubstituted aromatic ring B. Ring A is symmetrical, with 2 doublets at  $\delta$  7.32  
144 ( $J = 8.7$  Hz, H-2/H-6) and  $\delta$  6.75 ( $J = 8.7$  Hz, H-3/H-5). The *trans* configuration of the double  
145 bond can be ascertained by the very large coupling constant between the two protons at  $\delta$  6.90  
146 ( $J = 16.5$  Hz, H- $\alpha$ ) and  $\delta$  6.74 ( $J = 16.5$  Hz, H- $\beta$ ), and the B ring is symmetrical as well and  
147 was characterized by a singlet at  $\delta$  6.46 (H-2'/H-6'). In the same way as we identified a  
148 hydrated side chain in the moracins series, the main difference here between **9** and **10** is in the  
149 side chain in position 4', the double bond of which is also hydrated. This has been established  
150 by the observation of methylene group H-1'' at  $\delta$  2.66 instead of  $\delta$  3.28 and the apparition of  
151 a second methylene H-2'' at  $\delta$  1.68. In addition, the two methyl groups H-4'' and H-5''  
152 became equivalent at  $\delta$  1.25. The chromatography collected quantities was too low to observe  
153 heteronuclear  $^1\text{H}$ - $^{13}\text{C}$  HSQC / HMBC correlations and direct  $^{13}\text{C}$  chemicals shifts by  
154  $^{13}\text{C}$ /DEPTQ sequence. However, the above-described data in comparison with those of  
155 arachidin 2 are sufficient to ascertain identification of compound **10** as *trans*-4'-(3-hydroxy-3-  
156 methylbutyl)-oxyresveratrol. We named this new compound arachidin 4.

157

158 **Table 2**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopic data for stilbenes **9** and **10** in  $\text{CD}_3\text{OD}$

159

160 Compounds **11** and **12** both isolated as brownish syrups presented the ion peak at  $m/z$   
161 489.1540  $[\text{M} + \text{H}]^+$  in HREIMS indicating that they are isomers with molecular formulas  
162  $\text{C}_{28}\text{H}_{24}\text{O}_8$  (calcd 489.1544). The  $^1\text{H}$ -NMR allowed us to identify a 3,5-dihydroxyphenyl group  
163 and two distinct 2,4-dihydroxyphenyl groups in both compounds. By comparison of the  
164 respective spectral and chemical data with those described in the literature, compound **11** was



165 identified as alboctalol (Bates et al., 1997). Compound **12** has an  $[\alpha]_D^{20}$  value of  $-7.4^\circ$  (c  
166 0.004, CH<sub>3</sub>OH). It was clear that **12** was a diastereoisomer of **11** with equivalent H-18/H-22  
167 protons at  $\delta$  6.01 (Table 3). In **11**, H-18/H-22 pair gives a doublet at a strong upfield shift of  $\delta$   
168 5.77 typical of the  $\pi$ -stacking effect of the neighboring 2,4-dihydroxyphenyl groups. In  
169 addition, on this aliphatic ring, the main differences with **11** are on methylene H-5 and  
170 methines H-6, H-7 and H-8. H-5<sub>ax</sub> at  $\delta$  3.19 exhibited a broad triplet with large couplings ( $J =$   
171 13.7 Hz) with the gem H-5<sub>eq</sub> and the vicinal H-6 suggesting that the 6-aryl group should be  
172 equatorial and proton H-6 axial. This observation was corroborated by the multiplicity of H-  
173 5<sub>eq</sub> signal at  $\delta$  2.72. This signal is a doublet of doublet with a large coupling constant  $J = 15.6$   
174 Hz with H-5<sub>ax</sub> and a small coupling constant  $J = 3.0$  Hz with H-6<sub>ax</sub>. Signal of H-6<sub>ax</sub> at  $\delta$  3.51  
175 is a broad triplet of doublet with two large coupling constants  $J = 11.6$  Hz with H-5<sub>ax</sub> and H-  
176 7 and a small coupling constant  $J = 2.1$  Hz with H-5<sub>eq</sub>. This pattern indicates that the 7-aryl  
177 group is equatorial and H-7 axial. H-7<sub>ax</sub> at  $\delta$  3.41 exhibited one doublet of doublet with one  
178 large coupling constant ( $J = 11.3$  Hz) with H-6<sub>ax</sub> and a second rather large coupling constant  
179 ( $J = 8.2$  Hz) with H-8 indicating that the 8-aryl group might be equatorial and proton H-8  
180 axial. These assumptions were confirmed by NOESY experiment with cross peaks observed  
181 between H-5<sub>eq</sub> and H-6<sub>ax</sub>, H-6<sub>ax</sub> and H-8<sub>ax</sub>, H-6<sub>ax</sub> and H-18, H-8<sub>ax</sub> and H-22 and between H-5<sub>ax</sub>  
182 and H-16, H-7<sub>ax</sub> and H-16, H-7<sub>ax</sub> and H-28 (Figure 2). All data permitted to confirm that we  
183 had isolated a new epimer of alboctalol (**11**) therefore named (-)-epialboctalol (**12**).

184

185 **Table 3** <sup>1</sup>H and <sup>13</sup>C NMR spectroscopic data for distilbenes **11** and **12** in CD<sub>3</sub>OD

186

187 **Figure 2** Pertinent NOE interactions observed for (-)-epialboctalol (**12**) from NOESY  
188 experiment

189

190 In addition to these moracins and stilbenoids, we isolated flavanones steppogenin (**14**) (Lee et  
191 al., 2001), katuranin (**15**) (Lee et al., 2001) and dihydromorin (**16**) (Su et al., 2002), together  
192 with  $\beta$ -sitosterol (**17**) (Basnet et al., 2003, Aldrich Library of <sup>13</sup>C and <sup>1</sup>H FT NMR spectra,  
193 1992) and resorcinol (**18**) (Aldrich Library of <sup>13</sup>C and <sup>1</sup>H FT NMR spectra, 1992). These  
194 known compounds were identified by comparison of the respective spectral and chemical data  
195 with those described in the literature.

196

197 Essentially three classes of compounds were isolated in this study: moracins, stilbenes and  
198 flavanones. Only resorcinol **18** and  $\beta$ -sitosterol **17** do not belong to these classes. These two  
199 compounds are widely distributed in nature and cannot be viewed as chemotaxonomic  
200 markers.

201

202 Moracin N, M and P have been isolated before from *Morus alba*. In general, it was found  
203 from the literature that *Morus* genus is purveyor of moracins (Tagasuki et al., 1979; Hirakura  
204 et al., 1986; Basnet et al., 1993; Nguyen et al., 2009). The only one exception is the isolation  
205 of moracin M from *Artocarpus dadah* (Su et al., 2002).

206

207 Among stilbenes, *trans*-oxyresveratrol was isolated from various plants including *Morus* sp.  
208 and *Artocarpus* sp. (Hirakura et al, 1986; Su et al, 2002; Shimizu et al., 1998; Song et al,  
209 2009). *Trans*-resveratrol was isolated from many sources including the Moraceae *Cudrania*  
210 *javanensis* classified today as *Maclura cochinchinensis* (Murti et al., 1972, Chapman & Hall,  
211 2006). The distylbene artogomezianol **13** is a constituent of *Artocarpus gomezianus* roots and  
212 albolactol **11** was isolated from heartwood of *Morus alba* (Likhitwitayawuid and Sritularak  
213 2001, Ferlinahayati et al., 2008).

214

215 Regarding flavonoids, it has been described that many Moraceae can produce steppogenin  
216 (El-Sohly et al, 1999; Su et al, 2002; Sheu et al., 2005). Katuranin was also isolated from  
217 various biological sources in *Morus* and *Maclura* genera (El-sohly et al., 1999, Lee at al.,  
218 2009) and dihydromorin was isolated from *Morus*, *Artocarpus*, and *Maclura* genera (Shimizy  
219 et al., 1998, El-Sohly et al, 1999, Su et al., 2002).

220

221 It has been hypothesized before that stilbenes are the major types of compounds isolated from  
222 Moraceae and may be useful chemotaxonomic markers (Rowe and Conner, 1979). Also,  
223 Schultz has shown that stilbenoids play an important role in the high natural durability of  
224 *Maclura pomifera* wood (Schultz et al., 1990). Stilbenes are known as fungicide, termicides  
225 and bactericide (Hart and Shrimpton, 1979; Likhitwitayawui and Sritularak, 2001; Javasinghe  
226 et al., 2004), and may also exhibit antioxidant properties (Dani et al., 2008; Iacopini et al.,  
227 2008; Luo et al., 2005). If it is reasonable to believe that stilbenes are responsible for *Bagassa*  
228 *guianensis* heartwood natural durability based on literature precedents, stilbenes can be  
229 considered as a secondary chemotaxonomic marker here indicating that *Bagassa* is related to  
230 *Morus*, *Artocarpus*, and *Maclura* genera. In Weiblen classification, *Artocarpus* belongs to the  
231 Artocarpeae tribe and *Maclura* belongs to the Moreae sensu largo tribe, and both Moreae and  
232 Artocarpeae tribes are rather closely related genetically.

233 The peculiarity of *B. guianensis* in comparison with other Moraceae is the very high  
234 proportion of moracins. In this matter, it can be hypothesized that *Bagassa* genus is closely  
235 related to *Morus* and that moracins are specific to these two genera. These findings are in  
236 agreement with Weiblen genetic-based classification where both *Bagassa* and *Morus* belong  
237 to the Moreae sensu stricto tribe. It should be mentioned that the *Sorocea* genus, which also  
238 belongs to the Moreae s. s. tribe, has been investigated before in the literature and apparently

239 does not contain moracins (see for example Ferrari et al., 2003; Ross et al., 2008). This  
240 observation speaks in favor of a very close relationship between *Bagassa* and *Morus*.

241

### 242 3. Concluding remarks

243 Studies of defensive wood chemicals in *Bagassa guianensis* allowed us to identify large  
244 amount of diversely functionalized stilbenes presumably responsible for wood natural  
245 durability. In addition, it was found based on the presence of moracins that *Bagassa* is very  
246 closely related to *Morus* genus, therefore corroborating Weiblen phylogenetic classification  
247 where *B. guianensis* belongs to the Moreae s. s. tribe rather than to the Artocarpeae tribe.

248

### 249 4. Experimental

#### 250 4.1 General experimental procedure

251 The  $^1\text{H}$  and  $^{13}\text{C}$ -NMR spectra were recorded on a Bruker Avance DRX500 spectrometer ( $^1\text{H}$ -  
252 500.13 MHz) equipped with a 5 mm triple resonance inverse Cryoprobe TXI ( $^1\text{H}$ - $^{13}\text{C}$ - $^{15}\text{N}$ ),  
253 with z gradient. Spectra were recorded with 1.7 mm NMR capillary tube in 40  $\mu\text{L}$  of 99.99%  
254  $\text{CD}_3\text{OD}$  solvent ( $\delta_{1\text{H}}$  3.31 ppm -  $\delta_{13\text{C}}$  49.00 ppm) at 300 K. The  $^1\text{H}$  (500 MHz) and  $^{13}\text{C}$  NMR  
255 (125 MHz) data are reported in ppm downfield from tetramethylsilane. Coupling constants are  
256 in Hz and s stands for singlet, d for doublet, t for triplet, q for quartet, m for multiplet and br  
257 for broad. Hydrogen connectivity (C, CH,  $\text{CH}_2$ ,  $\text{CH}_3$ ) information was obtained from edited  
258 HSQC and/or DEPTQ-135 experiments. Proton and carbon peak assignments were based on  
259 2D NMR analyses (COSY, NOESY, HSQC and HMBC). HREI-MS were performed using a  
260 QStar Elite mass spectrometer (Applied Biosystems SCIEX, Concord, ON, Canada) equipped  
261 with an ESI source operated in the positive ion mode. The capillary voltage was set at 5,500  
262 V, the cone voltage at 20 V and air was used as the nebulizing gas (20 psi). In this hybrid  
263 instrument, ions were measured using an orthogonal acceleration time-of-flight (oa-TOF)

264 mass analyzer. Analyst software version 2.1 was used for instrument control, data acquisition  
265 and data processing. The accurate mass measurements were performed in triplicate with two  
266 internal calibrations. Direct sample introduction was performed at a 5  $\mu\text{L}/\text{min}$  flow rate using  
267 a syringe pump. The UV spectra were recorded on a Perkin-Elmer Lambda 5  
268 spectrophotometer . Optical rotations were measured with a Perkin-Elmer 241 polarimeter  
269 equipped with a sodium lamp (589 nm) and a 1 dm cell. The HPLC separations were  
270 performed on a Supelco Discovery<sup>®</sup> HS PEG column (250  $\times$  21.1 mm, 5  $\mu\text{m}$ ) using a Waters  
271 system equipped with a W600 pump and a W2996 photodiode array absorbance detector. The  
272 samples were injected manually through a Rheodyne injector and the flow rate was 15  
273  $\text{mL}\cdot\text{min}^{-1}$ . Silica gel 60 (35-70  $\mu\text{m}$ ) and analytical TLC plates (Si gel 60 F 254) were  
274 purchased from SDS (France). All other chemicals and solvents were analytical grade and  
275 purchased from SDS (France).

#### 276 *4.2 Plant Material*

277 *Bagassa guianensis* was collected in Régina, French Guiana. A voucher specimen is kept at  
278 the herbarium of Cayenne (CAY-RA13), French Guiana.

#### 279 *4.3 Extraction and isolation*

280 The dried powdered heartwood of *Bagassa guianensis* (140 g) was extracted with ethyl  
281 acetate (3  $\times$  500 mL) at room temperature to give a crude extract which was fractionated first  
282 on a silica gel column chromatography with polarity gradient of hexane/ethyl acetate  
283 mixtures: 80/20; 50/50; 20/80; 0/100. 9 fractions numbered F1 to F9 were obtained. Fractions  
284 F1 to F5 were purified on HPLC with a linear gradient of hexane/isopropanol, by the  
285 following method: 70:30 changing over 2 min to 60:40, then to 40:60 at 10 min and pure  
286 isopropanol at 15 min and remaining as is for 5 min. The fractions F6 and F9 were analyzed  
287 and purified with an isocratic method: 30:70 hexane/isopropanol. These methods allowed us  
288 to isolate moracin M **1** (6.2 mg; w/w 0.019%), moracin N **2** (6.7 mg; w/w 0.020%), 6-*O*-

289 methyl-moracin M **3** (3.3 mg; w/w 0.010%), 6-*O*-methyl-moracin-N **4** (9.1 mg; w/w 0.027%),  
290 moracin Z **5** (5.2 mg; w/w 0.016%), moracin P **6** (1.2 mg; w/w 0.003), *trans*-resveratrol **7**  
291 (12.6 mg; w/w 0.038%), *trans*-oxyresveratrol **8** (112.3 mg; w/w 0.343%), arachidin 2 **9** (5.1  
292 mg; w/w 0.015%), arachidin 4 **10** (0.4 mg; w/w 0.001%), alboctalol **11** (0.5 mg; w/w  
293 0.001%), (-)-epialboctalol **12** (5.4 mg; w/w 0.016%), artogomezianol **13** (12.7 mg; w/w  
294 0.038%), steppogenin **14** (11.5 mg; w/w 0.035%), katuranin **15** (1.5 mg; w/w 0.004%),  
295 dihydromorin **16** (20.4 mg; w/w 0.062%), the  $\beta$ -sitosterol **17** (8.4 mg; w/w 0.025%) and the  
296 resorcinol **18** (1.8 mg; w/w 0.005%). Compounds 1-6, 9-10 and 17-18 were obtained from  
297 the purification of the fractions F1-F5 while compounds 7-8 and 11-16 were isolated from the  
298 fractions F6-F9.

#### 299 4.3.1 6-*O*-Methyl-moracin M (**3**)

300 Yellowish amorphous powder; HR-EIMS  $[M + H]^+$   $m/z$  257.0805  $[M + H]^+$  (calcd 257.0808);  
301  $^1H$  and  $^{13}C$  NMR (500 MHz; CD<sub>3</sub>OD) see table 1.

#### 302 4.3.2 6-*O*-Methyl-moracin N (**4**)

303 Yellowish amorphous powder; HR-EIMS  $[M + H]^+$   $m/z$  325.1437  $[M + H]^+$  (calcd 325.1434);  
304  $^1H$  and  $^{13}C$  NMR (500 MHz; CD<sub>3</sub>OD) see table 1.

#### 305 4.3.3 Moracin Z (**5**)

306 Yellowish amorphous powder; HR-EIMS  $[M + H]^+$   $m/z$  343.1542  $[M + H]^+$  (calcd 343.1540);  
307  $^1H$  and  $^{13}C$  NMR (500 MHz; CD<sub>3</sub>OD) see table 1.

#### 308 4.3.4 Arachidin 4 (**10**)

309 Colorless syrup; HR-EIMS  $[M + H]^+$   $m/z$  315.1592  $[M + H]^+$  (calcd 315.1591);  $^1H$  and  $^{13}C$   
310 NMR (500 MHz; CD<sub>3</sub>OD) see table 2.

#### 311 4.3.5 (-)-Epialboctalol (**12**)

312 Brownish syrup;  $[\alpha]_D^{20}$   $-7.4^\circ$  (c 0.004, CH<sub>3</sub>OH); HR-EIMS  $[M + H]^+$   $m/z$  489.1540  $[M + H]^+$   
313 (calcd 489.1544);  $^1H$  and  $^{13}C$  NMR (500 MHz; CD<sub>3</sub>OD) see table 3.

314 The 3 known moracins M (**1**), N (**2**) and P (**6**) and the other known compounds 7-9, **11**, and  
315 **13-18** were identified by comparison of their physical and spectral data with those reported in  
316 the literature.

317

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322

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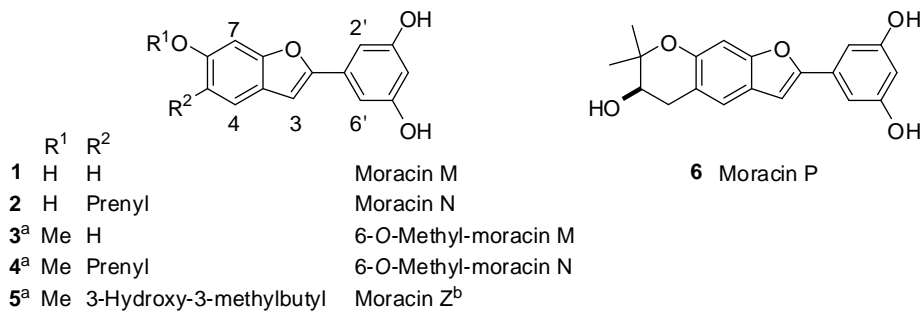
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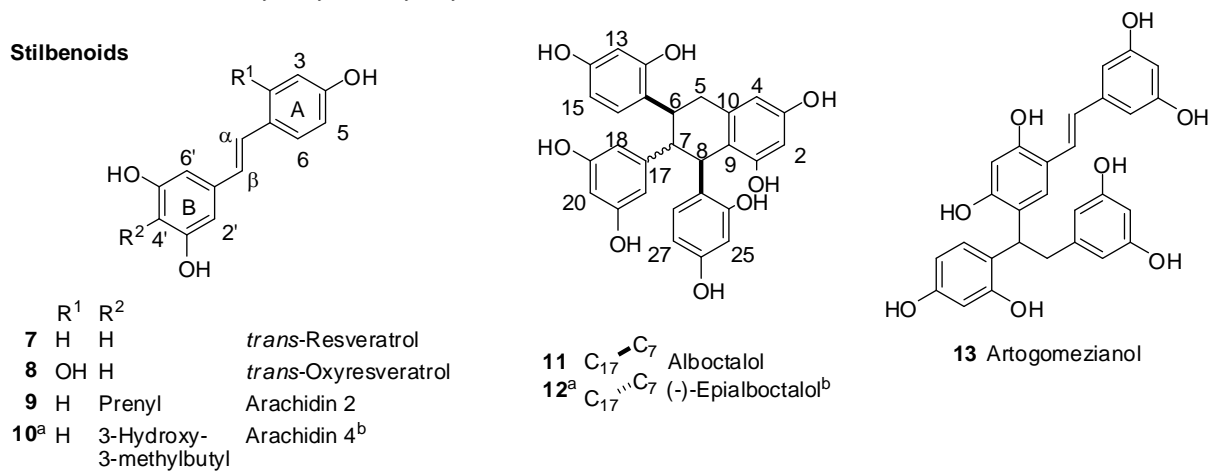
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452 **Figures and legends**

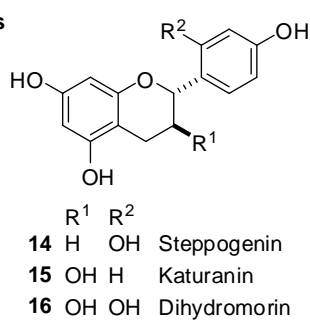
**Moracins**



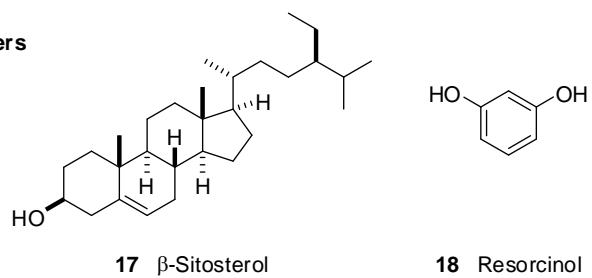
**Stilbenoids**



**Flavanones**



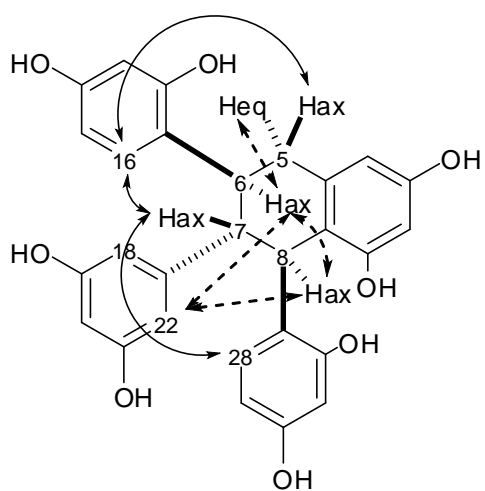
**Others**



453

454 **Figure 1** Compounds **1-18** isolated from *Bagassa guianensis* (Moraceae). (a) New  
 455 compounds; (b) New names.

456



457  
458

459 **Figure 2** Pertinent NOE interactions observed for (-)-epialboctalol (**12**) from NOESY  
460 experiment

461

462

463 **Tables**464 **Table 1**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopic data for moracins **3-5** in  $\text{CD}_3\text{OD}$ 

Atom	<b>3</b>		<b>4</b>		<b>5</b>	
	$\delta_{\text{C}}$	$\delta_{\text{H}}$ ( <i>J</i> in Hz)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ ( <i>J</i> in Hz)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ ( <i>J</i> in Hz)
2	156.5	-	156.2	-	156.2	-
3	96.5	6.95, d (0.6)	102.1	6.90, s	102.0	6.91, d (0.6)
4	121.9	7.43, d (8.5)	121.3	7.25, s	121.6	7.30, s
5	112.9	6.85, dd (8.5, 2.1)	127.5	-	128.6	-
6	159.6	-	157.4	-	157.5	-
7	102.0	7.09, brd (2.0)	94.7	7.09, s	94.7	7.09, s
8	157.0	-	155.7	-	155.8	-
9	123.7	-	123.0	-	123.1	-
1'	133.6	-	133.9	-	133.6	-
2'/6'	104.0	6.78, d (2.1)	103.9	6.77, d (2.1)	103.5	6.77, d (2.1)
3'/5'	159.7	-	159.9	-	160.0	-
4'	103.5	6.25, t (2.1)	103.5	6.24, t (2.1)	103.4	6.25, t (2.1)
1''	-	-	29.7	3.34, brd (7.3)	26.7	2.73, m
2''	-	-	124.3	5.32, tm (7.3)	45.5	1.74, m
3''	-	-	132.7	-	71.5	-
4''	-	-	17.8	1.73 brs	28.9	1.27, s
5''	-	-	26.0	1.74 brs	28.9	1.27, s
MeO	56.0	3.85, s	56.2	3.88 s	56.0	3.89, s

465

466

467 **Table 2**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopic data for stilbenes **9** and **10** in  $\text{CD}_3\text{OD}$ 

Atom	<b>9</b>		<b>10</b>
	$\delta_{\text{C}}$	$\delta_{\text{H}}$ ( <i>J</i> in Hz)	$\delta_{\text{H}}$ ( <i>J</i> in Hz)
1	130.6	-	-
2	128.6	7.31, d (8.6)	7.32, d (8.7)
3	116.5	6.75, d (8.6)	6.75, d (8.7)
4	158.1	-	-
5	116.5	6.75, d (8.6)	6.75, d (8.7)
6	128.6	7.31, d (8.6)	7.32, d (8.7)
$\alpha$	128.3	6.88, d (16.3)	6.90, d (16.5)
$\beta$	127.2	6.74, d (16.3)	6.74, d (16.5)
1'	137.6	-	-
2'	105.7	6.46, s	6.46, s
3'	157.2	-	-
4'	116.0	-	-
5'	157.2	-	-
6'	105.7	6.46, s	6.46, s
1''	23.3	3.28, d (7.1)	2.66, m
2''	124.6	5.23, tm (7.1)	1.68, m
3''	131.4	-	-
4''	26.0	1.62, brs	1.25, s
5''	18.0	1.75, brs	1.25, s

468

469



Atom	<b>12</b>		<b>11</b>
	$\delta_{\text{C}}$	$\delta_{\text{H}}$ ( <i>J</i> in Hz)	$\delta_{\text{H}}$ ( <i>J</i> in Hz)
1	156.7	-	-
2	101.8	6.10, d (2.2)	6.32, d (2.2)
3	156.2	-	-
4	107.3	6.19, d (2.2)	6.32, d (2.2)
5 <sub>ax</sub>	40.1	3.19, brt (13.7)	2.98, dd (16, 14)
5 <sub>eq</sub>		2.72, dd (15.6, 3.0)	2.53, dd (16.3, 4.3)
6 <sub>ax</sub>	40.3	3.51, brtd (11.6, 2.1)	3.75, dt (14, 3.7)
7 <sub>ax</sub>	56.2	3.41, dd (11.3, 8.2)	-
7 <sub>eq</sub>	-	-	3.28, d (3.3)
8 <sub>ax</sub>	44.1	4.42, d (8.2)	4.67, brs
9	119.6	-	-
10	142.2	-	-
11	123.7	-	-
12	156.4	-	-
13	103.3	6.16, d (2.2)	?
14	156.4	6.12, dd (8.4, 2.3)	6.13, dd (8.4, 2.3)
15	107.3	-	-
16	129.7	6.82, d (8.2)	6.44, d (8.2)
17	149.2	-	-
18	108.4	6.01, d (1.9)	5.77, d (1.9)
19	157.9	-	-
20	100.8	5.93, t (2.2)	6.02, t (2.2)
21	157.9	-	-
22	108.4	6.01, d (1.9)	5.77, d (1.9)
23	125.2	-	-
24	156.1	6.76, d (8.2)	6.25, d (8.2)
25	103.2	6.23, dd (8.2, 2.5)	6.04, dd (8.2, 2.5)
26	156.7	-	-
27	108.1	6.19, d (2.2)	6.25, d (2.2)
28	131.2	-	-