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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 β -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

41

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 ^1H and ^{13}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 ^1H spectrum composed of one doublet at δ 6.78 for H-
88 2'/H-6' and a triplet at δ 6.25 for H-4'. These protons are coupled to each other with a 4J
89 coupling of 2.1 Hz. In addition, ^{13}C spectrum indicates the presence of two equivalent aryl
90 hydroxyl groups at δ 159.7. The 3,5-dihydroxyphenyl moiety was linked to C-2 by the
91 observation of a long range ^1H - ^{13}C correlation between H-2'/H-6' and C-2 at δ 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 δ 7.43 ($J = 8.5$ Hz), a doublet of
94 doublet at δ 6.85 ($J = 8.5$ and 2.0 Hz) and a doublet at δ 7.09 ($J = 2.0$ Hz), respectively. On
95 the furan ring H-3 gives a doublet at δ 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 δ 3.85 (3H, s)
98 and the presence of crosspeak at δ 56.2 in the ^1H - ^{13}C HSQC spectra that compound **3** was a
99 moracin M methyl ether. The ^1H - ^{13}C long-range HMBC spectra gave a crosspeak with C-6 at
100 δ 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** ^1H and ^{13}C NMR spectroscopic data for moracins **3-5** in CD_3OD

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 ^1H and ^{13}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 ^1H NMR data of **4** (Table 1) demonstrated
111 the presence a methoxy group on C-6 in the benzofuran ring, with a signal at δ 3.88 (3H, s), a
112 crosspeak at δ 56.2 in the ^1H - ^{13}C HSQC experiment and a crosspeak with C-6 at δ 157.4 in
113 the ^1H - ^{13}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 δ 3.34 to
122 δ 2.73 and the apparition of a methylene H-2'' at δ 1.74 in place of the vinyl proton at δ 5.52;
123 in addition, the two methyl groups H-4'' and H-5'' became equivalent at δ 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 δ 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 δ 7.32
144 ($J = 8.7$ Hz, H-2/H-6) and δ 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 δ 6.90
146 ($J = 16.5$ Hz, H- α) and δ 6.74 ($J = 16.5$ Hz, H- β), and the B ring is symmetrical as well and
147 was characterized by a singlet at δ 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 δ 2.66 instead of δ 3.28 and the apparition of
151 a second methylene H-2'' at δ 1.68. In addition, the two methyl groups H-4'' and H-5''
152 became equivalent at δ 1.25. The chromatography collected quantities was too low to observe
153 heteronuclear ^1H - ^{13}C HSQC / HMBC correlations and direct ^{13}C chemicals shifts by
154 ^{13}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** ^1H and ^{13}C NMR spectroscopic data for stilbenes **9** and **10** in CD_3OD

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 ^1H -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° (c
166 0.004, CH₃OH). It was clear that **12** was a diastereoisomer of **11** with equivalent H-18/H-22
167 protons at δ 6.01 (Table 3). In **11**, H-18/H-22 pair gives a doublet at a strong upfield shift of δ
168 5.77 typical of the π -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_{ax} at δ 3.19 exhibited a broad triplet with large couplings ($J =$
171 13.7 Hz) with the gem H-5_{eq} 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_{eq} signal at δ 2.72. This signal is a doublet of doublet with a large coupling constant $J = 15.6$
174 Hz with H-5_{ax} and a small coupling constant $J = 3.0$ Hz with H-6_{ax}. Signal of H-6_{ax} at δ 3.51
175 is a broad triplet of doublet with two large coupling constants $J = 11.6$ Hz with H-5_{ax} and H-
176 7 and a small coupling constant $J = 2.1$ Hz with H-5_{eq}. This pattern indicates that the 7-aryl
177 group is equatorial and H-7 axial. H-7_{ax} at δ 3.41 exhibited one doublet of doublet with one
178 large coupling constant ($J = 11.3$ Hz) with H-6_{ax} 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_{eq} and H-6_{ax}, H-6_{ax} and H-8_{ax}, H-6_{ax} and H-18, H-8_{ax} and H-22 and between H-5_{ax}
182 and H-16, H-7_{ax} and H-16, H-7_{ax} 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** ¹H and ¹³C NMR spectroscopic data for distilbenes **11** and **12** in CD₃OD

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 β -sitosterol (**17**) (Basnet et al., 2003, Aldrich Library of ^{13}C and ^1H FT NMR spectra,
193 1992) and resorcinol (**18**) (Aldrich Library of ^{13}C and ^1H 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 β -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 ^1H and ^{13}C -NMR spectra were recorded on a Bruker Avance DRX500 spectrometer (^1H -
252 500.13 MHz) equipped with a 5 mm triple resonance inverse Cryoprobe TXI (^1H - ^{13}C - ^{15}N),
253 with z gradient. Spectra were recorded with 1.7 mm NMR capillary tube in 40 μL of 99.99%
254 CD_3OD solvent ($\delta_{1\text{H}}$ 3.31 ppm - $\delta_{13\text{C}}$ 49.00 ppm) at 300 K. The ^1H (500 MHz) and ^{13}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, CH_2 , 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[®] HS PEG column (250 \times 21.1 mm, 5 μm) 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 μm) 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 β -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; CD₃OD) 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; CD₃OD) 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; CD₃OD) 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; CD₃OD) see table 2.

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

312 Brownish syrup; $[\alpha]_D^{20}$ -7.4° (c 0.004, CH₃OH); HR-EIMS $[M + H]^+$ m/z 489.1540 $[M + H]^+$
313 (calcd 489.1544); 1H and ^{13}C NMR (500 MHz; CD₃OD) 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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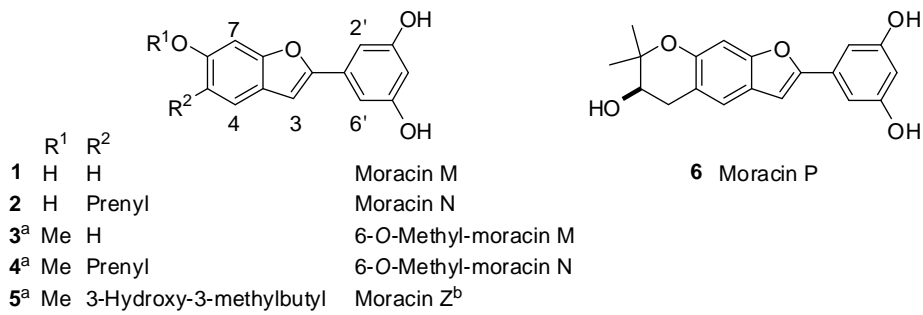
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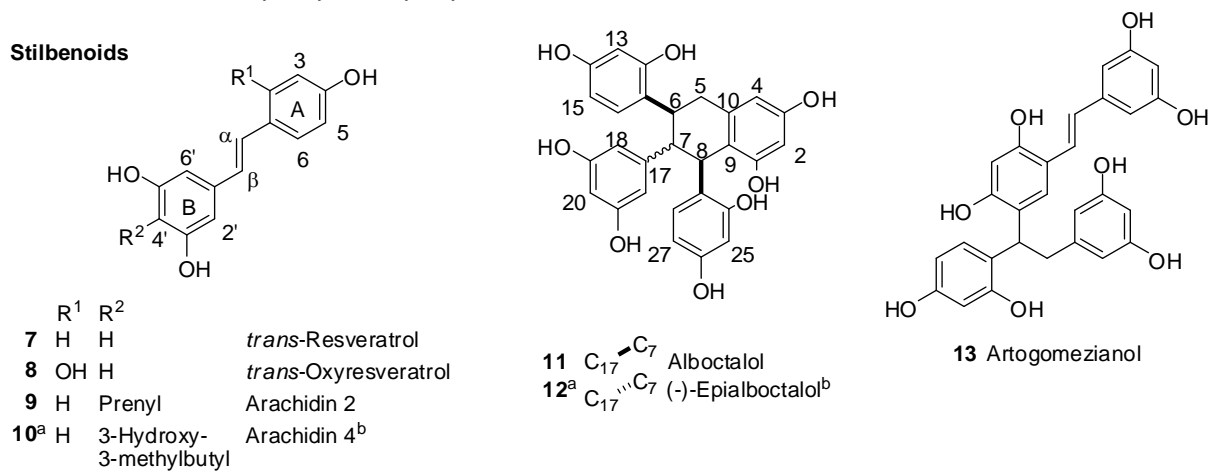
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452 **Figures and legends**

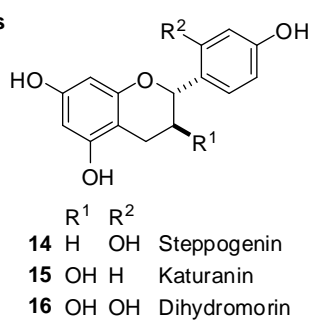
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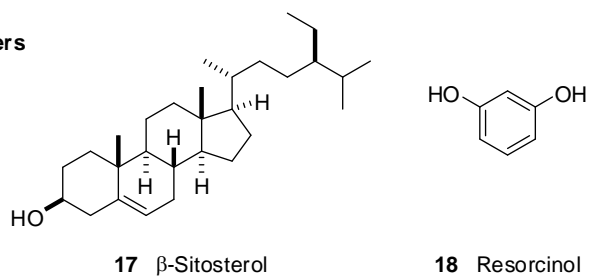
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Flavanones



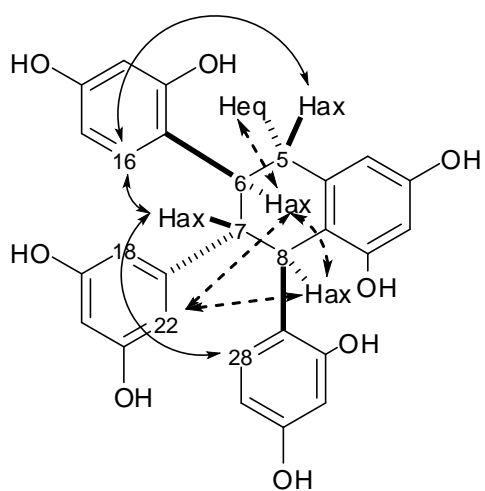
Others



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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** ^1H and ^{13}C NMR spectroscopic data for moracins **3-5** in CD_3OD

Atom	3		4		5	
	δ_{C}	δ_{H} (<i>J</i> in Hz)	δ_{C}	δ_{H} (<i>J</i> in Hz)	δ_{C}	δ_{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** ^1H and ^{13}C NMR spectroscopic data for stilbenes **9** and **10** in CD_3OD

Atom	9		10
	δ_{C}	δ_{H} (<i>J</i> in Hz)	δ_{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)
α	128.3	6.88, d (16.3)	6.90, d (16.5)
β	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	12		11
	δ_{C}	δ_{H} (<i>J</i> in Hz)	δ_{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 _{ax}	40.1	3.19, brt (13.7)	2.98, dd (16, 14)
5 _{eq}		2.72, dd (15.6, 3.0)	2.53, dd (16.3, 4.3)
6 _{ax}	40.3	3.51, brtd (11.6, 2.1)	3.75, dt (14, 3.7)
7 _{ax}	56.2	3.41, dd (11.3, 8.2)	-
7 _{eq}	-	-	3.28, d (3.3)
8 _{ax}	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	-	-