野八角的化学成分

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[摘要] 目的: 研究八角科 Illiciaceae植物野八角 *Illicium simonsii* 茎叶的化学成分。方法: 应用硅胶、Sephadex LH-20, Rp-C_8, Rp-C_{18}等各种色谱技术进行分离纯化, 根据化合物的理化常数和波谱数据鉴定其结构。结果: 从野八角茎叶的 95%乙醇提取物中分离得到 14个化合物, 通过波谱数据和理化常数分别鉴定为 ficusesquilignan A (**1**), 醉鱼草醇 C (**2**), 醉鱼草醇 D (**3**), leptolepisol A (**4**), acernikol (**5**), aviculin (**6**), 山柰酚 (**7**), 槲皮素 (**8**), 槲皮素-3-*O*-α-*L*-吡喃鼠李糖苷 (**9**), 花旗松素-3-*O*-β-*D*-吡喃木糖苷 (**10**), benzyl-2-*O*-β-*D*-glucopyranosyl-2, 6-dihydroxybenzoate (**11**), 2, 4-dihydroxy-3, 6-dimethylmethylbenzoate (**12**), biondinin C (**13**), 莽草酸 (**14**)。结论: 除化合物 **9**, **14**外, 其余化合物均为首次从该植物中分离得到。

[关键词] 八角属; 野八角; 木脂素; 黄酮; 化学成分

野八角 *Illicium simonsii* Maxim. 为八角科 Illiciaceae八角属灌木或小乔木, 产于我国云南、四川、贵州及印度和缅甸等地。八角属的化学成分前人已经作过较系统的研究, 主要含有倍半萜类和苯丙素类化合物[1]。野八角的化学成分主要包括黄酮、倍半萜内酯、二苯基新木脂素、三苯基新木脂素、挥发油等[2-5]。野八角的根、叶、果实均可入药, 煮水可杀虫、灭蚤虱、治胃寒作吐、膀胱疝气及胸前胀痛、疥疮等[6], 果实富含挥发油可作为食用香料, 主要成分为 *L*-柠檬烯, 有止咳、祛痰、镇痛和抑菌的功效[7]。为了更好的开发利用野八角资源, 本研究对干燥野八角茎和叶的 95%乙醇提取物, 依次用石油醚、氯仿、正丁醇萃取后, 从氯仿和正丁醇萃取部分分离得到 14个化合物。分别鉴定为 ficusesquilignan A (**1**), 醉鱼草醇 C (**2**), 醉鱼草醇 D (**3**), leptolepisol A (**4**), acernikol (**5**), aviculin (**6**), 山柰酚 (**7**), 槲皮素 (**8**), 槲皮素-3-*O*-α-*L*-吡喃鼠李糖苷 (**9**), 花旗松素-3-*O*-β-*D*-吡喃木糖苷 (**10**), benzyl-2-*O*-β-*D*-glucopyranosyl-2, 6-dihydroxybenzoate (**11**), 2, 4-dihydroxy-3, 6-dimethylmethylbenzoate (**12**), biondinin C (**13**), 莽草酸 (**14**)。除化合物 **9**, **14**外, 其余化合物均为首次从该植物中分离得到。

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1 仪器与材料

质谱由英国 Micromass产 VG Auto Spec-3000型质谱仪测定; EIMS用 70ev电子轰击源; FAB-MS采用负离子电离源; ^{1}H-NMR, ^{13}C-NMR (DEPT) 采用 Bruker AM-400 (400 MHz) 和 DRX-500 (500 MHz) 核磁共振光谱仪, 以 TMS为内标测定; 柱色谱硅胶 (200~300目) 和硅胶 H及薄层色谱硅胶 GF_{254}均为青岛美高化工厂生产; Sephadex LH-20为 Pharmacia公司产品; Rp-C_8, Rp-C_{18}薄层板和柱层析材料购自 Merck公司; 显色剂为 10% H_2SO_4-乙醇溶液。试验材料采自云南省昆明市, 由中国科学院昆明植物研究所雷立公博士鉴定为八角科八角属植物野八角 *I. simonsii* Maxim., 标本存放于中国科学院昆明植物研究所抗病毒与天然药物化学研究组, 编号为 2006-07-02。

2 提取与分离

干燥野八角茎和叶 7.5 kg, 粉碎后用 95%乙醇回流提取 3次, 每次 2 h, 滤液合并浓缩至浸膏。所得浸膏加水混悬, 依次用石油醚、氯仿、正丁醇萃取, 回收溶剂后得到石油醚部分 (300 g), 氯仿部分 (134 g), 正丁醇部分 (300 g)。其中氯仿部分经硅胶色谱柱 (1 kg 9.5 cm × 40 cm) 分离, 以氯仿-甲醇 (100∶0, 95∶5, 90∶10, 80∶20, 70∶30, 60∶40, 0∶100)梯度洗脱, 每 1 500 mL为 1个流分。经硅胶 TLC检查, 合并相同流分, 得 9个流分 (A~I)。对各个流分经硅胶, Rp-C_8, Rp-C_{18}色谱柱分离, 分别用石油醚-乙酸乙酯, 石油醚-丙酮, 氯仿-甲醇, 氯仿-丙

酮,甲醇-水系统反复洗脱,以 Sephadex LH-20纯化,得到化合物 **1** (15 mg), **2** (11 mg), **3** (10 mg), **4** (8 mg), **5** (13 mg), **7** (9 mg), **8** (20 mg), **13** (20 mg), **14** (50 mg)。正丁醇部分 (300 g)溶解于水后经大孔树脂 D101色谱柱(9 cm × 90 cm),以乙醇-水(0∶100, 20∶80, 40∶60, 80∶20, 100∶0)梯度洗脱,所得各流分经 TLC检查后合并为 4个流分 (J~M)。对各个流分经反复分离纯化得到化合物 **6** (5 mg), **9** (60 mg), **10** (41 mg), **11** (17 mg), **12** (30 mg)。

3 结构鉴定

化合物 **1** 白色胶状物, $[\alpha]_D^{22} = -13.0°$ (*c* 0.17, $CHCl_3$); FAB-MS *m/z* 583 $[M-H]^-$; ^{1}H-NMR (CD_3OD, 400 MHz) δ 6.97 (1H, d, *J* = 1.6 Hz, H-2″), 6.97 (1H, s, H-2′), 6.83 (2H, d, *J* = 8.0 Hz, H-6′, H-6″), 6.80 (2H, d, *J* = 8.0 Hz, H-5′, H-5″), 6.70 (2H, s, H-2, H-6), 4.73 (1H, d, *J* = 3.6 Hz, H-7), 4.22~4.30 (3H m, H-9a, H-9′a, H-9″a), 3.86~3.93 (4H, m, H-9b, H-9′b, H-9″b, H-8″), 3.55~3.59 (1H, m, H-7″), 3.12 (2H, m, H-8, H-8′), 3.87 (6H, OMe × 2), 3.83 (6H, OMe × 2); ^{13}C-NMR (CD_3OD, 100 MHz) δ 139.3 (C-1), 104.6 (C-2, C-6), 154.9 (C-3, C-5), 136.4 (C-4), 87.6 (C-7), 56.2 (C-8), 73.3 (C-9), 134.2 (C-1′), 111.7 (C-2′), 149.5 (C-3′), 147.7 (C-4′), 116.5 (C-5′), 121.1 (C-6′), 87.6 (C-7′), 55.7 (C-8′), 73.2 (C-9′), 134.1 (C-1″), 111.3 (C-2″), 149.0 (C-3″), 147.2 (C-4″), 116.0 (C-5″), 120.5 (C-6″), 74.2 (C-7″), 87.8 (C-8″), 62.1 (C-9″), 57.0 (OMe × 2), 56.8 (OMe), 56.7 (OMe)。与文献 [8]报道的 ficusesquilignan A基本一致。

化合物 **2** 白色胶状物, $[\alpha]_D^{22} = -8.0°$ (*c* 0.08, $CHCl_3$); FAB-MS *m/z* 613 $[M-H]^-$; ^{1}H-NMR (CD_3OD, 400 MHz) δ 6.94 (1H, d, *J* = 2.0 Hz, H-2″), 6.75 (1H, d, *J* = 7.0 Hz, H-5″), 6.70 (1H, d, *J* = 8.0 Hz, H-6″), 6.66 (2H, s, H-2′, H-6′), 6.65 (2H, s, H-2, H-6), 4.73 (1H, d, *J* = 3.6 Hz, H-7), 4.22~4.30 (3H, m, H-9a, H-9′a, H-9″a), 3.86-3.93 (4H, m, H-9b, H-9′b, H-9″b, H-8″), 3.55-3.59 (1H, m, H-7″), 3.12 (2H, m, H-8, H-8′), 3.80 (6H, OMe × 2), 3.30 (6H, OMe × 2); ^{13}C-NMR (CD_3OD, 100 MHz) δ 133.0 (C-1), 104.1 (C-2, C-6), 149.3 (C-3), 136.0 (C-4), 149.3 (C-5), 87.2 (C-7), 55.5 (C-8), 72.9 (C-9), 133.7 (C-1′), 104.4 (C-2′, C-6′), 154.5 (C-3′, C-5′), 139.0 (C-4′), 87.2 (C-7′), 55.4 (C-8′), 72.9 (C-9′), 133.0 (C-1″), 111.3 (C-2″), 149.3 (C-3″), 148.6 (C-4″), 115.6 (C-5″), 120.6 (C-6″), 74.0 (C-7″), 87.6 (C-8″), 61.6 (C-9″), 56.6 (OMe × 2), 56.3 (OMe × 2)。与文献 [9]报道的醉鱼草醇 C数据基本一致。

化合物 **3** 白色胶状物, $[\alpha]_D^{22} = -4.0°$ (*c* 0.10, $CHCl_3$); FAB-MS *m/z* 643 $[M-H]^-$; ^{1}H-NMR (CD_3OD, 500 MHz) δ 6.68 (2H, s, H-2, H-6), 6.67 (2H, s, H-2′, H-6′), 6.66 (2H, s, H-2″, H-6″), 4.91 (1H, m, H-7″), 4.77 (1H, d, *J* = 4.0 Hz, H-7), 4.74 (1H, d, *J* = 4.0 Hz, H-7′), 4.27-4.34 (3H, m, H-9a, H-9′a, H-8″), 3.92 (3H, m, H-9b, H-9′b, H-9″a), 3.87 (6H, OMe × 2), 3.84 (6H, OMe × 2), 3.82 (6H, OMe × 2), 3.63 (1H, m, H-9″b), 3.16 (2H, m, H-8, H-8′); ^{13}C-NMR (CD_3OD, 125 MHz) δ 136.2 (C-1), 104.2 (C-2, C-6), 149.3 (C-3, C-5), 138.8 (C-4), 87.1 (d, C-7), 55.7 (d, C-8), 72.9 (C-9), 136.2 (C-1′), 104.6 (C-2′, C-6′), 154.4 (C-3′, C-5′), 133.0 (C-4′), 87.2 (C-7c), 5514 (C28c), 7219 (C29c), 13310 (C21d), 10513 (C22d, C26d), 14819 (C23d, C25d), 13518 (C24d), 7413 (C27d), 8716 (C28d), 6118 (C29d), 5618 (OMe@3), 5617 (OMe@3)。以上数据与文献 [9]报道对醉鱼草醇 D数据基本一致。

化合物 **4** 白色无定型粉末, $[A]_D^{20} = -518b$ (*c* 0117, MeOH); ESI2MS *m/z* 591 $[M+Cl]^-$; ^{1}H2NMR (CD_3OD, 400MHz) Ð 6199 (1H, s, H22d), 6193 (1H, s, H22c), 6189 (1H, d, *J* = 716 Hz, H26d), 6184 (1H, d, *J* = 814 Hz, H25c), 6181 (1H, d, *J* = 814 Hz, H26c), 6173 (1H, s, H26), 6171 (2H, m, H24, H25d), 5149 (1H, d, *J* = 610 Hz, H22), 4180 (1H, d, *J* = 610 Hz, H27d), 4136 (1H, m, H28d), 3186 (1H, m, H29da), 3184 (3H, s, OMe), 3181 (3H, s, OMe), 3177 (1H, m, H23aa), 3174 (3H, s, OMe), 3175 (1H, m, H23ab), 3156 (1H, m, H29db), 3142 (2H, m, H25c), 3131 (1H, m, H23), 2162 (2H, t, *J* = 712 Hz, H25a),

1181 (2H, m, H-25b); ^{13}C-NMR (CD$_3$OD, 100 MHz) δ: 8816 (C-22), 5515 (C-23), 6510 (C-23a), 11719 (C-24), 12916 (C-24a), 13715 (C-25), 3219 (C-25a), 3518 (C-25b), 6212 (C-25c), 11410 (C-26), 14512 (C-27), 14714 (C-27a), 13710 (C-21c), 11117 (C-22c), 14819 (C-23c), 15119 (C-24c), 11913 (C-25c), 11818 (C-26c), 13410 (C-21d), 11110 (C-22d), 14816 (C-23d), 14619 (C-24d), 11516 (C-25d), 12110 (C-26d), 7410 (C-27d), 8611 (C-28d), 6212 (C-29d), 5617 (-OMe), 5614 (-OMe), 5613 (-OMe)。以上数据与文献[10]报道的 leptolepisol A数据基本一致。

化合物 **5** 白色无定型粉末, $[\alpha]_D^{18}$ = + 910° (*c* 0118, MeOH); ESI-MS *m/z* 585 [M - H]$^-$; ^{1}H-NMR (CD$_3$OD, 400 MHz) δ: 6196 (1H, s, H-22d), 6177 (1H, dd, *J* = 116, 810 Hz, H-26d), 6174 (1H, s, H-26c), 6172 (2H, m, H-24, H-25d), 6171 (2H, s, H-22c, H-26c), 5154 (1H, d, *J* = 610 Hz, H-22), 4190 (1H, d, *J* = 510 Hz, H-27d), 4123 (1H, m, H-28d), 3190 (1H, m, H-29da), 3186 (3H, s, -OMe), 3181 (3H, s, -OMe), 3179 (1H, m, H-23aa), 3178 (6H, s, -OMe@2), 3175 (1H, m, H-23ab), 3158 (1H, m, H-29db), 3156 (2H, m, H-25c), 3145 (1H, m, H-23), 2162 (2H, t, *J* = 712 Hz, H-25a), 1191 (2H, m, H-25b); ^{13}C-NMR (CD$_3$OD, 100 MHz) δ: 8816 (C-22), 5517 (C-23), 6510 (C-23a), 11719 (C-24), 12915 (C-24a), 13712 (C-25), 3219 (C-25a), 3518 (C-25b), 6212 (C-25c), 11411 (C-26), 14512 (C-27), 14714 (C-27a), 13916 (C-21c), 10318 (C-22c, C-26c), 15416 (C-23c, C-25c), 13612 (C-24c), 13317 (C-21d), 11113 (C-22d), 14816 (C-23d), 14618 (C-24d), 11516 (C-25d), 12016 (C-26d), 7410 (C-27d), 8713 (C-28d), 6116 (C-29d), 5617 (-OMe), 5616 (-OMe@2), 5613 (-OMe)。以上数据与文献[11]报道的 acernikol数据基本一致。

化合物 **6** 白色无定型粉末, $[\alpha]_D^{18}$ = + 4011° (*c* 0107, MeOH); ^{1}H-NMR (C$_5$D$_5$N, 500 MHz) δ: 7111 (1H, d, *J* = 810 Hz, H-25c), 6197 (1H, s, H-22c), 6190 (1H, s, H-23), 6189 (1H, s, H-26), 6183 (1H, d, *J* = 810 Hz, H-26c), 5119 (1H, br s, H-21d), 4167 (1H, m, H-29a), 4154 (1H, m, H-29ca), 4138 (1H, m, H-29b), 4130 (1H, m, H-29cb), 4111~4137 (4H, m, H-22d, H-23d, H-24d, H-25d), 3178 (3H, s, -OMe), 3170 (1H, m, H-27c), 3160 (3H, s, -OMe), 3148 (2H, m, H-27), 3114 (1H, m, H-28c), 2141 (1H, m, H-28), 1156 (3H, d, *J* = 510 Hz, H-26d); ^{13}C-NMR (C$_5$D$_5$N, 125 MHz) δ: 2811 (C-21), 13714 (C-22), 11718 (C-23), 14616 (C-24), 14818 (C-25), 11217 (C-26), 3316 (C-27), 3912 (C-28), 6413 (C-29), 13411 (C-21c), 11314 (C-22c), 14711 (C-23c), 14612 (C-24c), 11615 (C-25c), 12218 (C-26c), 4717 (C-27c), 4418 (C-28c), 6710 (C-29c), 10216 (C-21d), 7215 (C-22d), 7311 (C-23d), 7410 (C-24d), 7013 (C-25d), 1816 (C-26d), 5611 (-OMe), 5517 (-OMe)。与文献[12]中报道化合物 avicularin数据一致。

化合物 **7** 黄色无定型粉末, ^{1}H-NMR (CD$_3$OD, 400 MHz) δ: 8109 (2H, d, *J* = 716 Hz, H-22c, H-26c), 6189 (2H, d, *J* = 811 Hz, H-23c, H-25c), 6139 (1H, s, H-26), 6117 (1H, s, H-28); ^{13}C-NMR (CD$_3$OD, 100 MHz) δ: 14810 (C-22), 13516 (C-23), 17715 (C-24), 16015 (C-25), 9913 (C-26), 16515 (C-27), 9415 (C-28), 15812 (C-29), 10415 (C-210), 12318 (C-21c), 13016 (C-22c, C-26c), 11613 (C-23c, C-25c), 16214 (C-24c)。与文献[13]报道的化合物山柰酚数据一致。

化合物 **8** 黄色针状晶体 (甲醇), mp 310~312 ℃, ^{1}H-NMR [(CD$_3$)$_2$CO, 500 MHz] δ: 7165 (1H, s, H-22c), 7152 (1H, d, *J* = 816 Hz, H-26c), 6186 (1H, d, *J* = 816 Hz, H-25c), 6139 (1H, s, H-28), 6117 (1H, s, H-26); ^{13}C-NMR [(CD$_3$)$_2$CO, 125 MHz] δ: 15612 (C-22), 13518 (C-23), 17519 (C-24), 16018 (C-25), 9812 (C-26), 16410 (C-27), 9314 (C-28), 14718 (C-29), 10310 (C-210), 12210 (C-21c), 11516 (d, C-22c), 14619 (C-23c), 14511 (C-24c), 11511 (C-25c), 12010 (C-26c)。与文献[14]报道的槲皮素数据一致。

化合物 **9** 黄色无定型粉末, ^{1}H-NMR (C$_5$D$_5$N, 400 MHz) δ: 7170 (1H, d, *J* = 813 Hz, H-26c), 7168 (1H, s, H-22c), 7129 (1H, d, *J* = 813 Hz, H-25c), 6164 (1H, s, H-28), 6127 (1H, s, H-26), 5108 (1H, br s H-21d), 4166 (1H, m, H-25d), 4128~4142 (3H, m, H-22d, H-23d, H-24d), 1147 (3H, d, *J* = 610 Hz, H-26d); ^{13}C-NMR (C$_5$D$_5$N, 100

MHz) δ: 157.17 (C-22), 136.11 (C-23), 179.11 (C-24), 163.10 (C-25), 99.17 (C-26), 165.18 (C-27), 94.16 (C-28), 158.12 (C-29), 105.15 (C-210), 122.13 (C-21c), 116.15 (C-22c), 147.14 (C-23c), 150.18 (C-24c), 117.11 (C-25c), 122.12 (C-26c), 104.11 (C-21d), 72.12 (C-22d), 72.16 (C-23d), 73.14 (C-24d), 72.11 (C-25d), 18.15 (C-26d)。与文献[15]报道的化合物槲皮素-3-*O*-2,4-二-*O*-乙酰基-α-L-吡喃鼠李糖苷一致。

化合物 **10** 黄色无定型粉末, ^{1}H-NMR (C_5D_5N, 400 MHz) δ: 7.59 (1H, s, H-22c), 7.23 (1H, d, *J* = 8.10 Hz, H-25c), 7.18 (1H, d, *J* = 8.10 Hz, H-26c), 6.41 (1H, s, H-28), 6.34 (1H, s, H-26), 5.83 (1H, d, *J* = 8.10 Hz, H-22), 5.31 (1H, d, *J* = 7.16 Hz, H-23), 4.93 (1H, d, *J* = 6.10 Hz, H-21d), 4.47 (1H, dd, *J* = 12.10, 4.10 Hz, H-25da), 4.20 (1H, m, H-24d), 4.15 (1H, dd, *J* = 7.16, 7.12 Hz, H = 3d), 4.08 (1H, dd, *J* = 7.12, 6.14 Hz, H-22d), 3.69 (1H, m, H-25db); ^{13}C-NMR (C_5D_5N, 100 MHz) δ: 82.18 (C-22), 76.14 (C-23), 194.12 (C-24), 165.13 (C-25), 97.14 (C-26), 169.12 (C-27), 96.14 (C-28), 163.13 (C-29), 102.14 (C-210), 128.11 (C-21c), 116.10 (C-22c), 147.16 (C-23c), 148.12 (C-24c), 116.17 (C-25c), 119.19 (C-26c), 103.14 (C-21d), 73.18 (C-22d), 76.19 (C-23d), 70.19 (C-24d), 66.14 (C-25d)。以上数据与文献[16]报道的化合物花旗松素-3-*O*-β-D-吡喃木糖苷一致。

化合物 **11** 白色胶状物, FAB-MS *m/z* 405 $[M-H]^-$; ^{1}H-NMR (CD_3OD, 500 MHz) δ: 7.48 (2H, d, *J* = 7.15 Hz, H-23c, H-27c), 7.37 (1H, dd, *J* = 7.15, 7.15 Hz, H-25c), 7.30 (2H, dd, *J* = 7.15, 7.15 Hz, H-24c, H-26c), 7.25 (1H, dd, *J* = 8.13, 8.12 Hz, H-25), 6.73 (1H, d, *J* = 8.13 Hz, H-24), 6.58 (1H, d, *J* = 8.12 Hz, H-26), 5.40 (2H, s, H-21c), 4.93 (1H, d, *J* = 7.16 Hz, H-21d), 3.85 (1H, m, H-26da), 3.67 (1H, m, H-26db), 3.30~3.45 (4H, m, H-22d, H-23d, H-24d, H-25d); ^{13}C-NMR (CD_3OD, 125 MHz) δ: 170.10 (C-21), 110.17 (C-22), 159.18 (C-23), 107.18 (C-24), 129.12 (C-25), 111.16 (C-26), 158.12 (C-27), 68.11 (C-21c), 137.13 (C-22c), 129.15 (C-23c, 7c), 129.12 (C-24c, 6c), 134.10 (C-25c), 102.17 (C-21d), 74.19 (C-22d), 78.13 (C-23d), 71.12 (C-24d), 77.19 (C-25d), 62.15 (C-26d); 与文献[16]报道的化合物 benzyl-2,2′,2″,2‴-2-glucopyranosyl-2,2,6,6-tetra-2-hydroxybenzoate数据本一致。

化合物 **12** 白色无定型粉末; ^{1}H-NMR ($CDCl_3$, 500 MHz) δ: 6.20 (1H, s, H-25), 3.91 (3H, s, OMe), 2.46 (3H, s, H-29), 2.09 (3H, s, H-28); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ: 108.15 (C-21), 163.11 (C-22), 105.12 (C-23), 158.10 (C-24), 110.15 (C-25), 140.11 (C-26), 172.16 (C-27), 7.16 (C-28), 24.11 (C-29), 56.15 (OMe)。与文献[17]报道的2,4-二-tert-butyl-5-hydroxy-3,6-dimethyl-2-methylbenzoate数据基本一致。

化合物 **13** 白色无定型粉末, $[\alpha]_D^{20}$ = -22.13° (*c* 0.09, MeOH); EI-MS *m/z* 300 ($M^{+\cdot}$); ^{1}H-NMR ($CDCl_3$, 500 MHz) δ: 7.62 (1H, d, *J* = 15.19 Hz, H-27c), 7.43 (2H, d, *J* = 8.17 Hz, H-22c, H-26c), 6.87 (2H, d, *J* = 8.17 Hz, H-23c, H-25c), 6.33 (1H, d, *J* = 15.19 Hz, H-28c), 5.01 (1H, m, H-22), 2.41 (1H, m, H-23a), 2.03 (1H, m, H-26a), 1.82 (1H, m, H-23b), 1.77 (1H, m, H-25a), 1.71 (1H, m, H-24), 1.38 (1H, m, H-25b), 1.28 (1H, m, H-26b), 0.92 (3H, s, Me-27), 0.89 (3H, s, Me-27), 0.87 (3H, s, Me-21); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ: 48.19 (C-21), 80.13 (C-22), 36.18 (C-23), 44.19 (C-24), 28.10 (C-25), 27.12 (C-26), 47.18 (C-27), 13.16 (Me-21), 18.18 (Me-27), 19.17 (Me-27), 126.18 (C-21c), 130.10 (C-22c, C-26c), 115.19 (C-23c, C-25c), 158.13 (C-24c), 144.16 (C-27c), 115.11 (C-28c), 168.16 (C-29c)。与文献[18]报道的化合物 bisondinin C 数据基本一致。

化合物 **14** 白色无定型粉末, EI-MS *m/z* 174 ($M^{+\cdot}$); ^{1}H-NMR (C_5D_5N, 500 MHz) δ: 7.58 (1H, br s, H-22), 5.13 (1H, br s, H-23), 4.78 (1H, m, H-24), 4.41 (1H, m, H-25), 3.45 (1H, dd, *J* = 17.19, 4.17 Hz, H-26a), 2.96 (1H, dd, *J* = 17.19, 5.15 Hz, H-26b); ^{13}C-NMR (C_5D_5N, 125 MHz) δ: 170.12 (COOH), 131.11 (C-21), 139.13 (C-22), 68.15 (C-23), 73.12 (C-24), 67.14 (C-25), 32.15 (C-26)。以上波谱数据与文献[4]报道的莽草酸一致。

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Studies on chemical constituents of Illicium simonsii

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[Abstract] **Objective** To study the chemical constituents of the *Illicium simonsii*. **Method** The stems and leaves of *I. simonsii* were extracted with 95% EtOH. The EtOH extract was dispersed in H_2O and extracted with petroleum, $CHCl_3$ and BuOH, successively. The $CHCl_3$ and BuOH fractions were isolated and purified by column chromatography on silica gel, Sephadex LH-20, $Rp\text{-}C_8$ and $Rp\text{-}C_{18}$. The isolated compounds were identified on the basis of spectral analyses (including MS, ^{1}H-NMR, ^{13}C-NMR). **Result** Fourteen compounds were isolated from the stems and leaves of *I. simonsii*, which were characterized as ficusesquilignan A (**1**), buddlenol C (**2**), buddlenol D (**3**), leptolepisol A (**4**), acernikol (**5**), aviculin (**6**), kaempferol (**7**), quercetin (**8**), quercetin-3-*O*-*α*-L-rhamnopyranosyl-(1→6)-*β*-D-glucopyranoside (**9**), taxifolin-3-*O*-*β*-D-xylopyranoside (**10**), benzyl-2-*O*-*β*-D-glucopyranosyl-2, 6-dihydroxybenzoate (**11**), 2, 4-dihydroxy-3, 6-dimethyl-methylbenzoate (**12**), biondinin C (**13**), shikimic acid (**14**). **Conclusion** Except compounds **9** and **14**, all the other compounds were obtained from *I. simonsii* for the first time.

[Key words] *Illicium*; *Illicium simonsii*; lignans; flavonoids; chemical constituents

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