Diterpenoids from *Isodon japonicus*

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【ABSTRACT】 **AIM**: To study the chemical constituents of *Isodon japonicus*. **METHOD**: We isolated and elucidated the chemical constituents using chromatographic techniques and spectral analysis. **RESULT** and **CONCLUSION**: Twenty diterpenoids including three new *ent*-kauranoids (**1-3**) and a pair of epimers of new *ent*-abietanoid (**4** and **5**) were isolated and identified. These five new diterpenoids are 7β, 15β, 16β-trihydroxy-6β, 17-diacetoxy-7α, 20-epoxy-*ent*-kaurane (**1**), 16(*S*)-6β, 11α, 17-trihydroxy-6, 20-epoxy- 1α, 7-olide-6, 7-*seco*-*ent*-kaur-15-one (**2**), 11α-dihydroxy-1α-acetoxy-7, 20-olide-6, 7-*seco*-*ent*-kaur-16-en-15-one (**3**), 15(*S*)-3α, 17, 18-trihydroxy-*ent*-abieta-7(8)-en-15, 16-acetonide (**4**), 15(*R*)-3α, 17, 18-trihydroxy-*ent*-abieta- 7(8)-en-15, 16-acetonide (**5**), and named maoyecrystals C-E, G and H, respectively. The ^{13}C NMR data of lasiokaurin (**13**) is reported in this paper for the first time.

【KEY WORDS】 *Isodon japonicus*; Labiatae; *Ent*-kauranoid; *Ent*-abietanoid; Maoyecrystals C-E, G and H
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1 Introduction

In our previous phytochemical investigation on *Isodon japonicus* (Burman f.) Hara which is a folk medicine as anti-bacterial, anti-inflammatory and stomachic agents, even anthelmintic in many places of China and Japan[1], two new *ent*-kauranoids maoyecrystal A and B have been reported[2]. The further search for more bioactive constituents led to the isolation of 20 diterpenoids including three new *ent*-kauranoids maoyecrystal C-E (**1-3**) and a pair of epimers of new *ent*-abietanoid maoyecrystal G and H (**4** and **5**). On the basis of the spectroscopic analysis (including extensive 2D NMR and MS) and comparison with reported data, they were elucidated as 7β, 15β, 16β-trihydroxy-6β, 17-diacetoxy-7α, 20-epoxy-*ent*-kaurane (**1**), 16(*S*)-6β, 11α, 17- trihydroxy-6, 20-epoxy-1α, 7-olide-6, 7-*seco*-*ent*-kaur-15-one (**2**), 11α-dihydroxy-1α-acetoxy-7, 20- olide-6, 7-*seco*-*ent*-kaur-16-en-15-one (**3**), 15(*S*)-3α, 17, 18-trihydroxy-*ent*-abieta-7(8)-en-15, 16- acetonide (**4**), 15(*R*)-3α, 17, 18-trihydroxy-*ent*-abieta-7(8)-en-15, 16-acetonide (**5**), trichorabdal H (**6**), isodonoiol (**7**), isodonal (**8**), rabdosin B (**9**), enmenol (**10**), 1α-*O*-β-*D*-glucopyranoyl-enmenol (**11**), shikokianin (**12**), lasiokaurin (**13**), jiuhuanin A (**14**), epinodosin (**15**), isodocarpin (**16**), rabdosinate (**17**), rabdoepigibberellolide (**18**), wikstroemioidin B (**19**), and lushanrubescensin J (**20**). The ^{13}C NMR data of lasiokaurin (**13**) is reported in this paper for the first time.

2 Experimental

2.1 *Plant Material and Instruments*

The leaves of *I. japonicus* were collected in Tongbai mountains of Henan province in August 2001, and air-dried. The identity of plant material was verified by Prof. Zhong WenLin, and a voucher specimen (20010831-KIB-Lin) is deposited in the Herbarium of the Department of Taxonomy, Kunming Institute of Botany, Chinese Academy of Sciences.

Melting points were measured on an XRC-1 micro melting point apparatus and were uncorrected. Optical rotations were taken on a JASCO DIP-370 digital polarimeter. UV absorptions were obtained on a Shimadzu UV-2401 PC UV-VIS recording spectro-photometer. IR spectra were determined on a Bio-Rad FtS-135 spectrophotometer with KBr pellets. MS were recorded on a VG Auto Spec-3000 spectrometer. 1D- and 2D-NMR spectra were run on Brucker AM-400 and DRX-500 instruments with TMS as internal standard.

2.2 *Extraction and Isolation*

The dried and powdered leaves (10 kg) were extracted with 70% Me_2CO (15000 ml × 3) and filtered.

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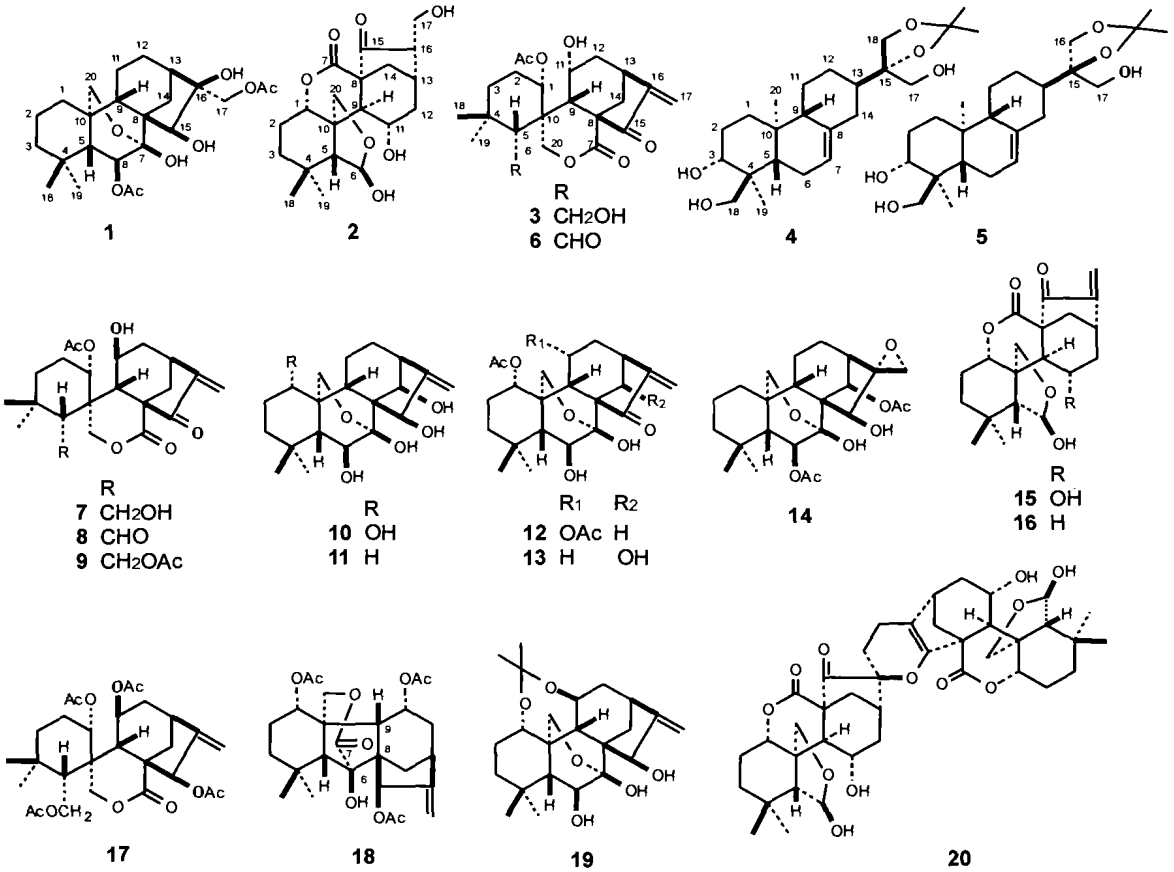
And then, the filtrate was concentrated and extracted with petroleum ether and EtOAc in turn. The EtOAc extract (374 g) was applied to column chromatography over silica gel (100 ~ 200 mesh, 3.0 kg) column eluting with a gradient system of $CHCl_3$-MeOH (1:0, 10:1, 9:1, 8:2, 7:3) to yield fractions I-X on basis of TLC. Fraction I (20 g) afforded **19** (200 mg), **18** (100 mg), **17** (80 mg), **12** (107 mg), and **9** (255 mg) in turns after being chromatographed over silica gel column eluting with CH_2Cl_2/2-propanol (100:1). Fraction II (182 g) was subjected to column chromatography over silica gel eluting with $CHCl_3$-MeOH (50:1) to obtain six fractions (Frs. 1-6). Compounds **8** (724 mg), **6** (112 mg), and **7** (512 mg) were isolated in turns from Fr. 1 by column chromatography over silica gel ($CHCl_3$-MeOH, 50:1). In the same way, compounds **13** (2.1 g), **14** (176 mg), **3** (15 mg), **16** (149 mg), and 1 (26 mg) were yielded in turns from Fr. 2, and compounds **15** (4.2 g), 2 (18 mg) and **20** (35 mg) from Fr. 4. Fraction III gave the mixture of **4** and **5** (7 mg) after repeated column chromatography over silica gel ($CHCl_3$/2-propanol, 30:1). Compounds **10** (29 mg) and **11** (33 mg) were obtained from fraction IV by similar column chromatography over silica gel and recrystallization.



3 Identification

Maoyecrystal C (**1**), a white amorphous powder, $[\alpha]_D^{25.7}$ −14.4° (*c* 0.104, pyridine); $UV\lambda_{max}^{MeOH}$ no absorption; $IR\upsilon_{max}^{KBr}$ cm^{-1} 3518, 3474, 3310, 2923, 2885, 1737, 1438, 1383, 1260, 1059. ^1H NMR (C_5D_5N) δ8.40 (1H, s, OH-7β), 5.65 (1H, d, *J* = 4.8 Hz, H-6α), 5.43 (1H, s, OH-16β), 5.05 (1H, d, *J* = 3.0 Hz, OH-15β), 4.47 (1H, d, *J* = 8.8 Hz, H-17a), 4.38 (1H, d, *J* = 3.0 Hz, H-15α), 4.35 (1H, d, *J* = 8.8 Hz, H-17b), 4.07 (1H, d, *J* = 7.6 Hz, H-20a), 3.97 (1H, d, *J* = 7.6 Hz, H-20b), 2.40 (2H, overlap, H-9β and H-3α), 2.24 (1H, dd, *J* = 3.2, 8.0 Hz, H-13α), 2.17 (3H, s, OAc), 2.02 (1H, dd, *J* = 3.2, 10.4 Hz, H-14α), 1.92 (3H, s, OAc), 1.89 (1H, d, *J* = 10.4 Hz, H-14β), 1.60 (1H, d, *J* = 4.8 Hz, H-5β), 1.56 (1H, m, H-12α), 1.37 (1H, m, H-11α), 1.34-1.22 (5H, overlap, H-1β, H_2-2, H-3β and H-12β), 1.18 (1H, m, H-11β), 1.08 (3H, s, Me-19), 0.95 (1H, m, H-1α) and 0.86 (3H, s, Me-18). EI-MS (70eV) *m/z* (rel. int. %) 452 $[M]^+$ (2), 434 (4), 410 (4), 392 (24), 374 (13), 332 (24), 319 (42), 260 (28), 180 (50), 151 (100). **1** was determined to possess a molecular formula $C_{24}H_{36}O_8$ (calcd 452.2410) by the molecular ion peak at *m/z* 452.2416 in the HREIMS spectrum. In the ^{13}C NMR spectrum (Tab 1) of **1**, besides four carbon

signals for two acetoxy groups, there were 20 signals for the skeleton of an 7,20-epoxy-*ent*-kaurane deduced from the characteristic signals of two methyls (C-18 and 19), three methines (C-5,9 and 13), three quaternary carbons (C-8,10 and 4), an oxymethylene (C-20) and a hemiketal group (C-7). Comparison of the ^{1}H and ^{13}C NMR data of **1** with those of maoyerabdosin (a known 7,20-epoxy-*ent*-kauranoid also isolated from this plant[3]) suggested **1** as 1-dehydroxy-maoyerabdosin, which was supported by the HMBC and ROESY spectral evidences (Fig 1). The 7, 20-epoxy group was confirmed by the HMBC correlations of H_2-20 with C-7. These two acetoxy groups were linked to C-6 and C-17 by the HMBC correlations of H-6 and H_2-17 with their two carbonyl carbons, respectively. The OAc-6β, OH-15β and OH-16β were determined by the key ROESY correlations of H-6α/Me-19, H-15α/H-14β and H-13α/H_2-17. Therefore, compound **1** was elucidated as 7β, 15β, 16β-trihydroxy-6β, 17-diacetoxy-7α, 20-epoxy-*ent*-kaur-15-one.

Tab 1 ^{13}**CNMR data of compounds 1-5(C_5D_5N, δ)**

	1	2	3	4 *and* 5	13
1	30.2(*t*)	77.1(*d*)	79.1(*d*)	38.1(*t*)	75.9(*d*)
2	18.3(*t*)	23.9(*t*)	24.2(*t*)	27.8(*t*)	25.6(*t*)
3	40.6(*t*)	37.0(*t*)	40.2(*t*)	73.6(*d*)	38.5(*t*)
4	33.1(*s*)	31.6(*s*)	33.9(*s*)	42.9(*s*)	33.9(*s*)
5	55.3(*d*)	54.0(*d*)	53.5(*d*)	43.0(*d*)	60.7(*d*)
6	74.5(*d*)	102.2(*d*)	59.2(*t*)	23.4(*t*)	74.5(*d*)
7	95.1(*s*)	170.2(*s*)	171.5(*s*)	120.6(*d*)	98.3(*s*)
8	52.4(*s*)	57.8(*s*)	58.7(*s*)	137.3(*s*)	62.5(*s*)
9	41.5(*d*)	53.0(*d*)	46.1(*d*)	52.9,52.8(*d*)*	52.7(*d*)
10	35.5(*s*)	50.8(*s*)	45.5(*s*)	35.3(*s*)	40.1(*s*)
11	14.5(*t*)	63.0(*d*)	64.4(*d*)	25.8(*t*)	18.4(*t*)
12	19.0(*t*)	32.7(*t*)	42.4(*t*)	27.3(*t*)	30.5(*t*)
13	36.1(*d*)	31.1(*d*)	35.2(*d*)	42.5,42.4(*d*)*	43.8(*d*)
14	25.0(*t*)	34.8(*t*)	30.0(*t*)	36.4(*t*)	73.4(*d*)
15	71.5(*d*)	213.0(*s*)	202.6(*s*)	85.9,85.8(*s*)*	209.1(*s*)
16	76.9(*s*)	59.0(*d*)	151.4(*s*)	68.9,68.8(*t*)*	152.9(*s*)
17	70.5(*t*)	58.4(*t*)	117.8(*t*)	64.3,64.2(*t*)*	119.6(*t*)
18	31.7(*q*)	32.9(*q*)	33.7(*q*)	67.6(*t*)	33.9(*q*)
19	20.2(*q*)	23.1(*q*)	23.7(*q*)	13.0(*q*)	21.9(*q*)
20	65.1(*t*)	73.8(*t*)	68.7(*t*)	15.9(*q*)	63.5(*t*)
OAc	170.5(*s*)		170.2(*s*)		170.1(*s*)
	169.3(*s*)		21.6(*q*)		21.4(*q*)
	21.5(*q*)				
	20.9(*q*)				
Isopropyliden				109.3(*s*)	
				27.6(*q*)	
				27.1(*q*)	

* *signals exchangeable*

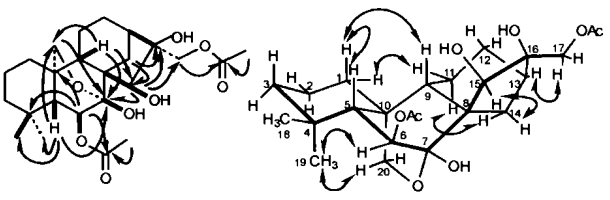


Fig 1 Key HMBC and ROESY correlations of 1

Maoyecrystal D (**2**), colorless needles; mp (250℃, $[\alpha]_D^{20}$ -120.0° (*c* 0.800, MeOH); $UV\lambda_{max}^{MeOH}$ 205 nm; $IR\upsilon_{max}^{KBr}$ cm^{-1} 3520, 3238, 2966, 2888, 1755, 1712, 1457, 1338, 1294, 1266, 1252, 1055, 979. ^{1}H NMR (C_5D_5N) δ 9.06 (1H, s, OH-6β), 7.41 (1H, s, OH-11α), 6.59 (1H, s, OH-7β), 5.73 (1H, s, H-6α), 4.91 (1H, dd, *J* = 6.0, 10.4 Hz, H-1β), 4.53 (1H, m, H-11β), 4.41 (1H, d, *J* = 11.0 Hz, H-20a), 4.27 (1H, d, *J* = 11.0 Hz, H-20b), 4.29 (1H, brs, H-17a), 4.10 (1H, br s, H-17b), 3.16 (1H, s, H-5β), 3.08 (1H, m, H-16β), 2.99 (1H, m, H-13α), 2.88 (1H, overlap, H-9β), 2.83 (1H, overlap, H-14β), 2.66 (1H, m, H-12β), 2.09 (1H, m, H-12α), 2.03 (1H, m, H-14α), 1.90-1.84 (2H, overlap, H_2-2), 1.37-1.26 (2H, overlap, H_2-3), 0.96 (6H, s, Me-18 and Me-19). EI-MS (70eV) *m/z* (rel. int. %) 380 $[M]^+$ (1), 362 (13), 344 (100), 332 (6), 314 (10), 298 (6), 286 (8), 149 (100). **2** was determined to possess a molecular formula $C_{20}H_{28}O_7$ by the $[M + Na]^+$ peak at *m/z* 403.1731 (calcd 403.1732) in the HRESIMS spectrum. In the ^{13}CNMR spectrum (Tab 1) of **2**, there were 20 signals for the skeleton of 6-hydroxy-1, 7-olide-6, 20- epoxy-6, 7-seco-*ent*-kaurane suggested by the characteristic signals of two methyls (C-18 and 19), three methines (C-5,9 and 13), three quaternary carbons (C-8, 10 and 4), an oxymethylene (C-20), a hemiacetal carbon (C-6), and a significant downfield oxymethine (C-1). Comparison of the ^{1}H and ^{13}CNMR data of **2** with those of epinodosin[4] (**15**, one of major constituents of this plant) indicated that **2** was very identical with **15** except for only one difference at C-16 that the exomethylene group at C-16 of **15** was replaced by a hydroxymethyl group in **2**, which was approved by the HMBC and ROESY spectral evidences (Fig 2). The 16α-CH_2OH was determined by the HMBC correlations of H_2-17 with C-15 and C-13, and the NOEs of H-16β/H-13β and H_2-17/12α, which was also confirmed by the obvious upshift of C-12 at δ 32.7 caused by the steric compress effect between H_2-17 and H-12α[5]. The α-orientation of H-6 was proved by the NOE of H-6/Me-19. Similarly, H-1β and H-11β were confirmed by the NOEs among H-1, H-11 and H-14β. Thus, compound **2** was assigned as 16(*S*)-6β, 11α, 17-trihydroxy-6, 20-epoxy-1α, 7-olide-6, 7-*seco*-*ent*-kaur-15-one.

Maoyecrystal E (**3**), a white amorphous powder, $[\alpha]_D^{27.9}$ + 41.5° (*c* 0.217, pyridine); $UV\lambda_{max}^{MeOH}$ 231 nm; $IR\upsilon_{max}^{KBr}$ cm^{-1} 3400, 2955, 1742, 1709, 1642, 1370, 1275, 1128, 1052. ^{1}H NMR (C_5D_5N) δ 6.80 (1H, d, *J* = 6.2 Hz, OH-11α), 6.48 (1H, s, OH-6), 5.99 (1H, s, H-17a), 5.74 (1H, dd, *J* = 3.0, 12.0 Hz, H-1β), 5.37 (1H, s, H-17b), 5.19 (1H, d, *J* = 12.0 Hz, H-20a), 5.02 (1H, overlapped by

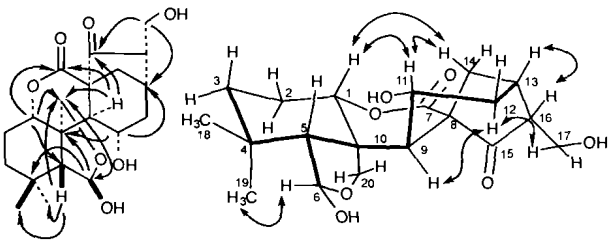


Fig 2 Key HMBC and ROESY correlations of 2

H_2O peak, H-11β), 4.89(1H, d, J = 12.0 Hz, H-20b), 3.85(2H, overlap, H_2-6), 3.54(1H, d, J = 12.0 Hz, H-14α), 3.33(1H, d, J = 3.0 Hz, H-9β), 3.16(1H, dd, J = 4.8, 9.2 Hz, H-13α), 2.65(1H, dd, J = 4.8, 12.0 Hz, H-14β), 2.47(1H, dd, J = 9.2, 14.4 Hz, H-12β), 2.19(3H, s, OAc), 2.15(1H, m, H-2α), 1.98-1.92(3H, overlap, H-5β, H-2β and H-12α), 1.37-1.30(2H, overlap, H_2-3), 0.88(3H, s, Me-18), 0.76(3H, s, Me-19). EI-MS(70eV) m/z (rel. int. %) 406 $[M]^+$ (61), 388(45), 364(6), 346(18), 237(36), 219(36), 121(66), 55(100). **3** was determined to possess a molecular formula $C_{22}H_{30}O_7$ (calcd 406.1992) by the molecular ion peak at m/z 406.2007 in the HREIMS. Similar to **1** and **2**, compound **3** was also regarded as a diterpenoid with a kaurane skeleton. Further analysis of the characteristic lactonic carbonyl signal at δ_C 171.5(s) due to C-7 and two noticeable oxymethylenes [one emerged at δ_C 59.2(t) and δ_H 3.85(2H, overlap) assignable to C-6/H_2-6, and the other resonated at δ_C 68.7(t) and δ_H 5.19/4.89(d, J = 12.0 Hz) attributable to C-20/H_2-20], along with the consideration on the structures of the diterpenoids also isolated from this plant, indicated **3** as a 6-hydroxy-7, 20-olide-6, 7-seco-*ent*-kauranoid. Comparison of the ^1H and ^{13}C NMR data of **3** with those of isodonoiol[3] (**7**, a known analogue also isolated this time) not only confirmed the above deduction, but also established **3** as 11-epiisodonoiol, which was approved by the key ROESY correlations of H-11 with H-1β and H-9β showing the presence of OH-11α. Then, compound **3** could be regarded as 6, 11α-dihydroxy-1α-acetoxy-7, 20-olide-6, 7-*seco*-*ent*-kaur-16-en-15-one, which structure was very consistent with the relational correlations (Fig 3) in the HMBC and ROESY spectra of **3**.

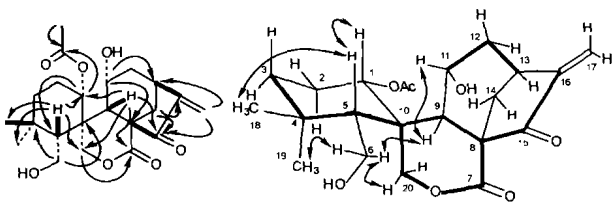


Fig 3 Key HMBC and ROESY correlations of 3

The mixture of *Maoyecrystals G* and *H* (**4** and **5**), a white amorphous powder, $[\alpha]_D^{27.9}$ + 29.4° (*c* 0.494, MeOH); UVλ_{max}^{MeOH} 204 nm; IRυ_{max}^{KBr} cm^{-1} 3434, 2984, 2935, 2889, 1699, 1558, 1380, 1054. ^1H NMR(C_5D_5N) δ 5.40 and 5.36 (each 1H, br s, H-7), 4.22(2H, overlap, H-16a), 4.20 (2H, overlap, H-3β), 4.10-4.06 (4H, overlap, H-16b and H-18a), 3.96-3.92(4H, overlap, H_2-17), 3.64(2H, d, J = 10.4 Hz, H-18b), 2.60 and 2.56 (each 1H, d, J = 14.8 Hz, H-14α), 1.88(4H, overlap, H-5β and H-13α), 1.50 (12H, br s, Me of the isopropyliden group), 1.12(6H, br s, Me-19), 0.91 and 0.89(each 3H, s, Me-18). EI-MS(70eV) m/z (rel. int. %) 394 $[M]^+$ (16), 379(40), 363(58), 336(20), 321(100), 218(83), 305(31), 287(40), 269(46), 262(74), 244(52), 229 (39), 145 (69), 131 (100). They were determined to possess the molecular formula $C_{23}H_{38}O_5$ (calcd 394.2697) by the molecular ion peak at m/z 394.9760 in the HREIMS. In the ^1H and ^{13}C NMR spectra, besides the signals of the isopropyliden group, there were signals more than those of a diterpenoid. Especially in the ^{13}C NMR spectrum, there were five extra signals being in pairs with another five ones of the rest 20 signals which included three methyls (C-18, 19 and 20), three methines (C-5, 9 and 13) and two quaternary carbons (C-4 and 10), suggesting a tricyclic diterpene skeleton. Comparison of these ^1H and ^{13}C NMR data with those of laxiflorin O[6] (an *ent*-abietanoid isolated from *I. eriocalyx* var. *laxiflora*) indicated that these were a pair of *ent*-abietane epimers differed from laxiflorin O only at C-15 and C-16, which was confirmed by the HMBCs of H-3 with C-18 and C-19, H-7 with C-5 and C-9, H_2-17 with C-13, and the relational NOEs (Fig 4) in the ROESY spectrum. An iospropyliden group was linked at C-15 and

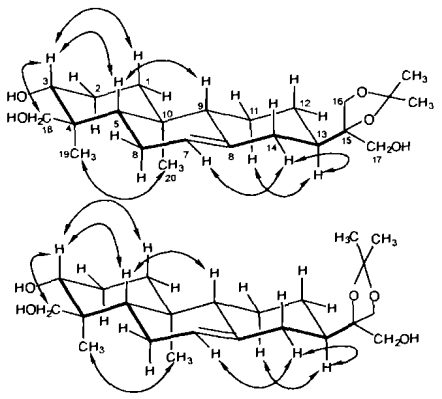


Fig 4 Key ROESY correlations of 4

C-16 of **4** and **5**, which was proved by the HMBCs of H-13 with C-15, C-16, and H_2-16, H_2-17 with C-13. Careful assignment of these ^{13}C NMR data with the aid of 2D-NMR spectroscopic methods achieved that those above-mentioned five pairs of carbon signals were assigned to C-9, C-13, C-15, C-16 and C-17, and the signals for the

other carbons of this pair of epimers were completely identical, indicating that compounds **4** and **5** were 15-epimers as displayed in Fig 4. These relational signals appearing in close pairs with a proportion of 1∶1 could exchange for **4** and **5**.

These 15 known diterpneoids were determined by comparison of their NMR data with reference data as trichorabdal H[4] (**6**), isodonoiol[3] (**7**), isodonal[3] (**8**), rabdosin B[4] (**9**), enmenol[7] (**10**), 1α-*O*-β-*D*-glucopyranoyl-enmenol[7] (**11**), shikokianin[4] (**12**), lasiokaurin[4] (**13**), jiuhuanin A[4] (**14**), epinodosin[4] (**15**), isodocarpin[4] (**16**), rabdosinate[4] (**17**), rabdoepigibberellolide[4] (**18**), wikstroemioidin B[4] (**19**), and lushanrubescensin J[8] (**20**). Accordingly, the ^{13}C NMR data of lasiokaurin (**13**) was assigned as present in Table 1 for the first time.

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毛叶香茶菜中的二萜化合物

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【摘　要】 **目的**: 对河南产毛叶香茶菜化学成分进行研究。**方法**: 运用各种色谱技术和波谱分析对其化学成分进行分离鉴定。**结果**: 分离鉴定了 20 个二萜化合物。**结论**: 化合物 1-3 为三个新的对映-贝壳杉烷二萜类化合物, 结构分别为 7β, 15β, 16β-三羟基-6β, 17β-二乙酰氧基-7α, 20-环氧-对映-贝壳杉烷(**1**)、16(*S*)-6β, 11α, 17β-三羟基-6, 20-环氧-1α, 7β-内酯-6, 7-断裂-对映-贝壳杉-15 酮(**2**)和 6α, 11α-二羟基-1α-乙酰氧基-7, 20-内酯-6, 7-断裂-对映-贝壳杉-16-烯-15-酮(**3**), 依次命名为毛叶香茶菜丙素、丁素和戊素; 化合物 **4** 和 **5** 为一对新化合物, 其结构为 3α, 15α, 1β6, 17β, 18β-五羟基-对映-松香-7(8)-烯的丙酮化物, 其丙酮化缩合部分互为对映体, 分别命名为毛叶香茶菜庚素(**4**)和辛素(**5**)。

【关键词】 毛叶香茶菜; 唇形科; 对映-贝壳杉烷; 对映-松香烷; 毛叶香茶菜丙、丁、戊、庚和辛素