SHORT REPORT

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Lignoids Isolated from *Nectandra turbacensis* (Kunth) Nees (Lauraceae)

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Abstract: A new 7,8-secolignan, as well as seven known compounds; were isolated from *Nectandra turbacensis* (Kunth) Nees (Lauraceae) (leaves and root bark). These compounds were identified as, one secolignan, turbacenlignan A (**1**); four diaryldimethylbutane lignans: *meso*-monomethyl dihydroguaiaretic acid (**2**), *threo*-dihydroguaiaretic acid (**3**), schineolignin B (**4**), and austrobailignan-5 (**5**); and three 7,7'-epoxylignans: henricine (**6**) and the identifiable mixture of veraguensin (**7**) and galgravin (**8**). Compounds **1-8**, were first isolated from *Nectandra turbacensis* (Kunth) Nees (Lauraceae) (leaves and root bark) and compounds **1, 6-8**, were isolated for the first time from *Nectandra* genus.

Keywords: *Nectandra turbacensis*; Lauraceae; Secolignan; Epoxylignans; Diaryldimethylbutane lignans; Chemotaxonomy.

1. Plant Source

The species *Nectandra turbacensis* (family: Lauraceae), known as "yellow Laurel", is distributed in some Latin American countries, especially Bolivia, Brazil, Mexico, Costa Rica, Cuba, Honduras, Jamaica, Peru, Puerto Rico, Colombia and Venezuela [1]. No ethnobotanical uses nor biological activity have been reported for this species, however, other species of the genus have ethnobotanical uses, such as antifungal, antidiarrheal, analgesic and antirheumatic [2, 3], anti-inflammatory, febrifuge, hypotensive, and energetic [4], among others. About the reported biological activity of the genus, antitumor activity (*Nectandra rigida*), antimalarial activity (*N. cuspidate* and *N. salicifolia*), activity against cardiovascular disease (*N. salicifolia*) [2] and antiplasmodial activity (*N. salicifolia*) [5]assays have been reported. In this paper, a 7,8-Secolignan, named turbacenlignan A (**1**) as well as seven known compounds (lignans) [(**2**), (**3**), (**4**), (**5**), (**6**), (**7**), and (**8**)]; were isolated from *Nectandra c turbacensis* (Kunth) Nees (Lauraceae) (leaves and root bark).

The plant material used for the phytochemical study is the *Nectandra turbacensis* species leave, collected in the city of Santa Marta (Magdalena, Colombia), in the village of Bonda (+11° 14'13.20") in March 2010; assisted by botanist Edwino Carbonó of the University of Magdalena (Colombia) and determined by Adolfo Jara Muñoz biologist at the National University of Colombia. *A voucher* specimen (COL-556717) was deposited in the herbarium of our institute [Colombian National Herbarium of the Institute of Natural Sciences].

2. Previous Studies

2,6-diaryl-3,7-dioxabicyclo[3.3.0]octanes lignans (furofuran) such as: (+)-sesamin, (+)-demethoxyexcelsin, (+)-piperitol, (+)-methoxypiperitol and (1*R*,2*S*,5*R*)-2-(3'-methoxy-4',5'-

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methylenedioxyphenyl)-3,7-dioxa-6-oxobicyclo[3.3.0]octane, have been reported from *N. turbacensis* [6].

3. Present Study

Dried and powdered leaves and root bark of *Nectandra turbacensis* were macerated (independently) with 96% ethanol, then concentrated under vaccum using a rotary evaporator at a temperature of 40°C, yielding 80 g of extract (root bark) and 90 g of extract (leaves); which were fractionated by flash column chromatography using hexane-ethyl acetate gradient and then washed with methanol, obtaining 20 fractions (in both cases) marked from *NtrbEtOH-1* to *NtrbEtOH-20* (root bark) and *NtlEtOH-1* to *NtlEtOH-20* (leaves). From *NtrbEtOH-2* (300 mg) fraction the secolignan **1** (25 mg) and compound **2** (30 mg), were isolated; from fraction *NtrbEtOH-3* (200 mg), compound **3** (24 mg) was obtained [in both cases using a mixture of hexane: acetone (9:1 to 7:3)], from fraction *NtrbEtOH-5* (180 mg), compound **6** (27 mg) was isolated using a mixture of toluene: ethyl acetate (9:1 to 85:15); while fraction *NtrbEtOH-6* (170 mg) gave the identifiable mixture of compounds **7** and **8** (70 mg of mixture, 90/10%, **7**/**8**) using the same solvent mixture. From NtlEtOH-2 (260 mg) fraction, compound **4**, was isolated; whereas, from fraction *NtlEtOH-3* (180 mg), compound **5** [in both cases using a mixture of hexane: acetone (9:1 to 7:3)]. A *Sephadex LH-20* column was used to further purify (in MeOH) the compounds.

Compound **1** was obtained as a colorless oil with a positive specific rotation, $[\alpha]_D^{24}$ +33 (c= 0.5, $CHCl_3$), and its molecular formula was assigned as $C_{22}H_{24}O_8$ based on the ^{13}C NMR and ^1H NMR spectroscopic data and quantitative elemental analysis. The IR spectrum exhibited absorption bands from phenyl (1594 cm^{-1}) and carbonyl (1707 cm^{-1}) moieties. Previous studies have reported the presence of this type of secondary metabolites (7,8-secolignans) isolated from species *Schisandra* (family Schisandraceae), such as marphenol B [7], schisandlignans A–C [8] and neglectahenols A-D [9], which showed similar shift values to the compound **1**; however, the compounds are distinguished by the presence of a hydroxyl group in the structure of marphenol B, which is replaced by a methoxy group in compound **1**.The ^1H NMR data for **1** (Table 1) showed signals for 24 hydrogens, and the ^{13}C NMR spectrum (Table 1) and DEPT experiments revealed the presence of 22 carbon, corresponding to two substituted benzene systems (3,4,5-trimethoxyphenyl and piperonyl), two carbonyl carbons (δ_C 164.7, C-7; 209.8, C-8), two methine carbons [δ_H 5.92 (1H, d, *J*= 10.1 Hz, H-7'); 3.17 (1H, dq, *J*= 10.1, 7.1 Hz, H-8'); δ_C 78.4, 52.5], and two methyl groups [δ_H 2.24 (3H, s, H-9), 0.97 (3H, d, *J*=7.1 Hz, H- 9'); δ_C 28.8, 13.9], three methoxyl groups [δ_H 3.86 (6H, s, OMe-3' and OMe-5'), 3.81 (3H, s, OMe-4'); δ_C 56.3, 60.9]. In the $^1H-^1H$ COSY spectrum, the presence of a −CH(H-7')−CH(H-8')−CH_3(H-9')− unit was evident (Figure 2), which were in accordance with the molecular formula $C_{22}H_{24}O_8$ and structural formula suggested (Figure 1). In the HMBC spectrum of **1**, H-9 [δ_H 2.24 (3H, s)] was correlated to C-8 (δ_C 209.8) and C-8' (δ_C 52.5), which indicated that a methyl ketone moiety (δ_C 209.8 and 28.8) is linked to C-8'. Additionally, H-7' [δ_H 5.91 (1H, d, *J* = 10.1 Hz)] was correlated to C-1' (δ_C 133.9), C-2' (δ_C 104.4), C-6' (δ_C 104.4), and C-7 (δ_C 164.7) in the HMBC spectrum, which indicated the linkage of C-7' to the 3,4,5-trimethoxyphenyl unit and the linkage of C-7 to the 3,4-methylenedioxyphenyl unit via an ester oxygen (Figure 2).

The relative configuration at C-7' and C-8' was determined as *threo* due to the coupling constant between H-7' [δ_H 5.92(d, *J* = 10.1 Hz, 1H)] and H-8' [δ_H 3.17 (dq, *J* = 10.1, 7.1 Hz, 1H)] which is also the same as *rel*-(7'*R*,8'*S*)-3,4-methylenedioxy-3',4'-dimethoxy-7,8-seco-7,7'-epoxylignan-7,8-dione [7, 8, 10]. The above information implied that **1** should be a 7,8-secolignan [8, 9]. Thus, the structure of **1** was established as: *=rel-(7'S,8'R)-3',4',5'-trimethoxy-3,4-methylenedioxy-7,8-seco-7,7'-epoxylignan-7,8-dione*; and named as turbacenlignan A, **1**.

Turbacenlignan A (*=rel-(7'S,8'R)-3',4',5'-trimethoxy-3,4-methylenedioxy-7,8-seco-7,7'-epoxylignan-7,8-dione*; **1**). White amorphous powder. $[\alpha]_D^{24}$ +33 (c=0.5,$CHCl_3$). IR (KBr): 3419, 3091, 2930, 2852, 1707, 1594, 1507, 1489, 1444, 1368, 1276, 1126, 1070, 824. ^1H- and ^{13}C-NMR (Table 1).

The compounds **2** [11]; **3** (24 mg) [12, 13]; **4** [18]; **5** [19, 20]; **6** [14]; **7** and **8** (70 mg of mixture, 90/10%, **7**/**8**) [15-17]; whose chemical structures (Figure 1) were established by analyses of spectroscopic data (1D and 2D NMR), and by comparison with spectroscopic data in the literature; they were also isolated. The presence of some of these compounds [(**3**, *m/z*=330.2); (**5**, *m/z*=326.2); and (**8,** *m/z*=372.0)] in the ethanol extract was initially determined by GC-MS.

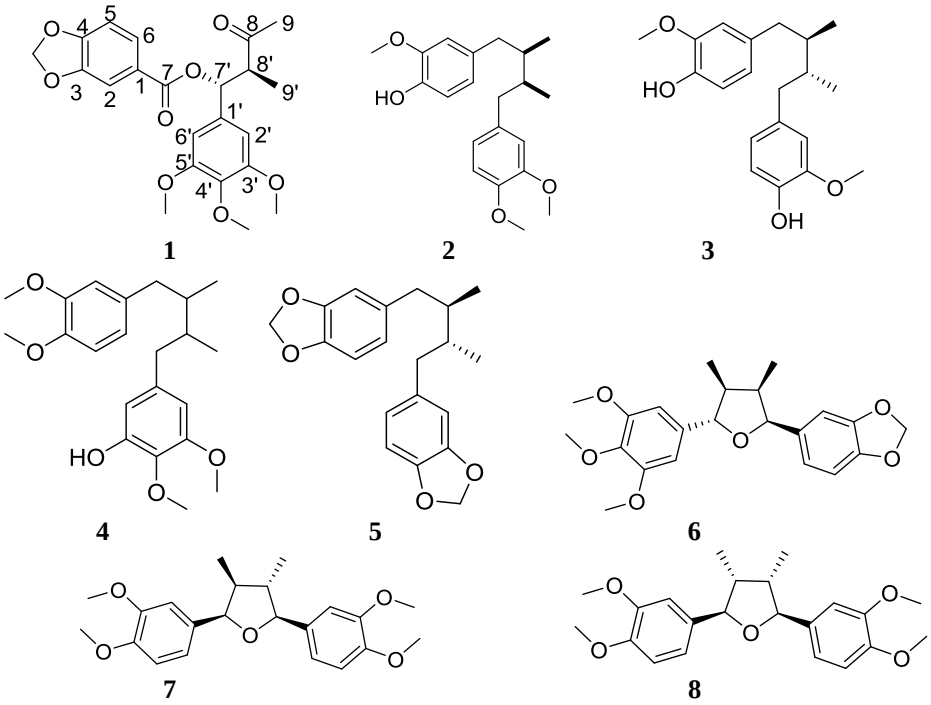

Figure 1. Structures of compounds **1**–**8.**

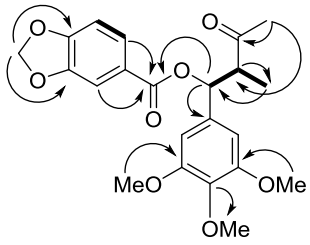

Figure 2. ^{1}H,^{1}H-COSY (—), Key HMBC (→) correlations of compound **1.**

Table 1. ^{1}H and ^{13}C NMR chemical shifts of compounds **1** (at 400 MHz ^{1}H and100 MHz ^{13}C in $CDCl_3$, δ in ppm, *J* in Hz).

Position (H)	δ_H	δ_C
1	-----	123.9
2	7.41 (1H, *d*, *J*= 1.6)	109.6
3	-----	147.6
4	-----	152.0
5	6.82 (1H, *d*, *J*= 8.2)	108.2
6	7.60 (1H, *dd*, *J*= 8.2, 1.6)	125.8
7	-----	164.7
8	-----	209.8
9	2.24 (3H, *s*)	28.8
1'	-----	133.9
2'	6.61 (1H, *s*)	104.4
3'	-----	153.5
4'	-----	138.2
5'	-----	153.5
6'	6.61 (1H, *s*)	104.4
7'	5.92 (1H, *d*, 10.1)	78.4
8'	3.17 (1H, dq, *J*= 10.1, 7.1)	52.5
9'	0.97 (3H, *d*, *J*= 7.1)	13.9
OCH_2O	6.03 (2H, *s*)	102.0
3'-OMe	3.86 (3H, *s*)	56.3
4'-OMe	3.81 (3H, *s*)	60.9
5'-OMe	3.86 (3H, *s*)	56.3

This work corresponds to the first report of this type of secondary metabolites (specifically; secolignan, and 7,7'-epoxylignans) found in the species *N. turbacensis* and *Nectandra* genus, and correspond to the compounds **1**, **2**, **3**, **4**, **5**, and **6** (Figure 1). Also becomes the first study of the root bark and leaves of the species (it had only been studied bark and wood of the trunk) [6]. Isolation of lignans and neolignans from *Nectandra* genus, such as dihydrobenzofurans [21]; 2,5-diaryltetrahydrofurans-type lignans; bicyclo [3.2.1] octanoids neolignans; 3,3'-neolignan; diaryldimethylbutane lignans, among others; have been previously reported. The presence of this type of secondary metabolites (lignans and neolignans) is consistent with the statement made by Rohwer [1], which states that the presence of phenylpropanoids and dimerization products (dehydrodieugenole, lignans and neolignans) correspond to the most common secondary metabolites in the genus [1]. However, the isolation of other types of secondary metabolites have also been reported [4, 22-24].

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Supporting Information

Supporting Information accompanies this paper on http://www.acgpubs.org/RNP

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