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Note

A NAPHTHOQUINONE DERIVATIVE FROM *TECTONA GRANDIS* (LINN.)

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A new naphthoquinone derivative has been isolated, along with a number of prenylnaphthoquinone congeners, from the heartwood of *Tectona grandis* (Linn.). It was characterized as dehydro- α -isodunnione (**1**) by careful analysis of its spectral data.

Keywords: *Tectona grandis* (Linn.); Verbenaceae; Naphthoquinone; Dehydro- α -isodunnione

INTRODUCTION

Tectona grandis (Linn.) belongs to the family Verbenaceae and is popularly known as teak or sagwan. It occurs in all tropical and subtropical regions. Its wood oil is used to treat eczema and ringworm, while wood-ash is applied to swollen eyelids [1]. Earlier phytochemical work on this plant led to the isolation of several quinonoid derivatives [2–8]. The present paper deals with the isolation and characterization of a new naphthoquinone derivative from the heartwood of this plant.

RESULTS AND DISCUSSION

From the chloroform extract of the heartwood of *T. grandis*, a new naphthoquinone derivative (**1**) has been isolated together with previously reported compounds, *viz.* lapachol [2], tecomaquinone-I [3], deoxylapachol [4], tectoquinone [5], dehydro- α -lapachone [6] and tectol [3]. Compound **1** was obtained as pale yellow needles, mp 183–85°C. Elemental analysis and molecular weight determination established the molecular formula as C₁₅H₁₂O₃, corresponding to ten double bond equivalents. The mass spectrum exhibits a molecular ion peak at *m/z* 240, also corresponding to a molecular formula C₁₅H₁₂O₃.

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TABLE I ^1H and ^{13}C NMR data of **1–3***

Position	1		2	3
	δ_{H}	δ_{C}	δ_{C}	δ_{C}
1	–	179.0	178.1	180.2
2	–	148.9	158.2	170.7
3	–	122.9	130.7	122.9
4	–	180.2	181.8	164.8
5	8.32 m	125.4	125.6	124.2
6	7.81 m	126.7	133.8	131.6
7	7.81 m	126.5	132.4	134.7
8	8.32 m	125.7	125.7	129.4
9	–	131.4	131.1	130.6
10	–	133.5	133.2	126.6
1'	–	124.1	45.1	44.2
2'	–	62.8	91.4	126.0
3'	1.58 s	26.8	25.8	86.8
4'	1.58 s	26.8	20.6	27.7
5'	4.90 sbr	110.0	14.2	27.7
	4.92 sbr			

* Measured in CDCl_3 at 300 MHz for ^1H and 22.5 MHz for ^{13}C NMR.

A prominent peak at m/z 239 is due to the loss of a H radical from the molecular ion. Other prominent peaks at m/z 211 and 183 are due to successive loss of two CO molecules from the rearranged ion. A base peak at m/z 153 is probably derived by elimination of two methyl radicals from the ion at m/z 183.

The UV spectrum of **1** shows absorption bands at 309 and 352 nm, exhibiting the presence of a quinonoid chromophoric moiety, which was confirmed by the IR spectrum displaying peaks at 1685 and 1642 cm^{-1} . Its ^1H NMR spectrum in CDCl_3 exhibits a pair of broad singlets at δ 4.90 and 4.92, corresponding to two exomethylene protons. This assignment is supported by the ^{13}C NMR chemical shifts of C-1' and C-5' carbons (δ 124.1 and 110.0 respectively). A sharp singlet at δ 1.58 integrated for six protons in the ^1H NMR spectrum is attributed to a gem-dimethyl group attached to an oxygenated carbon atom; this is supported by the downfield signal (δ 62.8) of C-2'. The remaining four protons resonating as multiplets at δ 7.81 and 8.32 ppm reveal their aromatic nature (Table I).

On the basis of above findings, compound **1** can be formulated as dehydro- α -isodunnione (**1**) (Fig. 1). More conclusive evidence for this structure is provided by its ^{13}C NMR spectrum, which shows signals for 15 carbon atoms, including one degenerate signal for two methyl groups. The ^{13}C NMR data were analyzed by analogy with the reported values for the structurally similar naphthoquinones, *viz.* α -dunnione (**2**) and dehydrodunnione (**3**), isolated from the plantlets and cultured cells of *Streptocarpus dunnii* [9].

EXPERIMENTAL

General Experimental Procedures

Melting points were determined with an electrothermal melting point apparatus and are uncorrected. The UV spectrum was recorded on a Hitachi U-2000 spectrophotometer, while the IR spectrum was taken on an FT-IR Magna-500 Nicolet spectrometer. ^1H (300 MHz) and ^{13}C NMR (22.5 MHz) spectra were recorded on Bruker DRX-300 and JEOL FX 90Q instruments, respectively, using CDCl_3 as solvent and TMS as internal standard. EIMS data were generated on a JEOL JMS-D-300 spectrometer. Column chromatography was run on

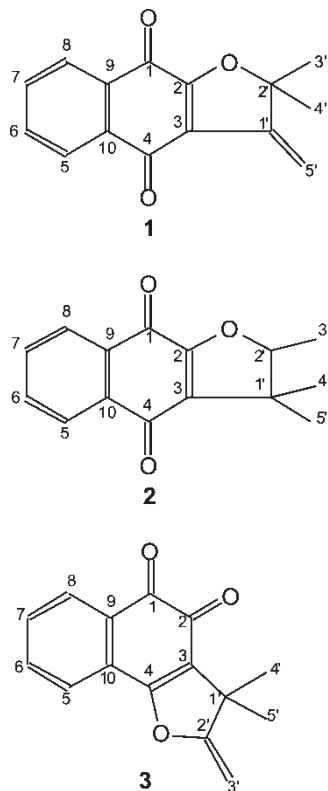


FIGURE 1 Structures 1–3.

neutral alumina (Acme Synthetic Chemicals) while TLC was conducted on Kieselgel 60F₂₅₄ plates (E-Merck).

PLANT MATERIAL

The plant material was collected at Sawai Madhopur district of Rajasthan, India and botanically identified by Professor P.S. Jain, Department of Botany, University of Rajasthan. A voucher specimen has been deposited in the herbarium, Department of Botany, University of Rajasthan, Jaipur, India.

EXTRACTION AND ISOLATION

The air-dried heartwood shavings of *Tectona grandis* (3 kg) were extracted with CHCl₃ on a boiling-water bath for 3 × 12 h. The concentrated extract, after taking in diethyl ether, was then separated into acidic and neutral fractions using 2 N Na₂CO₃ solution. The Na₂CO₃-soluble part, on neutralization with 6 N HCl, gave lapachol (10 g). The Na₂CO₃-insoluble part, on column chromatography over neutral alumina (deactivated with 10% aq. AcOH), gave five fractions. Fraction A (light petroleum (60–80°C)–C₆H₆ 3:1), after crystallization from MeOH, yielded tecomaquinone-I (250 mg). Fraction B (light petroleum–C₆H₆ 1:1) was further separated by preparative TLC (C₆H₆) to give deoxylapachol (70 mg)

and tectoquinone (340 mg). Fraction C (C_6H_6) after crystallization from light petroleum– $CHCl_3$ mixture afforded dehydro- α -lapachone (300 mg). The residue of fraction D (C_6H_6 –EtOAc 3:1) was purified by preparative TLC (CH_2Cl_2) to give dehydro- α -isodunnione **1** (125 mg). Column chromatography of fraction E (C_6H_6 –EtOAc 1:1) afforded tectol (150 mg). Compound **1** was obtained as pale yellow needles from light petroleum– $CHCl_3$ (1:1), mp 183–85°C. UV (EtOH) λ_{max} (nm) ($\log \epsilon$): 309 (1.593), 352 (1.221). IR (KBr) ν_{max} (cm^{-1}): 1685, 1642 (C=O), 1592, 1371, 1342, 1314, 750. 1H and ^{13}C NMR data, see Table I. EIMS m/z 240 $[M]^+$ (4), 239 $[M - H]^+$ (6), 211 $[239 - CO]^+$ (5), 183 $[211 - CO]^+$ (3), 168 $[183 - CH_3]^+$ (5), 153 $[168 - CH_3]^+$ (100). Elemental analysis, found (%) C 74.8, H 4.7; calcd for $C_{15}H_{12}O_3$, C 75.0, H 5.0.

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