REFERENCES

1. Bhandari, P., Tandon, S. and Rastogi, R. P. (1980) *Phytochemistry* **19**, 1544.
2. Bose, A. K., Fujiwara, H., Kamat, V. S., Trivedi, G. K. and Bhattacharya, S. C. (1979) *Tetrahedron* **35**, 13.
3. Brewster, K., Harrison, J. M. and Thomas, D. I. (1979) *Tetrahedron Letters* 5051.
4. Cussans, N. J. and Huckerby, T. N. (1975) *Tetrahedron* **31**, 2719.
5. Chan, K. K., Giannini, D. D., Cain, A. H., Roberts, J. D., Porter, W. and Trager, W. F. (1977) *Tetrahedron* **33**, 899.
6. Tandon, S. and Rastogi, R. P. (1977) *Phytochemistry* **16**, 1991.
7. Tandon, S. and Rastogi, R. P. (1979) *J. Sci. Ind. Res.* **38**, 428.
8. Das, S. C., Sengupta, S. and Herz, W. (1973) *Chem. Ind.* 792.
9. Sengupta, S. and Das, S. C. (1978) *Chem. Ind.* 954.

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CRYSTAL STRUCTURE OF A LIGNAN FROM *JATROPHA GOSSYPIFOLIA*

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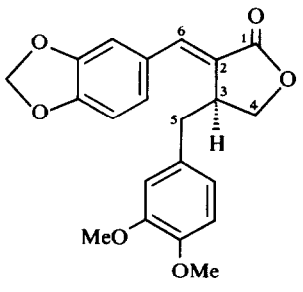
Key Word Index—*Jatropha gossypifolia*; Euphorbiaceae; 2-piperonylidene-3-verytryl-3*R*-γ-butyrolactone; X-ray analysis.

From the petrol extract of *Jatropha gossypifolia* (stem, roots and seeds) we have isolated a new lignan (**1**), $C_{21}H_{20}O_6$ (M^+ 368.126), mp 129° (C_6H_6), $[\alpha]_D^{25°}$ +87° ($CHCl_3$). The structure of this compound has been unambiguously settled from its X-ray crystallographic analysis.

The functionality of this lignan was revealed by its spectroscopic properties. The IR spectrum showed characteristic peaks for an α,β-unsaturated γ-lactone (1725 cm^{-1}), an olefinic double bond (1630 cm^{-1}), an aromatic nucleus (1595 and 1480 cm^{-1}) and a methylenedioxy group (910 cm^{-1}). The UV absorption of **1** (λ_{max}^{EtOH}: 333, 297, 288 and 223 nm; log ε 4.21, 3.98, 3.99 and 4.19) was closely similar to that of the lignan (−)-hibalactone (**2**), previously isolated from *Juniperus sabina* (Cupressaceae) [1], thereby indicating the presence of a dibenzylbutyrolactone skeleton with a double bond at the 2,6-position of the γ-butyrolactone ring. Several structural features of **1** could be ascertained from its 80 MHz ^1H NMR spectrum ($CDCl_3$). The spectrum revealed the presence of two OMe groups (δ 3.88, 3 H, *s* and 3.85, 3 H, *s*), one methylenedioxy group (6.04, 2 H, *s*), six aromatic protons (7.1–6.8, *m*) and one olefinic proton at C-6 (7.5, *s*). The other signals appeared at δ 4.27 (2 H at C-4, *d*, J = 4.1 Hz), 3.9–3.5 (1 H at C-3, *m*), 3.03 (1 H at C-5, *d*, J = 4 Hz) and 2.64 (1 H at C-5, *d*, J = 9.2 Hz). The compound was cleaved under electron impact and the fragmentation pattern revealed several details about the molecule. The characteristic ion peaks appeared at *m/z* 368, 217, 152, 151 (base peak), 135 and 28. The peaks at *m/z* 217 and 151 resulted from the benzylic cleavage at the 3–5 position. All the spectroscopic data suggested that the structure of the new lignan is **1**.

The structure of **1** was further corroborated from its



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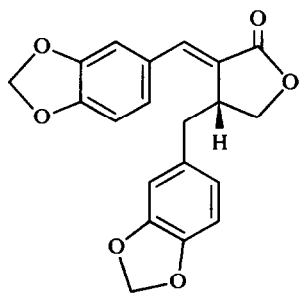

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crystal structure analysis by X-ray diffraction. The intensities were collected on an automatic four-circle diffractometer Phillips PW 1100, with Cu-Kα radiation selected by a graphite monochromator. The system was orthorhombic; the crystals belong to the space group $P2_12_12_1$ with cell parameters: $a = 25.822$, $b = 8.824$ and $c = 7.901$ Å. The structure was solved by application of the phase function [2], symbolic addition [3] and direct method [4]. The molecule is illustrated in Fig. 1.

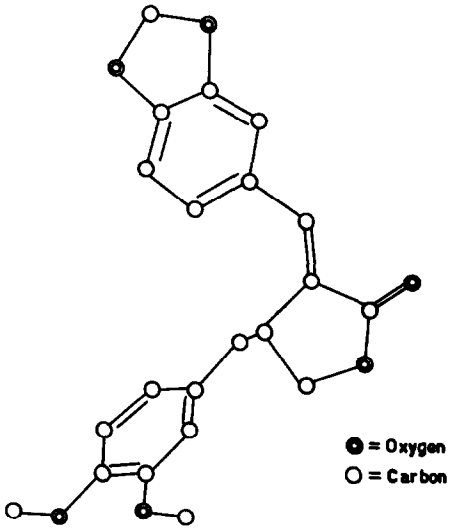

Fig. 1.

A survey of the literature revealed that the properties of the new lignan showed similarities with suchilactone (**3**) [5], which was previously reported as a degradation product of helianthoidin (**4**) [6]. As compounds **1** and **3** exhibit opposite rotation, they must differ in their steric configuration at C-3, the only chiral centre in the compound. Hence the lignan occurring in *Jatropha gossypifolia* is 2-piperonylidene-3-verytryl-3*R*-γ-butyrolactone. This is the first report of the occurrence of a lignan in the genus *Jatropha*.

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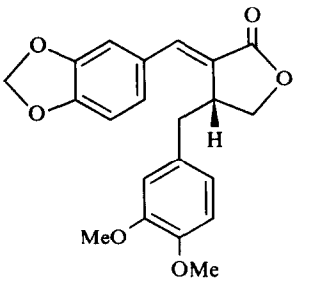

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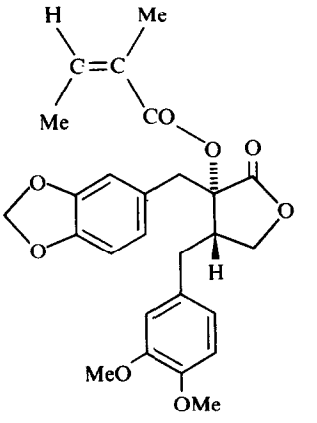

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REFERENCES

1. Schrecker, A. W. and Hartwell, J. L. (1954) *J. Am. Chem. Soc.* **76**, 4896.
2. Riche, C. (1973) *Acta Crystallogr. Sect. A* **29**, 133.
3. Karle, I. L. and Karle, J. (1964) *Acta Crystallogr. Sect. A* **20**, 849.
4. Germain, G., Main, P. and Woolfson, M. M. (1971) *Acta Crystallogr. Sect. A* **27**, 368.
5. Ghosal, S., Kumarswamy, C., Chauhan, R. P. S. and Srivastava, R. S. (1973) *Phytochemistry* **12**, 2550.
6. Burden, R. S., Combie, L. and Whiting, D. A. (1969) *J. Chem. Soc. C* 693.