

JATROLACTOL, A NEW LIGNAN FROM JATROPHA GOSSYPIFOLIA¹

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A new lignan, Jatrolactol has been isolated from the aerial parts of *Jatropha gossypifolia*. The structure of the compound was derived from its spectroscopic (1D and 2D NMR) data and chemical evidence.

Jatropha gossypifolia Linn (Euphorbiaceae), a small shrub, grows in different parts of India. Various medicinal and pesticidal activities of the plant are well known.²⁻⁵ The most valuable application of the plant is in the treatment of cancerous growth^{2,4,5} and as an insecticide³. Its major chemical constituents have been reported to be lignans and diterpenoids^{4,5}.

In continuation of our work⁶⁻¹¹ on the constituents of *J. gossypifolia* we report herein the isolation and characterization of a new lignan, Jatrolactol (**1**) together with the known compounds, Jatrophan (**2**)^{6,7} and gadain (**3**)⁷ from the aerial parts of the plant.

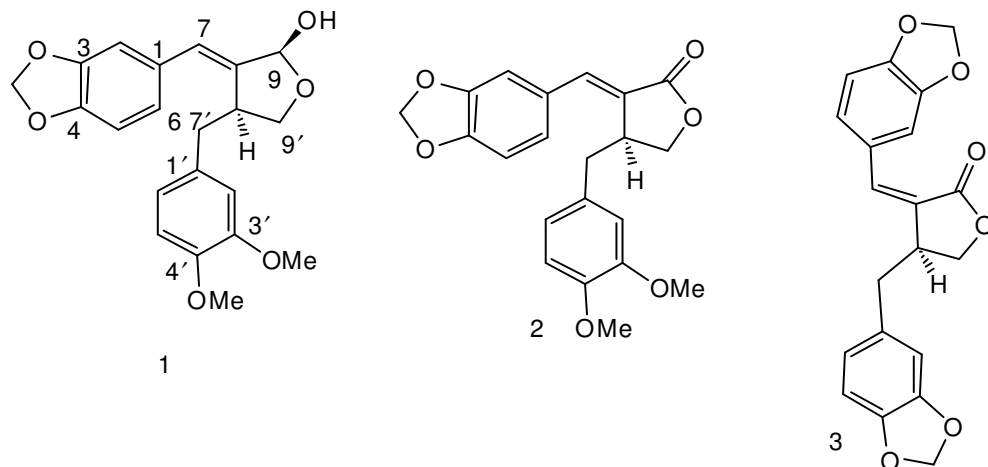
Jatrolactol (**1**) was obtained as a colorless viscous mass. Its molecular formula was assigned to be C₂₁H₂₂O₆ from its elemental analysis, ¹H and ¹³C NMR spectra and LSIMS (m/z 371 [M+H⁺]). Its IR spectrum showed the presence of hydroxyl group and unsaturation in the molecule. The ¹H and ¹³C NMR spectral data of **1** (vide experimental) indicated that the molecule is structurally related to the known constituent, Jatrophan (**2**)^{6,7}. Both the compounds contain two 1,3,4-trisubstituted aromatic rings and a trisubstituted olefinic double bond along with one

methylenedioxy and two methoxy groups. However, instead of a lactone ring present in **2** a lactol group is present in **1**. H-9 in **2** appeared at δ 5.32 in its ¹H NMR spectrum while C-9 at 108.4 in the ¹³C NMR spectrum. The HMBC spectrum suggested the correlations between H-7 (6.52) and C-9 as well as between H-9 and C-7 (120.6). The NOESY experiment on **2** showed that H-7 is related to H-9 and the latter to H-8' (2.91). However, H-7 did not show any correlation to H₂-7' (2.83-2.62). These 2D NMR experiments clearly suggested that the *trans* (*E*)-double bond is present at C-7-C-8 and the stereo configuration of both H-9 and H-8' is same.

Jatrolactol (**1**) on oxidation with Fetizon's reagent¹² afforded Jatrophan (**2**)^{6,7} thus confirming the structure and stereochemistry of the new lignan **1**.

Experimental

Column chromatography was carried out on silica gel (BDH, 100-120 mesh) and TLC with silica gel GF₂₅₄. The solvents were of commercial grade. Optical rotations were determined with a Jasco DIP 360 digital polarimeter. The spectra were recorded with the



following instruments; IR: Perkin-Elmer spectrophotometer; NMR: Varian Gemini 200 MHz and ESIMS: VG Micromass 7070H (70eV).

The aerial parts of *J. gossypifolia* were procured from Birbhum, West Bengal in June, 2012. The air-dried plant materials (5kg) were powdered and extracted with CH_2Cl_2 -MeOH (1:1) at room temperature. The extraction was continued thrice, each extraction was performed for 120 hr using 5 lit of the mixture of solvents. The total extract was concentrated under reduced pressure to generate a greenish gummy material (24.5g). The residue (24g) was purified by column chromatography using solvents of increasing polarity from hexane through EtOAc. Gadain (**3**) (20 mg), Jatrophan (**2**) (24mg) and Jatrolactol (**1**) (28 mg) were eluted with hexane-EtOAc (1:1), hexane-EtOAc (2:3) and EtOAc respectively. The first two compounds were identified by direct comparison (m.p. $[\alpha]_D$, TLC and co-TLC) with authentic samples available in our laboratory^{6,7}.

Jatrolactol (1) : Colorless viscous mass; $[\alpha]_D^{25} = +126.3$ (c 1.50, CHCl_3); IR : 3414, 1627, 1592, 1484, 925 cm^{-1} ; ^1H NMR (200 MHz, CDCl_3): δ 6.87 (1H, dd, $J=8.0, 2.0$, Hz, H-6), 6.83 (1H, d, $J=2.0$ Hz, H-2), 6.72 (1H, d, $J=8.0$ Hz, H-5), 6.70 (1H, $J=8.0$ Hz, H-5'), 6.65 (1H, dd, $J=8.0, 2.0$ Hz, H-6'), 6.52 (1H, short m, H-7), 6.02 (2H, s, $-\text{OCH}_2\text{O}-$), 5.32 (1H, d, $J=1.6$ Hz, H-9), 3.78 and 3.74 (3H, each, s, 2x-OMe), 3.43-3.36 (2H, m, H_2-9'), 2.91 (1H, m, H-8'), 2.83-2.62 (2H, m, H_2-7'); ^{13}C NMR (50 MHz, CDCl_3): δ 148.1 (C-3), 147.3 (C-4), 147.0 (C-3'), 145.8 (C-4'), 135.5 (C-8), 129.7 (C-1), 128.4 (C-1'), 122.5 (C-6), 120.8 (C-6'), 120.6 (C-7), 113.4 (C-5), 112.3 (C-5'), 109.2 (C-2), 108.4 (C-9), 108.2 (C-2'), 101.2 ($-\text{OCH}_2\text{O}-$), 68.6 (C-9'), 55.7 (-OMe), 55.5 (-OMe), 38.4 (C-8'), 35.6 (C-7'); LSIMS: m/z 371 $[\text{M}+\text{H}]^+$. [Found : C, 68.27, H, 5.93 $\text{C}_{21}\text{H}_{22}\text{O}_6$ requires C, 68.12, H, 5.95%].

Oxidation of Jatrolactol (1) to Jatrophan (2)

Jatrolactol (**1**) (15 mg) was dissolved in benzene (10 ml) and Fetizon's reagent (200 mg) was added. The mixture was refluxed for 2 hr under nitrogen using

Dean-Stark apparatus. The mixture was cooled and filtered. The filtrate was concentrated and the residue was subjected to column chromatography over silica gel to obtain pure Jatrophan (**2**) (9 mg). The product was identified by direct comparison (m.p. $[\alpha]_D$, TLC and co-TLC) with an authentic sample.

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