

## LAGEFLORIN, A PENTACYCLIC TRITERPENE FROM *LAGERSTROEMIA PARVIFLORA*

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**Key Word Index**—*Lagerstroemia parviflora*, Lythraceae, hop-21(22)-en-3,20-dione; lageflorin

**Abstract**—A new pentacyclic triterpene has been isolated from the whole plant of *Lagerstroemia parviflora* and the structure has been elucidated as **1** from detailed analyses of spectroscopic data.

### INTRODUCTION

Occurrence of several interesting chemical constituents [1, 2] including alkaloids [3] in the genus, *Lagerstroemia* led us to re-examine *L. parviflora* which afforded a new pentacyclic triterpene designated lageflorin (**1**). The structure of the compound, **1** was deduced from analysis of its spectral data.

### RESULTS AND DISCUSSION

Chromatography of the concentrated *n*-hexane extract of the whole plant of *Lagerstroemia parviflora* Roxb. over silica gel afforded a crude material in benzene–chloroform (1:1) to 2% methanolic chloroform eluates. The concentrated fractions on rechromatography over Tswett column followed by elution with petrol–benzene (2:3) mixture furnished lageflorin. It was crystallized from petrol–benzene mixture, mp 346–348° and was found to be homogeneous on TLC and by mass spectrometry.

Lageflorin,  $C_{30}H_{46}O_2$  ( $M^+$  438),  $R_f$  0.31 (benzene–chloroform; 3:1, silica gel G),  $\lambda_{max}$  244 nm (optical density, 0.953) responded to Liebermann–Burchardt colour reaction for triterpenes and showed the presence of a cyclohexanone moiety ( $1715\text{ cm}^{-1}$ ) in its IR spectrum. The compound does not contain any hydroxyl function as was evidenced from the IR spectrum, as also by its failure to form an acetate. The second oxygen function is therefore present either as keto-carbonyl or an epoxide. The absence of any oxirane proton in the  $^1\text{H NMR}$  spectrum of the compound clearly indicated that the second oxygen function occurs as a ketonic function. The presence of a band at  $1750\text{ cm}^{-1}$  in the IR spectrum of the compound confirmed that the ketonic function forms a part of a cyclopentanone ring in lageflorin.

The  $^1\text{H NMR}$  spectrum of the compound revealed all the structural features of the molecule. It showed the presence of six tertiary methyls, each appearing as a singlet, at  $\delta$  0.81, 0.85 (6H), 0.88, 0.91 and 0.99. The  $^1\text{H NMR}$  spectrum also exhibited signals at  $\delta$  1.44 (methylene protons) and at  $\delta$  1.99 (3H, singlet) and 2.11 (3H, singlet). The latter two signals clearly indicated the presence of an isopropylidene group [ $(\text{Me})_2\text{C}=\text{C}<$ ] in

the molecule of lageflorin. That the isopropylidene system is in conjugation with the five-membered ring carbonyl was apparent from the UV absorption maximum at 244 nm as also from the down-field shift of the isopropylidene methyls in the  $^1\text{H NMR}$  spectrum of the compound.

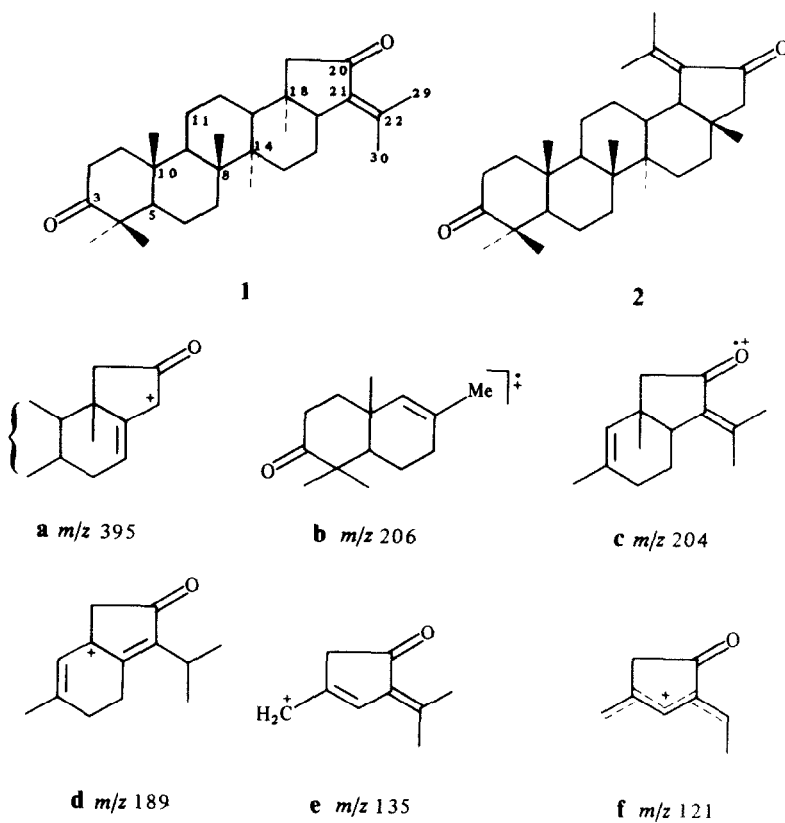
The above spectral and physical data of the compound led to the structure **1** or **2** for lageflorin. The lupene structure **2** for lageflorin was rejected from mass spectrum as it lacked the ion peaks at  $m/z$  218 and 232 characteristic for such skeleton [4]. The mechanism of the formation of the ion fragments at  $m/z$  395, 206, 204, 189, 135 and 121 corresponding to species **a**, **b**, **c**, **d**, **e**, and **f** could be best explained in terms of the hopene structure **1** for lageflorin.

### EXPERIMENTAL

Plant material was procured and identified by Dr S. R. Das (Survey Officer, Regional Research Institute (Ay.), Calcutta 700009). A voucher specimen of the plant material has been deposited at the Department of Chemistry, Calcutta University. Mps uncorr, UV spec EtOH, IR. KBr,  $^1\text{H NMR}$  (80 MHz)  $\text{CDCl}_3$ , TMS as int. standard, MS 70 eV, CC and TLC silica gel (BDH, 60–120 mesh) and silica gel G (Merck) respectively. The analytical sample was dried *in vacuo* over  $\text{P}_2\text{O}_5$  for 24 hr.

**Isolation of lageflorin (1)** The dried whole plant material (2 kg) of *L. parviflora* was crushed and extracted with *n*-hexane. After evapn of the solvent, the crude extract was chromatographed over silica gel with the solvents of increasing polarity. Benzene– $\text{CHCl}_3$  (1:1) to 2%  $\text{CHCl}_3$  in MeOH eluates on rechromatography on a Tswett column using silica gel yielded lageflorin in petrol–benzene (2:3) eluates. It was crystallized from petrol–benzene mixture to furnish colourless needles of lageflorin (**1**), mp 346–348°, yield 0.001% (Found C, 82.42, H, 10.14;  $C_{30}H_{46}O_2$  requires C, 82.19, H, 10.50;  $m/z$  (rel. int.) 438 ( $M^+$ , 56), 423 (22), 395 (48), 206 (52), 205 (28), 204 (28), 203 (29), 189 (100), 137 (20), 135 (53), 121 (62)).

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