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UMBELLIFERAE

EXTRACTIVES OF *LIGUSTICUM ELATUM*

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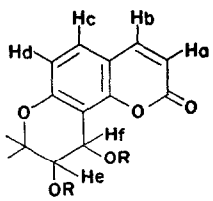
Plant. Ligusticum elatum. Previous work Essential oil [1]

Present work. Air dried roots were extracted with light petroleum (40–60), and the extract chromatographed over alumina Petrol eluation afforded anomalin (I) $C_{24}H_{26}O_7$, *m/e* 426 (M^+) m p. 175–76° (from acetone–petrol), λ_{max}^{EtOH} 223, 320 nm., ν_{max}^{KBr} 1722, 1605, 1390 and 1380 cm^{-1}. NMR ($CDCl_3$) 3·75 τ (1H, d, J = 9 5 cps, Ha); 2·45 τ (1H, d, J = 9·5 cps, Hb), 2 58 τ (1H, d, J = 8·5 cps; Hc); 3·24 τ (1H, d, J = 8 5 cps, Hd), 4 52 τ (1H, d, J = 5 cps; He); 3·24 τ (1H, d, J = 5 cps; Hf), 3·7–4 05 τ (2H, m, side chain olefinic protons); 8 0 τ (12H, m, four olefinic methyls of side chain) and 8 53 and 8·54 τ (3H each, s, gem dimethyl)

The petrol–benzene (1 3) eluate gave β-sitosterol (m.p and mixed m.p.). Rechromatography of the benzene eluate over deactivated alumina gave colourless crystalline material shown by TLC to be a mixture of three components, separated by preparative TLC (Silica gel G) using benzene–acetone (4 1) *Trans* khellactone (II) $C_{14}H_{14}O_5$ m p 186°; λ_{max}^{EtOH} 223, 327 nm, ν_{max}^{KBr} 3350, 1700, 1380, 1370 and 827 cm^{-1}; NMR ($CDCl_3$), 3·8 τ (1H, d, J = 9 5 cps, Ha); 2·4 τ (1H, d, J = 9 5 cps; Hb), 2·72 τ (1H, d, J = 8 cps, Hc); 3·25 τ (1H, d, J = 8·8 cps; Hd), 4·98 τ (1H, d, J = 6·5 cps, Hf), 6·15 τ (1H, d, J = 6·5 cps; He), 8 49 and 8 69 τ (3H each, s, gem dimethyl) Acetate $C_{18}H_{18}O_7$ m p 161–62° (from acetone–water).



(I) R=R'=–CO–C(CH$_3$)=CHCH$_3$
(II) R=R'=H (*trans*-khellactone)
(III) R=R'=H (*cis*-khellactone)

Cis-khellactone (III) $C_{14}H_{14}O_5$ m p 174°, λ_{max}^{EtOH} 211, 328 nm, ν_{max}^{KBr} 3500, 3350, 1705, 1390, 1380 and 840 cm^{-1}, NMR ($CDCl_3$), 3 76 τ (1H, d, J = 9·5 cps, Ha), 2·39 τ (1H, d, J = 9·5 cps; Hb), 2·69 τ (1H, d, J = 8 cps, Hc); 3 24 τ (1H, d, J = 8 cps, Hd); 4·78 τ (1H, d, J = 4 5 cps, Hf), 6·13 τ (1H, d, J = 5 cps; He), 8 58 and 8·54 τ (3H each, s, gem dimethyl). Acetate –$C_{18}H_{18}O_7$ m.p. 132–34°

Further extraction of the defatted plant with EtOH gave mannitol

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[1] Y K SARIN, *Per Essential Oil Records* **56**, 217 (1965)

Key Word Index—*Ligusticum elatum*, Umbelliferae, coumarins, anomalin, khellactone