12-Nonacosanone in Seeds of Laserpitium siler L.

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During our study on the seed constituents of Laserpitium siler L., we have isolated some time ago a crystalline compound of m.p. 74.5 °C showing the frequency of 1706 cm⁻¹ in its infrared spectrum. We have now identified this substance as 12-nonacosanone by mass spectrometry. The high resolution measurement gave for the molecular ion a value of 422.4493 which corresponded to the composition C₂₉H₅₈O (calculated 422.4487). The cleavage of the ionized molecule in the neighborhood of the carbonyl group gave rise to acylium ions C₁₁H₂₃C=O⁺ and C₁₇H₃₅C=O⁺ of mass values 183 (b.p.) and 267 resp. The products of the McLafferty rearrangement afforded peaks of m/e 282 and 198 (C₁₉H₃₈O and C₁₃H₂₆O) resp., which were accompanied by satellites of the protonated particles. The substance was subjected to Clemenson reduction in order to verify the normal character of the carbon chain. The reaction product was identified as n-nonacosane by mass spectrometry.

Aliphatic ketones are of relatively scarce occurrence in plant material. The occurrence of 12-nonacosanone in Nature is also interesting from the chemotaxonomic viewpoint since 10-nonacosanone has been isolated from the stalk wax of the species Laserpitium latijolium L. by Huneck (for mass spectroscopy data of 10-nonacosanone see the paper of Beckmann and Schüelle).

The mass spectra were measured in AEI-Mass Spectrometer MS 902 at 70 eV. The high resolution measurement were within 5 ppm.

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3 S. Huneck, Naturwissenschaften 47, 160 [1960].
