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SHORT REPORTS

THE ESSENTIAL OIL OF *INULA RACEMOSA*

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Abstract—The essential oil of *Inula racemosa* was found to contain mainly sesquiterpenes (*ca* 60%), although the most abundant constituent was heptadeca-1,8,11,14-tetraene (aplotaxene) at *ca* 22%. Phenylacetonitrile (*ca* 2%) was also detected.

INTRODUCTION

Inula racemosa is a member of the Compositae. It grows in the temperate and alpine western Himalayas, and it is common in Kashmir. The roots are widely used locally in indigenous medicine as an expectorant and in veterinary medicine as a tonic [1]. Previously, Singh *et al.* reported the isolation of two sesquiterpene lactones, alantolactone and isoalantolactone, by low-temperature crystallization of extracts of *I. racemosa* [2]. This report deals with the analysis of the essential oil obtained from the roots of the plant.

RESULTS AND DISCUSSION

The essential oil of the roots of *I. racemosa* was obtained by steam distillation in 0.05% yield as a dark brown liquid. It had the following physical properties: specific gravity, 0.9003; refractive index, 1.5385 at 31°; viscosity, 2.2009 at 23°; acid value, 20.7020; ester value, 150.4; optical rotation, inactive. The volatile constituents of the oil were examined by routine temperature programmed GC and identified as far as possible by high sensitivity GC/MS. The results are given in Table 1. Where positive identities are given, the mass spectra of sample components agreed well with those in the literature, e.g. [3, 4], within instrumental variability. Literature [4, 5] Kováts retention indices of most of these components (determined on the same phase as employed in this project) are included in the table, and these serve as limited supportive evidence of identity.

From Table 1 it can be seen that the essential oil contained 28 main (i.e. > 0.1%) components, of which 15 (comprising *ca* 48% of the sample) were positively identified, with a further 8 (*ca* 44%) partially characterized. The latter were all sesquiterpenes, mainly alcohols and aldehydes, which are notoriously difficult to identify by routine GC/MS alone. None of these partially characterized constituents was one of the more common members of these groups of compounds. Most of the constituents of the essence were, in fact, sesquiterpenes, in total 17, making up *ca* 60% of the oil. However, the most abundant constituent of all, by some margin, was not a terpene, and this was heptadeca-1,8,11,14-tetraene (*ca* 22%). Although this component co-eluted in the GC with 2-phenylethanol, it was clear from the mixed mass spectrum obtained on GC/MS that the alcohol was a minor constituent. As well as this tetraene, a related compound, heptadeca-1,8,11-triene, was also identified (at *ca* 3% of the essence). These two compounds, also known as aplotaxene and dihydroaplotaxene, respectively, have previously been identified in the root oil of *Cirsium japonicum* [6], and it has been suggested that these types of compounds could be intermediates in the biosynthesis of C_{17}-acetylenic compounds from oleic acid [7]. The mass spectra of heptadeca-1,8,11,14-tetraene and heptadeca-1,8,11-triene have been reported [6], and those obtained in this work agreed near perfectly. Whether these relatively unusual essential oil constituents bestow any specific beneficial properties on the plant is unknown at present.

One other interesting component of the oil is phenylacetonitrile (benzyl cyanide) at *ca* 2% of the sample. Again, the mass spectrum obtained in this work matched very well with that in the literature, e.g. [8]. Phenylacetonitrile often originates from benzylglucosinolate, although benzyl isothiocyanate would then also be expected as a co-product [8], and none could be detected. Phenylacetonitrile alone (i.e. without benzyl isothiocyanate) has also been found in sugar beet [9], and it was shown to possess auxin-like growth activity in the leaves and roots [10]. Clearly, it could therefore have a similar function in *I. racemosa*.

Table 1. Constituents of the essential oil of *Inula racemosa*

Component*	R_t (min)	Kovàts index (literature)†	% Relative abundance
p-Cymene	9.5	1272	0.4
2-Furfural	15.5	1449	0.3
Norbornyl acetate	16.8	1476	0.1
Benzaldehyde	18.0	1502	0.1
Sesquiterpene hydrocarbon	18.5	—	0.3
β-Elemene	20.0	1618	4.1
α-Pinene oxide	21.3	—	0.3
α-Humulene	22.5	1718	1.0
α-Farnesene	23.8	—	0.2
ar-Curcumene	25.0	1790	1.6
Heptadeca-1,8,11-triene	25.9	—	3.1
α-Ionone	27.1	—	6.6
Heptadeca-1,8,11,14-tetraene + 2-phenylethanol	27.5	— 1859	24.9
Phenylacetonitrile	28.8	1880	2.1
β-Ionone	29.1	1918	2.2
Sesquiterpene alcohol (M_r = 220)	30.7	—	3.7
Sesquiterpene	34.0	—	3.8
Sesquiterpene aldehyde (M_r = 218)	35.5	—	6.4
Sesquiterpene aldehyde (M_r = 218)	36.1	—	7.1
Sesquiterpene aldehyde (M_r = 218)	38.0	—	8.2
Sesquiterpene alcohol (M_r = 220)	42.0	—	8.4
Sesquiterpene alcohol (M_r = 220)	51.0	—	5.8

*Five unidentified components were also detected, all present in > 0.1%.
†Literature [4, 5].

Previously determined sesquiterpene lactones of *Inula*, such as alantolactone and neoalantolactone [2], could not be detected in *I. racemosa*, although efforts were made to locate them.

EXPERIMENTAL

Sample preparation. Roots of *Inula racemosa* were purchased from local markets in Srinagar, Kashmir, and 20 kg were subjected to conventional steam distillation, when 50 l. of distillate were collected. The essential oil was extracted from the distillate with $CHCl_3$, the extract dried ($MgSO_4$) and the solvent removed under reduced pressure to yield a dark brown oil (10.2 g).

GC. FID-GC: 5.5 m × 4 mm i.d. glass column packed with Carbowax 20 M (10% on Chromosorb W, AW and DMCS treated); N_2, 40 ml/min; temp. programme, 70–200° at 4°/min; detector and injection point heaters, 300 and 200°, respectively.

GC/MS. A Kratos MS25 instrument was used, linked on-line to a Kratos DS50 data processing system. GC conditions were as above, but with He as carrier gas. The single-stage all-glass jet separator was at 250°. Significant operating parameters of the MS were: ionization voltage, 70 eV; ionization current, 100 μA; source temp., 225°; accelerating voltage, 1.33 kV; resolution, 1000; scan speed, 3 sec/decade (repetitive throughout run).

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