ACTA CHROMATOGRAPHICA, NO. 19, 2007

GC–MS ANALYSIS OF BIOLOGICALLY ACTIVE COMPOUNDS IN COSMOPOLITAN GRASSES

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SUMMARY

Essential oils of *Lolium perenne* and *Bromus hordeaceus* (family *Poaceae*) were obtained by hydrodistillation and analysed by gas chromatography–mass spectrometry, a powerful tool for qualitative and quantitative analysis of essential oil components. Both oils were found to be rich in eugenol and methyleugenol.

INTRODUCTION

The family of grasses is, perhaps, of all groups in the plant world, the most important to mankind; paradoxically, however, little is known about them [1]. There are over 9000 known species of the *Poaceae* grass family. Commonly known grass plants include maize, wheat, rice, and rye, and grasses have been a dominant worldwide source of human food throughout history. Agricultural grasses grown for human food production are called cereals. Cereals constitute the major source of food energy for humans, and perhaps the major source of protein, and include rice in South Asia, maize in Central and South America, and wheat and barley in the Americas and North Eurasia. Many other grasses are also grown as forage and fodder for animal food.

Grasses are very modern food supplements and the composition of these plants should be investigated. Lemon grass (*Cymbopogon citratus*) is now a widely cultivated plant in tropical areas of America and Asia. Its oil is used as a culinary flavouring, as a scent, and as medicine. Lemon grass is principally taken as tea to remedy the digestive problems diarrhoea and stomach ache [2].

There have been few chemical investigations of the essential oils of *Lolium perenne* and *Bromus hordeaceus*. The objective of this study was to establish a procedure for isolating volatile compounds from these two very common kinds of grass. This is the first report on the composition of the essential oils of these grasses.

EXPERIMENTAL

Plant Material

Lolium perenne and *Bromus hordeaceus* plant material was collected in a local park in Łódź, Central Poland.

Isolation of the Essential Oil

The fresh plant material was submitted to hydrodistillation for 2 h in a Clevenger-type apparatus. Samples of the essential oils obtained were dissolved in dichloromethane for GC–MS analysis.

GC–MS Analysis

An Agilent model 6890 GC interfaced to a 5973 mass selective detector was used for mass spectral identification of the components of the oils. HP-5MS capillary columns (30 m × 0.25 mm × 0.25 µm film thickness) were used for GC. The oven temperature was maintained at 60°C for 6 min then programmed to 240°C at 5° min^{-1}. The carrier gas was helium, at a flow rate of 0.9 mL min^{-1}, and the injection volume was 1 µL. In mass spectrometry electron-impact ionization was performed at an electron energy of 70 eV.

Compound Identification

Components of the oils were identified by comparison of their mass spectra and retention indices with those published in the literature [3,4] and contained in the NIST ’98 MS computer library (Wiley).

RESULTS AND DISCUSSION

Gas chromatography–mass spectrometry (GC–MS) is a useful tool for quantitative and qualitative analysis of a wide range of relatively volatile compounds, and the technique has been widely applied in medical, biological, and food research.

The chemical profiles of the oils, the amount (%) of the individual components, and gas chromatographic and mass spectral data are summarized in Table I.

Table I

Gas chromatographic and mass spectral data for the essential oils of *Lolium perenne* and *Bromus hordeaceus*

No.	Compound	R_t (min)	Molecular mass	Molecular formula	Percentage area		MS fragment ions	
					Lolium perenne	*Bromus hordeaceus*	*Lolium perenne*	*Bromus hordeaceus*
1	β-Linalool	12.04	154	$C_{10}H_{18}O$	0.3	1.0	137, 93, 71, 55, 69	93, 71, 121, 55, 80
2	Estragol	15.40	148	$C_{10}H_{12}O$	5.2	5.9	148, 147, 121, 117, 133	148, 121, 133, 77, 91
3	Isosafrole	18.74	162	$C_{10}H_{10}O_2$	–	2.1	–	178, 162, 104, 135, 77
4	Eugenol	20.24	164	$C_{10}H_{12}O_2$	24.1	19.1	164, 149, 131, 103, 77	164, 149, 131, 103, 77
5	Methyl cinnamate, *trans*	20.97	162	$C_{10}H_{10}O_2$	18.5	31.2	131, 162, 103, 161, 77	131, 162, 103, 77, 51
6	Methyleugenol	21.61	178	$C_{11}H_{14}O_2$	16.6	30.3	178, 147, 163, 107, 179	178, 147, 163, 91, 103
7	(*E*)-7-Octadecene	23.67	252	$C_{18}H_{36}$	7.6	–	97, 55, 83, 69, 57, 111	–
8	*n*-Octadecane	24.44	254	$C_{18}H_{38}$	5.0	2.1	57, 71, 85, 55, 99	57, 71, 85, 55, 69
9	Myristicin	24.75	192	$C_{11}H_{12}O_3$	1.1	1.0	192, 91, 165, 161, 119	192, 165, 91, 131, 119
10	Elemicin	25.80	208	$C_{12}H_{16}O_3$	–	1.3	208, 193, 57, 91, 209	208, 193, 77, 209, 133
11	(−)-Spathulenol	26.53	220	$C_{15}H_{24}O$	1.3	–	119, 205, 93, 147, 105	–
12	Bisomel	27.10	270	$C_{17}H_{34}O_2$	3.3	–	228, 102, 229, 211, 60	–
13	*τ*-Cadinol	28.94	222	$C_{15}H_{26}O$	–	3.1	–	161, 204, 162, 105, 81
14	Ar-tumerone	30.04	216	$C_{15}H_{20}O$	4.4	2.7	83, 119, 216, 201, 132	83, 119, 216, 132, 201
15	Tumerone	30.24	218	$C_{15}H_{22}O$	1.0	–	83, 105, 120, 119, 91	–
	Total				88.4	99.8		

Twelve components were identified in the oil of *Lolium perenne*. The major components of the oil were eugenol (24.1%), *trans*-methyl cinnamate (18.5%), and methyleugenol (16.6%). Eleven compounds were identified in the oil of *Bromus hordeaceus*. *trans*-Methyl cinnamate (31.2%) was the most abundant component, followed by methyleugenol (30.3%) and eugenol (19.1%).

The composition of the oils is interesting because aliphatic compounds accounted for 16.8% of the total oil for *Lolium perenne* but only 3.1% of that for *Bromus hordeaceus*.

Comparison of the volatile compounds of *Lolium perenne* oil with those in the *Bromus hordeaceus* oil shows there are qualitative and quantitative differences between the two oils. These chemical differences most probably arose because the oils were obtained from different plant subspecies. The oils of both species are rich in eugenol and methyleugenol, and the phenols present at high concentrations can be considered as substitutes for *Lolium perenne* and *Bromus hordeaceus* oils in medicinal applications. Eugenol is known to be an antioxidant in oleaginous foods, and is used as an antiseptic in odontology for root (canal) therapy, as an anticarminative, antispasmodic, and antiseptic in pharmacology, and as an antimicrobial agent.

CONCLUSION

This report identifies *Lolium perenne* and *Bromus hordeaceus* (cosmopolitan grasses) as new sources rich in eugenol.

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