

GC-MS ANALYSIS OF THE ESSENTIAL OIL OF THE FRUIT OF *Bunium persicum*

B. E. Abduganiev, Ya. V. Rashkes,*
and V. N. Plugar'

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The fruit of *Bunium persicum* Boiss (zira) is an extremely popular seasoning for meat dishes in Central Asia. It is also widely used in folk medicine [1]. The composition of the essential oil of *B. persicum* has been studied by A. S. Sadykov [sic] et al., and by the GLC method they established the presence of nine compounds of the C₁₀ series, two of which — *p*-cymene and cumaldehyde — were isolated in the pure form and identified [2].

We have studied the essential oil of this plant once more, with the aid of chromato-mass spectrometry using a capillary column and the computer treatment of the spectra, including a library search program, without the use of standards or the preparative isolation of pure components.

MS 25RF instrument (Kratos) with a Carlo Erba 5163 chromatograph, a 0.3 mm × 25 m WCOT column with the phase CP-Sil-5, programming of the temperature from 27 to 100°C and from 100 to 250 °C at rates of 5 and 10 deg/min, respectively, carrier gas He, rate of flow 3 ml/min, temperature of the EI/CI source 250°C. DS-90 data-processing system.

The essential oil of the fruit of the Okpar variety of *B. persicum*, gathered in the Kulyarb province of the Republic of Tadzhikistan was obtained by steam distillation in a yield of 2.75%. Under the chromatographic conditions given above we observed 13 peaks. As result of the library search, nine compounds were identified unambiguously, while the mass spectra corresponding to the apices of four chromatographic peaks did not exclude the presence of alternative structures.

In the quantitative respect, agreement about six components is observed in the two sets of results. We did not detect camphor and the linear monoterpenoids citral and citronellol. At the same time, by the GC-MS method we found seven new compounds. The main feature of the previous results [2] is the predominance of aromatic derivatives of the C₁₀ series, with a considerable contribution of bicyclic terpenes having a pinane skeleton. In the second set of results, the first of the features mentioned is retained, but at the same time there was a redistribution in favor of the oxidation products of *p*-cymene and cumaldehyde. The presence of oxidized products was characteristic for the material to which these results relate. Thus, two compounds each with a mol. mass 150 made up almost half the total. The spectrum of the first of them agreed well with that of an aldehyde of the safranane series — safranal — but it may also correspond to limonenone, which is biogenetically close to the material under consideration. The second compound was identified as myrtenal — an α -pinene derivative.

Thus, in the case under consideration, α -pinene and a product of its oxidation were more common than β -pinene, in contrast to the essential oil studied previousl [2]. At the same time, the spectrum assigned to α -pinene resembles to no small degree the spectra of the menthadienes (β - or γ -terpinenes). The total material contained products of the oxidation of terpinenes or of limonene. The spectrum of one of the compounds contained an intense peak of the (M - 31)⁺ ion, and, consequently, its molecule included a hydroxymethylene group, like perillyl alcohol (*p*-mentha-1,8(9)-dien-7-ol). Another alcohol corresponded to terpinenol-4 (4-methyl-1-(1-methylethyl)cyclohex-3-en-1-ol).

Two minor components, with mol. masses of 150 and 152, were not identified.

A peak of the sesquiterpenoid γ -cadinene was observed in the high-temperature part of the chromatogram.

* Deceased.

TABLE 1. Comparison of GLC [2] and GC-MS Results on the Composition of the Essential Oil of *B. persicum* Fruit

Compound	Mol. mass	Element. composition	Amount, %	
			GLC [2]	GC-MS
<i>p</i> -Cymene	134	C ₁₀ H ₁₄	19.15	2.8
β -Pinene	136	C ₁₀ H ₁₆	4.20	0.2
Limonene	"	"	0.92	0.9
α -Pinene (β - and γ -terpinenes)	"	"	2.10	10.4
Cumaldehyde	148	C ₁₀ H ₁₂ O	40.66	29.8
Thymol	150	C ₁₀ H ₁₄ O	1.31	1.1
Safranal (limonenone)	"	"	—	22.3
Myrtenal	"	"	—	24.2
Unidentified	"	"	—	1.1
Unidentified	"	"	—	0.7
Perillyl alcohol	"	"	—	5.0
Citral	"	"	0.39	—
Camphor	"	"	1.75	—
Citronellol	156	C ₁₀ H ₂₀ O	7.90	—
Terpinenol-4	154	C ₁₀ H ₁₈ O	—	1.0
γ -Cadinene	204	C ₁₅ H ₂₄	—	1.4

Thus, the possibility has been shown of the rapid identification of the main components of essential oils. For a more reliable identification of them by the GC-MS method, a computer search must be combined with an analysis of literature information on the relative retention times of monoterpenoids in the capillary GLC regime.

REFERENCES

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2. Yu. D. Sadykov [sic], M. Kubanov, Kh. Khafizov, and Yu. M. Begovatov, Dokl. Akad. Nauk Tadzh. SSR, **21**, No. 5, 33 (1978).