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COMPONENT COMPOSITION OF *Crambe orientalis*

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Crambe orientalis L. (*C. amabilis* Butk. et Majlun) belongs to the family Cruciferae, is a perennial herbaceous plant of height 30–80 cm, and grows wild in the Caucasus (eastern and southern foothills) and Central Asia (Tian-Shan, west) [1, 2] on dry stony and pebbly slopes in the lower and middle mountain belts and as a weed in plantings. The chemistry of this species of *Crambe* is little studied. Only the presence in the plant of phospholipids, vitamin C, trace elements [3], and fatty oil [4] has been reported. Seeds and fruit are rich (up to 25–35%) in fatty oil, which was shown to contain myristic, palmitic, stearic, oleic, arachic, arachidonic, erucic, linoleic, linolenic, palmitoleic, lignocerinic, eicosanoic, and eicosadienoic acids [4]. The fatty oil is suitable as food. Leaves and runners are used in the Caucasus as an antiscorbutic agent and in food as asparagus [5]. *C. orientalis* was introduced to Samarkand Oblast. The harvest of greens reaches 375–425 Cwt/ha [6]. It was tested as a promising feed plant [7, 8].

Alkaloids from this plant species were not previously studied. Plants of the family Cruciferae typically contain S-containing alkaloids [9]. The alkaloid composition of *C. orientalis* has not been reported. Only brief information on the alkaloid composition of *C. kotschyana* is available [10].

We studied the alkaloids and other low-molecular-weight metabolites of *C. orientalis* collected in the vicinity of Gazalkent, Tashkent Oblast. Quantitative determination of total alkaloids from roots and the aerial part collected at the end of vegetation (October 2010) found contents of 0.064 and 0.06%, respectively, of the air-dried raw material weight. Total alkaloids were extracted from the aerial part of the plant collected from this site.

The mixture of bases were extracted and isolated from the aerial part of the plant (11 kg) by EtOH (85%, 8×). The combined and condensed alcohol extracts were worked up with H_2SO_4 solution (5%, 6×). The acidic extracts were washed with benzene and made basic with NH_4OH solution (conc.) until the pH was 10–11. The alkaloids were extracted with $CHCl_3$ (6×). The $CHCl_3$ extracts were dried over anhydrous Na_2SO_4. The solvent was distilled off to afford total alkaloids (7.0 g). Analogously the mixture of bases (4.0 g) was obtained from roots (6 kg).

The $CHCl_3$ total alkaloids from the aerial part and roots that were obtained from this process were chromatographed over a column of silica gel with elution by hydrocarbons:$CHCl_3$ (1:1, system 1) to produce five fractions with similar R_f values. Rechromatography of these produced homogeneous fractions and isolated two known oily alkaloids with R_f 0.5 (goitrin) and 0.3 (goitridin) (TLC, silica gel, system 1) that were isolated previously from *C. kotschyana* [11].

The mother liquor from the $CHCl_3$ total was analyzed by GC–MS. Table 1 presents the results. The principal component of the mother liquor was buten-1-isothiocyanate (allyl isothiocyanate, allyl mustard oil). The hydrocarbons *n*-undecane and 4-methylhexene-1 were also detected.

The basic solution continued to show a reaction with silicotungstic acid for the presence of nitrogenous bases after separation of total tertiary bases. The aqueous alkaline solution remaining after isolation of total alkaloids was evaporated and taken to dryness (water-soluble fraction).

According to GC–MS analysis, this fraction consisted mainly of *N*-ethylpyrrolidin-2-one (Table 1).

Other low-molecular-weight metabolites of this plant were studied by extracting roots (2.1 kg) with EtOH (85%, 8×). The combined extracts were condensed to produce total extractive substances that were diluted with distilled H_2O (1:1 ratio) and worked up successively with extractive benzine (1), $CHCl_3$ (2), EtOAc (3), and *n*-BuOH (4). This produced four fractions, three of which (2–4) were analyzed by GC–MS (Table 1). The $CHCl_3$ fraction contained buten-1-isothiocyanate, *n*-undecane, 1-(ethylsulfinyl)-1,3-butadiene, and 5-isopropylidene-3-hydroxy-4-(2′-methylpropionyl)furanone-2 (principal component).

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TABLE 1. GC–MS Analysis of Fractions from *Crambe orientalis*

Fraction No.	Component	Mass spectrum, *m*/*z*	Retention time, min
1	Buten-1-isothiocyanate	113 (M^+), 86 (13), 72 (100), 55 (23)	4.615
2	*n*-Undecane		6.77
3	1-(Ethylsulfinyl)-1,3-butadiene	130 (M^+, 12), 114 (30), 85 (100), 71 (3), 57 (18)	10.834
4	5-Isopropylidene-3-hydroxy-4-(2′-methylpropionyl)furanone-2	210 (M^+, 28%), 182 (46), 153 (32), 124 (19), 95 (52), 70 (100)	24.069
5	2-Methoxyhexene-2	114 (M^+, 15), 85 (100), 70 (10), 55 (83), 41 (22)	10.829
6	3-Methoxy-4-hydroxystyrene	150 (M^+, 100), 135 (75), 107 (33), 77 (27), 53 (8)	12.168
7	*N*-Ethylpyrrolidin-2-one	113 (M^+, 85), 98 (100), 84 (34), 70 (47), 58 (76)	6.262
8	5-Methylfurancarboxyaldehyde-2	110 (M^+, 100), 84 (11), 70 (16), 53 (52)	4.328

The EtOAc fraction showed the presence of buten-1-isothiocyanate and the hydrocarbons *n*-undecane, 2-methoxyhexene-2 ($C_7H_{14}O$), and 3-methoxy-4-hydroxystyrene.

The principal component of the BuOH fraction was the hydrocarbon *n*-undecane. The GC–MS also detected buten-1-isothiocyanate, *N*-ethylpyrrolidin-2-one, and 5-methylfurancarboxyaldehyde-2 (Table 1).

The GC–MS analytical data that were obtained from a library search were confirmed by mass spectra of the detected compounds. Table 1 presents the results.

The component composition of the aerial part and roots of *C. orientalis* were similar and differed little from each other.

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