LIPIDS AND LIPOPHILIC COMPONENTS OF THE AERIAL PART OF Daucus sativus

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UDC 547.915:665.33

The benzene extract of the aerial part of Daucus sativus is analyzed. Sterols, aliphatic alcohols and their esters, triterpenes, and isoprenes make up >50% of the extract mass. Carotenoids, α -tocopherol, and other biologically active substances are also observed.

Key words: Daucus sativus, lipids, fatty acids, carotenoids, alcohols.

The aerial part of most plants contains biologically active substances such as triterpenes, aliphatic and isoprenic alcohols and sterols and their esters, carotenoids, tocopherols, essential fatty acids, etc. These possess various pharmacological activity. Tonic effects on the central nervous and cardiovascular systems and antitumor, antihypercholesteremic, analgesic, and anti-inflammatory activities have been found [1-5]. It was also found that these compounds normalize lipid exchange [3].

Therefore, we analyzed several samples of two varieties (Early-ripening and Jizak) of the aerial part of *Daucus sativus* (Hoffm.) Roche (seed carrot) of the Apiaceae (celery) family for the presence of biologically active substances. For this, air-dried and ground raw material was extracted with benzene to isolate the total lipids and lipophilic substances, which make up 0.7-0.9% of the mass of starting material. The acid number of the extracted substances is 11.0-14.6 mg KOH. The carotenoid content varied in the range 600-1056 mg%.

The composition of the extracted substances was established using carrot tops, which are harvesting waste. The total lipids and lipophilic substances were isolated from this material by benzene. They were separated into fractions by column chromatography (CC) on silica gel. The substances were identified by qualitative reactions and spectral characteristics. Their content was determined gravimetrically.

It was found that aliphatic alcohols, isoprenes, triterpenes, and sterols make up \sim 35% of the extract mass; esters of aliphatic alcohols and sterols with fatty acids, 25.0%; triacylglycerides, free fatty acids, hydrocarbons, tocopherols, carotenoids, and esters of phthalic acid, 20.0%; unidentified substances, 20.0%.

The composition of fatty acids obtained from the total lipid extract was as follows according to GLC, % of acid mass: 10:0, 0.7; 12:0, 10.7; 14:0, 3.2; 15:0, 3.2; 16:0, 6.0; 16:1, 2.3; 17:0, 1.7; 18:0, 13.6; 18:1, 4.2; 18:2, 15.1; 18:3, 35.0; 20:0, 4.3. According to mass spectra, five molecular ions with m/z 340, 368, 396, 424, and 452 were found in addition to the acids noted above. These are assigned to saturated components in the series 22:0-30:0.

The essential acids 18:2 and 18:3 make up >50.0% of the total fatty acids.

Mass spectra of esters exhibit peaks for molecular ions; groups of fatty-acid fragment peaks [RCO0]⁺, [RCO]⁺, [RCO₂H₂]⁺ of the series 10:0-30:0, 18:1, and 18:2; and fragment peaks corresponding to aliphatic alcohols $C_{16:0}$, $C_{18:0}$, $C_{20:0}$, and $C_{21:0}$ and β -sitosterol. According to the mass spectrum, the molecular ion with m/z 676 belongs to the ester of β -sitosterol with 18:2 acid. The remaining peaks correspond to esters of saturated aliphatic alcohols and fatty acids.

Separation of the total extracted substances by CC isolated two fractions of phthalic-acid esters. The mass spectrum of the less polar phthalate fraction contained base peaks characteristic of dioctylphthalate. Esters of lower molecular weight, octylpentyl- and octylbutylphthalates, which can be assigned to lower-molecular-weight esters, were identified in the more polar phthalate fraction.

The tocopherol fraction contained peaks that belong to α -tocopherol.

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The mass spectrum of the alcohol fraction has peaks with m/z 426 (M⁺), 411, 218, and 203, which unambiguously indicate the presence of α - and/or β -amyrins and C_{18:0} and C_{20:0} aliphatics (m/z 252 and 280 [M - 18]⁺) and isoprenic alcohols of geranylgeraniol [M⁺, 290], farnesol [M⁺, 222], and phytol [M⁺, 296].

 β -Sitosterol (m/z 414 [M⁺]), stigmasterol (m/z 412 [M⁺]), and campesterol (m/z 400 M⁺]) were identified in the sterol fraction.

EXPERIMENTAL

GLC was performed on a Chrom 41 instrument with a flame-ionization detector. A 2000×4 mm column packed with 17% PEGS on Chromaton W was used at 198°C with He carrier gas.

CC of the extract was carried out on a L 100/250 mesh silica-gel column with elution by hexane with a gradually increasing concentration of diethylether (10, 20, 30, 40, 50, 100%).

Total lipids were hydrolyzed by 10% KOH in CH₃OH with boiling for 1 h using 1 g extract per 10 mL of alkaline solution.

The carotenoid content was established using method FS 42-2067-83 [6].

The acid number was determined by the literature method [7].

Mass spectra (MS) of the substances were recorded on an MX-1310 instrument at 40/50 eV ionizing-electron energy and ionization-chamber temperature 170/100°C.

MS of esters, m/z (I_{rel} , %): 706 (0.5), 704 (0.5), 676 (0.8), 648 (2.7), 634 (0.5), 632 (0.3), 620 (5.7), 618 (0.8), 606 (0.8), 592 (11.1), 590 (1.6), 578 (1.3), 564 (100.0), 550 (3.2), 548 (1.6), 546 (1.1), 536 (39.7), 534 (14.3), 522 (17.5), 508 (25.4), 506 (5.0), 494 (27.0), 480 (12.7), 466 (15.9), 452 (17.5), 438 (23.8), 424 (27.0), 410 (25.4) [M]⁺; 435-155 [RCO]⁺; 453-173 [RCOOH₂]⁺, 396, 294-224 [R' - 1]⁺.

MS of nonpolar fraction of phthalate esters, *m/z*: 390 (M⁺), 279, 261 (octyl-), 167, 149, 83, 70, 57, 43, 41. MS of polar fraction of phthalate esters, *m/z*: 348 (M⁺), 279, 261 (octyl-), 237, 219 (pentyl-), 223, 205 (butyl-), 167,

149, 113, 112, 85, 83, 81, 77, 71, 70, 57, 55, 43, 41.

MS of tocopherol fraction, *m*/*z* (*I*, %): 430 (M⁺, 44.4), 205 (15.6), 177 (11.1), 165 (100.0), 164 (44.4).

MS of aliphatic and triterpenic alcohols, *m/z*: 426, 419, 411, 390, 378, 372, 346, 336, 323, 316, 306, 296, 290, 280, 278, 263, 256, 252, 250, 222, 218, 208, 203, 201, 196, 193, 189, 185.

MS of sterols, *m/z* (*I*_{rel}, %): 414 (M⁺, 69), 412 (M⁺, 100), 400 (M⁺, 7), 397, 396, 394, 385, 382, 381, 379, 374, 369, 367, 351, 324, 315, 314, 300, 289, 273, 271, 255, 231, 213.

REFERENCES

- 1. S. N. Hooper, R. F. Chandler, E. Lewis, and W. D. Jamilson, *Lipids*, 17, 60 (1982).
- 2. R. F. Chandler, S. N. Hooper, D. L. Hooper, W. D. Jamilson, and E. Lewis, *Lipids*, 17, 102 (1982).
- 3. E. P. Parfent'eva, Yu. K. Vasilenko, L. I. Lisevitskaya, and E. T. Oganesyan, Vopr. Med. Khim., 174 (1980).
- 4. A. K. Bhattacharaya, *Experientia*, **38**, 1037 (1982).
- 5. S. P. Kochhar, Prog. Lipid Res., 22, 161 (1983).
- 6. Addendum to the USSR State Pharmacoepia, Xth Ed., Moscow (1986), Vol. 3, p. 321.
- 7. Handbook of Research Methods, Technical Monitoring, and Production Accounting in the Oil—Fat Industry [in Russian], VNIIZh, Leningrad (1967), Vol. 1, Book 2, p. 887.