Blackberry Flavor Components of Commercial Essence

A commercial essence of Evergreen blackberries (*Rubus ulmifolius inermis*) was extracted with ethyl chloride. Sixteen volatile compounds were identified in the extract by combined gas chromatography-mass spectrometry. Compounds identified included acetals, esters, alcohols, ketones, terpenes, and an aromatic.

The flavor components of blackberries have received little attention. Nursten and Williams (1967) omitted blackberries from their review of fruit flavor components for lack of published results.

Characterization of commercial fruit essences provides a valuable preliminary approach to studying fruit flavors, since quantities of volatile compounds greater than those readily isolated in the laboratory are available for analysis. However, the possibility of encountering artifacts resulting from commercial conditions must not be disregarded by the investigators.

EXPERIMENTAL METHODS

An essence of Evergreen variety blackberries (*Rubus ulmifolius inermis*) was obtained from a commercial juice-concentrating operation. The essence was observed to have characteristic fresh blackberry aroma. Extraction of a sodium chloride-saturated 100-ml portion of essence with three 50-ml portions of redistilled ethyl chloride was carried out in a separatory funnel at 0° C. The ethyl chloride extract was dried overnight over anhydrous sodium sulfate, and then concentrated at room temperature in a pear-shaped flask fitted with a drying tube. About 25 μl of an oily mixture having an intense blackberry aroma was obtained.

Separation of the mixture was accomplished with gas-liquid chromatography (glc) on a 300-ft by 0.01-in. i.d. stainless steel capillary column coated with butanediol succinate. The column was programmed from 75° to 200° C at a rate of 4° C per min, and then held at 200° C for 1.5 hr. For tandem operation with an Atlas CH-4 mass spectrometer, the end of the capillary column was connected directly to the double ion source without the use of a helium separator, and the glc effluent was continuously monitored by the 20-eV ion source. Spectra of detectable components were obtained by means of the 70-eV ion source.

RESULTS AND DISCUSSION

The compounds identified in this study are listed in Table I. A dimethoxyallylbenzene which had the same glc retention time and mass spectral fragmentation pattern as authentic 3,4-dimethoxyallylbenzene was found in the essence. Although the position of the methoxy substituents is not known with certainty at this time, the musty odor of dimethoxyallylbenzene would seem to be important to the characteristic flavor of blackberries. A number of compounds were not identified. Further work is in progress to provide additional identifications, and to relate these data to fresh blackberries.

Table I. Compounds Identified by Gas Chromatography and Mass Spectrometry in a Commercial Blackberry Essence

Compound	Relative Retention Time Authentic	Unknown
1,1-Dimethoxyethane[a]	0.92	0.91
Ethyl acetate[a]	0.98	0.96
1,1-Diethoxyethane[a]	0.99	0.96
Ethanol[a]	1.00	1.00
2-Hydroxy-2-methyl-3-butene[a]	1.11	1.09
2-Methylbutanol[a]	1.16	1.21
2-Heptanone[b]	1.00	1.00
2-Heptanol[b]	1.24	1.25
1-Hexanol[b]	1.33	1.39
Cyclohexanol[b]	1.56	1.53
Linalool[c]	0.80	0.83
Terpinen-4-ol[c]	0.91	0.91
Borneol[c]	1.00	0.99
α-Terpineol[c]	1.00	1.00
Carvone[c]	1.06	1.06
Dimethoxyallylbenzene[c]	1.33	1.30

[a] t_R/t_R ethanol. [b] t_R/t_R 2-heptanone. [c] t_R/t_R α-terpineol

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Richard A. Scanlan
Donald D. Bills
Leonard M. Libbey

Department of Food Science and Technology
Oregon State University
Corvallis, Ore. 97331

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