

Loganberry Flavor Components of Commercial Essence

Acetaldehyde, 2-heptanone, ethyl acetate, ethyl butyrate, linalool, and α -terpineol were identified in a commercial essence of loganberry (*Rubus*

ursinus var. *loganobaccus*). An additional 14 carbonyls, seven esters, seven alcohols, one acid, and an ether were tentatively identified.

Due to the scarcity of information concerning the flavor components of loganberry, experiments were conducted to define chemically the compounds that contribute to the odor of a commercial grade loganberry essence. This knowledge could lead to a more realistic quality control of the product by food processors and could also be an aid for plant breeders when developing more productive varieties.

EXPERIMENTAL SECTION

An essence of loganberries (*Rubus ursinus* var. *loganobaccus*) was obtained from a commercial juice-concentration operation. The loganberry condensate was concentrated approximately 150 times. The recovered essence was colorless and possessed the characteristic fresh loganberry odor.

A portion of the 150-fold loganberry essence was analyzed for carbonyl compounds. This was accomplished by converting the carbonyls to the 2,4-dinitrophenylhydrazone derivatives, separating the resulting derivatives into classes using magnesium oxide adsorption columns (Schwartz *et al.*, 1962), and finally separating each class of carbonyls by chain length using hexane-acetonitrile-Celite partition columns (Corbin and Schwartz, 1960).

The identity of the individual carbonyl compounds was determined by comparing their characteristics on both partition columns and paper chromatography with that of known compounds. In some cases the identity was confirmed by mass spectrometry (ms).

A portion of the loganberry essence was extracted with ethyl chloride, the ethyl chloride was removed, and the resulting extract was subjected to analysis by gas chromatography (gc). Separation of the volatile constituents was accomplished using two 9-ft by $\frac{1}{8}$ in. stainless steel columns packed with 20% diethylene glycol succinate (DEGS) and Apiezon M on Celite 545. Tentative identification of the separated components was made by comparing their gc retention times with those of authentic compounds. Further credence to this method of identifying compounds was accomplished by repeating the separation using Apiezon M, a relatively nonpolar stationary phase. The identity of some components was confirmed using the tandem gc-ms technique described by Scanlan *et al.* (1970).

RESULTS AND DISCUSSION

A list of carbonyl compounds identified in this study is presented in Table I. Conclusive identification of acetaldehyde and 2-heptanone was made by ms. With the exception of acetaldehyde (1333 ppb) and acetone (150 ppb), all of the carbonyl compounds were below 50 ppb in the original loganberry. It is not known what significance these compounds might play in the characteristic odor of loganberries.

The compounds identified by gc retention times and gc-ms are listed in Table II. The retention time of compounds listed in Table II agreed to within at least 5% of the retention time of known compounds chromatographed on both polar and nonpolar analytical columns. In most cases the error did not exceed 2%.

Olfactory analysis of the various separated components issuing from the effluent splitter on the gc instrument indicated that the characteristic odor of loganberry is concentrated in the relatively high boiling volatile com-

Table I. Carbonyl Content of a Commercial Loganberry Essence

Compound	ppb ^a	Compound	ppb ^a
Acetaldehyde	1333	<i>n</i> -Heptanal	19
Propanal	6	Hept-2-enal	2
Acetone	160	2-Heptanone	27
<i>n</i> -Butanal	37	<i>n</i> -Nonanal	22
<i>n</i> -Pentanal	37	<i>n</i> -Decanal	20
Pent-2-enal	2	Undecanal	13
<i>n</i> -Hexanal	29	Dodecanal	19
Hex-2-enal	15	Tridecanal	19

^a Concentration of carbonyls in single-strength loganberry juice.

Table II. Compounds Tentatively Identified by Gas Chromatography in a Commercial Loganberry Essence

Ether	2-Methyl-1-butanol
Acetaldehyde ^a	Amyl alcohol
Ethyl acetate ^a	Hexyl acetate
Propyl propionate	Methyl heptanoate
Ethyl butyrate ^a	1-Hexanol
2,2-Dimethyl-1-pentanol	Methyl octanoate
3-Methyl-3-pentanol	Octan-2-ol
Ethyl valerate	Ethyl octanoate
1-Butanol	Linalool ^a
2-Heptanone ^a	α -Terpineol ^a
Methyl hexanoate	Hexanoic acid

^a Verified by mass spectrometry.

pounds. This includes linalool and α -terpineol, both conclusively identified by ms.

Additional work is needed to identify the remaining compounds in the relatively low boiling fraction of loganberry essence.

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