logical route for the formation of the C_n δ-lactones, it is not clear why, in contrast to γ-lactones, the only δ-lactones observed were those of equal carbon numbers to the parent fatty acids.

In contrast to the above argument, preferential oxygen attack toward the center of the fatty acid chain was concluded by Brodnitz et al. (1968), who chemically cleaved the reduced esters of oxidized methyl palmitate and analyzed the resulting mono- and dibasic acids, and by Selke et al. (1975), who heated tristearin in a stainless steel "microroom" and analyzed the volatiles by gas chromatography. The apparent contradiction may be due to the different oxidative conditions and analytical techniques employed by different investigators. On the other hand, it should also be kept in mind that hydroperoxides decompose rapidly at elevated temperatures. Higher amounts of specific hydroperoxides collected after thermal oxidation may reflect their relative stability rather than their selective formation.

ACKNOWLEDGMENT

The authors thank Regina Whiteman and Francois Gouin for their technical assistance.

LITERATURE CITED

Brodnitz, M. H.; Nawar, W. W.; Fagerson, I. S. *Lipids* **1968**, *3*, 65.
Crossley, A.; Heyes, T. D.; Hudson, J. F. *J. Am. Oil Chem. Soc.* **1962**, *39*, 9.
Endres, J. G.; Bhalerao, V. R.; Kummerow, F. A. *J. Am. Oil Chem. Soc.* **1962**, *39*, 159.
Jewell, N. E.; Nawar, W. W., submitted for publication in *J. Am. Oil Chem. Soc.*, 1980.
Kleinau, H. J.; Neitzel, C. *Fette, Seifen, Anstrichm.* **1970**, *72*, 1025.
Lien, Y. C.; Nawar, W. W. *J. Food Sci.* **1973**, *39*, 911.
Nawar, W. W.; Champagne, J.; Dubravcic, M.; LeTellier, R. *J. Agric. Food Chem.* **1969**, *17*, 645.
Selke, E.; Rohwedder, W. K.; Dutton, H. J. *J. Am. Oil Chem. Soc.* **1975**, 52, 232.
Witchwoot, A.; Nawar, W. W., University of Massachusetts, unpublished data, 1980.

Received for review April 17, 1980. Accepted August 11, 1980. The work was supported in part by University of Massachusetts Experiment Station Project No. 443 and a grant from the Army.

Isolation and Identification of Volatile Compounds from Baked Potatoes

Edward C. Coleman,[1] Chi-Tang Ho,* and Stephen S. Chang

The volatile flavor components were isolated from 540 lb of Idaho Russet Burbank baked potatoes. Extensive gas chromatographic analysis yielded 420 fractions. The odor of each chromatographic fraction was evaluated, and the fractions were identified by infrared and mass spectrometry. A total of 228 compounds was identified. The compounds identified in the volatiles of baked potatoes included hydrocarbons, acids, alcohols, aldehydes, esters, lactones, ethers, furans, halogenated hydrocarbons, ketones, pyrazines, oxazoles, thiazoles, and miscellaneous heterocycles. The most important compounds in baked potato flavor are the pyrazines, oxazoles, thiazoles, and a furanone.

The volatile flavor compounds isolated from baked potatoes have not been extensively studied because of the difficulty involved in obtaining an isolate from such a mild but characteristic flavor. Self and Rolley (1963) compared the total number of volatiles produced by baking with the total number of volatiles produced by boiling potatoes. They reported an increase in the amount of 2- and 3-methylbutanal during baking, which were thought to arise from the Strecker degradation of isoleucine and leucine, respectively.

Buttery et al. (1973) reported the identification of 45 compounds, mostly pyrazines and aliphatic aldehydes, as volatile flavor components of Washington Russet Burbank potatoes. The authors consider the following compounds to be the most important to baked potato aroma: 2-ethyl-3,6-dimethylpyrazine, methional, deca-*trans*,*trans*-2,4-dienal, and, possibly, 2-ethyl-3,5-dimethylpyrazine. These compounds have been previously identified by Deck et al. (1973) in potato chip aroma.

Pareles and Chang (1974) identified 16 compounds in the volatiles of baked potato. They have found that 2-isobutyl-3-methylpyrazine, 2,3-diethyl-5-methylpyrazine, and 3,5-diethyl-2-methylpyrazine, taken as a mixture, have an odor close in character to baked potato aroma.

The present study is a systematic chemical analysis of the volatile flavor components isolated from a natural baked potato flavor.

EXPERIMENTAL SECTION

Isolation of the Volatile Compounds from Baked Potatoes. The potatoes used for this study were Idaho Russet Burbank potatoes purchased from a local supermarket.

The potatoes used for baking were freed from adhering soil particles by thorough washing and scrubbing. After potatoes were baked whole with skin wrapped with aluminum foil at 205 °C for 105 min, the volatile compounds were isolated by the apparatus previously described by Chang et al. (1977). Nitrogen gas was used to remove the volatile compounds from baked potatoes. The samples and nitrogen gas were kept at 65 °C during the isolation period. The true aroma of baked potatoes was collected from the head space of the food as it exists under normal conditions; the flavor was not isolated from a water slurry of baked potatoes. Since the concentration of the flavor components in the space above the food is extremely low and a genuine baked potato aroma is very mild, it became necessary to run 18 isolations of 30 lb each. Isolations were run for 48 h. A total of 540 lb of baked potatoes was used. The total volatile isolate collected in traps cooled with dry ice and

Department of Food Science, Cook College, Rutgers, The State University of New Jersey, New Brunswick, New Jersey 08903.
[1]Present address: Whitestone, NY 11357.

0021-8561/81/1429-0042$01.00/0 © 1981 American Chemical Society

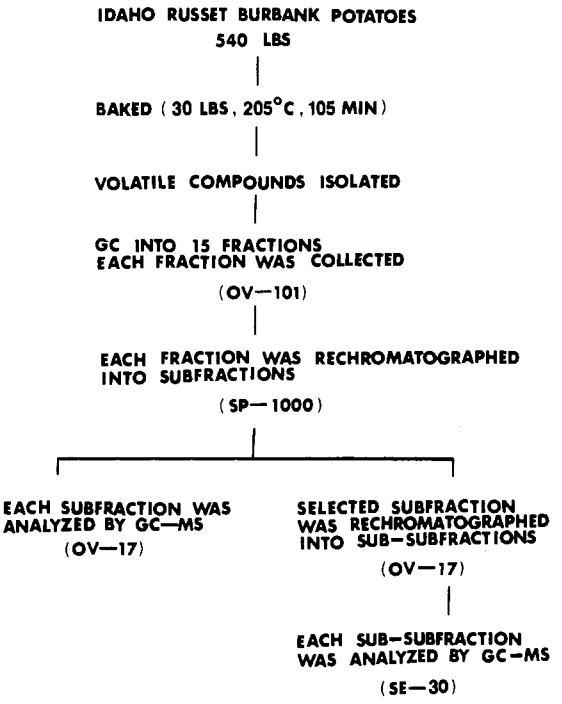

Figure 1. Flow diagram of the steps taken in the analysis of the baked potato volatiles.

acetone was treated in a manner similar to that described by Herz and Chang (1966). The condensate (pH 7) was saturated with NaCl and extracted with anhydrous ethyl ether. The ether extract (9000 mL) was dried with anhydrous sodium sulfate and then concentrated down to a final volume of 3 mL with the use of a 30-plate Oldershaw column and a 200-plate spinning band still. A flow diagram indicating the steps taken in the analysis of the baked potato volatiles is given in Figure 1.

Fractionation of the Flavor Isolate. The initial preparative chromatography of the baked potato flavor isolate was performed on a Beckman GC-55 gas chromatograph equipped with a flame ionization detector, fitted with a $^1/_8$ in. o.d. × 12 ft stainless steel column packed with 10% OV-101 on 80–100-mesh Chromosorb W. The flow rate was 30 mL/min with a column temperature which was programmed from 40 to 250 °C at a rate of 2.5 °C/min. The chromatogram (Figure 2) was divided into 15 broad fractions. Each broad fraction was successively collected according to the method of Thompson et al. (1978).

A second fractionation was performed on all 15 broad fractions using a $^1/_8$ in. o.d. × 12 ft stainless steel column packed with 10% SP-1000 liquid stationary phase on 80–100-mesh Chromosorb W. A third chromatography was performed on selected subfractions using a $^1/_8$ in. o.d. × 12 ft stainless steel column packed with 10% OV-17 liquid stationary phase on 80–100-mesh Chromosorb W. A total of 420 fractions were collected.

Identification of Gas Chromatographic Fractions. Each fraction in sufficient quantity for infrared spectroscopy was analyzed on a Beckman AccuLab 4 infrared spectrophotometer. A Hewlett-Packard instrument, Model 5992, mass spectrometer with a splitter interfaced with a Hewlett-Packard 5730 gas chromatograph was used for GC–MS analysis. A $^1/_8$ in. o.d. × 12 ft stainless steel column packed with 10% OV-17 was used for fractions which were chromatographed 2 times and a $^1/_8$ in. × 12 ft stainless steel column packed with 10% SE-30 was used for fractions which were fractionated 3 times. The flow rate was 28 mL/min, and the column temperature was programmed to provide maximum resolution of each fraction analyzed.

The procedure for the identification of the gas chromatographic fractions by the combination of infrared and mass spectrometry has been described previously (Deck et al., 1973).

Relative Concentration. The relative concentration of each chromatographic fraction was estimated by calculating the areas of the gas chromatographic peaks. The value of ethyl acetate, the most abundant compound, was defined as 1.00. The concentrations of other peaks relative to the concentration of ethyl acetate were listed in Table I.

RESULTS AND DISCUSSION

A total of 228 compounds was identified in the volatile flavor isolated from 540 lb of baked potatoes. Table I lists the compounds identified, indicating their fraction numbers and relative concentrations. The compounds identified consisted of 29 pyrazines, 17 ketones, 13 acids, 23 aldehydes, 22 alcohols, 19 esters, 14 halogen compounds, 3 thiazoles, 7 ethers, 2 oxazoles, 9 furans, 5 sulfur compounds, 11 nitrogen compounds, 14 saturated hydrocarbons, 38 unsaturated and aromatic hydrocarbons, and

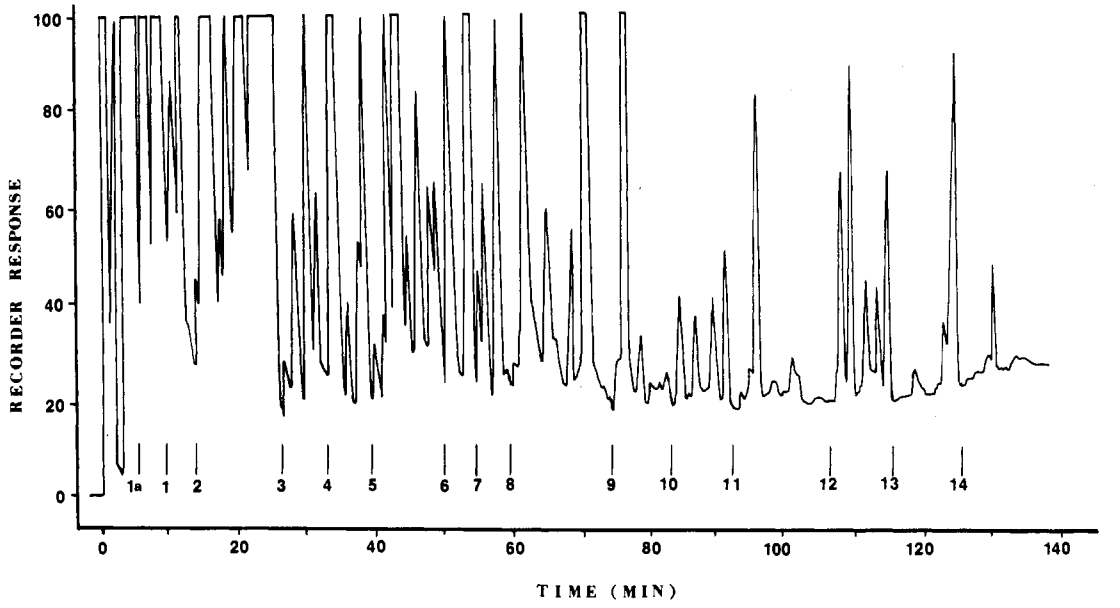

Figure 2. Broad gas chromatographic fractions of baked potato flavor.

Table I. Volatile Compounds Identified in Baked Potato Flavor

fraction no.	identifn	MS spectral identifn	IR spectral identifn	rel concn
	Saturated Hydrocarbons			
1-1-6	2,4-dimethylheptane	yes	no	0.06
11-7	2,6,9-trimethylundecane	yes	no	0.05
11-6	2,6,10-trimethylundecane	yes	no	0.11
10-8	4,6-di-n-propyldodecane	yes	yes	0.13
14-14	1-cyclopentyl-4-octyl-dodecane	yes	no	0.06
8-7	2-methyltetradecane	yes	no	0.09
11-5	2,6,10,14-tetramethylpentadecane	yes	no	0.09
12-21	5,7-dimethylhexadecane	yes	no	0.03
12-7	7,9-dimethylhexadecane	yes	no	0.06
12-23	2,6,11,15-tetramethylhexadecane	yes	yes	0.09
14-1	9-octylheptadecane	yes	yes	0.09
7-3	3-methyleicosane	yes	no	0.09
1-3-6	methylcyclopentane	yes	no	0.06
8-8	cyclododecane	yes	no	0.05
	Unsaturated and Aromatic Hydrocarbons			
2-9-3	3,5,5-trimethyl-1-hexene	yes	yes	0.07
7-3	2-ethyl-3-octene	yes	yes	0.16
7-14	4-ethyl-3-octene	yes	no	0.09
12-12	1-octadecene	yes	yes	0.12
6-4	1,4-dimethyl-4-vinylcyclohexene	yes	no	0.09
6-4	3-carene	yes	no	0.08
10-11	*trans,trans*-farnesene	yes	no	0.14
9-10	γ-humulene	yes	yes	0.13
8-16	limonene	yes	yes	0.19
6-4	myrcene	yes	no	0.08
8-18	β-phellandrene	yes	yes	0.12
8-20	β-pinene	yes	no	0.07
3-6	benzene	yes	no	0.01
2-6	toluene	yes	no	0.01
3-6	1,2-dimethylbenzene	yes	yes	0.21
3-7	1,3-dimethylbenzene	yes	no	0.07
3-6	1,4-dimethylbenzene	yes	yes	0.28
5-6	isopropylbenzene	yes	no	0.07
6-6	*tert*-butylbenzene	yes	no	0.16
8-17	*sec*-butylbenzene	yes	no	0.05
7-6	1,2,3,5-tetramethylbenzene	yes	no	0.07
8-18	hexamethylbenzene	yes	no	0.07
5-6	1-methyl-4-ethylbenzene	yes	no	0.07
10-13	nonylbenzene	yes	no	0.04
6-1	*o*-cymene	yes	yes	0.21
6-1	3-ethylstyrene	yes	yes	0.20
6-4	3,4-dimethylstyrene	yes	no	0.09
9-19	biphenyl	yes	no	0.06
10-24	diphenylmethane	yes	no	0.05
6-6	1-methylindan	yes	yes	0.21
6-6	4,5,7-trimethylindan	yes	no	0.09
9-18	1,2-dimethylnaphthalene[a]	yes	no	0.17
9-19	1,3-dimethylnaphthalene[a]	yes	no	0.06
10-19	2,7-dimethylnaphthalene	yes	no	0.05
10-15	2-isopropylnaphthalene[a]	yes	yes	0.31
10-25	1,3,8-trimethylnaphthalene	yes	no	0.04
10-26	1,4,5-trimethylnaphthalene	yes	no	0.07
9-14	1,4,6-trimethyl-1,2,3,4-tetrahydronaphthalene[a]	yes	no	0.06
	Acids			
1a-17-1	acetic acid	yes	no	0.07
2-13	propanoic acid	yes	no	0.06
1-1-2	2-methylpropanoic acid	yes	yes	0.60
1-4-2	butanoic acid	yes	yes	0.23
2-9-3	3-methylbutanoic acid	yes	yes	0.07
1-3-3	pentanoic acid	yes	yes	0.27
1a-17-1	2-methylpentanoic acid	yes	yes	0.07
1a-4-6	3-methylpentanoic acid	yes	no	0.09
1a-11	4-methylpentanoic acid	yes	no	0.05
2-7-10	hexanoic acid	yes	no	0.07
1a-17-2	2-methylhexanoic acid	yes	yes	0.09
1a-14	heptanoic acid	yes	yes	0.15
2-9-3	2-ketoadipic acid	yes	yes	0.07
	Alcohols			
1a-4-2	methanol	yes	no	0.06
1a-14	ethanol	yes	yes	0.14
1-2-1	2-butanol	yes	yes	0.21
3-12	3-methyl-1-pentanol	yes	yes	0.20
3-16	2-methyl-2-pentanol	yes	yes	0.33
1-2-7	2,4-dimethyl-3-pentanol	yes	no	0.09
1a-17	*cis*-2-pentenol	yes	yes	0.15

Table I (*Continued*)

fraction no.	identifn	MS spectral identifn	IR spectral identifn	rel concn
1-4-7	4-methyl-4-pentenol	yes	no	0.09
1-1-6	2-methyl-3-penten-2-ol	yes	no	0.06
1-4-7	2-methyl-1-penten-3-ol	yes	no	0.03
1a-4-3	heptanol	yes	no	0.07
8-8	3,6-dimethyl-3-octanol	yes	no	0.05
12-7	2-isobutyloctanol	yes	no	0.07
10-20	dodecanol	yes	no	0.06
12-17	hexadecanol	yes	no	0.07
1a-10	cyclohexanol	yes	yes	0.13
13-7	2-tetradecyloxyethanol	yes	no	0.03
11-5	hexahydrofarnesol	yes	yes	0.20
5-17	benzyl alcohol	yes	yes	0.13
7-12	trimethylbenzyl alcohol	yes	yes	0.10
9-16	3-methoxy-4-isopropylbenzyl alcohol	yes	no	0.08
8-20	naphthol	yes	no	0.04
	Aldehydes			
1-4-2	2-methylpropanal	yes	yes	0.33
1-1-3	2-methyl-2-propenal	yes	no	0.05
1-5-4	3-methyl-1-butenal	yes	yes	0.17
2-7-5	2-methyl-2-butenal	yes	no	0.06
1a-4-3	3-methyl-2-butenal	yes	no	0.07
2-7-7	pentanal	yes	yes	0.08
2-7-7	2-pentenal	yes	yes	0.08
9-16	4-methyl-2-phenyl-2-pentenal	yes	no	0.08
2-12-4	hexanal	yes	yes	0.27
2-7-7	*trans*-3-hexenal	yes	yes	0.21
5-10	2-ethylhexanal	yes	yes	0.16
10-10	5-methyl-2-phenylhexanal	yes	no	0.07
2-8	heptanal	yes	yes	0.63
6-1	nonanal	yes	yes	0.56
14-14	undecanal	yes	no	0.03
1-4-2a	hexadecanal	yes	no	0.05
12-17	octadecanal	yes	no	0.05
4-9	benzaldehyde	yes	yes	0.58
7-13	ethylbenzaldehyde	yes	yes	0.16
7-12	2,5-dimethylbenzaldehyde	yes	no	0.10
5-15	2-phenylacetaldehyde	yes	yes	0.03
9-15	*p*-methoxycinnamaldehyde	yes	no	0.06
8-20	salicylaldehyde	yes	no	0.04
	Esters and Lactones			
1-4-1	ethyl acetate	yes	yes	1.00
1a-6	1-methylpropyl acetate	yes	yes	0.15
1a-7	butyl acetate	yes	no	0.09
2-8	2-methylbutyl acetate	yes	no	0.06
1a-3	pentyl acetate	yes	no	0.05
3-9	hept-1-enyl 2-acetate	yes	no	0.09
1a-8	methyl 2-methylbutanoate	yes	no	0.10
1a-12	methyl pentanoate	yes	yes	0.10
2-9-3	2-methylbutyl pentanoate	yes	no	0.07
5-12	methyl 2-methylpentanoate	yes	yes	0.07
1-3-3	methyl hexanoate	yes	yes	0.11
10-22	allyl hexanoate	yes	no	0.09
1a-18	methyl octanoate	yes	yes	0.11
1a-17-1	methyl nonanoate	yes	no	0.07
10-19	diethyl phthalate	yes	no	0.09
13-7	diisobutyl phthalate	yes	no	0.03
12-19	diisobutyl isophthalate	yes	yes	0.14
10-28	phthalic anhydride	yes	yes	0.14
8-18	4-pyridoxic acid lactone	yes	no	0.08
	Ethers			
1a-3	methyl ether	yes	no	0.05
3-3	ethyl isopropyl ether	yes	yes	0.49
2-4	ethyl pentyl ether	yes	no	0.12
7-14	methyl nonyl ether	yes	no	0.09
10-17	diethylene glycol diethyl ether	yes	yes	0.24
11-11	1-ethoxy-1-propoxyethane	yes	no	0.09
2-3	1,1-diethoxyisopentane	yes	yes	0.13
	Furans			
3-14	2-furaldehyde	yes	yes	0.41
4-10	5-methyl-2-furaldehyde	yes	yes	0.14
5-1	2-acetylfuran	yes	yes	0.14
5-12	2-propionylfuran	yes	yes	0.07
5-3	2-pentylfuran	yes	yes	0.13
5-5	*trans*-2-(2-pentenyl)furan	yes	no	0.26
5-12	methyl furoate	yes	yes	0.07

Table I (*Continued*)

fraction no.	identifn	MS spectral identifn	IR spectral identifn	rel concn
3-12	2,5-dimethyltetrahydrofuran	yes	yes	0.20
2-11	2-methyltetrahydrofuran-3-one[a]	yes	yes	0.21
	Halogen Compounds			
2-12-4	chloroform	yes	no	0.21
1a-5-1	1,1,1-trichloroethane	yes	yes	0.13
1a-5-3	tetrachloroethylene	yes	yes	0.12
1-1-2	2-chloropropane	yes	no	0.05
4-4	1-chloro-2-methylbutane	yes	no	0.07
3-8	1-chloroheptane	yes	yes	0.07
4-3	1,1-dichloroheptane	yes	yes	0.20
13-7	1-chlorohexadecane	yes	yes	0.04
10-13	*o*-chloroaniline	yes	yes	0.04
11-12	*p*-chloroaniline	yes	yes	0.19
10-25	2-chlorobiphenyl	yes	no	0.03
1-6-5	trichloroacetic acid	yes	yes	0.03
11-6	2-bromo-5-ethylnonane	yes	no	0.11
12-6	1-iodooctadecane	yes	no	0.09
	Ketones			
2-3	acetone	yes	yes	0.12
1-3-1	4-methyl-2-pentanone	yes	yes	0.20
1-1-1	5-methoxy-2-pentanone	yes	no	0.06
2-8	4-methyl-3-penten-2-one	yes	no	0.07
2-5	2,6-dimethyl-3-penten-2-one	yes	yes	0.16
3-8	2-heptanone	yes	yes	0.07
1-5-9	4-heptanone	yes	no	0.04
1-5-9	2-methyl-4-heptanone	yes	no	0.04
2-9-1	2,6-dimethyl-4-heptanone	yes	yes	0.13
5-6	2-methyl-2-hepten-6-one	yes	no	0.07
5-6	3-octen-2-one	yes	no	0.07
9-6	4-decanone	yes	yes	0.15
1a-8	cyclopentanone	yes	yes	0.10
3-10	2,5-dimethyl-2-cyclopentenone	yes	yes	0.09
8-10	2-acetyl-3,3-dimethylcyclohexanone	yes	no	0.07
5-15	1-phenyl-1,2-propanedione	yes	no	0.03
5-4	*p*-methyl acetophenone	yes	no	0.08
	Oxazoles			
3-9	2,4,5-trimethyloxazole[a]	yes	yes	0.09
5-4	5-acetyl-2,4-dimethyloxazole[a]	yes	yes	0.09
	Pyrazines			
3-10	methylpyrazine	yes	yes	0.18
4-6	2,3-dimethylpyrazine	yes	yes	0.21
4-5-2	2,5-dimethylpyrazine	yes	yes	0.33
7-9	2,6-dimethylpyrazine	yes	yes	0.09
8-19	ethylpyrazine	yes	yes	0.13
5-1	2-ethyl-3-methylpyrazine[a]	yes	yes	0.19
5-7	2-ethyl-5-methylpyrazine	yes	yes	0.10
5-7	2-ethyl-6-methylpyrazine	yes	yes	0.10
5-8	2,3,5-trimethylpyrazine	yes	yes	0.17
5-5	2,3-diethylpyrazine	yes	yes	0.26
6-3	2-ethyl-3,6-dimethylpyrazine[a]	yes	yes	0.83
6-3	2-ethyl-3,5-dimethylpyrazine[a]	yes	yes	0.21
6-2	2-ethyl-6-vinylpyrazine[a]	yes	yes	0.26
8-14	2-butyl-3-methylpyrazine	yes	no	0.18
8-13	2-butyl-6-methylpyrazine	yes	yes	0.13
7-8	2-isobutyl-3-methylpyrazine[a]	yes	yes	0.21
7-9	2,3-diethyl-5-methylpyrazine[a]	yes	yes	0.09
7-9	3,5-diethyl-2-methylpyrazine[a]	yes	yes	0.09
8-17	2-ethyl-6-propylpyrazine	yes	no	0.07
7-8	2-ethyl-3,5,6-trimethylpyrazine[a]	yes	no	0.11
8-12	2,3-dimethyl-5-butylpyrazine[a]	yes	yes	0.07
8-10	2,5-dimethyl-3-butylpyrazine[a]	yes	no	0.07
8-12	2,6-dimethyl-3-butylpyrazine[a]	yes	no	0.09
8-17	2-methyl-6,7-dihydro-5*H*-cyclopentapyrazine[a]	yes	yes	0.06
7-11	5-methyl-6,7-dihydro-5*H*-cyclopentapyrazine[a]	yes	no	0.21
8-16	3,5-dimethyl-6,7-dihydro-5*H*-cyclopentapyrazine[a]	yes	yes	0.07
8-10	5,7-dimethyl-2,3,4,7,8-hexahydroquinoxaline[a]	yes	no	0.07
8-12	2,3,6-trimethyl-5-hydroxycyclopentapyrazine	yes	no	0.23
	Thiazoles			
9-13	2,5-dimethyl-4-ethylthiazole	yes	no	0.19
8-10	2,5-dimethyl-4-butylthiazole	yes	no	0.13
7-7	2,5-diethyl-4-methylthiazole[a]	yes	no	0.19

Table I (*Continued*)

fraction no.	identifn	MS spectral identifn	IR spectral identifn	rel concn
	Miscellaneous Nitrogen-Containing Compounds			
2-11	2-aminopyridine	yes	yes	0.13
3-2	2-acetylpyridine	yes	no	0.03
5-8	2-acetylpyrrole	yes	yes	0.14
5-13	*N*-methyl-2-formylpyrrole	yes	yes	0.05
4-7	*N,N*-diethylformamide	yes	yes	0.19
5-10	*N,N*-diethylacetamide	yes	no	0.13
11-16	diphenylamine	yes	yes	0.16
10-24	thymine	yes	no	0.05
5-3	cyanobenzene	yes	no	0.05
11-11	2-amino-4-nitrotoluene	yes	no	0.09
2-10	2-aminopentane	yes	yes	0.18
	Miscellaneous Sulfur-Containing Compounds			
10-17	thiophene	yes	yes	0.08
5-16	2-formylthiophene	yes	no	0.07
8-20	2-butyl-5-ethylthiophene	yes	yes	0.04
8-8	2-ethylhexyl mercaptan	yes	no	0.05
9-14	2-isopropylbenzimidazole	yes	no	0.06
	Miscellaneous Oxygen-Containing Compounds			
11-8	2-propyl-1,3-dioxolane	yes	no	0.19
1-3-6	2,4,6-trimethyl-1,3,5-trioxane	yes	yes	0.25

[a] Key compound in baked potato flavor.

2 miscellaneous compounds. Many of the compounds identified are being reported for the first time in potato flavor. The pyrazines, oxazoles, and thiazoles were found to be the most important classes of compounds in a genuine baked potato flavor.

Pyrazine Compounds. The most important class of compounds identified was the pyrazine compounds. Many of the pyrazines are being reported for the first time in baked potato or potato flavor. 2-Ethyl-6-vinylpyrazine was described as buttery, baked, and potato-like. 2-Ethyl-3-methylpyrazine contributed a pleasant earthy and nutty note to the total flavor. The alkylated five- and six-membered bicyclic pyrazines, namely, 5-methyl-6,7-dihydro-5*H*-cyclopentapyrazine, 5,7-dimethyl-2,3,4,7,8-hexahydroquinoxaline, 2-methyl-6,7-dihydro-5*H*-cyclopentapyrazine, 3,5-dimethyl-6,7-dihydro-5*H*-cyclopentapyrazine, and 2,3,6-trimethyl-5-hydroxycyclopentapyrazine, contribute very pleasant earthy, baked-potato-like aromas.

Oxazoles and Thiazoles. A number of thiazoles and oxazoles have been identified in coffee (Vitzthum and Werkhoff, 1974) and meat aroma (Peterson et al., 1975; Wilson et al., 1973). These two classes of heterocyclic compounds contributed important earthy and nutty notes to the total flavor of baked potato. 2,4,5-Trimethyloxazole and 5-acetyl-2,4-dimethyloxazole are being reported in potato for the first time.

Three thiazoles were identified in the volatile flavor of baked potato: 2,5-dimethyl-4-butylthiazole; 2,5-diethyl-4-methylthiazole; 2,5-dimethyl-4-ethylthiazole. The thiazoles have earthy, baked aromas similar to the pyrazines with the same alkyl-substituted groups.

Furans. Nine furan compounds were identified in baked potato flavor. *trans*-2-(2-Pentenyl)furan was identified for the first time in a food system by comparing its spectra with that of the authentic compound which was synthesized in our laboratory (Smagula et al., 1979). 2-Methyltetrahydrofuran-3-one was also identified. This furan may form in baked potato via a mechanism which involves the thermal degradation of thiamin. In general, the furans have green and fruity notes and may contribute to the total flavor of baked potatoes.

Other Heterocyclic Compounds. Three thiophenes, two pyrroles, two pyridines, one dioxolane, and one trioxane were identified in baked potato flavor. Many heterocyclic compounds have been reported in the aroma of coffee (Stoffelsma et al., 1968), meat (Ohloff and Flament, 1978a), and other foodstuffs (Ohloff and Flament, 1978b). Two oxygen-containing heterocyclic compounds, 2-propyl-1,3-dioxolane and 2,4,6-trimethyl-1,3,5-trioxane, are being reported for the first time in potato flavor.

Halogen Compounds. Fourteen halogen compounds, many are being reported for the first time in a food system, were identified in the volatiles of baked potato (Ho and Coleman, 1981).

Carboxylic Acids. Thirteen acids were identified in the volatile flavor of baked potatoes. The acids were characterized as having painty, fruity, acidic, and green notes. The acids in baked potatoes are formed as thermal oxidative decomposition products of the fat or by deamination of amino acids.

Esters and Lactones. Nineteen esters and one lactone were identified. Most of the esters were characterized as having green and fruity notes. In baked potato, the esters are formed as a result of esterification of the various alcohols and acids present in the flavor. 4-Pyridoxic acid lactone was identified. Lactones are thermal decomposition products of fats and have been identified in a number of food systems, including meat (Watanabe et al., 1971).

Alcohols. A large number (22) of alcohols was identified. Most of the simple straight-chain alcohols had green, painty odors. Some high molecular weight alcohols like hexadecanol and hexahydrofarnesol were identified. The mechanism by which most of the alcohols in baked potato is formed involves the decomposition of the hydroperoxides of the unsaturated fatty acids, and some may also form by the reduction of the carbonyl compounds which are present in baked potato flavor. Hydrofarnesol, a terpenoid alcohol, may originally be present in potatoes.

Aldehydes and Ketones. Seventeen ketones were identified. The simple saturated ketones, like 2-heptanone and 4-heptanone, were characterized as having painty, green, and fruity aromas. 2-Acetyl-3,3-dimethylcyclohexanone is a cyclic ketone which is being reported for the first time and was evaluated as having a buttery and earthy type aroma.

Twenty-three aldehydes were identified in baked potato flavor. A number of saturated aldehydes from C_4 to C_{10}

were identified and contributed buttery, green, and sour notes. It is interesting to note that no decadienals which have been previously identified in potato chips (Chang et al., 1977) and baked potato (Pareles and Chang, 1974) and contribute fried aromas to a flavor were identified in the genuine baked potato flavor analyzed in this research. The aldehydes found in baked potato flavor are formed by the decomposition of the hydroperoxides of the unsaturated fatty acids found in potato and by the Strecker degradation of many of the amino acids present in potato.

Saturated Hydrocarbons. Fourteen saturated hydrocarbons were identified. A number of these high molecular weight compounds contributed weak earthy and burnt aromas. These compounds are of little importance to the flavor.

Unsaturated Hydrocarbons. Thirty-eight unsaturated and aromatic hydrocarbons were identified in the volatile flavor of baked potato. The most interesting were the substituted naphthalenes. Seven naphthalenes were identified and characterized as possessing earthy notes which may be important to the total flavor of baked potatoes.

CONCLUSION

A natural and genuine baked potato flavor was isolated from 540 lb of baked potatoes as they exist under normal conditions. Baked potato flavor is a very mild flavor but is extremely complex; extensive chromatographic analysis yielded over 420 fractions. A total of 228 compounds was identified in baked potato flavor by a combination of infrared and mass spectrometry. The most important compounds in baked potato flavor (Table I, footnote *a*) are the pyrazines, oxazoles, thiazoles, and a furanone. The alkylated five- and six-membered bicyclic pyrazines were of particular interest because they are being reported for the first time in potato flavor and they contribute very pleasant earthy, baked-potato-like aromas. A chemical structure–flavor relationship was perceived among the trisubstituted pyrazines, thiazoles, and oxazoles. Nitrogen- and/or sulfur- and/or oxygen-containing heterocyclic compounds with identical substituents were found to have similar odor characteristics.

A number of alkyl-substituted naphthalenes were identified in the volatiles of baked potato flavor and were characterized as possessing flavor notes which contribute to the total flavor. Also, fourteen halogen compounds were identified in baked potato flavor which is interesting when their possible precursors are postulated. Potatoes, which contain a large number of amino acids and sugars, provide a reservoir of raw materials which yield a number of interesting flavor compounds under baking conditions to produce the very mild but characteristic flavor.

The identification of the volatile components of a natural food flavor like baked potato is significant because the pool of compounds which may be used to produce a synthetic baked potato flavor is increased and information on the volatile flavor compounds may also be of assistance to food processors in the quality control of baked potato and potato products. The quantitative data provided would be helpful to flavor chemists involved in the reconstitution of a natural baked potato flavor.

ACKNOWLEDGMENT

We thank Joan B. Shumsky for her excellent secretarial aid.

LITERATURE CITED

Buttery, R. G.; Guadagni, D.; Ling, L. C. *J. Sci. Food Agric.* **1973**, *24*, 1125.
Chang, S. S.; Vallese, F.; Hwang, L. S.; Hsieh, O.; Min, D. B. S. *J. Agric. Food Chem.* **1977**, *25*, 450.
Deck, R. E.; Pokorny, J.; Chang, S. S. *J. Food Sci.* **1973**, *38*, 345.
Herz, K. O.; Chang, S. S. *J. Food Sci.* **1966**, *31*, 937.
Ho, C.-T.; Coleman, E. C. *J. Agric. Food Chem.* **1981**, companion paper in this issue.
Ohloff, G.; Flament, I. *Heterocycles* **1978a**, *11*, 663.
Ohloff, G.; Flament, I. *Fortschr. Chem. Org. Naturst.* **1978b**, *36*, 231.
Pareles, S. R.; Chang, S. S. *J. Agric. Food Chem.* **1974**, *22*, 339.
Peterson, R. J.; Izzo, H. J.; Jungermann, E.; Chang, S. S. *J. Food Sci.* **1975**, *40*, 948.
Self, R.; Rolley, H. *J. Sci. Food Agric.* **1963**, *14*, 8.
Smagula, M. S.; Ho, C.-T.; Chang, S. S. *J. Am. Oil Chem. Soc.* **1979**, *56*, 516.
Stoffelsma, J.; Sipma, G.; Kettenes, D. K.; Pypker, J. *J. Agric. Food Chem.* **1968**, *16*, 1000.
Thompson, J. A.; May, W. A.; Paulose, M. M.; Peterson, R. J.; Chang, S. S. *J. Am. Oil Chem. Soc.* **1978**, *55*, 897.
Vitzthum, O. G.; Werkhoff, P. *J. Food Sci.* **1974**, *39*, 1210.
Watanabe, K.; Sato, V. *Agric. Biol. Chem.* **1971**, *35*, 756.
Wilson, R. A.; Mussinan, C. J.; Katz, I.; Sanderson, A. *J. Agric. Food Chem.* **1973**, *21*, 873.

Received for review May 21, 1980. Accepted October 10, 1980. This work was performed as a part of NJAES Project No. 10205 supported by the New Jersey Agricultural Experiment Station, Hatch-Regional Funds, NE-116. Paper of the Journal Series, New Jersey Agricultural Experiment Station, Cook College, Rutgers, The State University of New Jersey, New Brunswick, NJ 08903.