PERFUMER & FLAVORIST

GRAS Flavor Chemicals—Detection Thresholds

By John C. Leffingwell and Diane Leffingwell
Leffingwell & Associates, Canton, Georgia

The relative intensity of individual chemical odorants and flavorants is a subject that daily confronts those involved in the creation of fragrances and flavors. The actual measurement of such intensities has largely been restricted to the determination of "threshold values of detection." This is the value determined by panelists (usually a minimum panel of sixteen or more) at which the odor or flavor of a "pure" odorant can be detected. The measurement of threshold values is dependent on a number of factors: (a) experimental methodology, (b) screening of panelists for specific anosmia, (c) experience of panelists, (d) purity of odor/flavor chemical, and (e) sex and age makeup of panel and (f) the media in which the odorant is evaluated.

Addressing these points, one should be aware that various published values for detection thresholds—even reported from the same group of workers—do not always agreee exactly.

Regarding methodology, suffice it to say there are several generally accepted methods—e.g., the procedure described by Guadagni and Buttery[122], the procedure of Amoore[123] and others. A case in point regarding the effect of methodology on an odorant threshold determination is the example of Damascenone reported in 1978 by Ohloff on the components of Bulgarian Rose Oil[86](see also footnote 126 relative to the original threshold report).

"Continuing the determinations of threshold values of minor components, Pickenhagen found that the actual threshold of ß-damascenone is by a factor of 10^3 lower than reported here (10 ppb). The error is due to the fact that, at a certain level, which exceeds its threshold by a factor of around 1000, ß-damascenone seems to have a fatiguing

0272-2666/91/0001-0101$04.00/00—

Perfumer & Flavorist (ISSN 0272-2666)
An Allured Publication
Volume 16, Number 1

JANUARY/FEBRUARY 1991

effect and stays in the mouth. Thus by determining the threshold by a double triangle test against water, with descending concentrations, tasters frequently indicate the product to be in the blank too. The now found threshold concentration is 0.009 ppb and was determined using descending concentrations."

Now, this experiment also points out another problem—semantics—is the value determined a "flavor threshold" or an "odor threshold?" Ohloff appears to have intermixed values determined by different methodologies in some of his tabulations[37,86] and resolved the problem simply by labeling them as "threshold values." This is also the case in other publications[71] where reported "odor" thresholds may, in fact, be "flavor" thresholds. For the purist, this may be incorrect, but in most cases, detection thresholds determined by an acceptable procedure will provide the practicing flavorist a starting point from which to build his own judgements. Detection thresholds reported and discussed here are restricted to determinations in aqueous media.

For volatile non-ionizable odorants, such as damascenone, we believe that whether detected by smelling (external) or by placing in the mouth (internal) that the threshold determined is that of the "odor." However, with materials, such as isovaleric acid or trimethylamine which ionize in water—"taste" as well as "odor" may complicate the determination depending on technique. Similarly, non-volatile materials, such as caffeine and glycine, which have no odor, can only be evaluated based on the flavor or taste. Suffice it to say that in the tabulation presented in this review, we consider that the variations in reported "odor" and "flavor" thresholds reflect primarily different methodologies. However, one particularly disturbing factor is prevalent in the literature. A number of workers will simply list chemical odor detection thresholds in publications and not indicate which have been newly determined, redetermined or simply restated based on prior published work.

If the values presented are consistent with earlier published values, of course, there is no concern, but when a threshold value for a product like benzaldehyde, which had previously been accepted as 350 ppb[10,45], suddenly is stated to be 3500 ppb,[88] one wonders if this is a "typographical" error or not. Similarly, the threshold value for 2-methylpyrazine has recently been listed as 60 ppb[10] when earlier publications indicated it to be 60000 ppb[32,120] and the lowest other reported value is 30000 ppb.[124]

Selection of panelists for determination of threshold values is of some interest since it is now generally accepted that women are more sensitive to odors than men. This was demonstrated by Koelega (118) and statistically seems to be confirmed by The National Geographic Smell Survey conducted in late 1986.[47] Age of respondents also appears to play a major role in acuity, with definite decreases occurring past age 50.[47,112] A series of papers from the conference on "Nutrition and the Chemical Senses in Aging" held in 1989 and published in the New York Academy of Science Annals provides insight into possible reasons for this loss of sensitivity.[112-115] Loss of sensitivity with age is not just restricted to detection threshold levels but also to impairment of the ability to discriminate foods and odors.[116,117] In addition, Amoore[38] reported that screening of 764 laboratory employees for one or more of six anosmia types resulted in 3% to 47% specific anosmias in various (odor) categories, with a general anosmia to all odors of 0.2%. In particular, the "urinous" odor of 5-α-Androst-16-en-3-one showed 47% of respondants as being anosmic while the "malty" odor of isobutyraldehyde showed 36% anosmics and the nature identical musk omega-cyclopentadecanolide (also known as Thibetolide or Exaltolide), 12% anosmics (as measured with aqueous solutions at sixteen times the "normal" threshold level).

Thus, with the caveat that a threshold detection level for one individual is not a threshold level for all, we can now begin to examine the utility of such reported values in the world of the practicing flavorist.

Guadagni et. al.[28] proposed the concept of "odor units" as a measure to assess the relative importance of individual chemical components present in a more complex aroma mixture. Since most foods consist of 70-90% water, the odor unit (U_o) value is obtained by dividing the concentration "C" (in ppb) of the chemical odorant in water by the thresold concentration "T" (in ppb) for that particular

chemical in water.

$$U_O = C/T$$

In theory, it has been presumed that the probability of a chemical odor being detected should be greater the larger the number of odor units for that chemical that are present. This concept has been tested rather successfully by scientists at the Western Regional Research Center of the USDA in Albany, California for a number of food flavors. Guadagni et al.(121) also suggested that the odor unit value for a mixture of volatile chemical odorants present in an aroma mixture was equal to the sum of the number of odor units for each of the individual constituents.

$$U_o \text{ (mixture)} = U_{o1} + U_{o2} + U_{o3} + \ldots.$$

It should be recognized that this simplistic approach is an approximation. For example, increases of odor intensity are often not directly linear with concentration(119) and any synergistic effects which may occur from the admixture of flavor chemicals cannot be accounted for by this approach. But, in the absence of anything better—and considering that, in most cases, the odor unit approach works—this technique is a very valuable tool for the flavor chemist. Utilization of the odor unit concept for assessing the relative importance of flavor chemicals determined in the analysis of volatile chemicals in a natural product now seems obvious. Why then has this procedure found such little actual use?

Many flavorists have been posed with the problem of duplicating the "natural" aroma/flavor profile of a product from compositional data determined by the highly sophisticated analytical techniques now available. But if one is faced with a chromatogram identifying 450 components (many of which may not be GRAS), the easy solution is to either forget the analysis and rely on the age-old art of pure creativity or to make a very complicated flavor. If the flavorist ignores the detailed analysis he risks being labeled as uncooperative, unappreciative and sin of all sins—unscientific.

The concept of utilizing odor units and threshold values at least provides both the analytical scientist and the creative flavorist the opportunity to constructively collaborate in the conversion of an impractical aroma reconstruction from hundreds of chemicals (most of which are probably of minor importance) to a handful which are likely to be the key components (even if only present in the original aroma in trace quantities). All of a sudden, that impractical analysis may be usable afterall, especially with a little creative flavor work to round out the rough edges.

In recent years, a number of examples of this concept have been published in the scientific journals. Yet few flavorists actually utilize the technique because the necessary threshold values required to construct the odor unit values are spread out in various journals (and in many cases are not reported in consistent units—ppb, ppm, mg/liter, millimoles/mole, micrograms/kilogram, molar concentrations and log molar concentrations, etc.). In the table at the end of this article, we have provided a series of detection threshold values, all in the same units (ppb), so that a quick assessment as to the relative strength can be made by those utilizing the table.

In preparing this article, we realized that without at least one practical example of the utility of using threshold data and the odor unit concept that this tabulation would probably gather dust on the shelves of most flavorists.

An example of using threshold data and the odor unit concept in constructing a flavor is shown for cooked rice. Table I lists the quantitative values of 17 major components of cooked rice (out of more than 100 reported in the literature). In this example (Buttery, 1988), all of the components reported here are GRAS with the exception of 2-acetyl-1-pyrroline whose odor threshold value is known to be 0.1 ppb.

TABLE I

MAJOR VOLATILE AROMA CONSTITUENTS OF COOKED RICE (10)

FEMA No.	Chemical	Concentration (in ppb)	Odor Threshold	No. of Odor Units
2858	2-Phenethyl alcohol	90	1000	0.09
2557	Hexanal	12	5	2.4
2782	Nonanal	3	1	3
3739	4-Vinylphenol	2	10	0.2
2675	4-Vinylguaiacol	2	3	0.7
2362	Decanal	2	2	1
3317	2-Pentylfuran	1	6	0.2
2797	Octanal	0.9	0.7	1.3
2540	Heptanal	0.7	3	0.2
2127	Benzaldehyde	0.7	350	0.002
	2-Acetylpyrroline	0.6	0.1	6
3165	(E)-2-Heptenal	0.4	13	0.03
2567	Hexyl alcohol	0.4	2500	0.0002
3135	(E,E)-2,4-Decadienal	0.4	0.07	5.7
2789	Nonyl alcohol	0.2	50	0.004
3213	(E)-2-Nonenal	0.1	0.08	1.2
2366	(E)-2-Decenal	0.05	0.4	0.1

*Adapted from Buttery et. al., J. Agric. Food Chem., 36, 1007 (1988)

TABLE II

COOKED RICE FLAVOR RECONSTRUCTION

INGREDIENTS	RELATIVE AMOUNTS A	B
2-Phenethyl alcohol	90.00	90.00
Hexanal	12.00	12.00
Nonanal	3.00	3.00
Octanal	0.90	0.90
(E)-2-nonenal	0.10	0.10
Hexyl alcohol	0.40	0.40
(E,E)-2,4-Decadienal	0.40	0.40
2-Acetylthiazole	60.00	0.00
2-Acetylpyrazine	0.00	372.00
Total	166.80	478.80

Accordingly, from the table we find that even though phenethyl alcohol is present at levels 150 times higher than 2-acetylpyrroline, its odor unit value is only 1.5% as great. Obviously from the number of odor units, 2-acetylpyrroline (which possesses a strong popcorn aroma) and 2,4-decadienal with its fatty, tallowy character are two of the major flavor impact compounds of cooked rice. Since 2-acetylpyrroline is not GRAS, the creative flavorist could utilize either 2-acetylpyrazine, 2-acetyl thiazole or 2-acetylpyridine as these all have similar odor profiles. But which is mot cost effective? While none has a lower odor threshold than 2-acetylpyrroline (0.1 ppb), at least based on threshold data, it appears that 2-acetylthiazole with a threshold of 10 ppb is a better choice than 2-acetylpyrazine (threshold of 62 ppb). On a pure cost basis, 2-acetylpyridine (threshold level of 19 ppb) is the least expensive choice, however, its flavor is somewhat less desirable.

Having made the decision to evaluate both 2-acetylthiazole and 2-acetylpyrazine in applications, one needs to know the amount required to (theoretically) match the odor value contribution of the 2-acetylpyrroline to be replaced. In order to determine the concentration of 2-acetylthiazole necessary to have an odor unit value equal to the 2-acetylpyrroline in Table I (a value of 6 odor units), one uses the equation -

Concentration = Odor units x Threshold

wherein the threshold value utilized is that of 2-acetylthiazole (10 ppb):

Concentration = 6 x 10 ppb = 60 ppb (for acetylthiazole)

Similarly, one can apply the equation for 2-acetylpyrazine by using its threshold value (62 ppb):

Concentration = 6 x 62 ppb = 372 ppb (for acetylpyrazine)

Utilizing this technique, two cooked rice flavors were prepared with the goal of using no more than eight components.

Note that for the flavor chemicals employed (Table II), the units correspond to an exact replica of the amounts found (in ppb) from the analytical values in Table I, with the exception that the 2-acetylthiazole and 2-acetylpyrazine have been incorporated at levels which theoretically (based on odor unit values) replace the odor contribution of the non-GRAS component, 2-acetylpyrroline.

The two flavors "A" and "B" were diluted to a 0.5% solution each in benzyl alcohol and compared in odor to a commercial sample of Basmati Rice extract. Sample "B", although slightly stronger, was extremely close in odor profile to the commercial "aromatic" rice extract. Sample "A" possessed a more fatty character that was considered characteristic of non-aromatic cooked rice.

Sample "A" was added during cooking to unscented long grain cooked rice at a level of 166 ppb and compared to an unfortified control sample. The flavor of the fortified sample was judged to be well balanced and much richer in both aroma and taste, but possessed none of the characteristic "nutty" notes associated with the scented Basmati or Texamati types.

Sample "B" was added during cooking to unscented long grain cooked rice at a level of 478 ppb; the flavor of this sample was more aromatic, but not as "natural" in profile as sample "A". Panelists' comments indicated that while it possessed some of the notes of a Texamati sample, it lacked the nutty intensity. Compared to the unscented control rice, it was more aromatic, but slightly unbalanced.

Accordingly, with just two experiments, one of the two flavors (Sample "A"), provided a very good reconstituted cooked rice flavor. Sample "B", while not hitting the mark initially, was later modified into a Texamati-type flavor.

It should be noted that in the two synthetic rice flavors (Table II), the incorporation of 2-phenethyl alcohol and hexyl alcohol have negligible impact in the flavor and could theoretically be removed. Based on the odor unit concept, these two items contribute less than 0.5% to the sum of the odor unit values in these flavors.

In conclusion, odor detection threshold data can be useful in making judgements on use levels in flavor creation, as well as in planning flavor reconstructions. With the plethora of published data now available on the composition of natural food aromas, utilization of Guadagni's odor unit concept is an effective and inexpensive tool for simplifying the otherwise difficult problem of converting a complex flavor analysis into a "practical" flavor system.

In our labs, we have now collected threshold values in various media for about 22% of all chemicals which appear on the GRAS lists. Only detection thresholds in water media are provided in this tabulation.(125)

Address Correspondence to: John C. Leffingwell, Leffingwell & Associates, Route 1, Box 22, Arbor Hill Road, Canton, Georgia 30114

REFERENCES

1. Engle, K.-H., R. A. Flath, R. G. Buttery, T. R. Mon, D. W. Ramming and R. Teranishi, J. Agric. Food Chem., 36, 549-553 (1988)
2. Takeoka, G. R., R. A. Flath, T. R. Mon, R. Teranishi and M. Guentert, J. Agric. Food Chem., 38, 471-477 (1990)
3. Shaw, P. E., J. Tatum, T. Kew, C. Wagner Jr.and R. Berry J. Agric. Food Chem., 18, 343-345 (1970)
4. Fors, S. "Sensory Properties of Volatile Maillard Reaction Products And Related Compounds" in The Maillard Reaction in Foods and Nutrition, ACS Symposium Series 215, G. R. Waller and M. S. Feather, Editors, ACS, Washington, pp. 185-286 (1988)
5. Mulders, J. Z. Lebensm. Unters. Forsch., 151, 310-317 (1973)
6. Hartung, L. D., E. G. Hammond and J. R. Minor Livestock Waste Management Pollution Abatement, Int. Symp. Proc., 105-106 (1971)
7. Flath, R. A., D. R. Black, D. G. Guadagni, W. H.

McFadden and T. H. Schultz J. Agric. Food Chem., **15**, 29-35 (1967)
8. Harrison, G. J. Inst. Brewing, **76**, 486-495 (1970)
9. Mielgard, M. Master Brew. Assn. Am. Tech. Quart., **12**(3), 151-168 (1975)
10. Buttery, R. G., J. G. Turnbaugh and L. C. Ling, J Agric. Food Chem., **36**(5), 1006-1009 (1988)
11. Guadagni, D. G., R. G. Buttery and S. Okano, J. Sci. Food Agric., **14**, 761-765 (1963)
12. Amoore, J. E., L. J. Forrester and P. Pelosi, Chem. Senses & Flavor, **2**(1), 17-25 (1976)
13. Fazzalari, F. A., editor, Compilation of Odor and Taste Threshold Data, ASTM Data Series DS 48A (1978)
14. Lea, C. H., and P. A. T. Swoboda, Chem Ind. (London), 1289-1290 (1958)
15. Siek, T. J., I. A. Albin, L. A. Sather and R. C. Lindsay J. Food Sci., 34, 265 (1969)
16. Day, E. A., D. A. Lillard and M. W. Montgomery J. Dairy Sci., **46**, 291-294 (1963)
17. Amoore, J. E., L. J. Forrester and R. G. Buttery J Chem. Ecol., **1**, 299-310 (1975)
18. Griffiths, N. M., Chem. Senses Flavor, 1, 187 (1974); abstracted from reference 13. 19. Baker, R. A., J. Am. Water Works, **55**, 913-916 (1963)
20. Kieth, E. and J. Powers, J. Food Sci., **33**, 213-218 (1968)
21. Buttery, R. G., R. M. Seifert, D. G. Guadagni, D. R. Black and L. C. Ling J. Agric. Food Chem., **16**, 1009-1015 (1968)
22. Golovnja, R. V. and M. Rothe Nahrung, **24**, 129-139 (1980)
23. Guadagni, D. G., Am. Perf. Cosm., **82**, 43 (1967)
24. Lindsey, R. C., J. Dairy Sci., **52**, 1198 (1969); abstracted from reference 13.
25. Wick, E. L. Food Technology, **20**, 1549 (1966); abstracted from reference 13.
26. Patton, S., Food Research, **22**, 316 (1957); abstracted from reference 13.
27. Salo, P., J. Sci. Food Agric., **21**, 597 (1970); abstracted from reference 13.
28. Guadagni, D. G., R. G. Buttery and J. Harris, J. Sci. Food Agric., **17**, 142-144 (1966)
29. Amoore, J. E. and D. Venstrom, J. Food Sci., **31**, 118-128 (1966)
30. Wasserman, A. E., J. Food Sci., 31, 1005 (1966); abstracted from reference 13.
31. Boehlens, M. H. and J. van Gemert, Perfumer & Flavorist, 12(5), 31-43 (1987)
32. Guadagni, D. G., R. G. Buttery and J. Turnbaugh, J. Sci. Food Agric., **23**, 1435-1444 (1972)
33. Meijboom, P. W., J. Am. Oil Chem. Soc., **41**, 326-328 (1964)
34. van Gemert, L. J. and A. H. Nettenbreijer, Editors Compilation of Odor Threshold Values in Air and Water; RID, CIVO-TNO, Zeist, The Netherlands (1977)
35. Patton, S., J. Food Sci., **29**, 679 (1964)
36. Sega, G. M., M. J. Lewis and M. H. Woskow, Proc. Am. Soc. Brew. Chem., 156-164 (1967)
37. Ohloff, G., "Recent Developments in the Field of Naturally-Occurring Aroma Components", Prog. Chem. Org. Nat. Prod., 35, 431-527 (1978)

38. Amoore, J. E., Chem. Senses Flavor, 2(3), 267-281 (1976)
39. Palamand, S. R. and W. A. Hardwik, Master Brew. Assn., Am. Tech. Quart., 6, 117-128 (1968)
40. Pietrzak, E. W. A., Acta Aliment. Polonia, 2, 207 (1976); abstracted from reference 13.
41. Patton, S.J., Dairy Sci., 37, 446-452 (1954)
42. Manning, D. J., J. Dairy Res., 40, 63,73 (1973); abstracted from reference 13.
43. Takeoka, G., R. G. Buttery, R. A. Flath, R. Teranishi, E. L. Wheeler, R. L. Wieczorek & M. Guentert, "Volatile Constituents of Pineapple" in Flavor Chemistry: Trends and Developments, ACS Symp. Series 388, R. Teranishi, R. G. Buttery and F. Shahidi, editors, ACS, Washington DC, pp. 221-237 (1989)
44. Cartwright, L. C., Food Technology, 6, 372 (1952); abstracted from reference 13.
45. Buttery, R. G., R. M. Siefert, D. G. Guadagni and L. C. Ling, J. Agric. Food Chem., 19, 524-529 (1971)
46. Buttery, R. G., R. Teranishi, R. A. Flath and L. C. Ling "Fresh Tomato Volatiles" in Flavor Chemistry: Trends and Developments, ACS Symp. Series 388, R. Teranishi, R. G. Buttery and F. Shahidi, editors, ACS, Washington, DC, pp. 211-222 (1989)
47. Wysocki, C. J. and A. N. Gilbert, Ann. New York Acad. Sci., 561, 12-28 (1989)
48. Collins, E., J. Agric. Food Chem., 19, 533-535 (1971)
49. Tressl, R., Monatsschr. Brau., 32(5), 240-248 (1979)
50. Rosen, A. A., J. Water Pollut. Control Assn.,35,777(1963); abstracted from reference 13.
51. Koehler, P. E., M. E. Mason and G. V. Odell, J. Food Sci., 36, 816-818 (1971)
52. Buttery, R. G., R. M. Seifert, D. G. Guadagni and L. C. LingJ. Agric. Food Chem., 17, 1322-1327 (1969)
53. Brule, G., P. Dubois and T. Obretenov, Ann. Technol. Agric., 20, 305-312 (1971)
54. Bergia, H. W., Food Technology, 9, 23 (1955): abstracted from reference 13.
55. Kirimura, J., J. Agric. Food Chem.,, 17, 689 (1969): abstracted from reference 13.
56. Land, D. G., Referenced in ASTM Data Series DS 48A (ref. 13)
57. Swan, J. S. and S. M. Burtles, Chem. Soc. Rev., 7(2), 201-211 (1978)
58. Pittet, A., P. Rittersbacher and R. Muralidhara J.Agric. Food Chem., 18, 929-933 (1970)
59. Schutte, L., CRC Crit. Rev. Food Technol., 4, 457-505 (1974); see also ref. 104
60. Hoehn, E., As referenced in ASTM Data Series DS 48A (ref. 13)
61. Vernin, G. and G. Vernin, "Heterocyclic Aroma compounds in Foods: Occurrence and Organoleptic Properties" In "The chemistry of heterocyclic flavoring and aroma compounds", G. Vernin, editor, Ellis Horwood Ltd., Chichester, England, pp. 72-150 (1982)
62. Amoore, J. E., J. R. Popplewell and D. Whissell-Buechy J. Chem. Ecol., 1, 291-297 (1975)
63. Leonardos, G., L. M. Libbey, W. Y. Cobb and E. A. Day J. Air Pollution Control Assn., 19, 91-95 (1969)
64. Maga, J. A., Cereal Foods World, 18, 326 (1973); abstracted from reference 13.
65. Rothe, M., G. Wolm, L. Tunger and H. J. Siebert, Nahrung, 16, 483 (1972); Chem. Abstr. 78, 15568c (1973)
66. Griffiths, N. H., Nature, 243, 304 (1973)
67. Tatum, J. H., J. Food Sci., 40, 707 (1973); abstracted from reference 13.
68. Forss, D. A., "Odor and Flavor Compounds from Lipids" In Progress in the chemistry of fats and other lipids, Vol. XIII, Part 4, R. T. Holmann, editor, Pergamon Press, Oxford, p. 177 (1972)
69. Teranishi, R., R. Buttery and D. Guadagni, Geruch-und Geschmacjsstiffe, Proc. Int. Symp. Bad Pyrmont, F. Drawert, editor, Verlag Hans Carl, Nurumberg, pp. 177-186 (1975)
70. Pickenhagen, W, "Enantioselectivity in Odor Perception" in Flavor chemistry: Trends and Developments, ACS Symp. Series 388, R. Teranishi, R. G. Buttery and F. Shahidi, editors, ACS, Washington DC, pp. 151-157 (1989)
71. Peyron, L., "Recent Techniques in the Analysis of Heterocyclic Aroma Compounds in Food" in The chemistry of heterocyclic flavoring and aroma compounds, G. Vernin, editor, Ellis Horwood Ltd., Chichester, England, pp. 262-304 (1982) 72. Walker, N. and I. Gray J. Agric. Food Chem., 18, 346-352 (1970)
73. Siek, T. J., J. A. Albin, L. A. Sather and R. C. Lindsey J. Dairy Sci., 54, 1 (1971)
74. Anon, Givaudan Corporation, Product Data Sheet, 1986
75. Pyysalo, T., Materials and Processing Technology, Tech. Res. Center of Finland, Pub. 14, Helsinki (1976)
76. Takken, H., L. van der Linde, M. Boehlens and J. van Dort, J. Agric. Food Chem., 23, 638-642 (1975)
77. Tressl, R., R. Renner, T. Kossa and H. Koppler European Brew. Conv., Proc. 16th Congress, 693-707 (1977)
78. Seifert, R. M., R.G. Buttery, D. G. Guadagni, D. Black and J. Harris, J. Agric. Food Chem., 18, 246-249 (1970)
79. Deck, R. E. and S. S. Chang, Chem. Ind. (London), 1343-1344 (1975)
80. Vernin, G., Parfums. Cosmet. Aromes, 29(June/July), 77-87 (1979)
81. Buttery, R. G., D. G. Guadagni and R. Lundin, J. Agric. Food Chem., 24, 1-3 (1976)
82. Honkanen, E., Acta Chem. Scand., 18, 612 (1964)
83. Buttery, R. G., R. M. Seifert, L. C. Ling, E. L. Soderstrom, J. M., Ogawa and J. G. Turnbaugh, J. Agric. Food Chem., 30, 1208-1211 (1982)
84. Evans, C. D., H. A. Moser and C. D. List, J. Am. Oil Chem. Soc., 48, 495-498 (1971)
85. Tressl, R., "Formation of Flavor Components in Roasted Coffee" in "Thermal generation of asromas", ACS Symp. Series 409, T. H. Parliment, R. J., McGorrin and C.-T. Ho, editors, ACS, Washington DC, pp. 285-301 (1989)
86. Ohloff, G., Perfumer and Flavorist, 1(3), 11-22 (1978)
87. McGill, A. S., R. Hardy and J. R. Burt, J. Sci. Food Agric., 25, 1477 (1974)
88. Buttery, R. G., R. Teranishi, L. C. Ling and J. G. Turnbaugh, J. Agric. Food Chem., 38, 336-340 (1990)

89. Kazeniac, S. J. and R. M. Hall, J. Food Sci., 35, 519-530 (1970)
90. Kobayashi, A., "Sotolon - Identification, Formation and Effect on Flavor" in Flavor chemistry: trends and development, ACS Symp. Series 388, R., Teranishi, R. G. Buttery and F. Shahidi, editors, ACS, Washington DC, pp. 49-59 (1989)
91. Murray, K., J. Shipton and F. Whitfield, Chem. Ind. (London), 897-898 (1970)
92. Callabretta, P., Cosm. Perf., 90(June), 74-80 (1975)
93. Mulders, E. J., R. J. C. Kleipool and M. C. ten Noever de Brauw, Chem. Ind. (London), 613-614 (1976)
94. Schieberle, P. and W. Grosche, "Bread Flavor" in *Thermal generation of aromas*, ACS Symp. Series 409, T. H. Parliment, R. J. McGorrin and C.-T. Ho, editors, ACS, Washington DC, pp. 258-267 (1989)
95. Boehlens, M., P. de Valois, H. Wobben and A. van der Gen, J. Agric. Food Chem., **19**, 984-991 (1971)
96. Callabretta, P., Perfumer and Flavorist, **3**(3), 33-42 (1978)
97. Teranishi, R., "Odor and Molecular Structure" in *Gustation and Olfaction*, G. Ohloff and A. F. Thomas, ed., pp.165-177 (1971)
98. Seifert, R. M., et. al., J. Sci. Food Agric., **26**, 1844 (1975)
99. Berry, R. E., C. J. Wagner, Jr., and M. G. Moshonas J. Food Sci., **32**, 75 (1967)
100. Stark, W. and D. A. Forss, J. Dairy Res., **31**, 253 (1964)
101. Engen, S., J. Inst. Brew. Assn., **80**, 162 (1974); abstracted from reference 13.
102. Buttery, R. G., L. C. Ling, R. Teranishi and T. Mon J. Agric. Food Chem., **25**, 1227-1229 (1977)
103. Schmidlin-Meszaros, J., Alimenta, **10**, 39 (1971)
104. Schutte, L. "Precursors of Sulfur-Containing Flavor Compounds" in Fenroli's *Handbood of Flavor Ingredients*, T. E. Furia and N. Bellanca, editors, CRC Press
105. Mussinan, C. J., R. A. Wilson, I. Katz, A. Hruza and M. H. Vock, "Identification and Flavor Properties of Some 3-Oxazolines and 3-Thiazolines Isolated From Cooked Beef" in "Phenolic, sulfur, and nitrogen compounds in food flavor", ACS Symp. Series 26, G. Charalambous and I. Katz, editors, ACS, Washington DC, 1976
106. Demole, E., P. Enggist and G. Ohloff, Helv. Chem. Acta, **65**, 1785-1794 (1982)
107. Urbach, G., J. Dairy Res., 39, **42** (1972); abstracted from reference 13.
108. Buttery, R. G., R. Teranishi, R. A. Flath and L. C. Ling J. Agric. Food Chem., **38**, 792-795 (1990)
109. Nishimura, O. and S. Mihara, J. Agric. Food Chem., **38**, 1038-1041 (1990)
110. Flament, I., Food Rev. Int., **5**(3), 317-414 (1989)
111. Buttery, R., D. Guadagni, L. Ling R. Seifert and W. Lipton, J. Agric. Food Chem.,**24**, 829-832 (1976)
112. Cain, W. S. and J. C. Stevens, Annals New York Acad. Sci., **561**, 29-38 (1989)
113. Cowart, B. J, Annals New York Acad. Sci., **561**, 39-55 (1989)
114. Doty, R. L., Annals New York Acad. Sci., **561**, 76-86 (1989)
115. Stevens, J. C., Annals New York Acad. Sci., **561**, 87-93 (1989)
116. Schiffman, S. and M. Pasternak, J. Gerontol., **34**, 73-79 (1979)
117. Schiffman, S. and J. C. Leffingwell, Pharmacol. Biochem. Behav., **14**, 787-798 (1981)
118. Koelega, H. S. and E. P. Coster, Annals New York Acad. Sci., **237**, 234-346 (1974)
119. Koster, E. P., Perfumer and Flavorist, **15**(2). 1-12 (1990)
120. Teranishi, R., R. G. Buttery and D. G. Gaudagni, Annals New York Acad. Sci., **237**, 209-216 (1974)
121. Guadagni, D. G., R. G. Buttery, S. Okano and H. K. Burr, Nature (London), **200**, 1288-1289 (1963)
122. Guadagni, D. G. and R. G. Buttery, J. Food. Sci., **43**, 1346-1347 (1978)
123. Amoore, J. E., *Molecular basis of odor*, Charles C. Thomas, Springfield, IL, pp. 16-25 (1970)
124. Masuda, H. and S. Mihara, J. Agric. Food Chem., **36**, 584-587 (1988)
125. Threshold detection values abstracted from a more extensive list scheduled for release in supplement No. 1 of the Flavor-base database. "Flavor-base" is a trademark of Leffingwell & Associates.
126. The quotation from Ohloff's article (86) is from a note of explanation to clarify that the threshhold value originally reported for damascenone (10 ppb) in his lecture at the VII International Congress of Essential Oils at Kyoto, Japan in October of 1977 had been revised based on Pickenhagen's new determination.

Table III. Odor/Flavor Detection Threshold Data in PPB (Water)

FEMA No.	Name	Odor Threshold	Odor References	Flavor Threshold	Flavor References
2003	Acetaldehyde; Ethanal; Acetic aldehyde;	15-120	4,5,6,7,10,120		
2006	Acetic acid; Ethanoic acid;			22000	13,15
2008	Acetoin; 3-Hydroxy-2-butanone	800	88		
3326	Acetone; 2-Propanone; Propan-2-one; Dimethyl ketone;	500000	13,25,42	450000	37,68
2009	Acetophenone; Methyl phenyl ketone; Phenyl methyl ketone;	65	10		
3126	Acetylpyrazine; 2-Acetylpyrazine;	62	4,69		
3251	Acetylpyridine; 2-Acetylpyridine; Methyl 2-pyridyl ketone;	19	4,69,71		
3202	Acetylpyrrole; 2-Acetylpyrrole; Methyl pyrrolyl ketone;	170000	10		
3328	Acetylthiazole; 2-Acetylthiazole;			10	4,59,104
2042	Allyl sulfide; Diallyl sulfide;	32.5	13,40		
3471	Ambrox; (+)-Ambrox isomer;	2.6	70		
3471	Ambrox; (-)-Ambrox isomer; Ambroxan;	0.3	70		
3471	Ambrox; DL-Ambrox isomer; Synambran;	0.6	70		
2056	Amyl alcohol; 1-Pentanol; Pentyl alcohol;	4000	10,46,88		
2059	Amyl butyrate; n-Pentyl butanoate; Amyl butanoate;	210	2	1300	13,20
2097	Anisole; Methoxybenzene;	50	13,18		
2127	Benzaldehyde;	350-3500	10,45,88	1500	13,20
3616	Benzenethiol; Thiophenol; Phenyl mercaptan;	13500	13,19		
3256	Benzothiazole;	80	10		
2137	Benzyl alcohol;	10000	10	5500	13,20
2159	Bornyl acetate;	75	13,21		

Table III (con't). Odor/Flavor Detection Threshold Data in PPB (Water)

FEMA No.	Name	Odor Threshold	Odor References	Flavor Threshold	Flavor References
3478	Butanethiol; 1-Butanethiol;	6	4,13,19	0.004	4,22
2170	Butanone; 2-Butanone; Methyl ethyl ketone;	50000	13,25		
2174	Butyl acetate; n-Butyl acetate;	66	2,7		
2178	Butyl alcohol; Butanol; 1-Butanol; n-Butanol;	500	10		
2186	Butyl butyrate; Butyl butanoate;	100	2		
2201	Butyl hexanoate; Butyl caproate;	700	2		
2188	Butyl isobutyrate; n-Butyl 2-methylpropanoate;	80	2		
3393	Butyl methylbutyrate; n-Butyl 2-methylbutyrate	17	2		
2211	Butyl propionate; n-Butyl propanoate;	25-200	2,7,13		
3130	Butylamine; 1-Aminobutane;	50000	13,17		
2219	Butyraldehyde; Butanal; n-Butanal;	9-37.3	4,10,11,13,31		
2221	Butyric acid; n-Butanoic acid;	240	13,23	6200-6800	13,15,35
2249	Carvone; data for (-)-carvone	50	86		
2252	Caryophyllene; beta-Caryophyllene;	64	28,37		
2303	Citral; Geranial isomer	32	46,88		
2303	Citral; Neral isomer	30	46		
2309	Citronellol; (-)-Citronellol isomer	40	86		
3480	Cresol; 2-Methylphenol; o-Cresol;	650	13,19	2.5	13
3530	Cresol; 3-Methylphenol; m-Cresol;	680	13,19		
2337	Cresol; 4-methylphenol; p-Cresol;	55	10		
3639	Cyclocitral; beta-Cyclocitral isomer	5	46,88		
3420	Damascenone; beta-Damascenone;	0.002	46,88	0.009	86
3659	Damascone; alpha-Damascone;	1.5-100	70		
3659	Damascone; (+)-alpha-Damascone isomer;	100	70		
3659	Damascone; (-)-alpha-Damascone isomer;	1.5	70		
3135	Decadienal; trans,trans-2,4-Decadienal;	0.07	10,31,32,37,45		
2360	Decalactone; gamma-Decalactone; 4-Decanolide;	11	1	88	37,73
2361	Decalactone; delta-Decalactone; 5-Decanolide;	100	1	90-160	13,15,20,37,73
2362	Decanal; Aldehyde C-10; Decyl aldehyde;	0.1-2	10,11,13,31,37	7	13,14,31
2364	Decanoic acid; Capric acid;	10000	10,13,34	3500	13,35
2366	Decenal; 2-Decenal; (E)-2-Decenal;	0.3-0.4	10,13,21,31,32	230	31
2370	Diacetyl; 2,3-dioxobutane;	2.3-6.5	4,5,36,37,65	5.4	13,15
3137	Dimethoxyphenol; 2,6-Dimethoxyphenol; Syringol;	1850	13,30	1650	13,30
3536	Dimethyl disulfide; Methyl disulfide;	0.16-12	4,5,111	0.06-30	22,41,59,104
3275	Dimethyl trisulfide; Methyl trisulfide;	0.005-0.01	4,108,111	3	4,59,104
3268	Dimethylcyclopentadione; 3,4-Dimethyl-1,2-cyclopentadione	17-20	74,109		
3269	Dimethylcyclopentadione; 3,5-Dimethyl-1,2-cyclopentadione;	1000	74		
3664	Dimethylmethoxyfuranone; 2,5-Dimethyl-4-methoxy-3(2H)-furanone	0.03	37,75		
3271	Dimethylpyrazine; 2,3-Dimethylpyrazine;	2500-35000	4,10,32,76,120		
3272	Dimethylpyrazine; 2,5-Dimethylpyrazine;	800-1800	4,10,77,78,79		
3273	Dimethylpyrazine; 2,6-Dimethylpyrazine;	200-9000	4,32,49,76,120		
3274	Dimethylthiazole; 4,5-Dimethylthiazole;	450-500	4,80,81		
3541	Dimethyltrithiolane; 3,5-Dimethyl-1,2,4-trithiolane;			10	104
2400	Dodecalactone; gamma-Dodecalactone; 4-Dodecanolide;	7	1		
2401	Dodecalactone; delta-Dodecalactone; 5-Dodecanolide;			1000	13,20
2615	Dodecanal; Lauric aldehyde; Aldehyde C-12; Dodecyl aldehyde;	2	31	0.9	13,14
2614	Dodecanoic acid; Lauric acid;	10000	13		
3569	Ethoxymethylpyrazine; 2-Ethoxy-3-methylpyrazine isomer	0.8	124		
2414	Ethyl acetate;	5-5000	7,13,43	3000-6600	13,15,20
2415	Ethyl acetoacetate; Acetoacetic acid, ethyl ester;			520	13,20
2418	Ethyl acrylate;	67	13,19		
2419	Ethyl alcohol;	100000	7,13,23,43	52000	13,20
2422	Ethyl benzoate;	60	10		
2427	Ethyl butyrate; Ethyl butanoate;	1	2,7,13,43	450	13,20
2430	Ethyl cinnamate;			16	13,20
2437	Ethyl heptanoate;	2.2	2	170	13,20
2439	Ethyl hexanoate; Ethyl caproate;	1	2,43		
2428	Ethyl isobutyrate; Ethyl 2-methylpropanoate;	0.1	2,43,83		
2440	Ethyl lactate;	14000	13,27		
2443	Ethyl methylbutyrate; Ethyl 2-methylbutyrate;	0.1-0.3	2,7,13,43		
3343	Ethyl methylthiopropionate;				

Table III (con't). Odor/Flavor Detection Threshold Data in PPB (Water)

FEMA No.	Name	Odor Threshold	Odor References	Flavor Threshold	Flavor References
	Ethyl 3-methylthiopropionate;	7	43		
2451	Ethyl palmitate; Ethyl hexadecanoate; Ethyl cetylate;	>2000	10		
2452	Ethyl phenylacetate;	650	13,27		
2456	Ethyl propionate; Ethyl propanoate;	10	43		
2462	Ethyl valerate; Ethyl pentanoate;	1.5-5	2,7,13,43	94	13,20
2464	Ethyl vanillin; 3-Ethoxy-4-hydroxybenzaldehyde; Ethavan;	100	13,44		
3149	Ethyldimethylpyrazine; 2-Ethyl-3,5-dimethylpyrazine isomer	1	4,49		
3149	Ethyldimethylpyrazine; 2-Ethyl-3,6-dimethylpyrazine isomer	0.4-5	4,32,77,120		
3150	Ethyldimethylpyrazine; 3-Ethyl-2,6-dimethylpyrazine;	1	4,49		
2436	Ethylguaiacol; 4-Ethylguaiacol; 4-Ethyl-2-methoxyphenol;	50	57		
3151	Ethylhexanol; 2-Ethyl-1-hexanol; 2-Ethylhexan-1-ol;	270000	13,50		
3623	Ethylhydroxymethylfuranone; 2-Ethyl-4-hydroxy-5-methyl-3-furanone	43	74		
3280	Ethylmethoxypyrazine; 2-Ethyl-3-methoxypyrazine	0.4-0.425	4,78,120		
3154	Ethylmethylpyrazine; 2-Ethyl-5-methylpyrazine;	100	4,13,32,120		
3155	Ethylmethylpyrazine; 3-Ethyl-2-methylpyrazine;	130	4,13,32,120		
3546	Ethylmethylpyridine; 5-Ethyl-2-methylpyridine;	19000	13,50,61		
3281	Ethylpyrazine; 2-Ethylpyrazine;	6000-22000	4,13,32,51,120		
2465	Eucalyptol; Cineole; 1,8-Cineole; 1,8-epoxy-p-menthane;	12	13,29		
2467	Eugenol; 4-Allyl-2-methoxyphenol;	6-30	86,88		
2475	Eugenyl methyl ether; Methyl eugenol; Methyl eugenol ether;	820	86		
2478	Farnesol;	20	86		
2487	Formic acid;	450000	13,23	83000	13
2489	Furfural;	3000-23000	4,10,13,32,52	5000	4,53
2491	Furfuryl alcohol;			5000	4,53
2493	Furfuryl mercaptan;	0.005	85	0.04	4,22
3163	Furylmethylketone; 2-Furyl methyl ketone; 2-Acetylfuran;	10000	88	80000	4,13,53
2507	Geraniol; trans-3,7-Dimethyl-2,7-octadien-1-ol;	40-75	2,86		
2509	Geranyl acetate;	9	10,13,28		
3542	Geranyl acetone; 6,10-Dimethyl-5,9-undecadien-2-one;	60	10,45,46,88,120		
2513	Geranyl isobutyrate; Geranyl 2-methylpropanoate;	13	13,28		
2517	Geranyl propionate; Geranyl propanoate;	10	13,28		
2525	Glycerol; Glycerin;			4400000	13,54
3287	Glycine; Aminoacetic acid;			1300000	13,55
2532	Guaiacol; o-Methoxyphenol; o-Hydroxyanisole;	3-21	10,13,30	13	13,30
2539	Heptalactone; gamma-Heptalactone; 4-heptanolide;	400	1		
2540	Heptanal; Aldehyde C-7; Heptaldehyde; Heptyl aldehyde;	3	10,11,13,21,31	21	31
3348	Heptanoic acid;	3000	13		
2544	Heptanone; 2-Heptanone; Methyl amyl ketone;	140-3000	10,13,56,120	1000	13,56
3289	Heptenal; 4-Heptenal (cis and trans);	0.8-10	37,87		
3165	Heptenal; trans-2-Heptenal;	13	10,11,31,32,46	80	31
3289	Heptenal; (E)-4-Heptenal; trans-4-Heptenal;	10	37,87		
3289	Heptenal; (Z)-4-Heptenal; cis-4-Heptenal;	0.8	37,87		
3400	Heptenone; 3-Hepten-2-one; (E)-3-Hepten-2-one	56	120		
2548	Heptyl alcohol; 1-Heptanol; n-Heptanol; Alcohol C-7;	3	11,13	31	13,15
2550	Heptyl isobutyrate; Heptyl 2-methylpropanoate;	13	13,28		
3429	Hexadienal; (E,E)-2,4-Hexadienal; trans,trans-2,4-Hexadienal;	10-60	31,120		
2556	Hexalactone; gamma-Hexalactone; 4-Hexanolide; Hexan-4-olide;	1600	1		
2557	Hexanal; Aldehyde C-6; Caproic aldehyde;	4.5-5	7,10,11,31,45	16-76	13,14,15,31
2559	Hexanoic acid; Caproic acid;	3000	10,13,34,88	5400	13,35
2567	Hexanol; 1-Hexanol; Hexyl alcohol; Caproic alcohol; Alcohol C-6;	2500	2,10		
2560	Hexenal; 2-hexenal; Hex-2-enal; (E)-2-hexenal;	17	2,10,11,45,46		
2561	Hexenal; cis-3-Hexenal; (Z)-3-hexenal;	0.25	46,88		

Table III (con't). Odor/Flavor Detection Threshold Data in PPB (Water)

FEMA No.	Name	Odor Threshold	Odor References	Flavor Threshold	Flavor References
2563	Hexenol; 3-Hexen-1-ol; cis-3-Hexenol; (Z)-3-Hexenol;	70	2,13,45,46,88		
2565	Hexyl acetate;	2	2,7,13,83		
2568	Hexyl butyrate; Hexyl butanoate;	250	2		
3172	Hexyl isobutyrate; Hexyl 2-methylpropanoate;	6-13	2,13,28		
3499	Hexyl methylbutanoate; Hexyl 2-methylbutanoate;	22	2		
2576	Hexyl propionate; Hexyl propanoate;	8	2,13,28		
3696	Hydroxydecadienoic acid lactone; 6-Pentyl-alpha-pyrone;	150	1		
3549	Hydroxydihydrotheaspirane; 6-Hydroxydihydrotheaspirane;	0.2	86		
2593	Indole;	140	10		
2594	Ionone; alpha-Ionone;			0.4	13,20,37
2595	Ionone; beta-Ionone	0.007	23,32,37,45,88		
2055	Isoamyl acetate; 3-Methylbutyl acetate;	2	43		
2057	Isoamyl alcohol; 3-Methyl-1-butanol; Isopentyl alcohol;	250-300	10,46,88	170	13,20
2175	Isobutyl acetate;	66	7,13		
2179	Isobutyl alcohol; 2-Methyl-1-propanol;	7000	13,27		
2189	Isobutyl isobutyrate; 2-Methylpropyl 2-methylpropanoate;	30	2,13,28		
3132	Isobutylmethoxypyrazine; 2-Isobutyl-3-methoxypyrazine;	0.002-0.016	4,37,52,76,120		
3133	Isobutylmethylpyrazine; 2-Isobutyl-3-methylpyrazine;	35-130	4,13,32,76,120		
3134	Isobutylthiazole; 2-Isobutylthiazole;	2-3.5	4,13,45,46,89	3	4,59,104
2220	Isobutyraldehyde; 2-Methylpropanal;	0.1-2.3	4,12,32,38		
2222	Isobutyric acid; 2-Methylpropanoic acid;	8100	13,27		
3102	Isovaleric acid; 3-Methylbutanoic acid;	120-700	13,27,37,38,88		
3745	Jasmine lactone; Dec-7-en-5-olide;	2000	1		
2633	Limonene; d-Limonene;	10	13,37,45		
2635	Linalool;	6	13,28,37,45,88		
2656	Maltol; Veltol ; Corps praline;	35000	4,58	7100-13000	4,13,20,58
3153	Maple furanone; 5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone;	0.00001	90		
3700	Menthenethiol; 1-p-Menthene-8-thiol;	0.0001	106		
2667	Menthone; p-Menthan-3-one;	170	13,29		
3358	Methoxyisopropylpyrazine; 2-Methoxy-3-isopropylpyrazine isomer	0.002-10	4,76,52,92		
3358	Methoxyisopropylpyrazine; 2-Methoxy-5-isopropylpyrazine isomer	10	4,92		
2671	Methoxymethylphenol; 2-Methoxy-4-methylphenol; Creosol;	90	13,30	65	13,30
3433	Methoxymethylpropylpyrazine; 2-Methoxy-3-sec-butylpyrazine;	0.001	4,91		
3183	Methoxymethylpyrazine; 2-,5 or 6-Methoxy-3-methylpyrazine;	3-15	4,78,92		
3183	Methoxymethylpyrazine; 2-Methoxy-3-methylpyrazine;	3-7	4,78,92,120,124		
3183	Methoxymethylpyrazine; 5-Methoxy-2-methylpyrazine isomer	15	4,92		
3302	Methoxypyrazine; 2-Methoxypyrazine;	400-700	4,78,120,124		
2675	Methoxyvinylphenol; 2-Methoxy-4-vinylphenol; 4-Vinylguaiacol;	3	10		
2693	Methyl butyrate; Methyl butanoate;	60-76	2,43		
3362	Methyl furfuryl disulfide; Methyl 2-furylmethyl disulfide;	0.04	93,94		
2705	Methyl heptanoate;	4	28,43		
2708	Methyl hexanoate; Methyl caproate;	70-84	2,43		
2694	Methyl isobutyrate; Methyl 2-methylpropanoate;	7	43		
2716	Methyl mercaptan;	0.02	4,11,13	2	4,9,13,26
2719	Methyl methylbutyrate; Methyl 2-methylbutyrate;	0.25	43		
2720	Methyl methylthiopropionate; Methyl 3-methylthiopropionate;	180	43		
2728	Methyl octanoate; Methyl caprylate;	200	43		
3576	Methyl propenyl disulfide; Methyl 1-propenyl disulfide;			6.3	4,95,104
2745	Methyl salicylate;	40	46,88		

Table III (con't). Odor/Flavor Detection Threshold Data in PPB (Water)

FEMA No.	Name	Odor Threshold	Odor References	Flavor Threshold	Flavor References
2746	Methyl sulfide; Dimethyl sulfide; Methylthiomethane;	0.3-1.0	4,5,11,88	0.03-12	4,22
2752	Methyl valerate; Methyl pentanoate;	20	43		
2677	Methylacetophenone; 4-Methylacetophenone; p-Methylacetophenone	0.027	110		
3644	Methylbutyl acetate; 2-Methylbutyl acetate;	5	7,13		
2691	Methylbutyraldehyde; 2-Methylbutyraldehyde;	1	4,12		
2692	Methylbutyraldehyde; 3-Methylbutyraldehyde; Isovaleraldehyde;	0.2-2	4,12,78,88	170	20
2695	Methylbutyric acid; 2-Methylbutyric acid;			1600	13,20
2700	Methylcyclopentenolone; Cyclotene; Ketonarome; Corylone; MCP;	300	109		
3189	Methylfurfurylthiopyrazine; 2-Methyl-3-(furfurylthio)pyrazine	<1	4,96		
3189	Methylfurfurylthiopyrazine; 2-Methyl-5-(furfurylthio)pyrazine	<1	4,96		
3363	Methylheptadienone; 6-Methyl-3,5-heptadien-2-one;	380	10,13,45,88		
FDA	Methylheptenol; 6-Methyl-5-hepten-2-ol	2000	88		
2707	Methylheptenone; 6-Methyl-5-hepten-2-one;	50	46,88		
3578	Methylpropyloxathiane; *2-Methyl-4-propyl-1,3-oxathiane;*	2-4	70		
3578	Methylpropyloxathiane; (+)-cis-2-Methyl-4-propyl-1,3-oxathiane	2	70		
3578	Methylpropyloxathiane; (-)-cis-2-Methyl-4-propyl-1,3-oxathiane	4	70		
3309	Methylpyrazine; 2-Methylpyrazine;	60-105000	10,32,51,92,124		
3204	Methylthiazoleethanol; *4-Methyl-5-thiazoleethanol; Sulfurol;*	*10800*	*13,60*		
3206	Methylthioacetaldehyde; 2-Methylthioacetaldehyde;	16	13,45		
3208	Methylthiomethylpyrazine (mixture of isomers);	1-4	4,92,96		
3208	Methylthiomethylpyrazine; 2-Methylthio-3-methylpyrazine isomer	1-4	4,92,124		
3208	Methylthiomethylpyrazine; 5-Methylthio-2-methylpyrazine isomer	4	4,96		
3209	Methylthiophencarboxaldehyde; 2-Formyl-5-methylthiophene;			1	4,59
2747	Methylthiopropanal; 3-(Methylthio)-propanal; Methional;	0.2	4,13,32,88	0.05-10	4,59,41,104
2762	Myrcene;	13-15	13,21,28,37,97		
2763	Myristaldehyde; Tetradecanal; Aldehyde C-14 (Myristic);			60	13,14
2764	Myristic acid; Tetradecanoic acid;	10000	10,13,34		
2770	Nerol;	300	86		
3377	Nonadienal; (E,Z)-2,6-Nonadienal; trans,cis-2,6-Nonadienal;	0.01	31,120		
3212	Nonadienal; (E,E)-2,4-Nonadienal; trans,trans-2,4-Nonadienal;	0.09	120		
2782	Nonanal; Nonyl aldehyde; Aldehyde C-9;	1	10,11,13,31,98	6-12	13,14,31
2784	Nonanoic acid;	3000	10,13,34		
2789	Nonanol; 1-Nonanol; Nonyl alcohol; Alcohol C-9;	50	10		
2785	Nonanone; 2-Nonanone; Methyl heptyl ketone;	5-200	10,120		
3213	Nonenal; 2-Nonenal;	0.08-0.1	10,11,21,31,37	6	31
3580	Nonenal; cis-6-Nonenal;	0.02	37		
3166	Nootkatone; (+)-Nootkatone (the natural isomer)	0.8-1	37,70,86,99		
3166	*Nootkatone; (-)-Nootkatone (the unnatural isomer)*	600	70		
3214	Octalactone; delta-Octalactone; 5-Octanolide;	400	1		
2796	Octalactone; Gamma-Octalactone; 4-octanolide;	7	1	400	13,20
2797	Octanal; Caprylic aldehyde; Aldehyde C-8;	0.7	10,11,13,31,120	5-45	13,14,31
2799	Octanoic acid; Caprylic acid;	3000	10,13,34	5300	13,35
2800	Octanol; 1-Octanol; Octyl alcohol; Alcohol C-8;	110-130	10,13,19		
2802	Octanone; 2-Octanone;	50	10	150-1000	13,14,15
2803	Octanone; 3-Octanone;	*28*	*10*		
3215	Octenal; 2-Octenal;	3	10,13,31,32	90	31
2805	Octenol; 1-Octen-3-ol;	1	10		
3515	Octenone; 1-Octen-3-one;	0.005	108	0.1	37,68

Table III (con't). Odor/Flavor Detection Threshold Data in PPB (Water)

FEMA No.	Name	Odor Threshold	Odor References	Flavor Threshold	Flavor References
2806	Octyl acetate;	12	13,28		
2808	Octyl isobutyrate; Octyl 2-methylpropanoate;	6	13,28		
2832	Palmitic acid; Hexadecanoic acid;	10000	13		
2840	Pentadecalactone; omega-Pentadecalactone; 15-pentadecanolide;	1-4	13,38,62		
2842	Pentanone; 2-Pentanone;	70000	13,42		
3218	Pentenal; 2-Pentenal;	1500	46		
3584	Pentenol; 1-Penten-3-ol;	400	13,45,46,88		
3382	Pentenone; 1-Penten-3-one; Ethyl vinyl ketone;	1-1.3	13,45,46,32,88		
3417	Pentenone; 3-Penten-2-one;	1.5	10		
3317	Pentylfuran; 2-Pentylfuran;	6	4,52,88		
3383	Pentylpyridine; 2-Pentylpyridine;	0.6	4,102		
2858	Phenethyl alcohol; 2-Phenethyl alcohol;	750-1100	10,46,86,88		
3223	Phenol;	5900	13,19		
2874	Phenylacetaldehyde;	4	10,13,32,45,46		
2878	Phenylacetic acid;	10000	13,64		
2902	Pinene; alpha-Pinene;	6	13,28		
2903	Pinene; beta-Pinene;	140	13,28		
2908	Piperidine;	65000	13,17		
2911	Piperonal; Heliotropine;			3.9	13,20
3521	Propanethiol; 1-Propanethiol; n-Propyl mercaptan;	3.1	13,40	0.06	4,22
2928	Propanol; 1-Propanol; Propyl alcohol;	9000	7,13,23		
3227	Propenyl propyl disulfide; Propyl propenyl disulfide;			2.2	4,13,95
2922	Propenylguaethol; 2-Ethoxy-5-propenylphenol;	400	13,44		
2923	Propionaldehyde; Propanal;	9.5-37	10,11,13,31,120		
2924	Propionic acid; Propanoic acid;	20000	13,27		
2934	Propyl butyrate; Propyl butanoate;	18-124	2,7,13		
2958	Propyl propionate; Propyl propanoate;	57	2,7,13		
3231	Pyrazinyl methyl sulfide; 2-(Methylthiomethyl)-pyrazine;	20	4,96		
2966	Pyridine;	2000	10		
3386	Pyrrole;	49600	13,17		
3523	Pyrrolidine;	20200	13,17		
3470	Quinoline;	700	10,34		
2588	Raspberry Ketone; 4-(p-Hydroxyphenyl)-2-butanone; Oxanone;	100	37,103		
3236	Rose oxide; 4-Methyl-2-(2-methylpropen-1-yl)-tetrahydropyran	0.5	86		
3141	Sinensal; alpha-Sinensal;	0.05	37,97		
3634	Sotolon; Caramel furanone; 4,5-Dimethyl-3-hydroxy-2(5H)-furanone	0.001	90		
3035	Stearic acid; Octadecanoic acid;	20000	10,13		
3174	Strawberry furanone; 2,5-Dimethyl-4-hydroxy-3(2H)-furanone;	0.04	37,75		
3233	Styrene; Vinylbenzene;	730	13,19		
3045	Terpineol; alpha-Terpineol; p-Menth-1-en-8-ol;	330-350	2,21,37,86,88		
3046	Terpinolene; p-Menth-1,4(8)-diene;	200	13,21		
3237	Tetramethylpyrazine; 2,3,5,6-Tetramethylpyrazine;	1000-10000	4,51,96		
3322	Thiamine hydrochloride; (value for thiamine pure)			39	104
3066	Thymol; 5-Methyl-2-isopropylphenol;			50	13
3241	Trimethylamine;	0.37-1.06	13,17,38,66		
3473	Trimethylcyclohexanone; 2,2,6-Trimethylcyclohexanone;	100	2		
3525	Trimethyloxazoline; 2,4,5-Trimethyl-3-oxazoline;	1000	4,105		
3244	Trimethylpyrazine; 2,3,5-Trimethylpyrazine;	400-1800	4,80,92		
3325	Trimethylthiazole; 2,4,5-Trimethylthiazole;	50	4,80		
3294	Undecalactone; delta-Undecalactone; 5-Undecanolide;			150	13,20
3092	Undecanal; Aldehyde C-11 (undecylic);	5	11,13,31,120		
3245	Undecanoic acid; Undecylic acid;	10000	13		
3093	Undecanone; 2-Undecanone; Methyl nonyl ketone;	7	10,120		
3098	Valeraldehyde; Pentanal;	12-42	10,11,13,31,120	76	31
3101	Valeric acid; Pentanoic acid;	3000	13		
3107	Vanillin; 4-Hydroxy-3-methoxybenzaldehyde;	20-200	13,37,44,65	680	13,20
3739	Vinylphenol; 4-Vinylphenol;	10	10		