Table V. $F$ Values from ANOVA for the Mean Values of Objective Parameters of Four Carrot Entries Grown in Three Locations

| objective parameters | source of variation: entries | source of variation: locations |
|---|---|---|
| dry weight | 0.8 | 26.2**[a] |
| refractive index | 3.3 | 55.6** |
| carotenoids | 1.9 | 26.5** |
| fructose | 18.5** | 3.7 |
| glucose | 23.0** | 3.4 |
| sucrose | 5.4* | 17.7** |
| total sugars | 0.9 | 31.3** |
| α-pinene | 2.4 | 1.2 |
| β-pinene/sabinene | 3.6 | 0.1 |
| myrcene | 2.1 | 7.1 |
| α-phellandrene | 25.2* | 5.9 |
| α-terpinene | 5.2 | 0.4 |
| limonene | 14.1* | 0.3 |
| γ-terpinene | 2.5 | 0.0 |
| terpinolene | 90.5** | 28.3* |
| terpinen-4-ol | 3.6 | 0.9 |
| bornyl acetate | 1.3 | 1.8 |
| caryophyllene | 2.6 | 1.0 |
| γ-bisabolene (A) | 4.3 | 9.0 |
| γ-bisabolene (B) | 1.1 | 2.3 |
| total volatiles | 20.2* | 1.5 |

[a] (*) Significant at the 5% level; (**) significant at the 1% level.

the genotype or the environment. The levels of reducing sugars and terpinolene were genetically most variable and sucrose, α-phellandrene, limonene, and total volatiles displayed some genetic variation. Dry weight, refractive index, carotenoids, sucrose, total sugars, and terpinolene were most variable environmentally. Although the genetic diversity of entries and environmental diversity of growing sites in this experiment were large, it should be noted that these conclusions may only apply to the lines and locations tested. This reservation is most appropriate for the volatiles, which were only represented by two locations.

Volatiles and sugars appear to play an important part in carrot flavor. The true level of their contribution can only be determined by the reconstitution of an attribute with exogenous supplementation.

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# The Importance of Hydrophobic Properties of Organic Compounds on Their Taste Intensities: A Quantitative Structure-Taste-Intensity Study

Michael J. Greenberg

The relationship between taste intensity and physicochemical properties of organic compounds was investigated using the Hansch approach, a quantitative structure–activity relationship technique which utilizes linear free-energy relationship (LFER) parameters and multiple regression analysis. Literature taste threshold data for a homologous series of alcohols, ketones, and acids whose members had noncolinear hydrophobic, steric, and polar parameters were successfully correlated only with the hydrophobicity parameter log $P$, the log [$n$-octanol/water partition coeffecient]. Poor correlations were achieved with $E_s$, the Taft steric constant, and $\sigma^*$, the Taft polar constant. This indicates that taste intensity of homologues depends upon their hydrophobic rather than their steric and polar properties. Log $P$ also correlated well with taste intensity for a series of lactones, esters, and sulfamates, as well as taste intensity data for a wide variety of organic stimulants of different functionality. Addition of a hydrogen bonding indicator parameter, HB, to the equation relating taste intensity for a nonhomologous series of stimulants significantly improved the correlation.

Taste, like other biological processes, involves a substrate and receptor site interaction. The nature of the substrate–receptor interaction and how this interaction leads to perceived taste quality and intensity has yet to be elucidated. Early studies in taste involved the number, size, shape, and distribution of taste buds in various species as reviewed by Kare (1971).

Other studies have centered on whether there are four (or more) primary taste qualities (sour, sweet, salty, and bitter) and that there are specific receptors for each. The early work of Hänig (1901) indicated that the bitter mo-

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dality was generated in the posterior part of the tongue, the sweet one on the tip, the salty one on the anterior, and the sour modality on the sides of the tongue.

From electrophysiological data Kimura and Beidler (1961) found that perception of basic taste qualities results from a pattern of nerve activity coming from many cells and that specific receptor cells for sweet, sour, bitter, and salt do not exist. A recent review by Price and Desimone (1977) of inhibitor, cross-adaption, and electrophysiological data has produced evidence favoring the existence of the four primary tastes and specific receptors for each.

Other recent areas of study have centered on correlating chemical structure and taste type. This is particularly the case for sweetness as reviewed by Crosby (1976). A stereochemical model for compounds with sweet taste has been described by Shallenberger and Acree (1969). Vicinal hydroxyl groups of sugars in the staggered or gauche conformation as the stereochemical model for an AH, B unit was used to describe either intra- or an intermolecular hydrogen bond. It was determined that the AH proton to B orbital distance needed to be 3 Å for optimum sweetness. AH, B units have been identified in amino acids, chloroform, saccharin and in certain flavones and glycosides as reviewed by Shallenberger and Lindley (1977).

The research in the sweetener area as discussed by Beets (1978) has concluded that "the sweet modality has a narrow structural basis which is restricted to variants of a single combination of features of which the components and the parameters can only vary within fairly narrow limits". Beets (1978) also concluded that the bitter taste can be produced by practically all functional groups and the sour modality produced mostly by carboxylic and sulfonic acid groups.

Relatively little work has been reported on how taste intensity is dependent upon the physicochemical properties of the taste stimulant. An equation derived by Beidler (1954) related magnitude of (salt taste) electrical neural response and stimulus concentration. From this and other studies Beidler (1961) concluded that stimulus adsorption on the surface of the taste receptor results in a weak stimulus receptor complex, taste response is a function of sites occupied by the stimulus, and the number of taste receptor sites is finite and thus can be saturated. In later studies with acids, Beidler (1967, 1971) correlated acid sourness (rat electrophysiological recordings) with pH. Siek et al. (1971) failed to correlate vapor pressure with taste intensity of alcohol, ketone ester, and lactone stimulants. These authors felt that molecular size and stereochemistry may be important for determining taste intensity of those organic compounds.

The use of computer techniques in the correlation of biological activity with substrate physical–chemical properties has received much attention in the area of medicinal chemistry. The use of these techniques, denoted quantitative structure–activity relationships (QSAR), were developed mostly by Hansch and his co-workers and have been reviewed by Tute (1971), Purcell et al. (1973), and Dunn (1973).

The QSAR techniques involve correlating the logarithm of the reciprocal molar concentration of a bioactive compound required for a specific biological response such as $ED_{50}$ or $LD_{50}$ values with linear free-energy constants such as the Hammett constant ($\sigma$), a measure of aromatic substituent electronic effects, Taft polar constant ($\sigma^*$), a measure of substituent polar effects, the logarithm of the *n*-octanol/water partition coefficient (log *P*), a measure of hydrophobic–lipophilic effects, and the Taft steric constant ($E_s$), a measure of substituent steric effects.

In the area of taste, these techniques were used by Hansch and Deutsch (1966) to show that the relative sweetness to cane sugar of a series of substituted nitroanilines depended upon the hydrophobicity and electron donating ability of the substituents. Recently QSAR was applied by Boelens (1976) to study compounds with bitter almond and musk odors. A significant relationship between almond odor quality and the *n*-octanol/water partition coefficients and a molecular shape–volume parameter was achieved. A significant relationship between the partition coefficients and musk odor quality was reported for 16 musk odorants. More recently QSAR was applied by Greenberg (1979) in showing the dependence of odor intensity on the hydrophobic–lipophilic properties of odorants.

The object of this paper is to report the applicability of QSAR techniques such as those used by Hansch and his co-workers in establishing the primary physical–chemical property(s) important for determining taste intensity and to rationalize how this contributes to the process of taste. A secondary objective is to establish whether these techniques can be used to predict taste intensity regardless of taste type within and between homologous series of organic compounds. The premises for pursuing this study are as follows: (1) Taste intensity depends upon the organic stimulant's ability to partition from a medium in which it is dissolved into the saliva and membrane layers taste buds until it reaches a receptor site. (2) The hydrophobicity of the organic stimulant as measured by the log [*n*-octanol/water partition coefficient] (log *P*) can be used to quantitate these partitioning processes. (3) A relationship can be developed between log *P* and taste intensity by using multiple regression analysis. (4) The physical–chemical properties such as the Taft steric constant ($E_s$) and polar constant ($\sigma^*$) can be used to determine the importance of stimulant steric and polar effects on taste intensity. (5) The derived regression equations can be used to predict taste intensity of untested compounds.

## PROCEDURES

The procedures for doing this particular quantitative structure–activity relationship involve the following: (1) searching the chemical literature for taste detection threshold values of classes of organic compounds whose members have noncolinear steric, polar, and hydrophobic constants; (2) calculating or using reported steric (Taft steric constant), polar, and hydrophobic (log *P*) constants; and (3) correlating the log of the reciprocal molar concentration required for a threshold value denoted log ($1/c$) with the corresponding Taft polar, steric, and log *P* values.

Classes of chemical compounds having different functional groups and taste qualities, some of which are useful to the flavor industry, were selected for this initial study. Fourteen alcohols, ranging from ethanol to decanol, and 31 carbonyl compounds including ketones, lactones, esters, and aliphatic acids were studied. For each class of chemical compounds, literature threshold values obtained only from one laboratory were used in order to prevent errors associated with technique or methodology between laboratories that occur for threshold determinations as discussed by Guadagni et al. (1963) and Powers and Ware (1976).

The log [*n*-octanol/water partition coefficients] (log *P*) for compounds selected for this study were obtained from those reported by Hansch et al. (1971) or were calculated from fragmental constants as reported by Nys and Rekker (1974). The Taft steric ($E_s$) and polar ($\sigma^*$) constants were obtained from those values reported by Taft (1956).

Table I. Equations Relating Taste Intensity to Hydrophobic, Steric, and Electronic Parameters for Series Having Noncolinear Physicochemical Properties

| compd (medium) | eq no. | equation | $n$ | $R$ | $S$ | source[a] |
|---|---|---|---|---|---|---|
| alcohols (water) | 1 | $\log(1/c) = 0.87 \pm (0.36)\log P + 2.96 \pm (0.38)$ | 14 | 0.95 | 0.40 | A |
| | 2 | $\log(1/c) = -0.30 \pm (1.44)\Sigma E_s + 4.88 \pm (2.32)$ | 14 | 0.13 | 1.26 | A |
| | 3 | $\log(1/c) = -0.35 \pm (3.03)\Sigma\sigma^* + 4.48 \pm (0.81)$ | 14 | 0.07 | 1.27 | A |
| 2-alkanones (butter oil) | 4 | $\log(1/c) = -0.20 \pm (0.12)(\log P)^2 + 1.01 \pm (0.59)\log P + 2.88 \pm (0.58)$ | 9 | 0.87 | 0.39 | B |
| | 5 | $\log(1/c) = -1.72 \pm (2.18)E_s + 2.62 \pm (1.35)$ | 9 | 0.58 | 0.59 | B |
| | 6 | $\log(1/c) = -9.46 \pm (11.28)\sigma^* + 2.57 \pm (1.33)$ | 9 | 0.60 | 0.58 | B |
| carboxylic acids (butter oil) | 7 | $\log(1/c) = -0.57 \pm (0.26)\log P + 4.48 \pm (1.02)$ | 9 | 0.89 | 0.68 | B |
| | 8 | $\log(1/c) = 1.31 \pm (5.53)E_s + 3.70 \pm (3.49)$ | 9 | 0.21 | 1.48 | B |
| | 9 | $\log(1/c) = 11.94 \pm (27.36)\sigma^* + 4.27 \pm (3.30)$ | 9 | 0.36 | 1.41 | B |

[a] A, Siek et al. (1971); B, Siek et al. (1969).

Table II. Equations Relating Taste Intensity to Hydrophobic Properties for Series Not Having Noncolinear Physicochemical Properties

| compd (medium) | eq no. | equation | $n$ | $R$ | $S$ | source[a] |
|---|---|---|---|---|---|---|
| carboxylic acids (water) | 1 | $\log(1/c) = 0.25 \pm (0.23)\log P + 3.64 \pm (0.56)$ | 5 | 0.89 | 0.25 | A |
| γ-lactones (water) | 2 | $\log(1/c) = 0.91 \pm (0.74)\log P + 3.49 \pm (2.02)$ | 6 | 0.86 | 0.59 | A |
| γ-lactones (butter oil) | 3 | $\log(1/c) = 0.42 \pm (0.14)\log P + 3.69 \pm (0.38)$ | 6 | 0.97 | 0.11 | B |
| 2-alkanones (water) | 4 | $\log(1/c) = 0.62 \pm (0.38)\log P + 3.54 \pm (0.85)$ | 10 | 0.80 | 0.85 | A |
| | 5 | $\log(1/c) = -0.28 \pm (0.09)(\log P)^2 + 1.94 \pm (0.43)\log P + 2.74 \pm (0.36)$ | 10 | 0.98 | 0.29 | A |
| ethyl esters (water) | 6 | $\log(1/c) = -0.28 \pm (0.24)(\log P)^2 + 1.94 \pm (1.47)\log P + 3.54 \pm (1.24)$ | 7 | 0.89 | 0.72 | A |
| aldehydes (water) | 7 | $\log(1/c) + 0.34 \pm (0.17)\log P + 5.57 \pm (0.40)$ | 12 | 0.82 | 0.50 | A |
| | 8 | $\log(1/c) = -0.11 \pm (0.05)(\log P)^2 + 0.86 \pm (0.25)\log P + 5.40 \pm (0.42)$ | 12 | 0.96 | 0.28 | A |
| sulfamates (water) | 9 | $\log(1/c) = 0.68 \pm (0.45)\log P + 0.05 \pm (0.61)$ | 7 | 0.86 | 0.33 | C |

[a] A, Siek et al. (1971); B, Siek et al. (1969); C, Benson and Spillane (1976).

Table III. Equations Relating Hydrophobicity to Taste Intensity for a Wide Variety of Taste Stimulants

| compd (medium) | eq no. | equation | $n$ | $R$ | $S$ | source[a] |
|---|---|---|---|---|---|---|
| alcohols, aldehydes, ketones, lactones, acids, esters | 1 | $\log(1/c) = 0.54 \pm (0.17)\log P + 4.08 \pm (0.35)$ | 54 | 0.67 | 1.00 | A |
| | 2 | $\log(1/c) = 0.49 \pm (0.16)\log P + 0.43 \pm (0.38)\mathrm{HB} + 3.75 \pm (0.41)$ | 54 | 0.70 | 0.96 | A |
| | 3 | $\log(1/c) = -0.12 \pm (0.09)(\log P)^2 + 1.10 \pm (0.44)\log P + 3.74 \pm (\pm 0.33)$ | 54 | 0.72 | 0.95 | A |
| | 4 | $\log(1/c) = -0.13 \pm (0.08)(\log P)^2 + 1.09 \pm (0.42)\log P + 0.47 \pm (0.35)\mathrm{HB} + 3.36 \pm (0.31)$ | 54 | 0.80 | 0.89 | A |

[a] A, Siek et al. (1971).

For alcohols the $E_s$ and $\sigma^*$ values for the substituents bonded to the carbinol moiety were each summed and correlated against log $(1/c)$. For aldehydes and ketones the $E_s$ and $\sigma^*$ values for substituents bonded to the carbonyl group were each summed and correlated against log $(1/c)$. The use of $E_s$ and $\sigma^*$ has been reviewed by Shorter (1972).

The use of a hydrogen bonding indicator parameter (HB) in quantitative structure–activity relationships recently has been reviewed by Fujita et al. (1977). In that study it was found that an indicator parameter (HB) which represents the "extra" hydrogen-bonding effect on the biological activity is required in the Hansch-type correlations when the relative hydrogen-bonding effect of bioactive compounds on phases involved in the binding at the site of biological action differs from that in the $n$-octanol–$H_2O$ partitioning phases used as the reference to estimate hydrophobicity. Examples were presented in which the HB indicator parameter was used in correlating activity of gaseous anesthetics and the binding of phenyl $N$-methylcarbamates with acetylcholinesterase inhibition. In this study HB was used to ascertain whether it would improve the correlations involving series of congeners with substituents having appreciable association capability such as in nonhomologous series. Nonhydrogen bonders were assigned on HB value of 0, while hydrogen acceptors or donors were each assigned an HB value of 1.

Regression studies of the taste intensity data were carried out using the Continental Can Co. stepwise multiple regression program and the PDP-11-45 minicomputer (Digital Equipment Corp.).

## RESULTS AND DISCUSSION

A literature search yielded literature taste threshold data for series of aliphatic alcohols, methyl ketones, aliphatic aldehydes, γ-lactones, carboxylic acids, alkylsulfamates, and ethyl esters which were used in this study. No literature taste threshold data were available for series of py-

Table IV. Squared Correlation Coefficients for Equations Relating LFER Parameters to Alcohol Taste Threshold Data

| | log (1/c) | log P | $\Sigma E_s$ | $\Sigma \sigma^*$ |
|---|---|---|---|---|
| log (1/c) | 1.00 | 0.90 | 0.02 | 0.01 |
| log P | 0.90 | 1.00 | 0.02 | 0.02 |
| $\Sigma E_s$ | 0.02 | 0.02 | 1.00 | 0.98 |
| $\Sigma \sigma^*$ | 0.01 | 0.02 | 0.98 | 1.00 |

Table V. Squared Correlation Coefficients for Equations Relating LFER Parameters to Ketone Taste Threshold Data

| | log (1/c) | log P | $E_s$ | $\sigma^*$ |
|---|---|---|---|---|
| log (1/c) | 1.00 | 0.07 | 0.34 | 0.36 |
| log P | 0.07 | 1.00 | 0.38 | 0.47 |
| $E_s$ | 0.34 | 0.38 | 1.00 | 0.96 |
| $\sigma^*$ | 0.36 | 0.47 | 0.96 | 1.00 |

razines, thiazoles, mercaptans, and other important flavor compounds found in cooked foods such as meats and vegetables.

The results found relating this literature taste threshold data to log $P$, $E_s$, and $\sigma^*$ are presented in Tables I–III. For each equation $N$ is the number of compounds in the data set, $R$ is the correlation coefficient, and $S$ is the equation standard deviation. The numbers in parentheses are the calculated confidence intervals at the 95% level of confidence.

From the 11 sets of data in Tables I–III, very good correlations were achieved between log (1/c) and log $P$ and in one case with log $P$ and HB with 10 sets having an equation with a correlation coefficient greater than 0.85 which was least significant at the 95% level of confidence. Taste intensity of homologous series as well as for compounds with different functional groups were found to correlate well with log $P$, although correlations of the latter were improved by the addition of the hydrogen bonding parameter HB. For example, the results in Table III indicated that log $P$ and HB correlated well with taste threshold data for a data set of 54 compounds which include all the homologous series (water medium) listed in Table I and II determined by Siek et al. (1971).

Log $P$ correlated well with log (1/c) for each homologous series of stimulants in water as well as deodorized butter oil resulting in equations with similar coefficients. The major exception appears to be the carboxylic acids which had increasing taste intensity with increasing hydrophobicity in a water medium and decreasing taste intensity with increasing hydrophobicity in an oil medium.

Taste intensity was poorly related to $E_s$ or $\sum E_s$ for literature data sets whose hydrophobic and steric properties were not colinear. The results of these correlations are presented in Table I. The results in Table I, eq 2 indicate that $\sum E_s$ correlated very poorly with log (1/c) for a congeneric series of alcohols. Only 2% of the variance in the model was accounted for by $\sum E_s$ as opposed to 90% by log $P$. Thus the bulkiness of the substituents on the carbinol moiety does not determine the level of taste intensity. Similar results were found for the methyl ketone data in eq 5 and the carboxylic acid data in eq 8. These data indicate that the bulkiness of the substituents on the carbonyl moiety does not determine the level of taste intensity. The correlation matrix in Table IV–VI summarize all correlations of log (1/c) vs. $E_s$ (or $\sum E_s$) and verify the fact that $E_s$ and log $P$ are not colinear.

Taste intensity was also poorly correlated with $\sum \sigma^*$ or $\sigma^*$ for the alcohol, ketone, and acid sets whose polar and hydrophobic properties were not colinear. This indicates that the polar effects of the groups bonded to the carbinol

Table VI. Squared Correlation Coefficients for Equations Relating LFER Parameters to Acid Taste Threshold Data

| | log (1/c) | log P | $E_s$ | $\sigma^*$ |
|---|---|---|---|---|
| log (1/c) | 1.00 | 0.79 | 0.04 | 0.13 |
| log P | 0.79 | 1.00 | 0.34 | 0.49 |
| $E_s$ | 0.04 | 0.34 | 1.00 | 0.96 |
| $\sigma^*$ | 0.13 | 0.49 | 0.96 | 1.00 |

and carbonyl moieties do not affect the level of taste intensity. The correlation matrix in Tables IV–VI summarize all correlations of log (1/c) vs. $\sigma^*$. These tables verify the fact that log $P$ and $\sigma^*$ are not colinear.

The relationship of taste intensity and hydrophobicity offers insight into the mechanism of taste stimulation of organic compounds. In a review of taste receptor stimulation by Beidler (1961) and Beets (1978) it is known that the taste cell nucleus has a double membrane, each section of which is 75 Å thick and separated from the other by 100 Å. Microvilli are located at the apical end of the taste cell. It is believed by some workers in this area that a receptor taste stimulant interaction occurs on the surface of these microvilli. The ability of a taste stimulant to partition through the saliva layer, the membrane layers of the taste cell, and the microvilli will affect the concentration of the stimulant that reaches the binding sites and thus the degree of taste intensity. This had been speculated earlier by Beidler (1967) who found that the taste effectiveness (sourness) of a homologous series of acids increased with increasing chain length having an order of intensity of butyric > propionic > acetic > formic. Beidler felt that this order of intensity could be correlated with increasing lipid solubility, not hydronium ion concentration. Other workers such as Hough and Khan (1978) have shown that a 2000-fold increase in sweetness can result for sucrose by replacing hydroxyl groups at carbons 1′, 4, and 6′ with more lipophilic chloro groups. Kier (1972) identified a third binding site as being hydrophobic in nature to explain varying sweetness of amino acids and substituted nitroanilines.

Although many excellent correlations between taste intensity and log $P$ were observed, the question on whether log $P$ is linearly or parabolically related to taste intensity for a specific medium needs to be resolved. Six equations in Tables I–III linearly related log $P$ to taste intensity, while five parabolic relationships were observed which had an optimum hydrophobicity (log $P_o$) associated with maximum taste intensity. Log $P_o$ values observed for stimulants in water were 3.46 (eg 5, Table II), 3.46 (eg 6, Table II), 3.91 (eg 8, Table II), and 4.19 (eg 4, Table III). Compounds with log $P$ values of 3.5–4.2 seem to have maximum taste intensity in an aqueous medium.

As discussed by Cammarata and Rogers (1972), the more complex the biological system on which a series of bioactive compounds is tested, the more likely the biological activities will be found to be nonlinear with respect to partition coefficients. The rationale for this is that compounds with a particular partition coefficient ($P_o$) value achieve sufficient concentrations in a receptor compartment to lead to a maximum in biological response. Compounds with partition coefficients greater or less than $P_o$ tend to become involved in kinetic or energetic processes which cause decreased concentrations of the bioactive compound in the receptor compartment. The biological activities of simple test systems may at times show a nonlinear dependence with respect to partition coefficients, but this usually occurs when the bioactive substances are intrinsically of high lipophilicity, and a wide range of log $P$ values is represented by the series. It is possible that the observed linear relationships between taste intensity and log $P$ would

become parabolic if the authors would have studied data sets with compounds having larger log $P$ ranges such as 5–6. For example, the alcohol series had a log $P$ range of 3.7 with no taste stimulants having log $P$ values greater than 3.5, thus it cannot be ascertained whether there is a log $P_o$ value in the 3.5–4.2 log $P$ value range. Similar statements can be made for the lactone and sulfamate data. These series have narrow log $P$ ranges and few data points with log $P$ values greater than the observed log $P_o$. The carboxylic acid in butter oil data produced a relationship of decreasing taste intensity with increasing log $P$ values. This may be misleading since there is only one data point within the log $P$ value range of 0 to 1.5 where there seems to be a maxima in a parabolic curve.

Another area of further study is the effect of olfaction on taste threshold data. The flavor of food as discussed by Beidler (1961) is often associated not with the taste stimuli but with the odor that passes from the posterior oral cavity to the olfactory area of the nose. It is possible that taste threshold data may contain an olfactory contribution. The testing procedure by Siek et al. (1969) involved having panelists tasting samples that they could not categorize by sniffing. Panelists could detect one or two concentrations lower by tasting than they could by sniffing. Meijboom (1964) found that taste threshold values for aldehydes in paraffin oil were lower than for those for odor. This does not rule out a distillation effect in the mouth by volatile stimulants producing an odor response; however, this would not be the case for the "nonvolatile" sulfamate salts. Electrophysiological measurements of taste bud response to a congeneric series of strategically designed compounds would enhance the validity of the taste intensity–hydrophobicity relationships presented in this study.

## SUMMARY

The use of the QSAR technique known as the Hansch approach in the investigation of taste intensity and organic taste stimulant physicochemical properties has indicated that hydrophobic properties of congeneric series of compounds, not steric or polar properties, are highly correlated to the level of taste intensity. This was shown to be the case for literature taste threshold data determined at different laboratories using aqueous and oil media. The hydrophobicity term as measured by log $P$, the log [$n$-octanol/water partition coefficient], indicates that the ability of an organic taste stimulant to partition from the medium in which it is dissolved into the saliva and its ability to partition through membrane layers to reach receptor sites is highly correlated to taste intensity.

Further work is needed in this area before a general predictive equation can be derived relating taste intensity of compounds in a given media to log $P$ or log $P$ and HB. The question on whether log $P$ is linearly or parabolically related to taste intensity needs to be resolved. Data sets of taste stimulants (such as pyrazines, thiazoles, mercaptans and other pertinent flavor compounds) having large log $P$ ranges of 5–6 with noncolinear steric and polar properties need to be studied to resolve this issue. Predictive equations relating log $P$ to taste intensity have to be verified by electrophysiological data from taste receptor cell response to homologous series of alcohols, aldehydes, ketones, and acids. This information would conclusively establish the odor response contribution to taste threshold values.

Recently this laboratory had presented evidence that odor intensity was highly correlated to log $P$ for homologous and nonhomologous series of odorants (Greenberg, 1979). Further evaluations of log $P$ as a taste and odor intensity predicting tool should generate general equations relating log $P$ to odor and taste intensity for a wide range of important flavor compounds in specific media. Comparisons of log $P_o$ values for optimum odor and taste intensities of a given series of flavor compounds would aid synthetic organic chemists in designing novel flavor compounds having optimum odor and taste intensities.

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