

## **Structural Functions of Taste in the Sugar Series: Characteristics of Simple Chlorinated Sugars**

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### *ABSTRACT*

*The tastes of a number of chlorinated, deoxy and, in one instance, branched-chain (C-methyl) derivatives of simple sugars were examined in an effort to relate the sensory characteristics of defined lipophilic character in conformationally stable sugars. Conclusions are drawn in relation to existing theories of sweetness.*

### **INTRODUCTION**

A hypothesis as to the basic structural requirement for sweetness in sugar molecules has been proposed by Shallenberger & Acree (1971). They postulated an AH,B system consisting of a vicinal dihydroxy grouping, AH acting as an acid function and B as the proton acceptor, this binding to a commensurate AH,B system on the taste receptor to evoke a sweet taste. Studies on the structure–taste relationships in deoxy (Birch & Lee, 1974) and methyl ethers of sugars (Lindley & Birch, 1975) suggested that the AH function was probably located at C-4 with the C-3 hydroxyl acting as the B in an AH,B unit.

Lipophilicity as an important factor in high intensity sweetness was first observed by Deutsch & Hansch (1966) in the nitroaniline series. Kier (1972) extended this idea by defining a regio-specific lipophilic function in different classes of high intensity sweeteners, located at the apex of a triangle 3.5 Å from AH and 5.5 Å from B. Hough & Phadnis (1976) and

Hough & Khan (1978) explained the high sweetness of chloro sucroses by the presence of such a Kier template in these molecules.

In this paper we describe an investigation of the effect of lipophilicity on the sensory characteristics of simple, conformationally stable sugar molecules.

## EXPERIMENTAL

All sugars were commercially available or synthesised by classical methods in carbohydrate chemistry and purified by standard techniques to chromatographic standards of purity. Previously synthesised derivatives prepared in this way agreed in melting point and optical rotation with literature reports. Further, the structures of all compounds were confirmed by elemental analyses and nuclear magnetic resonance spectrometry.

Ten assessors were selected and trained (Spencer, 1971). Panelists were then instructed to place a small amount (mg) of the test material on the tongue and to classify it according to the following descriptors: no taste (0), trace sweet (trS), sweet (S), very sweet (SS), trace bitter (trB), bitter (B) and very bitter (BB). The results reported are those agreed by at least 70 % of the assessors in duplicate tasting sessions, i.e. at least 70 % of the assessors coincided with the descriptor (no averaging was performed).

## RESULTS AND DISCUSSION

The discovery of the very sweet taste of chloro sucroses was indeed surprising since all known previous modifications resulted in derivatives which were never sweeter than the parent sugar (Birch *et al.*, 1977). Hough & Phadnis (1976) explained the high sweetness of the chlorinated sucroses by assigning a tripartite template, with a chlorine atom acting as the lipophilic function, with dimensions similar to those predicted by Kier, as necessary for high intensity sweetness.

The sensory evaluation of a number of derivatised monosaccharides of conformationally stable sugars is shown in Table 1. Shallenberger & Lindley (1977) have argued a tripartite site for simple sugars—AH and B on carbons C-4 and C-3, respectively and a  $\gamma$ , or 'greasy', function at the primary methylene group. If this is the case and if, in fact, the reason given for the high sweetness of chloro sucroses is correct, then substitution at

**TABLE 1**  
Sensory Analysis of Monosaccharide Derivatives

Compound	Sweetness	Bitterness
(I) Methyl $\alpha$ -D-glucoside	S	0
(II) Methyl $\alpha$ -D-galactoside	S	0
(III) Methyl 6-chloro-6-deoxy $\alpha$ -D-glucoside	0	trB
(IV) Methyl 6-chloro-6-deoxy- $\alpha$ -D-galactoside	0	BB
(V) Methyl 4-chloro-4-deoxy- $\alpha$ -D-glucoside	S <sup>a</sup>	0
(VI) Methyl 4-chloro-4-deoxy- $\alpha$ -D-galactoside	trS	0
(VII) Methyl 3-chloro-3-deoxy- $\alpha$ -D-glucoside	trS	trB
(VIII) Methyl 3-chloro-3-deoxy- $\alpha$ -D-glucoside	trS	trB
(IX) Methyl 6-deoxy- $\alpha$ -D-glucoside	trS	0
(X) Methyl 6-(C-methyl)- $\alpha$ -D-glucoside	trS	0

<sup>a</sup> In direct comparison panelists found this compound sweeter than compound (I).

the C-6 of these sugars should lead to a compound of increased sweetness. Both compounds (III) and (IV) were, however, bitter and the galactose sugar (IV) was extremely bitter. These results are surprising and do not support the above reasoning. They do, however, agree with previous results on the free sugars (Dziedzic & Birch, 1981). Both 6-deoxy glucose (IX) and the branched-chain 6-(C-methyl) compound (X) showed a decrease in sweetness, although there was no bitterness detectable. Kubota & Kubo (1969) suggested an AH,B distance of 1.5 Å as a prerequisite for bitterness. This seems unlikely since all peracetates, for example, can only possess a 'B' function, i.e. a proton acceptor, so that bitterness may be associated with a conformationally appropriate B,B system. This may explain the intense bitterness of the galactose compound (IV).

The tastes of the 4-chloro compounds ((V) and (VI)) are interesting, particularly that of compound (V), where the panelists, in fact, noted an increase in sweetness upon chlorination. Such derivatisation cannot allow the accepted AH,B system to function since the AH has been replaced by a 'B', i.e. a chlorine atom. Previous work on methyl ethers of sugars showed that all mono-methyl ethers were at least trace sweet and that,

**TABLE 2**  
Sensory Analysis of Fructose and Sucrose Derivatives

<i>Compound</i>	<i>Sweetness</i>	<i>Bitterness</i>
(XI) Sucrose	SS	0
(XII) Fructose	SS	0
(XIII) 6',6-Dichloro-6',6-dideoxy sucrose	trS	0
(XIV) 6',6-Dideoxy sucrose	trS	0
(XV) 6-Chloro-6-deoxy fructose	S	trB
(XVI) 6-Deoxy fructose	trS	0

although the AH,B is usually located at the C-4 and C-3 positions, this may, in some cases, revert to the C-3 and C-2 positions, respectively (Lindley & Birch, 1975). A similar effect could explain the sweet taste of compounds (V) and (VI).

Table 2 shows the sensory characteristics of sucrose and fructose derivatives. Chlorination of the disaccharide molecule (XIII) reduced the sweet taste. A similar decrease in sweet taste was also noted for the dideoxy derivatives (XIV). Fructose derivatives were also evaluated since this moiety in chlorinated sucrose may well contain the glycopore (Dziedzic & Birch, 1981). Both the derivatives, however, showed a decreased sweetness response compared with the parent sugar.

## CONCLUSIONS

The rationale proposed to account for the high sweetness of chloro sucroses cannot be extended to simple sugars. None of the derivatives examined was very sweet; in fact, all of the test sugars (except for compound (V)) showed a decreased sweetness. The results support the hypothesis that, although lipophilicity is important for favourable partitioning onto a taste receptor (such as described by Deutsch & Hansch, 1966), the overall lipophilic vector is essential in governing the quality of taste.

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