

Supporting Information for
Detection and Identification of Natural and Artificial Sweeteners
Using a Colorimetric Sensor Array

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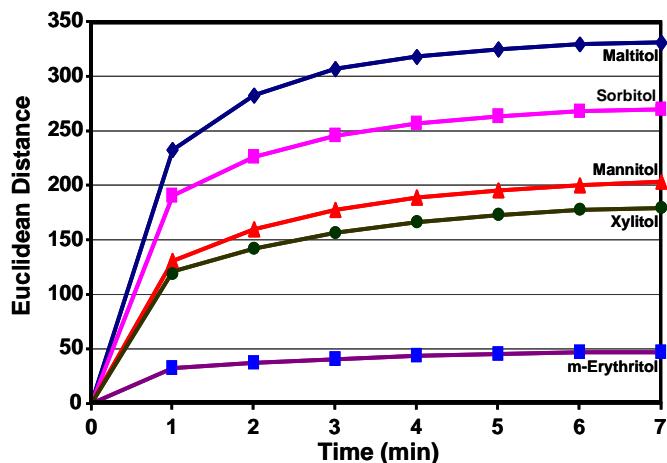


Figure S1. Response time curves for several sugar alcohols. The overall responses to a series of analytes commonly used as sweeteners, such as sorbitol and xylitol (found in “sugar free” gums) and maltitol (used in many hard candies and reduced-sugar ice creams) are shown.

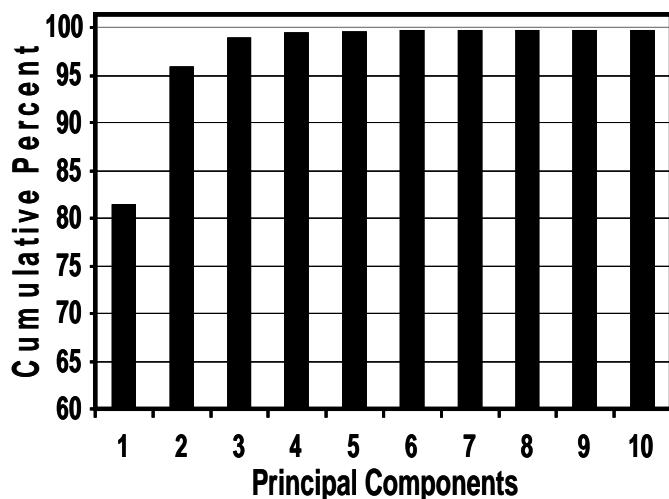


Figure S3. Scree plot from a principal components analysis for the detection and identification of fourteen natural and artificial sweeteners plus one control. Four dimensions required to define >99% of the total variance.

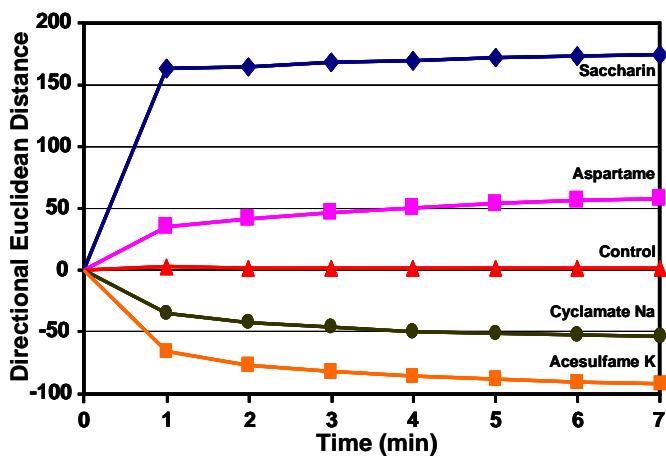


Figure S2. Response time curves for several artificial sweeteners. A directional Euclidean Distance was defined by offsetting the observed color changes by +255 to permit differentiation between positive and negative changes in RGB values, and the resulting Euclidean difference renormalized by subtraction of $(16 \cdot 255^2)^{1/2}$.

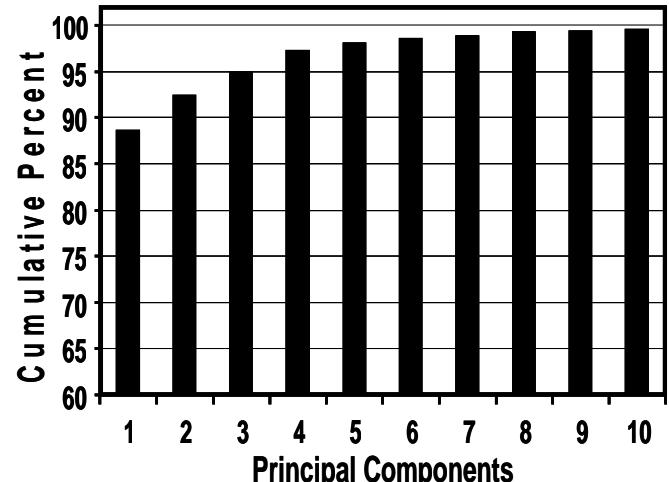


Figure S4. Scree plot from a principal components analysis for the detection and identification of individual serving packets of six different sweeteners plus one control. Four dimensions required to define >95% of the total variance and eight dimensions required for >99% of the total variance.

Table S1. Sweetener Packet Contents

Sweet'n LowTM: Nutritive Dextrose, 3.6% Saccharin, Cream of tartar, Calcium Silicate.
EqualTM: Dextrose, Maltodextrin, Aspartame.
SplendaTM: Dexrose, Maltodextrin, Sucralose.
StevitaTM: Stevia extracts (95%), Erythritol.
Sugar in the RawTM: Pure cane sugar (sucrose, molasses, "natural nutrients").

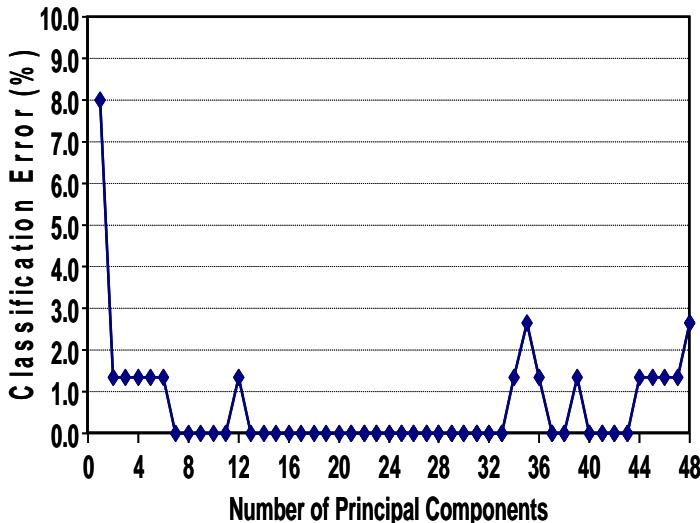


Figure S5. Classification error rates for Linear Discriminant Analysis (LDA) as a function of increasing numbers of principal components for the detection and identification of fourteen natural and artificial sweeteners plus one control. For each dimensionality, the LDA classification error was established using a "leave-one-out" cross validation. The error rate becomes zero at seven dimensions.

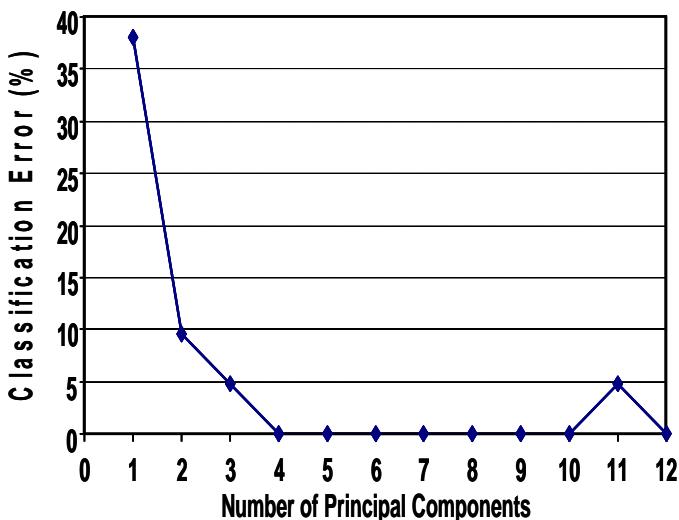


Figure S6. Classification error rate for Linear Discriminant Analysis (LDA) as a function of increasing numbers of principal components for the detection and identification of individual serving packets of six different sweeteners plus one control. For each dimensionality, the LDA classification error was established using a "leave-one-out" cross validation. The error rate becomes zero at four dimensions.

Table S2. Structures and placement of indicators.

1. Bromophenol Blue	2. Tetrabromophenol Blue	3. Bromochlorophenol Blue	4. Bromophenol Red
5. Bromopyrogallol Red	6. Bromocresol Green + Methyl Red (2:3)	7. Phenol Red	8. <i>m</i>-Cresol Purple
9. 3',3'',5',5''-Tetraiodophenolsulfonephthalein	10. Bromocresol Green	11. Cresol Red	12. Thymol Blue
13. Chlorophenol Red	14. Bromocresol Purple	15. Bromothymol Blue	16. 3,4,5,6-Tetrabromophenolsulfonephthalein

Table 3. Structures of Natural and Artificial Sweeteners.

Name	Structure
Acesulfame Potassium	
Aspartame	
Sodium Cyclamate	
m-Erythritol	
D-Fructose	
D-Glucose	
Lactitol	
Maltitol	
D-Mannitol	

Name	Structure
Ribitol (Adonitol)	
Saccharin	
D-Sorbitol	
Sucrose	
Xylitol	
Sucratose*	

* Not individually tested

Table S4. Color Difference Database for 14 natural and artificial sweeteners.

Table S5. Color Difference Database for six different types of sweetener packets.

R1	G1	B1	R2	G2	B2	R3	G3	B3	R4	G4	B4	R5	G5	B5	R6	G6	B6	R7	G7	B7	R8	G8	B8	R9	G9	B9	R10	G10	B10	R11	G11	B11	R12	G12	B12	R13	G13	B13	R14	G14	B14	R15	G15	B15	R16	G16	B16					
Splenda 1	143	14.8	-37	21.5	22.2	-7.7	12.5	-2.9	26.5	16.8	-3.0	2.7	1.7	-1.5	13.5	-0.2	-0.4	0.6	-0.5	0.4	0.5	-1.3	0.0	26.4	11.7	-6.5	42.8	11.2	0.0	0.2	-3.4	0.3	-2.2	-0.4	0.8	8.0	10.4	0.0	8.3	5.2	0.0	0.9	-0.7	0.0	1.2	-1.0	0.0					
Splenda 2	20.9	21.6	-4.9	18.1	22.4	-7.3	12.5	-3.3	3.0	28.4	18.7	-2.8	2.1	2.1	-1.7	13.3	0.0	-0.8	0.3	0.2	-0.8	0.6	-1.3	-0.9	27.1	12.6	-6.9	43.5	10.8	0.0	0.2	-3.3	0.0	-0.9	-2.3	4.3	7.3	10.9	0.0	7.7	5.3	0.0	-0.2	0.0	0.0	1.3	0.1	0.0				
Splenda 3	138	15.1	-5.1	18.1	22.6	-7.4	14.0	14.1	-3.1	30.1	13.1	-0.1	2.4	2.4	-2.4	13.6	0.5	-1.0	-0.6	-0.2	-0.4	-0.5	-1.2	0.1	24.7	13.8	-7.3	45.6	11.1	0.0	-0.1	-2.5	0.3	-0.2	-3.8	1.2	5.7	10.8	0.0	1.5	8.9	0.0	0.8	0.0	-0.2	-0.3	0.0					
Equal 1	22.9	26.9	-4.8	21.4	25.3	-6.9	16.1	15.2	-2.6	33.0	22.6	-1.3	1.0	1.5	-1.8	8.0	0.8	-0.9	-0.7	0.5	-0.1	0.7	1.2	26.9	9.3	-4.8	50.1	12.5	0.0	-0.8	12.3	1.1	2.1	6.3	-1.2	5.7	12.0	0.0	8.1	6.7	0.0	-0.7	0.2	0.0	-0.4	1.3	0.0					
Equal 2	22.6	25.7	-5.3	24.1	27.4	-7.9	24.2	21.5	-2.8	21.5	26.9	-2.8	2.3	2.8	-2.2	9.9	-0.4	-0.3	0.0	-0.6	-0.2	-0.2	-0.3	0.0	27.7	10.7	-5.6	49.9	12.3	0.0	-0.10	7.4	0.3	-0.8	4.6	7.6	5.8	12.4	0.0	9.1	6.8	0.0	-1.0	-0.4	0.0	-0.5	2.2	0.0				
Equal 3	19.4	21.7	-5.5	25.1	28.1	-8.3	21.3	20.0	-4.2	36.8	26.0	-2.0	2.0	2.3	-2.5	10.7	-0.3	-0.8	-0.4	1.1	-0.2	-1.9	-0.2	-0.1	28.6	12.6	-7.7	53.1	13.4	0.0	0.2	3.0	0.3	-1.0	0.6	3.3	7.0	13.4	0.0	11.6	8.6	0.0	-0.3	0.0	0.0	-0.1	1.9	0.0				
Stevia 1	0.4	0.0	-0.2	2.6	4.1	1.0	-0.6	0.3	-0.5	1.7	0.2	-1.2	0.0	-0.6	-0.2	3.6	-0.2	-0.6	0.6	0.2	0.2	1.3	0.2	0.3	5.5	0.8	0.2	-0.1	0.1	0.2	0.1	0.42	0.0	1.5	6.9	21	0.3	1.1	0.0	-0.2	0.0	0.3	3.2	0.0								
Stevia 2	-1.0	-1.0	0.8	-3.1	-6.1	3.4	-0.8	-0.9	0.3	0.1	3.8	0.0	-2.0	-0.8	0.7	-2.7	0.0	-0.1	-0.1	0.4	1.1	0.3	1.8	0.1	-1.9	-5.7	1.2	0.5	-0.1	0.0	0.0	0.2	0.1	0.6	0.4	0.0	-0.2	1.8	0.0													
Stevia 3	-0.6	-0.1	0.2	-2.6	-4.9	3.9	-0.2	-0.3	0.1	-1.3	-0.2	0.5	-1.0	-0.3	-0.4	-2.7	-0.1	0.0	-0.6	0.0	-0.3	0.8	0.6	1.1	-4.3	0.7	0.8	0.6	1.1	-0.5	-0.2	0.5	0.1	11	0.0	2.3	0.8	-0.5	1.5	3.0	0.0											
RawSugar 1	0.6	1.9	-0.8	-0.7	-1.1	2.2	0.3	1.6	-1.2	0.8	-0.8	-2.8	-1.0	-2.7	-4.2	-0.8	-0.9	-6.1	-2.9	-1.0	-0.7	-1.0	-0.6	-0.3	-0.1	-0.6	-0.3	-0.4	-0.4	-0.3	-0.4	-0.2	-0.0	-0.2	-0.4	-0.1	-0.5	-0.3	0.0													
RawSugar 2	-0.1	0.8	-0.9	0.2	-0.1	-1.4	0.5	1.7	-1.2	-3.0	-1.6	-2.5	-2.9	-0.1	-0.6	-5.7	-3.1	-0.6	-6.3	-1.5	-2.8	-0.2	-6.5	-2.7	9.4	1.5	0.0	-5.0	6.3	0.0	-1.8	10.0	-4.5	-31	0.7	0.0	-0.7	0.0	0.0	1.6	3.1	0.0	-0.5	-0.4	0.6	0.0						
RawSugar 3	2.2	4.7	-1.6	1.0	1.4	-1.4	1.2	3.3	-1.8	5.0	8.7	-1.0	-2.7	-1.0	-2.7	-3.2	-0.2	-1.1	-5.1	-2.7	-0.2	-4.5	-1.0	-2.3	-0.2	-5.9	-3.7	10.8	2.1	0.0	-4.4	7.7	0.0	-1.6	7.6	-24	-1.8	1.4	0.0	-0.2	0.4	0.0	-2.6	0.5	0.0	-4.3	0.6	0.0				
Domino 1	0.7	1.1	-1.0	4.1	6.2	1.1	0.1	0.3	-0.7	1.9	2.1	-0.4	-1.5	-0.9	-1.9	-0.1	-0.4	-2.6	0.2	0.0	-0.2	-0.3	0.3	0.1	-1.2	-1.2	-1.9	-1.9	-0.9	-0.2	-1.9	1.6	0.0	-0.3	0.0	-0.1	1.9	6	-0.9	0.0	-0.1	1.9	6	0.0								
Domino 2	0.4	0.9	-0.5	4.9	9.0	4.8	0.0	0.5	-0.8	3.5	6.6	-1.3	-1.4	-0.8	-1.2	-3.1	0.1	-0.7	-3.1	-0.4	0.0	-0.32	-0.2	-1.0	-1.3	-3.7	-0.5	1.1	-0.5	-0.3	-2.7	1.9	0.4	-2.7	5.6	3.5	-1.0	1.9	0.0	-2.1	3.3	0.0	-3.4	-0.1	-0.1	-2.7	15.8	0.0				
Domino 3	0.7	1.4	-1.0	3.5	5.6	0.7	0.1	0.7	-1.0	1.8	3.9	-1.0	-1.9	-0.6	-1.7	-3.3	-0.1	-0.8	-2.9	-0.6	-0.2	-24	-0.9	-4.6	-2.9	-1.3	2.5	0.4	1.1	2.3	1.0	0.4	-1.0	5.8	0.7	0.5	3.2	0.0	0.9	0.1	-1.3	0.3	-1.1	-1.6	11.9	0.0						
Control 1	0.1	1.1	-0.3	-0.2	1.4	-0.4	-0.1	1.1	-0.3	-0.5	0.2	0.0	0.0	-0.4	1.5	0.4	-0.4	0.0	-0.5	0.7	0.0	-1.0	0.0	0.0	-0.5	0.0	-0.5	0.0	-0.4	-0.4	0.0	-0.19	0.0	0.0	-0.8	-0.2	0.0	0.0	-0.4	0.0	-0.1	-0.6	0.0									
Control 2	0.5	1.0	-0.3	0.3	1.1	-0.3	0.1	1.0	0.0	-0.6	0.1	0.0	-0.3	0.1	-0.1	-0.5	-0.1	1.1	0.1	-0.1	-0.6	0.1	1.3	0.0	-0.1	-0.6	0.7	0.4	0.0	-0.8	0.2	0.0	-0.1	0.0	-0.1	0.0	-0.1	0.0	-0.1	-0.6	0.0											
Control 3	1.0	1.8	-0.6	1.7	2.4	-1.0	0.9	2.1	-0.4	1.1	1.1	0.0	0.0	0.2	0.0	2.6	0.1	-0.1	-0.1	-0.1	0.0	-0.15	-0.3	1.8	-0.4	-0.7	4.6	1.8	0.0	-0.3	-0.4	1.1	0.0	-0.7	0.0	1.1	0.5	0.0	-0.1	0.0	0.0	-0.8	0.4	0.0								
SwtnLo-1	14.3	13.9	-1.8	14.7	10.9	-0.4	16.1	15.7	-2.4	19.9	9.9	0.0	0.2	1.0	-1.6	3.9	0.0	-0.1	1.1	0.8	0.1	-0.4	-0.7	-1.9	14.4	9.2	-2.0	20.2	3.7	0.1	0.4	-0.3	0.0	2.8	1.4	0.0	-1.2	0.7	0.0	-0.2	0.8	0.0	-1.1	0.0	-0.2	0.8	0.0					
SwtnLo-2	15.7	16.2	-3.4	14.4	10.5	12.1	17.9	16.9	-2.3	19.1	10.4	-1.1	0.6	2.3	-1.2	5.1	0.1	-0.3	-0.9	-0.5	0.7	0.2	-0.6	-0.3	16.0	10.9	-5.7	17.8	3.7	0.0	-0.9	2.1	0.1	-1.4	1.9	3.2	0.0	0.3	0.5	0.1	-1.1	-1.1	0.0	-0.4	-0.8	0.0	-0.1	0.8	0.0			
SwtnLo-3	15.8	15.1	-1.5	15.3	11.0	-1.2	18.3	16.8	-1.7	21.0	12.0	0.0	1.2	1.6	-1.0	4.1	-0.1	-1.0	-0.6	0.1	-1.0	0.6	0.3	-1.0	14.3	9.8	-6.3	18.9	5.0	0.2	0.3	-0.2	-0.4	-0.9	-1.4	2.4	3.8	0.0	2.6	1.5	0.0	-0.4	-0.6	1.4	1.1	0.0	-0.6	0.4	-0.6	1.4	1.1	0.0