

Colorimetric Sensor Array for Soft Drink Analysis

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Fourteen commercial soft drinks have been analyzed using colorimetric sensor arrays made from a set of 25 chemically responsive dyes printed on a hydrophobic membrane. Digital imaging of the dye array before and after immersion provides a color change profile as a unique fingerprint for each specific analyte. The digital data library generated was analyzed with statistical and chemometric methods, including principal component analysis (PCA) and hierarchical clustering analysis (HCA). Facile identification of all of the soft drinks was readily achieved using comparison of the color change profiles or a PCA score plot. Using a HCA dendrogram, the misclassification rate was <2%, and even very similar sodas were easily differentiated. In addition, the monitoring of soft drinks as they degas or upon dilution also proved to be possible. This work demonstrates the potential of our colorimetric sensor array technology for quality assurance/control applications of sodas and perhaps other beverages as well.

KEYWORDS: Colorimetric sensor array; cross-responsive sensors; dyes; chemometrics; beverages; soft drinks; soda

INTRODUCTION

Quality control (QC) and quality assurance (QA) of food and beverages are extremely important both to industry and consumers. In the past decade, a variety of sensor techniques have been developed (1–11), and various applications have been achieved for the analyses of food and beverages (12–19). Generally, these so-called electronic tongue and electronic nose devices consist of an array of cross-responsive sensors and are inspired by the mammalian gustatory and olfactory systems (20–22) in which it is the *composite* response of the array that differentiates one analyte from another. Instead of a traditional component-by-component analysis (e.g., gas or liquid chromatography) (23), this approach is potentially less expensive and has found some applications in industrial practice. Most array sensors are based on conductive polymers or electrochemical sensors; a common limitation of such arrays, however, is their general lack of *chemical discrimination*, which makes differentiation among similar species problematic.

Recently, we have reported an optoelectronic approach that uses a colorimetric sensor array for the general detection, identification, and quantification of volatile organic compounds in the gas phase (24–30). The colorimetric sensor arrays are inexpensive disposables and, therefore, their reversibility is not an important issue (24). Because the sensor dyes and substrate upon which the dyes are printed are both hydrophobic, we have even been able to use this approach for the detection and differentiation of organic compounds dissolved in aqueous solutions without interference from the presence of 55 M water (30). The color change pattern of the dye array before and after

exposure to an analyte provides a color “fingerprint” for each specific analyte (**Figure 1**), and this simple array system makes facile identification of a wide variety of aqueous organic solutions possible over a concentration range of 10^{-5} –0.1 M.

Complex mixtures present no inherent difficulty for sensor arrays, in general, if they have sufficient *discriminatory power*. Obviously, the composite response of an array does not give a component-by-component analysis, but for the purpose of identification or quality control such an analysis is often not required. Beverages comprise an important class of complex mixtures, and carbonated soft drinks are, of course, one of the most consumed beverages in the world. Not surprisingly, there have been previous examinations of soft drinks by electronic tongue and nose devices (19, 31–33). For example, Gardner and co-workers developed a microsensor using surface acoustic waves (SAW) detection, which can monitor the decarbonation of cola versus time after opening (31). Legin and co-workers developed an electronic tongue that could distinguish among some soft drink samples (33). These methods, however, are either relatively low in discriminatory ability, expensive, or nonportable. In comparison, however, our colorimetric sensor array has an extremely high discriminatory power (27–30), a very low cost, and the potential for facile miniaturization. In this work, 14 different commercial soft drinks were examined using the colorimetric sensor array system in the liquid phase; in addition, the effects of decarbonation and dilution were also investigated for potential QA/QC applications.

MATERIALS AND METHODS

Sample Preparation and Instruments. Fourteen soft drinks were purchased from local supermarkets and were used directly and freshly

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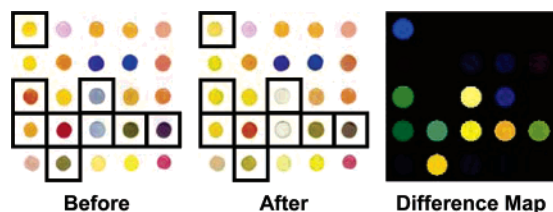


Figure 1. Image of the colorimetric sensor array before and after exposure to 7-Up. The dyes that changed color the most are marked with circles. For the purposes of effective visualization, the color range shown in these representations is expanded from RGB values of 10–41 (i.e., 5 bit) to 0–255 (i.e., 8 bit).

Table 1. pH Values of the 14 Commercial Soft Drinks Used

soft drink ^a	pH ^b	soft drink ^a	pH ^b
Coca-Cola Classic	2.50	Fanta	2.93
Diet Coke	3.38	Dr. Pepper	2.83
Pepsi	2.47	A&W Root Beer	4.67
Diet Pepsi	3.07	Canada Dry Tonic Water	2.56
Sprite	3.30	Canada Dry Club Soda	5.18
Diet Sprite	3.37	La Croix Sparkling Water	4.26
7-Up	3.24		
Diet 7-Up	3.77		

^a All product names are trademarks of or copyrighted by their respective manufacturers. ^b Measured immediately after opening.

from their containers. Loss of CO₂ was minimized by conducting parallel triplicate experiments immediately after the containers had been opened. NaH₂PO₄·H₂O and Na₂HPO₄ were dissolved in purified water (obtained using a NANOpure Ultrapure Water System, Barnstead International) to make a 0.3 M phosphate buffer solution at pH 7.0 [the same buffer as used in prior aqueous sensing (30)]. A ThermoOrion 920A-plus pH-meter was used for pH measurements; the pH values of the soft drinks used are listed in **Table 1**.

Sensor Array. The composition of the colorimetric sensor array was described previously (30) and was prepared following the previous procedure (24–26). This 5 × 5 array was optimized for detecting acidity in aqueous solutions, and the printed arrays are available commercially (array CSI.083) from ChemSensing, Inc. (Champaign, IL; www.chem-sensing.com).

Data Acquisition. Data acquisition was carried out using an ordinary flatbed scanner (Epson Perfection 1250) following previously reported procedures, described in the Supporting Information (30). In use, the array is first saturated in an aqueous liquid without dissolved organics (i.e., phosphate buffer) and imaged. After exposure to an analyte solution, rapid color changes in the dyes are readily observed and digitally imaged. All of the analyses of soft drink samples were conducted in triplicate. The colors of the solutions have no significant effects because the liquid layer between the sensor array and flatbed scanner is extremely thin (<100 μm).

Data Processing and Analysis. Simply subtracting the before-exposure image from the after-exposure image (red value after exposure to analyte minus red value before exposure, green minus green, blue minus blue) provides a color change profile for the analyte solution, as shown in **Figure 1**. The center of each dye spot is averaged to avoid edge artifacts using Photoshop or a customized analysis package, ChemEye (ChemSensing, Inc.). The color change profiles are simply a 3*N*-dimensional vector (where *N* = number of dyes) that can be easily analyzed by standard statistical and chemometric techniques. In addition to the triplicate data, an average response was also calculated for each analyte.

It is convenient to visually display these vectors as color change maps by representing each spot as the absolute value of its color change in RGB. For purposes of display, the color ranges of the images are expanded; RGB values of 10–41 (i.e., 5 bit) were expanded to 0–255 (i.e., 8 bit). This visual representation in no way affects the actual digital data used for chemometric analysis. The color change profiles were compiled into a library of 75-dimensional vectors (25 red, green, and

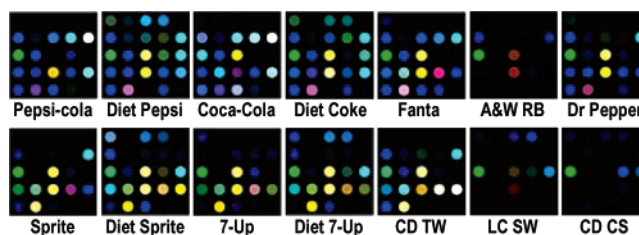


Figure 2. Average color change profiles from the colorimetric sensor array for 14 common soft drinks, Abbreviations: A&W RB, A&W Root Beer; CD TW, Canada Dry Tonic Water; CD CS, Canada Dry Club Soda; LC SW, LaCroix Sparkling Water. For the purposes of effective visualization, the color range shown in these representations is expanded from RGB values of 10–41 (i.e., 5 bit) to 0–255 (i.e., 8 bit); the complete digital data are provided as Supporting Information.

blue color changes) with 56 entries (4 for each of 14 analytes), which is provided in the Supporting Information.

Principal component analysis (PCA) and hierarchical clustering analysis (HCA) (34) were performed on the library using the Multi-Variance Statistical Package (MVSP, Kovach Computing Services, Anglesey, Wales; www.kovcomp.co.uk) software.

RESULTS AND DISCUSSION

Molecular recognition is, of course, a function of the interatomic, intermolecular, or interfacial interactions of the analyte with the sensor. Our colorimetric approach to molecular recognition (24–30) uses a cross-responsive array of chemically diverse dyes; the design of a colorimetric sensor array is based on stronger dye–analyte interactions rather than exclusively physical adsorption (as in most forms of chromatography and prior electronic nose technology). The chemically responsive dyes fall into three general classes: (1) metal ion containing dyes that respond to Lewis basicity (i.e., electron pair donation, metal ion ligation), (2) pH indicators (35) that respond to Brønsted acidity/basicity (i.e., proton acidity and hydrogen bonding), and (3) dyes with large permanent dipoles (e.g., zwitterionic solvatochromic dyes) that respond to local polarity (36). To some extent, of course, all dyes have some components of all three classes: that is, all dyes will have some Lewis acid/base interactions, nearly all will have some hydrogen bonding, and all have some response to solvent polarity. For aqueous analysis, it is important that the dyes chosen must be hydrophobic.

Colorimetric Sensor Array Responses. Average color change profiles were obtained for 14 common soft drinks as shown in **Figure 2**. Distinct and highly reproducible patterns were obtained for each soft drink. Among these, two simple carbonated waters *without* organic additives were examined: LaCroix Sparkling Water and Canada Dry Club Soda. (All product names are trademarks of or copyrighted by their respective manufacturers.) Upon examination of **Figure 2**, it is obvious that the strong responses from the complex mixtures present in other sodas do *not* primarily come from the dissolved CO₂, because the carbonated water samples gave much weaker responses than all of the other soft drinks. We are, however, able to discriminate easily even between these two carbonated waters on the basis of the slight differences in their CO₂ content (and resulting pH differences).

Principal Component Analysis. PCA is a mathematical transformation used to extract variance between entries in a data matrix by reducing the redundancy in the dimensionality of the data. It takes the data points (changes in RGB values for each of the dyes in the array) for all analytes and generates a set of orthogonal eigenvectors (principal components, PCs) for maxi-

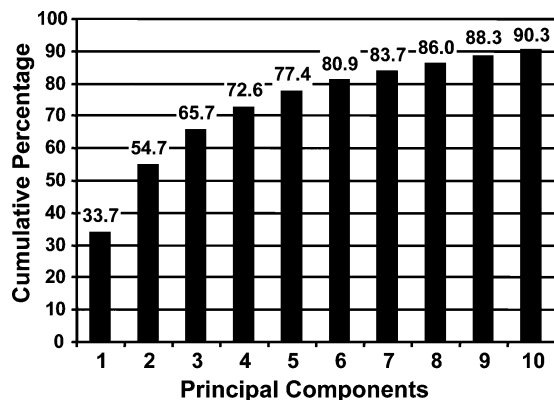


Figure 3. Scree plot of the cumulative percentage of variance for the 10 most important principal components obtained from the color change profile numerical data.

imum variance. The maximum total number of PCs equal to $3N - 1$, where N is the number of dyes in the array (i.e., 75 dimensions for the aqueous-phase sensor array used here). PCA essentially concentrates the data's variation among analytes into the minimum number of dimensions. Generally speaking, the larger the number of PCs necessary for a certain level of discrimination (e.g., 95% of the total data variability), the better the sensor will be able to discriminate among similar analytes (24).

As shown in **Figure 3**, 90% of all the data variance is contained in 10 dimensions of 75 total possible dimensions; 15 dimensions are required for 95% of the variance and 25 dimensions for 99%. In general, other electronic nose and electronic tongue techniques typically have 95–99% of discrimination in their first *two* dimensions. The high dimensionality (i.e., high dispersion) of the colorimetric sensor array demonstrates the unusually high level of chemical discrimination and, hence, an exceptional ability of the colorimetric sensor arrays to discriminate among very similar analytes.

A three-dimensional PCA score plot was obtained using the three most important PCs, which accounts for only 65.7% of the total variance (**Figure 4**). All of the triplicates plus the average of each soft drink sample were reasonably well clustered together and separated from those of other samples, which is surprising considering that less than two-thirds of the total variance is captured in **Figure 4**, and the resolution between classes is in fact better than can be shown using only three principal component dimensions. The relative locations in the PCA space reflect the response of the array, which is based on the differences in the concentrations of various organic compounds and the pH of each analyte, and the responses cannot be translated exactly into the actual taste for each type of soft drink. Nonetheless, the relative locations of the soft drink samples on the plot roughly reflect the differences in their tastes. For example, the data points for A&W Root Beer are relatively distant from those of the other soft drinks in the score plot, and likewise, the taste of root beer is also (subjectively) relatively different from that of other soft drinks. Conversely, Diet 7-Up and Diet Sprite (or 7-Up and Sprite, or Diet Coke and Diet Pepsi, etc.) are spatially close, and they *do* taste much alike.

Statistical Analysis and Error Analysis. A very standard statistical procedure, HCA, provides a better alternative for accurate representation and classification of high-dimensional data in that it uses the full dimensionality of the data in creating a classification dendrogram. HCA groups the analyte vectors according to their intervector distances in their full dimensional space (i.e., 75-dimensional). There exist various related methods

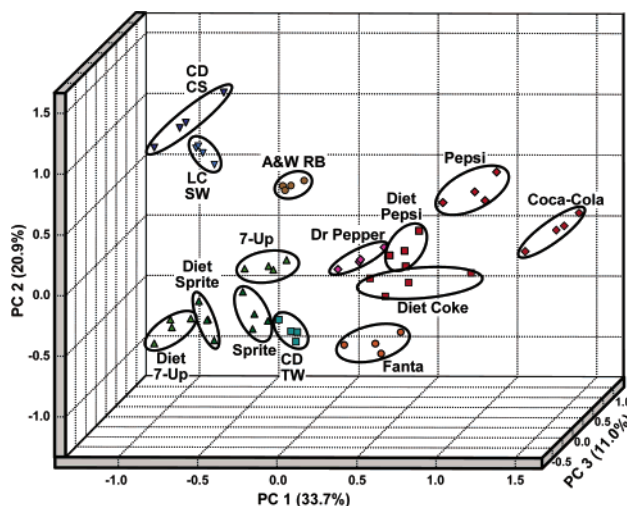


Figure 4. PCA score plot using the three most important principal components based on the data for the analysis of all soft drinks. Triplicate data plus their average are plotted for each soft drink. The resolution between classes is in fact much better than can be shown by these three principal components because they account for only 65.7% of the total variance. Abbreviations: A&W RB, A&W Root Beer; CD TW, Canada Dry Tonic Water; CD CS, Canada Dry Club Soda; LC SW, LaCroix Sparkling Water.

for defining clusters from the set of analyte vectors. The most common of these is the minimum variance method (Ward's method) (21), which we use here. The sum of the squared Euclidean distances (SEDs) from the group centroid to each of the vectors in that group is used to evaluate the variance within the group, and the groups with the minimum variance are clustered preferentially. Those clusters are then grouped together to form new larger scale clusters. The operation is performed repeatedly until only one supercluster remains. A dendrogram is generated in this fashion that shows quantitatively the similarities among the various analytes. An HCA dendrogram shows quantitatively the degree of similarity of the array responses among the various analytes using the data's full dimensionality. It also shows any misidentifications or overlap between individual measurements of analytes. In addition, once a database is established, any new unknown sample can be easily classified using the HCA dendrogram to identify the unknown or at least to identify the database entry closest to it.

As shown in the HCA dendrogram of all soft drinks (**Figure 5**), all of the samples were clustered correctly with a single misclassification (one Diet Sprite was mistakenly clustered with Diet 7-Up, these two, after all, being rather close in taste). Furthermore, the classes of sodas are distinct: colas separate from citrus flavors, diet from regular, etc. These results suggest that the HCA dendrogram may be used to identify unknown samples.

Commercial soft drinks are normally acidic, and their pH values do of course affect the response of the dye array. In soft drinks, CO_2 is supersaturated; as a consequence, even though the system is not closed in our trials, we can still measure a reproducible pH that does not change over the time of our testing. We find, moreover, that pH *does not play an overwhelming or even a predominant role* in determining the array's responses to the soft drinks. The pH values for all 14 soft drinks were measured using a pH-meter immediately after the containers had been opened (**Table 1**). The pH values of all the soft drinks are between 2.5 and 5.2. By comparing the pH values with the color change profiles (**Figure 2**) and the HCA

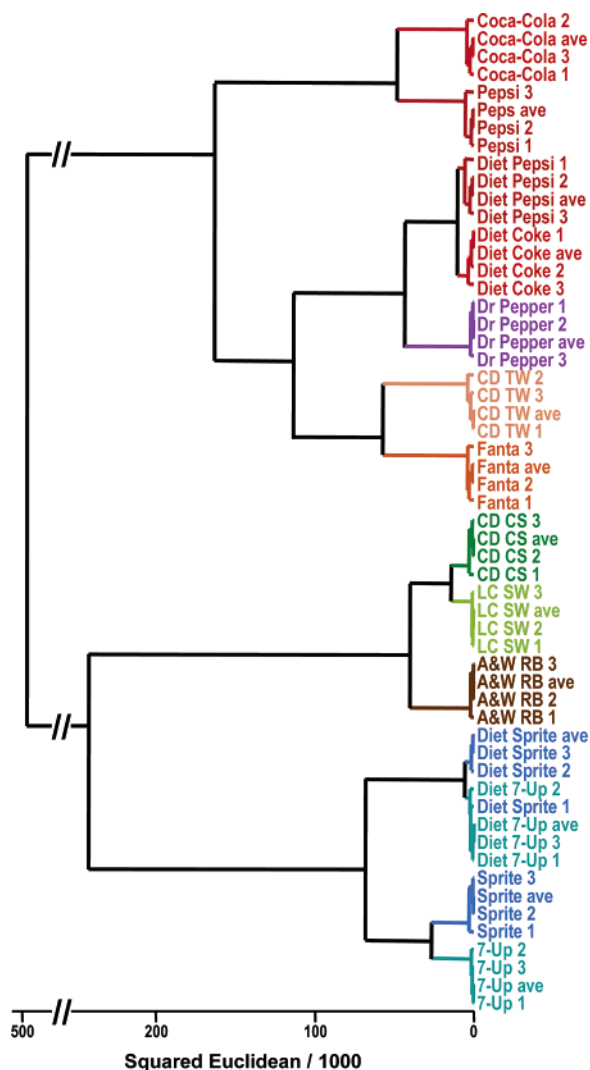


Figure 5. Hierarchical cluster analysis dendrogram for 14 soft drinks using Ward's method. All experiments were run in triplicates and an average generated thereof. After the beverage name, the trial number or "ave" (for average) is given. Abbreviations: A&W RB, A&W Root Beer; CD TW, Canada Dry Tonic Water; CD CS, Canada Dry Club Soda; LC SW, LaCroix Sparkling Water.

dendrogram (**Figure 5**) of the 14 soft drinks, clearly pH does not dominate the array response: for example, Diet Coke (pH 3.38) and Diet Pepsi (pH 3.07) are tightly grouped in the dendrogram, whereas Diet Sprite (pH 3.37) is quite distant from Diet Coke (the pH of which is essentially identical) and very close in the dendrogram to Diet 7-Up (pH 3.77). Even though pH is not predominant, changes in pH (or CO_2 concentration once the soda is below supersaturation), of course, will change the array response, as in the case of degassing (discussed later).

Testing the reproducibility and reliability of a multidimensional sensor array is much more complicated than that for single sensors. The work reported here is satisfactory for proof of concept, but there are insufficient replicates to produce a truly rigorous cross-validation, which must remain for future work. HCA provides an optimized model of the entire database; as we see in **Figure 5**, there is only a single case of misclassification in the 56 library entries (one Diet Sprite entry mistaken for Diet 7-Up), that is, a misclassification rate of 1.8%.

One of the major remaining sources of error with the colorimetric sensor arrays is in the reproducibility of the printing of the arrays, which (in these studies) were produced by transfer

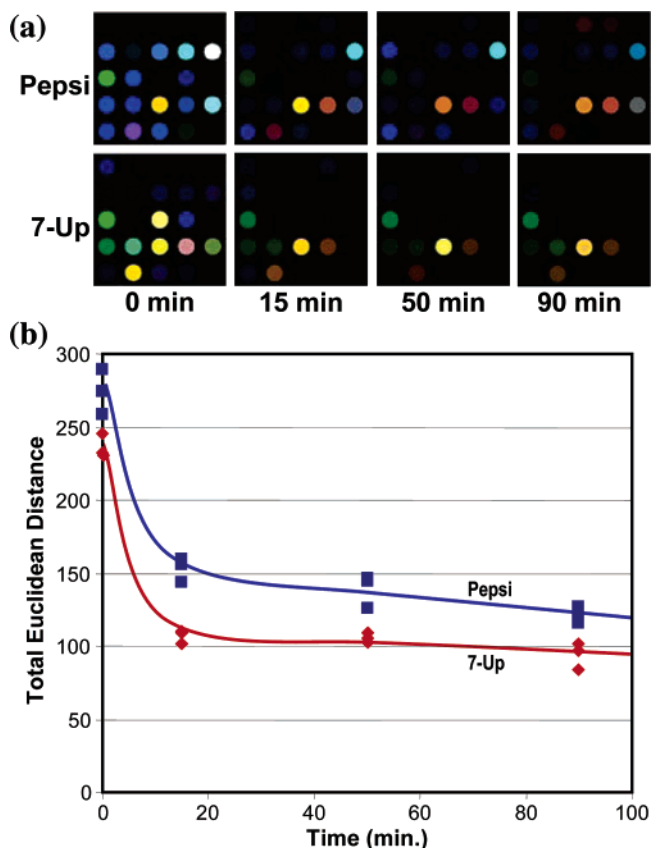


Figure 6. (a) Average color change profiles for Pepsi and 7-Up versus length of time of decarbonation by bubbling with argon gas for 15, 50, and 90 min at ~ 200 mL/min. The color range of the difference maps is expanded from RGB values of 10–41 (i.e., 5 bit) to 0–255 (i.e., 8 bit). (b) Total Euclidean distance (i.e., square root of the sum of the squares of each of the changes in the 108 dimensions) versus length of time of decarbonation. The trend lines are simply smoothed curves to guide the eye.

from an ink-well array to the hydrophobic membrane using an array of dipped stainless steel pins (24–30). The level of reproducibility in array printing, however, is improving rapidly using noncontact printing.

Quality Control/Quality Assurance. This work suggests that colorimetric sensor arrays might prove to be useful in QC and QA for soft drink production in the food and beverage industry. We have conducted two simple experiments along these lines for proof of concept: the effects on the colorimetric sensor array response of removal of CO_2 (i.e., decarbonation) and of dilution.

The array response (done in triplicate) was determined for two soft drinks, Pepsi and 7-Up, after degassing with an argon gas flow. As shown in **Figure 6**, the color change profiles of the array do respond to removal of CO_2 , and the changes in the array response are clearly distinguishable even by eye. Another set of experiments was conducted to determine the effect of watering on the array response. As shown in **Figure 7**, the color change profiles do change with increased dilution, and the changes are again clearly distinguishable. By using the total Euclidean distance as an overall measure of the array response, one can also generate monotonic (but obviously not linear) response curves, as shown in **Figures 6b** and **7b**. These results show the potential of the colorimetric sensor array technique for both qualitative and quantitative applications to QA/QC of soft drinks and perhaps other beverages as well.

In summary, we have successfully applied a new colorimetric sensor array methodology to the analyses of 14 common soft

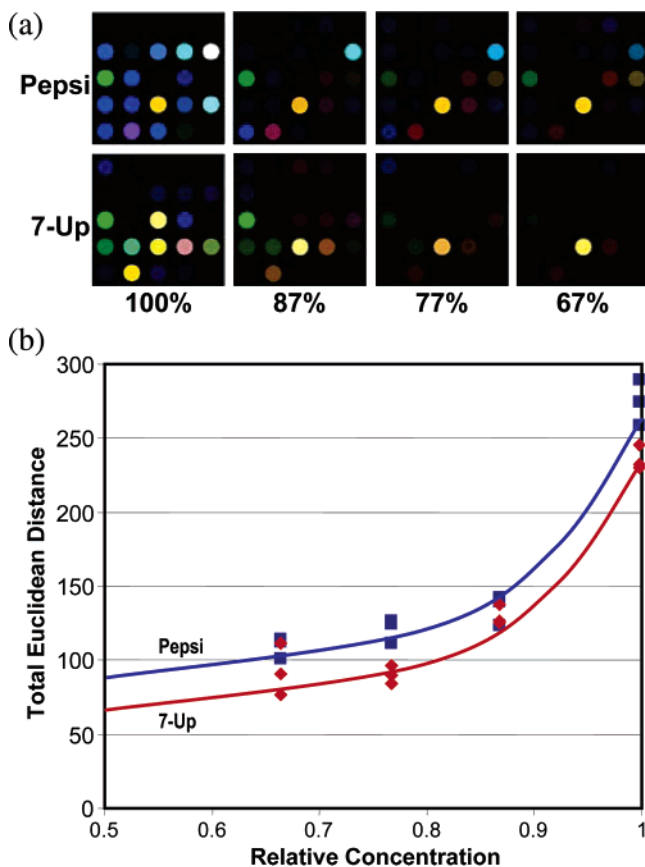


Figure 7. (a) Average color change profiles for Pepsi and 7-Up after dilution with purified water to the specified final relative concentration (e.g., 87% = 15 mL of water added to 100 mL of soda). The color range of the difference maps is expanded from RGB values of 10–41 (i.e., 5 bit) to 0–255 (i.e., 8 bit). (b) Total Euclidean distance versus dilution. The trend lines are simply smoothed curves to guide the eye.

drinks. A distinct and unique pattern can be obtained for each sample with very simple experiments using a very simple apparatus. The data can be analyzed using standard chemometrics methods, including PCA and HCA, and excellent discrimination can be obtained from either a PCA score plot or an HCA dendrogram. We have established in these studies that we can tell the difference even between very subtly different soft drinks with reasonable accuracy. Our preliminary results also suggest potential applications of the colorimetric sensor array to QC and QA in the food and beverage industry. In addition, the extremely high dimensionality of the data from our colorimetric arrays suggests that statistical correlations with the evaluations by organoleptic panels (i.e., people) may prove to be possible for quantitative prediction of human response. It is important to realize, however, that the colorimetric sensor array is based on the differences in the concentrations of various organic and inorganic components (including pH) of the analytes and that the array responses cannot be translated (at this time, at least) into an actual human perception of taste and smell.

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Supporting Information Available: More experimental details and the full digital database for sodas. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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