Atomic Absorption/Emission Spectrometry

Determination of Lead and Chromium Levels in Commercial and Home-Brewed Kombucha Health Tonic via Atomic Absorption Spectroscopy

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Kombucha tea is an alternative health tonic that is gaining popularity as a remedy for a broad spectrum of ailments. In a study found in the Australian Journal of Medicine, a married couple was admitted to a hospital with symptoms of lead poisoning in 1998. For six months the couple had been drinking Kombucha tea brewed in a ceramic vessel. Based on the data divulged in the study, we postulate that the highly acidic nature of the tea is responsible for elution of toxic metal oxides from the brewing vessel. To test for lead and chromium content in commercial and home brewed samples, flame atomic absorption spectroscopy was implemented. Detection limits for lead and chromium were calculated as 0.044 mg/L and 0.0242 mg/L. The analysis showed that the lead levels for GT’s was 0.035 mg/L, Brew Doctor was 0.119 mg/L, home-brew was 0.068 mg/L, and Mama Kombucha contained levels below the detection limit of the Flame AAS unit. Chromium levels were 0.0253 mg/L for GT and 0.0410 mg/L for the home-brew samples. Mama and Brew Doctor Kombucha both had levels below the detection limit for chromium content. The analyses of commercial and home-brewed Kombucha samples showed that the metals are detectable but were not above FDA regulations for lead and chromium content in food products.

Atomic Absorption Spectroscopy Investigation of Metals in Fireworks

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Two kinds of fireworks, Piccolo Petes and Ground Blooms, were analyzed for metal content after being lit off using atomic absorption spectroscopy. Strontium, cadmium and barium are the metals that were searched for. In one set of samples, water was used to dissolve the metal salts to simulate a water bucket used to douse the used fireworks around the holidays, while another set of samples nitric acid was used to get as much metal out as possible.

Results show that there is no cadmium metal found above the instruments detection limits in any samples. Strontium was found only in the Ground blooms, 6.6 mg/firework in the nitric solution and 1.1 mg/firework in the water. Barium was found in all samples, having 0.61 mg and 2.7 mg in each piccolo pete and ground bloom in nitric while only 0.20 found in the ground bloom in water. No barium was found in the piccolo petes in water. Results show that insignificant amounts of metals are leached into the water from used fireworks.
Safe Lead Concentrations in Reusable Safeway Bags: An ICP-AES Study

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This experiment was designed to determine the concentration of Pb in reusable Safeway bags. A method for textile pre-digestion was used, along with ICP to detect the Pb concentration within the sample. No Pb was found above the detection limit of 77 ppm. Concentrations below the detection limit were in the range of 31 ppm to 57.5 ppm. The federal limit for Pb in children’s products is 90 ppm; since the sample is well below this amount, the Safeway reusable bags contain safe amounts of Pb for both children and adults.

An analysis of the leaching of metals from cookware

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Iron, aluminum, chromium, nickel and zinc concentrations in aqueous solutions boiled in aluminum, cast iron and stainless steel pots were analyzed. Solutions of pH 5.7 and 3.0 were used for each pot. Analysis was carried out by inductively coupled plasma atomic emission spectroscopy. Significant leaching of iron and aluminum were observed, as well as a trend in increasing leaching with decreased pH. A t-test (t-table = 4.303) showed significant difference between the measured concentrations of the two solutions for aluminum (t-calculated = 11.4) and cast iron (t-calculated = 4340).

Concentration of As, Cd, Cr, and Pb in cigarettes, chewing tobacco, and shisha

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We conducted a comparison of metal contents in cigarettes, chewing tobacco, and shisha. We tested three cigarettes from a single pack, three samples from a container of wintergreen chewing tobacco, and three samples from a box of mint shisha. Samples were ground in a mortar and pestle, with chewing tobacco and shisha requiring liquid nitrogen. Each .5g sample was prepared by heated acid digestion for 18 minutes. Samples were analyzed by ICPAES.

Cigarettes were found to have an average concentration of 660.5 PPB for Pb, 1072 PPB for Cr, 3984 PPB for As, and 4245 PPB for Cd. Chew was found to have an average concentration of 259.4 PPB for Pb, 1014 PPB for Cr, 2577 PPB for As, and 870.0 PPB for Cd. Shisha was found to have an average concentration of 2098 PPB for Pb, 441.2 PPB for Cr, 2091 PPB for As, and 13490 PPB for Cd. Due to the
high standard deviations from the three samples of each sample type (Table 3), we fail to reject the null hypothesis that there is a difference between analyze concentrations between any two tobacco types.

**Quantitative Analysis of Copper Leachate from ACQ Treated Wood**

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Alkaline Copper Quaternary (ACQ) is a water-based wood preservative often used in pressure-treated lumber. Construction projects that are exposed to weather and soil contact utilize the treated wood because ACQ acts as a both fungicide and insecticide, leading to a slower degradation rate when compared to untreated wood. Our initial concern was copper leaching into the soil and affecting small-scale agricultural production. However, it was discovered that the greater danger concerning copper leachate is to aquatic life. As increasing quantities of debris enter construction and demolition (C&D) landfills – from hurricanes Katrina and Sandy, for example – treated wood can leach large amounts of copper into the soil and groundwater, polluting waterways and endangering aquatic life.

In order to test for ACQ leaching into the soil, Flame Atomic Absorption Spectrometry (FAAS) was used to detect copper concentrations in three ACQ-treated lumber samples (weather and soil exposure, weathering with no soil exposure, new wood sample) obtained from a one-year-old raised garden bed. Sawdust samples were prepared with concentrated nitric acid, subjected to microwave digestion, and then diluted with 2% nitric acid to achieve levels detectable by FAAS.

The FAAS analysis showed that average copper concentration in new wood (New) was 3.7 mg Cu/g wood, which was near the expected value of 3.75 mg Cu/g wood. The Cu concentrations in the remaining samples were 2.6 and 1.7 mg Cu/g wood for the weathered/no soil exposure (Not Exposed) and weathered/soil exposure samples (Exposed), respectively. The results demonstrate that ACQ treated wood will leach significant amounts of copper when weathered and exposed to soil, as is the case in C&D landfills.

**Comparison of Metal Concentrations in Organic vs. Non-organic Coffee Beans by ICP Atomic Emission Spectroscopy**

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Inductively Coupled Plasma Atomic Emission Spectrometry (ICP-AES) was used to measure the content of various heavy metals in two Guatemalan coffees; one organic and the other non-organic. Iron, copper, lead, and cadmium were tested for in each sample and while performing the analysis, nickel was also found to be present in detectable amounts with great contrast between levels found in the organic sample versus the non-organic sample. From the concentrations of the test solutions the amount of each metal per serving was back calculated for each sample. The levels between the organic
and non-organic were compared yielding concentrations which were: 2.3%, 3.2%, 10.6%, and 46% higher in the organic coffee for cadmium, copper, iron, and nickel respectively. An adequate comparison for lead could not be acquired because lead content was consistently below the detection limit of the instrument.

No Title

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The concentration of cadmium, nickel, zinc and lead in fine particulate street dirt was determined for both a Millipore water and a 0.5 M hydrochloric acid extraction via ICP-AES analysis. Samples were collected from two streets in Ashland, OR; Euclid Ave and Chapman St. There was a statistical difference between metals contents found at each site. HCl extraction pulled more metals from sediment than water. Solid phase metals did not exceed EPA guidelines for Zn. Dissolved metals did not exceed environmental regulations. These results are preliminary and suggest more research be done on this sediment to determine whether a threat is posed to the receiving water body.

Testing for Sufficient Filtration of Metal Contaminants in Sewage and Runoff Water Before and After Filtration

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Excess water from runoff during the rainy seasons or sewage must be cleaned before it can be reintroduced into the rivers. This is a multi-step process that involves disposing of the sludge from the primary influent (raw sewage), the use of bacteria cultured on river rock that consumes dissolved organic matter (secondary influent), and then disposal of the bacteria via chlorination/dechlorination (secondary effluent). The secondary effluent is then sent to a digester where the excess methane is burned off while the filtered water is warmed to approximately 80°C before being released into the local rivers as it is deemed safe for wildlife and plants. The samples used in this experiment were collected at various stages in the filtration process, which included the primary influent (raw sewage), primary effluent, and the secondary effluent.

Toxic metals have long been known to have a detrimental effect on the human body. Lead disrupts heme production in the body inhibiting the transportation of oxygen in the body, cadmium collects in the kidneys and interrupts the filtering process, copper is known to cause liver and kidney damage and finally, chromium exposure can lead to lung cancer and respiratory problems. The concentrations of toxic metals in these samples were examined using an ICP instrument. The values obtained were then compared to Oregon’s state standards for water safety and those measured in the past by the Corvallis Waste Water Management (CWWM). The final concentrations of Cu and Cr were
0.885 ng/mL and 3.021 ng/mL, respectively, while Cd and Pb were not detected. These values are well below the state standards set forth by the EPA and Oregon’s environmental standards.

Dirty Soil? : Heavy Metal Analysis of Organic Growers Club Farm Soil

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Soil from the Oregon State University Organic Growers Club farm was analyzed by ICP-AES for concentrations of Zinc (Zn), Lead (Pb), Chromium (Cr), and Cadmium (Cd). Samples were taken at varying distances from highway 34 which runs parallel to the vegetable plots. Both Pb and Cd were below their respective detection limits of 5.26 ug/g, Pb, and 4.69 ug/g, Cd. Soil concentrations of 58.6 to 70.5 ug/g and 31.0 to 45.8 ug/g were found for Zn and Cr respectively. Chromium was the only element to show a correlation between soil concentration and distance from the road with a two sample t-test, assuming equal variances comparing the samples closest and furthest from the road, yielding a p-value of 0.016.

Essential Elements Analysis in Meat and Veal

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The experiment involved the analysis of six essential minerals in both veal and beef. The motivation behind the experiment was to determine if veal was healthier than beef in terms of the six essential minerals tested for. These elements (Ca, K, P, Mn, Cu, and Se) are among fourteen that are considered crucial to the growth and production of bones, teeth, hair, blood, nerves, skin, and hormones. Imbalances in any of these may cause health issues and lead to deficiency diseases. Meat is among the main sources that contribute to the intake of essential minerals (other sources include vegetables, fruits, nuts, and legumes). In the U.S., projected beef product consumption was the second highest at 66 pounds per person just following projected chicken consumption at 87 pounds per person.

The minerals that were tested were potassium, calcium, manganese, copper, phosphorus, and selenium. Potassium, calcium, manganese, and phosphorus were chosen for their high concentration in milk and hay, the main food source for calves and cows, respectively. Lower concentrations of selenium and copper were thought to have been in veal due to a smaller period for accumulation of these metals. Three of the minerals (Mn, Cu, and Se) were not detected by the ICP-AES instrument in the diluted samples. For the minerals that were detected (Ca, P, K), there wasn’t a significant difference within a 95% confidence interval between beef and veal.
Comparison of Trace Metals in Organic and Non-Organic Cucurbita Seeds by Inductively Coupled Atomic Emission Spectrometry

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A method was developed on an inductively coupled plasma atomic emission spectrometer (ICP-AES), Liberty-150, to quantifiably measure the levels of five trace metals in two organic and non-organic species of Cucurbita (squash); acorn and butternut, to observe which species would ultimately be healthier. Following various calculations, the results yielded an elevated level of iron in the butternut organic species at 23.595 mg/kg of dry seed. Both non-organic species (butternut and acorn) conveyed elevated levels of copper valued at 13.757 and 32.308 mg/kg of dry seed respectively. Prepared samples for organic acorn squash were lost during analyte extraction, which influences the lack of a definitive conclusion for this experiment. The performance and recommended method established for the ICP-AES were advisable for the study implemented in this project based on the data collected.

Analysis of Elemental Mercury in Commonly Consumed Fish by ICP-AES

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The mercury content in canned Albacore tuna, canned eel, and fresh ahi tuna were analyzed using an ICP-AES. The samples were prepared by microwave digestion then diluted into 50 mL volumetric flasks before being run through the ICP-AES. The ICP was calibrated with a DL of 1.5 ppb. The eel had the highest mercury content with 0.523 ± .01ug Hg/g fish; canned albacore is second with 0.499 ± .098 ug Hg/ g fish, and the fresh ahi tuna had the least amount of mercury with 0.449 ± .066 ug Hg/g fish. All the values were within 1 standard deviation of the mean of the EPA’s accepted mercury level.

Macro- and Micro-mineral Determination in Fish

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This experimental analysis will be looking at the amount of essential dietary minerals (Ca, Mg, Cu, Zn, and Se) present in 3 different types of fish, in comparison to the price paid; the three types of fish in order of most expensive are Halibut, Cod, and Catfish. We formulated a hypothesis which stated that the price of the fish dictates the amount of minerals found in the fish. Two fillets of each type of fish will be acquired from the same location, and three samples will be run on each fillet. The fish samples were each blended and run through a microwave digestion, diluted, and then analyzed through
ICP-AES. A total of 36 samples were analyzed and their mineral concentrations were found, and from back calculations the mineral content was determined in the original fillets. This was in turn used in comparison to the price of each fillet to determine the amount of mineral per dollar paid for fillet. It was found that halibut had the highest amount of Ca per dollar at 11.23 mg/dollar. Cod had the highest amount of Mg at 18.38 mg/dollar and Se at 0.02286 mg/dollar. Catfish was found to have the highest amounts of Zn per dollar at 0.6278 mg/dollar as well as Cu at 0.2061 mg/dollar.

Carcinogenic Metal Concentration in Tobacco

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As, Cd, and Cr all have been found to exist in tobacco. We set out to find out how much of each of these metals were found in a typical additive and non-additive cigarette. Through the use of ICP-AES we were able to find the following concentrations of As in four different brands of cigarettes. American Spirit: 12185 ng/cig + 6.0%, Camel: 2291 ng/cig + 80%, Marlboro: 5915 ng/cig + 42%, Winston: 1376 ng/cig + 30%.

No Title or Names

The mineral concentrations of three types of cereal, both name brand and generic brand, were determined by Induced Coupled Plasma Atomic Emission Spectroscopy (ICP-AES). Cheerios, Corn Flakes, Fruit Loops, and their generic equivalents were tested for calcium, iron, magnesium, zinc, lead, and arsenic concentrations to determine if there is a difference between name brand cereals and generic cereals based on mineral concentrations. Samples were prepared by following a procedure very close to that of the oyster preparation from Experiment 4. The concentrations reported by the ICP were back calculated to find the mineral content in a serving size, and then compared to the concentrations reported by the cereal. Detection limits were determined by 2% HNO₃ and a recovery test was performed, although it didn’t produce usable data. A t-test determined that there is no statistical difference of average mineral content between name brand cereals and their generic equivalent, although the percent differences for each cereal type between the name brand and generic brand indicated some possible difference.
The amount of chlorophyll bound magnesium was measured in samples of commercial samples of baby spinach and kale leaves. Total magnesium content was measured by incineration of organic content from the leaves, with subsequent digestion of the ashes in concentrated nitric acid and quantification via atomic absorption spectroscopy (AAS). Selective extraction of chlorophyll bound magnesium was achieved via a solid phase extraction of chlorophyll from the leaves with acetone under grinding. The extracts were then concentrated under reduced pressure, dissolved with concentrated nitric acid, and quantified by AAS. The ratio of bound chlorophyll magnesium to total magnesium was found to be 2.67% and 6.70%, with plant concentrations found to be 681.9 µg/g and 262.5 µg/g for spinach and kale respectively.
UV-visible Spectrophotometry

Spectrophotometric Determination of Ethanol in Wine

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A single beam UV-visible spectrophotometer was used to determine the ethanol content in several wine samples by measuring the reduction of chromium (VI) to chromium (III). Four ethanol standards, ranging from 5% ethanol to 40% ethanol, were prepared with potassium dichromate, perchloric acid, and de-ionized water. The absorbance of chromium (VI) in the standards, three wine samples, and three sample blanks was determined using the spectrophotometer. Through the use of a calibration curve and the absorbance readings from the spectrophotometer, the ethanol content of each standard and sample was determined with percent errors ranging from 1.0% to 78.0%.

Analysis of Vitamin C of Frozen Green Beans using Multiple Cooking Methods

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Ascorbic acid (C₆H₈O₆) is a water soluble vitamin and is a necessary supplement because it cannot be synthesized by the human body. Vitamin C is needed in the diet to prevent scurvy, whose symptoms include hemorrhaging, joint pain and exhaustion. Frozen green bean samples and a vitamin C pill were attained and analyzed using various cooking methods. A spectrophotometer was used to measure the difference in absorbance values from a redox reaction with 2,6-Dichlorophenolindophenol (DCPIP). Values found for green beans samples fell below the detection limit of 0.287 mg/L and could not be quantified. The analysis for the vitamin C pill had a 38% loss after boiling for 5 minutes and a 48% loss from the listing on the tablets bottle.
This experiment was designed to determine three different things. The first was that sonication of beer during a solution preparation does not affect the measured alcohol content, the second was that the ADH method of determining alcohol concentration used in CH461 reflects the manufacturers stated amount, and finally, the third goal of this experiment was to determine a method for using the OOI CCD as a detector for this experiment (instead of a PMT). A calibration curve was set up using 3 standard ethanol solutions in testing the second hypothesis. The first and second hypotheses were tested using a OOI CCD as a photodetector. With regard to the first hypothesis the results of this experiment showed that only 1 out of three sonicated samples were significantly different than an unsonicated sample. As for the second hypothesis, one beer (Stella Artois) did not agree with the manufacturers value, while the other sample (Henry Weinhard’s Private Reserve) had mixed results: two sonicated samples agreed with the manufacturers posted value, while one sonicated and one unsonicated value were significantly different than the posted value.

Determination of Organic Compounds in Cigarette Smoke and Car Exhaust

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An examination of the organic gas constituents found in both car exhaust and cigarette smoke. This based on the hypothesis that both contain similar constituents and therefore have similar health affects on the human body. The sample was collected in evacuated gas cells and examined using a Nicolet 6700 inferred spectrophotometer. The cigarette smoke was found to contain more carbon monoxide and less carbon dioxide than the car. It also contained levels of methane and hydrogen cyanide, which the car exhaust did not. Calibration runs of CO₂ were run and calibration curves were created. According to the data from the samples the car exhaust has between 16% and 43% more carbon dioxide than cigarette smoke. The results of the experiment do not reveal whether car exhaust or cigarette smoke is more harmful to the human body. What is clear, however, is that both contain similar constituents at similar levels and additional studying into health comparisons would be warranted.
High Pressure Liquid Chromatography

The Determination of BPA in Canned Tomatoes

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To determine whether BPA is found in canned tomatoes, and in what amount, two canned tomato samples, Organic and Non-Organic, were prepared, as well as four standards of known BPA concentration and a blank, each consisting of fresh tomatoes. The samples were homogenized and a solid phase extraction was performed. Following evaporation with a rotary evaporator and reconstitution of the residue, the samples were run through High Pressure Liquid Chromatography (HPLC). Due to the over dilution of the samples, the BPA peaks were not present so the Organic, Non-Organic, 4 mg/kg, 10 mg/kg sample, and the 41 mg/mL solution samples were run Gas Chromatography-Mass Spectrometry (GC/MS), as it is more sensitive.

BPA was found in the Organic, Non-Organic, 4 mg/kg and 10 mg/kg on the GC/MS. However, the results allowed us to determine the presence of BPA qualitatively, but not quantitatively so it cannot be compared to literature values, nor can standard deviation be determined.

Determination of Gallic Acid in Selected Wines Using RP-HPLC

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Health benefits have been associated with moderate consumption of wine. However, winemaking includes a variety of grapes and fermenting processes. Reverse-phase HPLC with a mobile phase of 15:85 (v:v) methanol to aqueous was used to determine and compare the concentration of gallic acid, an antioxidant, in selected wines: Sauvignon Blanc, Rosé, Shiraz, Merlot, and Cabernet Sauvignon. Standards with a known concentration of gallic acid were run, and a calibration curve was formatted to deduce the concentration in the selected wines. The mean concentration of Sauvignon Blanc was 9.49 mg/L with a standard error of ± 4.4 mg/L. Respectively, the Rosé was 10.63 mg/L ± 4.40 mg/L; the Shiraz was 34.43 mg/L ± 4.24 mg/L; the Merlot was 41.27 mg/L ± 4.27 mg/L; and the Cabernet Sauvignon was 44.32 mg/L ± 4.30 mg/L.
Analysis of Vitamin D3 in Dog food

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The objective of this experiment was to determine the relative and absolute concentration of vitamin D3 (cholecalciferol) in three different brands of dog food. The dog foods analyzed were Dogswell Brand Happy Hips, Blue Buffalo, and Science Diet. The method included solid liquid extraction followed by liquid-liquid extraction of the D3 from the dog food. This extraction was run through high performance liquid chromatography. The results found quantitatively significant amounts of the target analyte. The results showed concentrations of 2.56E+2 ug/g for Blue Buffalo, 3.26E+2 ug/g for Science Diet, and 1.42E+2 ug/g for Dogswell. This indicates that Science Diet has the highest concentration of D3 followed by Blue Buffalo, and the lowest concentration belonging to Dogswell.

Concentration of Berberine in Oregon Grape (Berberis aquafolium) compared to Goldenseal (Hydrastis Canadensis L.)

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The concentration of berberine in a commercial Goldenseal root and a Wild-crafted Oregon grape root was determined using UV-visible Spectrophotometry and High Performance Liquid Chromatography (HPLC). In an attempt to indicate the cost effectiveness of using Oregon grape root as a wild source of berberine, the content of berberine in Oregon grape and Goldenseal root was used to determine the cost of berberine extracted from the two root samples. The Oregon grape and Goldenseal root studied were found to contain 2.23 mg/g and 24.6 mg/g of berberine, respectively. The cost of extracted berberine for Oregon grape and Goldenseal root was calculated to be 2.22 cents/mg and 1.68 cents/mg, respectively.
Polyphenolic Content in Organic & Nonorganic Red Delicious Apples

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Analysis of two pholyphenolic compounds, Catechin and Chlorogenic Acid, found in Red Delicious apples was accomplished via High Performance liquid Chromatography (HPLC). Standard dilutions of the compounds were analyzed and employed in order to create calibration curves, which produced equations of $Y = 2.43E+05X - 1.45E+04$ and $Y = 2.43E+05X - 1.45E+04$ for Chlorogenic Acid and Catechin, respectively. Samples of organic and nonorganic Red Delicious apples were then analyzed, and polyphenolic content was matched with the respective calibration curve, producing the total polyphenolic content found in each variation of the apple. Total polyphenolic content of organic and nonorganic Red Delicious apples was found to be 152.4 and 113.8 ug/g fresh weight, respectively. Due to the small discrepancy in concentration, the hypothesis of the organic variation of Red Delicious apples containing more polyphenolic content remains inconclusive.

Determination of Formaldehyde Concentration in Sunsilk Shampoo

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Determination of formaldehyde concentration of Sunsilk-Straight to Perfection shampoo was achieved using a standard addition process via high-performance liquid chromatography. Formaldehyde concentration was found to be $9.1E04$ ug/mL + $2.1E05$ ug/mL. A previous method using standard formaldehyde concentrations of 2.5—10 ug/mL was unsuccessful because the derivatization element 2,4-dinitrophenylhydrazine covered the formaldehyde peak. The covering of the formaldehyde derivative peak can be attributed to the delicate equilibrium that exists between formaldehyde and 2,4-DNPH. Further studies and revisions to techniques are needed to accurately measure formaldehyde concentrations.
Determination of Caffeine Concentrations in Over-the-Counter Migraine Medicines using HPLC

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High performance liquid chromatography has been used to determine the concentrations of caffeine in two migraine headache pain relievers, Kroger and Excedrin. It was hypothesized that the name brand Excedrin would contain more caffeine and thus could be more habit forming. The average values obtained in relation to the Kroger and Excedrin samples were 43.1 ± 1.84 mg per tablet, and 53.9 ± 4.31 mg per tablet. Both values obtained are significantly less than the literature value of 65 mg per tablet. The method used was modeled after the method found in the article “Quantitative HPLC Analysis of an Analgesic/Caffeine Formulation: Determination of Caffeine” by GK Ferguson.

HPLC Analysis of 4-methylimidazole in Soda Beverages with Caramel Coloring Agents

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This experiment was formulated to determine if there were measurable amounts of 4-MEI within a caramel colored soft drink, specifically Pepsi and Diet Pepsi. To do this, samples of soda were processed through solid phase extraction, and the concentrations of the new solutions were determined via High Pressure Liquid Chromatography (HPLC). The results of the HPLC after calculations show Pepsi having an average concentration of 139.2 ng/mL with a standard deviation of 10.8 ng/mL, Diet Pepsi having an average concentration of 224.7 ng/mL with a standard deviation of 12.5 ng/mL. The recovery sample suggests a 75% recovery of analyte after sample preparation is complete. Although the numbers do not match that of the literature, we did see 4-MEI concentrations in the samples, proving that it is in the soda, though not above the legal limit of 200 mg/kg.
DETERMINATION OF CAFFEINE AND THEOBROMINE LEVELS VIA HPLC IN THREE STARBUCKS ROASTS

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High performance liquid chromatography (HPLC) has been used to determine the concentrations of caffeine and theobromine in three different types of roasted Starbucks espresso beans, light, medium, and dark, and a non-Starbucks decaf roast for comparison. It was hypothesized that the lightest roast would contain the most caffeine and theobromine, therefore would provide more of an energy boost. The average values obtained in relation to the Starbucks samples were 64.83 ppm of caffeine and 0 ppm of theobromine for the light roast; 77.63 ppm of caffeine and 3.356 ppm of theobromine for the medium roast; 78.76 ppm of caffeine and 2.872 ppm of theobromine for the dark roast; and 1.88 ppm of caffeine and 2.321 ppm of theobromine for the non-Starbucks decaf roast. All values obtained are based off of the calibrations using the areas of the peaks. Calibrations were also run using the heights of the peaks and these values were within reason of the concentrations obtained before. The method used was modeled after the method found in the article “Determination of Caffeine in Coffee Products According to DIN 20481” by Edgar Naegele of Agilent Technologies Inc. in Waldbronn, Germany.
Bomb Calorimetry

Experimental Determination of Caloric Content in Budweiser Select 55

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The analysis of the caloric content of Budweiser Select 55 was determined by bomb calorimetry. The beer samples were lyophilized and then pressed into pellets. Using bomb calorimetry, the heat of combustion of each sample was determined. From three unique beer samples, each ran in duplicate, the average calculated caloric content was 9.29 ± 0.31 kcal/bottle. A 95% confident interval was found to lie between 8.96 and 9.61 kcal/bottle. This value is reported excluding ethanol content. Assuming 4% alcohol/vol, the energy from ethanol per bottle was estimated to be 79.4 kcal/bottle. Including the assumed energy content from alcohol, the total average caloric content of Budweiser Select 55 was 88.7 ± 0.31 kcal/bottle.
Gas Chromatography

GCMS Comparison of an Unknown Gunpowder and IMR-700x based on Nitroglycerin Content

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Nitroglycerin is one of the most critical energizers in a double base gunpowder. This report aims to confirm the identity of an unknown sample of gunpowder by comparison of nitroglycerin content to IMR 700x by GCMS due to its use in other reported literature. This is important to the safe use of the powder. Nitrosol 0.6 mg sublingual tablets were used as a standard for comparison. A SIM mode selection of M/Z [30, 46, 76, 89, 90, 101, 103, 165, 169] was selected based on detected components in preliminary testing. Development of methodology over two papers, (4, 5) was explored giving a final temperature scheme of T[100 C, 275 C] Hold = 3 Min., dT = 10 C / Min., T= 18+min. An acetone bracketing scheme of [.5 uL Ac, 1.0 ul sample, .5 uL Ac.] was implemented to insure constant injection volume. Samples were run on a HP 5890 Series II Chromatograph with an HP 598228 Ionization Gauge Controller with a C-18 Column. Calibration of IMR 700x for abundances of M/Z = 30 and 101 gave a percent difference over a [µ+ 3o] for X[30] = 2638 mg/ml, X[101] = 7879 mg/ml, S[30]= 43 mg/ml, S[101]= 1045 mg/ml a percent difference of 120% for the upper limit and 61% for the lower limit. Based on this, it is determined that the unknown powder is not IMR 700x. The low number of runs contributed to a large degree of variability, which could have impacted a false positive. There also exists the possibility that unforeseen matrix effects may have impacted detection of both fragments, artificially altering the calibration curves. Further studies would need to be performed to examine these the impact of these factors.

Analysis of Pesticides in Organic versus Non-organic Oranges

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In this experiment selected pesticide concentration in oranges via gas chromatography mass spectroscopy was determined on DB-5 column in 6890N network GC system with GEOL JMS-600H electron impact MS with the use of HPS MX Autoloader by 2 ul injection where detection limit was 1 ppm [ideal meant at low ppb]. Standards for calibration were determined for 50, 100, 200, and 400 ppb. Orange peel sample constituted by SPE (solid-phase extraction) by the use primary-secondary amine (PSA) was analyzed by double replication. Results were indeterminable. Expected concentrations of organic oranges are below 100 ppb and for non-organic to be above.
Elucidation of Methanol Concentrations in Commercial and Wine Fortifying Brandies

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The presence of methanol in brandy is something of interest for consumers of such distilled spirits. Detection and quantification of methanol in two commercial and two wine fortifying samples of brandy was achieved via the use of a GC with Flame Ionization Detector. Methanol levels in the Coelho Winery Stainless Steel, Coelho Winery Wood Barrel, Hennessey VS Cognac, and Christian Brothers brandies were 55.79 mg/100mL, 11.93 mg/100mL, 75.41 mg/100mL, and 11.31 mg/100mL, respectively. All the collected data is below the legal limit of 280 mg/100mL 40% abv.

Benzenes in Beverages

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In this experiment various commercial beverages were tested for benzene in nanograms per 25 mL sample. Through a method using purge and trap coupled with GC/MS benzene was able to be detected. A series of eight standards were used to form a calibration curve of abundance versus known concentration of the ions 51 m/z, 77 m/z, and 78 m/z using the scan mode. The samples tested were Aquafina Flavor Splash Citric Blend, Fruit20 Strawberry Flavored Water, and Safeway Select Diet Orange Soda. Each sample was put through the method two times using the SIM mode, searching only for 51 m/z, 77 m/z, and 78 m/z and one diet orange sample was run after being exposed to UV light for thirty minutes. In the scan mode the MS looks at each ion for 6 ms, in the SIM mode it looks at each ion for 100 ms.

To correct for the difference between the samples and the calibration curve, sample concentration was divided by 16.6. The concentration of the Aquafina was 0.026145 (+ 0.1) ng, the concentration of Fruit20 was 0.4902 (+ 0.02) ng, and the concentration of diet orange soda was 0.2477 (+ 0.481) ng and 0.03429 ng (UV). The limit of quantification was found to be 0.0867 ng, from the lowest standard. This method was developed after learning about the FDA study on the concentration of benzene a variety of other beverages.
Toluene Concentrations in Commercial Gasoline

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The purpose of this experiment was to compare the concentrations of toluene (gram/gallon) in commercial gasoline. Samples from two different gas stations were taken. One from Chevron Station, labeled GasA, and the other from the 76 Station, labeled GasB. Both samples were marked as regular unleaded with an 87 octane rating. The samples were prepared in dichloromethane (DCM) and an HP GCMS was used to analyze all of the samples. A standard addition of Toluene to one of the samples was used to determine the signal increase of our target analyte. The concentration of toluene for each sample was determined to be $1.80 \pm 0.03$ g/gal from the Chevron gasoline and $1.86 \pm 0.09$ g/gal from the 76 Station. Due to the fact that the concentrations of toluene are so close, we have determined that toluene is a very common octane booster in most types of gasoline.

Analysis of Accelerants in Fire Debris Using Gas Chromatography/ Mass Spectrometry

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Fire accelerants, such as gasoline and lighter fluid, can be detected from fire debris using Gas Chromatography/Mass Spectrometry (GC/MS). This method is important for helping forensic scientists determine what was used to start a fire. GC/MS of standard samples of gasoline and charcoal lighter fluid were analyzed against burnt cloth samples which were burned with either gasoline or charcoal lighter fluid. The presence of aromatic compounds helped determine if the cloth sample was burned with gasoline. Though the accelerant used in each cloth sample was determined by comparing the GC/MS spectra, further tests need to be run in order to confidently report the results.
Solid Phase Extraction

Dyes in mouthwash: separation and concentration

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Mouthwash was analyzed by completing a solid phase extraction (SPE) of individual dyes from three different brands; Swish, Kroger and Listerine. Yellow #5, Blue #1 and Red #33 were the dyes present in these mouthwashes. After SPE was performed on all the mouthwashes, concentrations of the dyes were determined. Using these concentrations, the molarity per bottle and grams per rinse were found for each dye which are reported later in this report. However, since correct standards were not available for Blue #1 and Red#33, the concentrations are marginally different than what was determined. Beer’s law and the use of Red #40 were used to estimate their concentrations. In Swish, the concentrations of Blue #1 and Red #33 were 2.00E-07 M and 9.36E-07 M. In Listerine, the concentrations of Blue #1 and Red #33 were 6.21E-09 M and 2.66E-06 M. In Kroger, the concentrations of Blue #1 and Yellow #5 were 3.95E-07 M and 7.37E-07 M.