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In advance of the Denver X-Ray Conference, we asked leading scientists who will be speaking at the conference about current trends and advances in X-ray fluorescence and X-ray diffraction. Here, these investigators discuss their work to advance these techniques and the sample preparation for such analyses, in areas such as photonics for telecommunications, steel structures, metals in pharmaceuticals, and imaging.

Analysis of Beverages by Total Reflection X-ray Fluorescence

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Total reflection X-ray fluorescence spectrometry (TXRF) is a well established and versatile multielement trace analytical method (1). Its ease of use and low detection limits make it an ideal tool for routine analysis of samples ranging from liquids and solids to biological tissues. The project presented in this short article was inspired by undergraduate research experience and showcases TXRF as an undergraduate teaching and research tool. When exposing undergraduate students to research one has to take into account the lack of laboratory experience of the student, in addition the project should spark and retain the interest of the student, and also maintain a high research standard. With this in mind, the subject of study were common beverages. Beverages such as juices are recommended as a means of delivering essential nutrients and trace elements to children and adults alike. Many of them are fortified and most are processed to remove unwanted residues and pulp or are reconstituted from concentrate. We purchased three common fruit juices—apple juice, cranberry juice, orange juice—and one bottle of lemonade for this study and compared their metal content to water obtained from a drinking fountain at the university. All fruit juices were pulp free and none of the beverages were from concentrate. Table I lists the name, origin, and daily values of the beverages stated on the label.

Table I: Beverage information as shown on the back label. All beverages were not from concentrate and the nutrition facts are listed for the bottle content of 340 mL.

Nutrition Facts	Apple Juice	Cranberry Juice	Orange Juice	Lemonade
Content	100% juice	27% juice, filtered water, sugar, natural flavors	100% juice	11% lemon juice, filtered water, cane sugar, natural flavor
Fat	0	0	0	0
Sugars	40 g	48 g	33 g	40 g
Total carbohydrates	43 g (14% DV)	49 g (16% DV)	37 g (12% DV)	43 g (14% DV)
Na	5 mg	25 mg	—	20 mg
K	340 mg (10% DV)	—	640 mg (18% DV)	—

Two sample preparation methods were compared with each other to examine the difference in trace metal content between the liquid part of the juice and the solid–liquid mixture that includes plant fibers. For the liquid-only element content, a 5-mL aliquot of the purchased beverages was centrifuged at 9000 rpm for 10 min and 1 mL of the supernatant was analyzed. For the solid–liquid mixture, a 1-mL aliquot of the beverages was diluted with the same amount of ultrapure water after shaking the bottle vigorously and then analyzed. Drinking fountain water was analyzed directly. For all samples gallium was used as the internal standard.

It was found that each purchased beverage contained a suite of common metals, with potassium and calcium having the highest concentrations and manganese, iron, copper, zinc, rubidium, and strontium present as traces. The concentrations of all detected metals varied not only between beverages, but also between the methods of preparation substantially. Drinking fountain water contained much lower concentrations of potassium and calcium, but comparable concentrations for the other metals were detected. This is not surprising because the plant tissue is enriched with potassium and calcium.

Figure 1 shows the concentrations of calcium (Figure 1a) and copper (Figure 1b) for all samples. Please note that the calcium concentrations are expressed in units of milligrams per liter and the copper concentrations in micrograms per liter. The fountain water concentration of calcium was a factor of 1000 smaller than for the other beverages. When calculated for the 340-mL bottle content and compared to daily intake values, the freshly pressed apple and orange juices delivered more calcium and copper. In fact, the copper amount delivered by one 340-mL bottle of orange juice is about a quarter of the daily recommended value for children and 10% for adults. (2). The juice that contributed substantially to daily intake values was 100% orange juice and only when the solids or pulp were included in the drink. All other beverages had only marginal daily amounts of the metals detectable by TXRF.

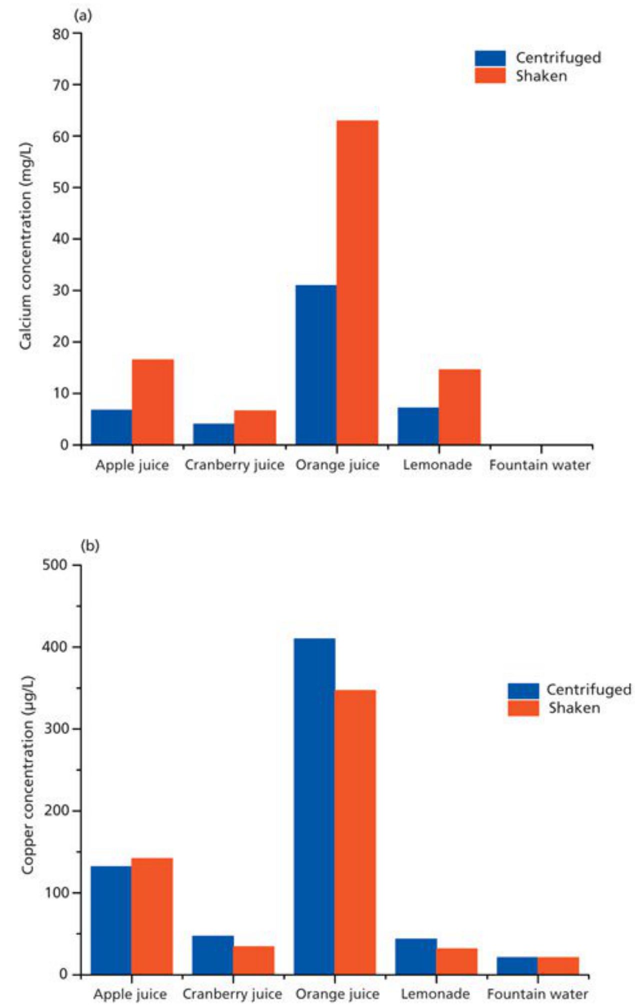

Figure 1: (a) Calcium and (b) copper concentrations in different beverages. The blue bars show the concentrations of the supernatant after centrifugation and the red bars the concentrations of the shaken beverages.

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References

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