Rapid profiling of tomatoes by infrared spectroscopy and chemometerics

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ABSTRACT

Tomatoes are the second most produced and consumed vegetable in the United States according to the USDA. The value of tomato production in the US totals over $2 billion since 2005. Current methods to analyze sugars and carotenoids in tomatoes are time and labor intensive and utilize harmful solvents making efficient assays for detection and quantification desirable. Our objective was to develop simple accurate and economical protocols to determine sugars and carotenoids by Attenuated Total Reflectance Infrared (ATR-IR) spectroscopy and multivariate analysis.

Samples were obtained from genetically diverse tomato varieties that encompassed commercial hybrids and elite parents used in tomato processing and fresh market industry. Fresh tomatoes were blended, aliquots (5 mL) centrifuged and infrared spectra collected using ATR-IR microspectroscopy from vacuum dried supernatant or paste applied directly to a handheld IR. Reference methods included HPLC for carotenoids and enzymatic kits for sugars. Partial least squares regression (PLSR) was used to create calibration models that correlated the chemical components in tomatoes with infrared spectra. Multivariate models accurately predicted sugars (glucose, fructose), using the supernatant with R-values > 0.94 and SECV <0.02 g/100g using the infrared region of 1200-900cm-1. By using infrared spectra collected from tomato paste, PLSR models predicted carotenoids content with R-value >0.95 and SECV of 0.5 for lycopene. ATR-IR could provide the tomato industry with a simple and high throughput method for chemical profiling of tomatoes that could lead to improved varieties with enhanced characteristics for industry and consumer demands.

INTRODUCTION

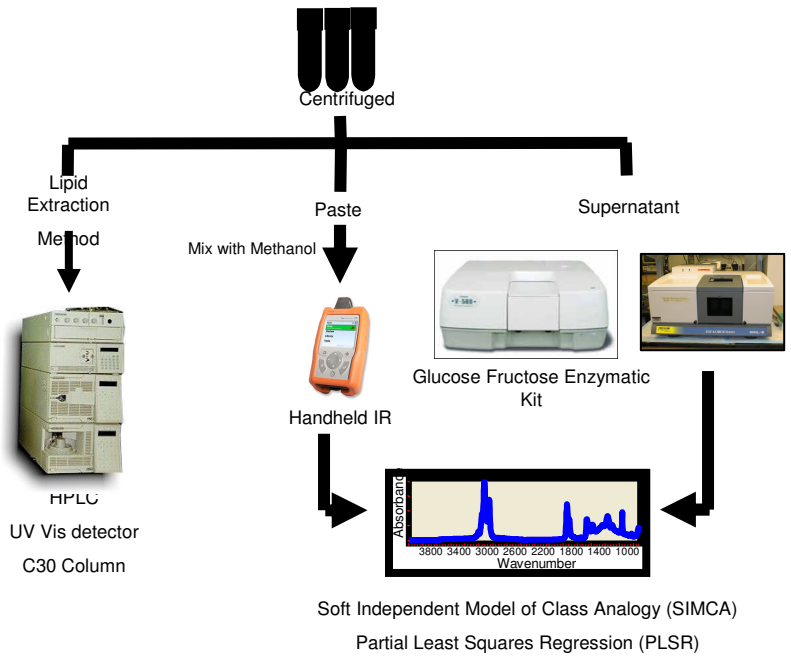
Ohio ranks fifth nationally in tomato production with 10,000 acres producing a crop with a value of $80 million. Fresh-market tomatoes are for the wholesale, retail and supermarket trade. Tomatoes are classified for use in fresh market and processing-tomato industries used for and they are based on their sugar and carotenoid content. Glucose and fructose are the major sugars in tomatoes are and give an indication of flavor quality. The predominate carotenoids in tomatoes are lycopene and β carotene. Lycopene is a fat soluble pigment that has antioxidant properties that play a critical role in disease prevention including cancer and cardiovascular disease. β carotene is one of the most common carotenoids in nature and is a known precursor of vitamin A. Due to these important health benefits plant breeders wish to maximize the caroenoid content of their products.

The carotenoid content and sugar levels are important factors in determining a tomatoes use and market price. The industry is looking for fast and reliable assays for the detection of these compounds. Infrared spectroscopy combined with multivariate analysis is a rapid accurate and cost effective and will greatly advance current analytical methods.

OBJECTIVES

To develop simple accurate and economical protocols to determine sugars and carotenoids by Attenuated Total Reflectance Infrared (ATR-IR) spectroscopy and multivariate analysis.

MATERAILS AND METHODS



RESULTS

Fig 1. Spectra of Different Carotenoids

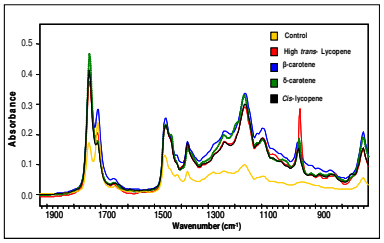


Figure 2 PLSR of Lycopene

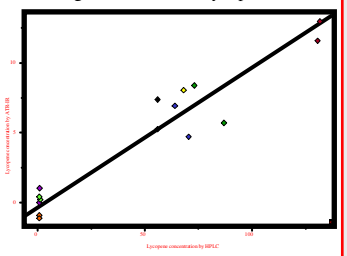


Figure 3 PLSR of Glucose

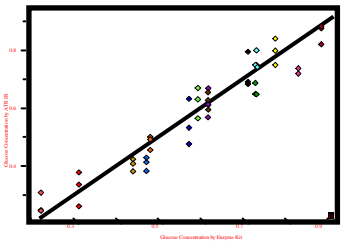


Figure 4 PLSR of fructose

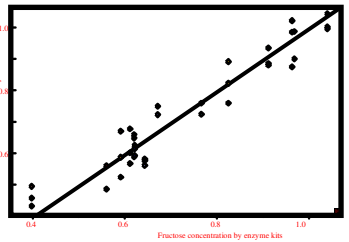


Figure 5 PLSR of Brix

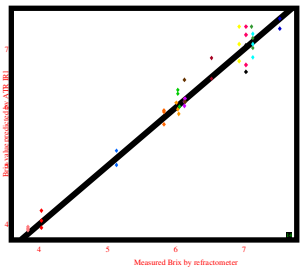
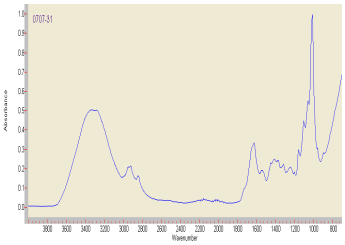


Figure 6 AR IR Spectra of tomato



DISCUSSION

•Calibration models, based on PLSR, were developed to relate the IR spectra with fructose, glucose, and brix content determined by enzymatic kits as a reference method.

Multivariate models accurately predicted sugars (glucose, fructose), using the supernatant with R-values > 0.94 and SECV <0.02 g/100g using the infrared region of 1200-900cm-1 (Figure 3-6)

•The *trans*-lycopene spectrum shows a unique band at 957cm^{-1} for lycopene (bending HC=CH out-of-plane vibrations) (Figure1)

•Calibration models, based on PLSR, were developed to relate the IR spectra with lycopene & β-carotene concentrations determined by the HPLC reference method. (Figure 2)

CONCLUSIONS

•ATR-IR spectroscopy with multivariate analysis has shown to be an easy, rapid, and robust technique for tomato profiling.

•This technique will allow for effective and efficient selection of tomato varieties with specific sugar and pigment contents.

•This technique will allow the tomato industry to rapidly and accurately determine the best use for various tomato varieties.

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