Title Profiling of nutritionally important carotenoids from genetically-diverse tomatoes by infrared spectroscopy

Author Daniel E. Rubio-Diaz, Thais De Nardo, Alejandra Santos, Susana de Jesus, David Francis and Luis E. Rodriguez-Saona

Citation Food Chemistry, Volume 120, Issue 1, 1 May 2010, Pages 282-289

Keywords Tomato; Carotenoids; Phenotype profiling; ATR-IR spectroscopy; Chemometrics

Abstract

An efficient and rapid protocol for profiling tomato carotenoids based on their specific vibrational spectroscopic signatures was developed. Twenty-four tomato varieties that included eight distinct combinations of genes affecting carotenoid concentration and content were grown and harvested in a replicated trial. Hexane was used to extract the lipid fraction from samples, and the extract was applied directly onto an ATR ZnSe crystal plate for spectra acquisition and injected in a reverse-phase HPLC system for carotenoid separation. Soft independent modelling of class analogy (SIMCA) was used to classify tomatoes based on unique infrared spectral signatures. Models exhibited tight and well-separated clusters (inter-class distances >3.0) that correlated well with the HPLC information, and demonstrated the capability of grouping the tomato varieties based on their carotenoid profile. Classification of lipid fractions was primarily based on the presence of *trans*-double bonds and their *cis* and *trans* conjugations. Major discriminating bands at 957 and 964 cm^{-1} were associated with bending *trans* HC=CH out-of-plane deformation vibrations. ATR-IR and multivariate analysis provided a simple and rapid tool for the identification of dietary carotenoids. This technique will facilitate the effective selection of tomato varieties with specific pigment content, improving the screening process for carotenoid-rich products.