**Title** Study of the suitability of HRMAS NMR for metabolic profiling of tomatoes: Application to

tissue differentiation and fruit ripening

Author Estela María Sánchez Pérez, María José Iglesias, Fernando López Ortiz, Isidro Sánchez Pérez

and María Martínez Galera

Citation Food Chemistry, Volume 122, Issue 3, 1 October 2010, Pages 877-887

Keywords H HRMAS NMR spectroscopy; Tomato ripening; Tomato tissues; Principal component

analysis

## **Abstract**

The feasibility of HRMAS NMR as an efficient technique for metabolic studies of tomato fruit and tomato tissues is described. A good-taste tomato variety from Almería (Spain) (commercial name Zayno) was chosen for this study. Fruits of three different ripening stages (green, turning and red) were selected, based on their external appearance. NMR data of whole fruits were obtained through <sup>1</sup>H HRMAS NMR spectra of tomato purée. Flesh, peel and seeds from mature red fruits were separately analysed. H HRMAS NMR spectra showed resolutions similar to that of solution <sup>1</sup>H NMR with the advantages of minimal sample manipulation and possibility of analysing polar and non-polar compounds simultaneously. Seeds could be clearly distinguished by visual comparison of the spectra. Tryacylglycerols, in which linoleic (47%) and oleic (28%) acyl chains preponderate, were the major components of seeds. By contrast, signals of fructose, glucose, citric acid, and the amino acids GABA, glutamine and glutamate dominated the spectra of flesh, peel and tomato purée. Principal components analysis, performed on the covariance matrix, revealed a clear separation between peel and flesh. Apart form the presence of the cutin biopolymer, peel showed a specific accumulation of sugar and sugar moieties related to pectin degradation, as well as glycosylated metabolites. Chemometric analysis also allowed the metabolic trajectory from green to red mature stages to be visualised. However, sample heterogeneity in the analysis of the whole fruit proved to be an important issue. The source of such heterogeneity was assigned to the presence of tissues of different hardness in the small amount of sample used. The presence of two clusters of samples at the turning stage indicated that the levels of certain metabolites could diverge significantly in fruits with almost identical appearance.