

Title

Comprehensive non-targeted screening and quantification of fruit juice constituents.

Authors

Lea Heintz, Markus Godejohann, Birk Schütz and Manfred Spraul

Bruker BioSpin GmbH, Silberstreifen, D-76287 Rheinstetten, Germany.

Abstract

Here we report a comprehensive, fast and sensitive new approach of non-targeted screening and quantification of fruit juice constituents, based on NMR and time-of-flight mass spectrometry.

This generic method allows sample profiling for origin authenticity, species purity or false labeling assessment through statistical evaluation of raw data, as well as subsequent quantification of target compounds.

The analysis of direct juice with NMR and of SPE extracts with UPLC-TOF/MS presents the advantage of covering a huge variety of compounds detected, from highly polar compounds like sugars and acids to middle and low polar compounds like vitamins, polyphenols and pesticides.

In particular, the mixed-mode solid-phase extraction presented allowed us to enrich more compounds with different chemical properties in comparison to classical reversed-phase extraction.

As an example, we show the results of juice screening, NMR quantification of highly concentrated constituents and UPLC/MS quantification of common pesticides used during fruit growing and storage.