ABSTRACT

The development of analytical methods for parallel characterization of multiple phytoconstituents is essential to advance the quality control of herbal products. While chemical standardization is commonly carried out by targeted analysis using gas or liquid chromatography-based methods, more universal approaches based on quantitative ^{1}H NMR (qHNMR) measurements are being used increasingly in the multi-targeted assessment of these complex mixtures. The present study describes the development of a 1D qHNMR-based method for simultaneous identification and quantification of green tea constituents. This approach utilizes computer-assisted ^{1}H iterative Full Spin Analysis (HiFSA) and enables rapid profiling of seven catechins in commercial green tea products. The qHNMR results were cross-validated against quantitative profiles obtained with an orthogonal LC-MS/MS method. The relative strengths and weaknesses of both approaches are discussed, with special emphasis on the role of identical reference standards in qualitative and quantitative analyses.

Keywords:

Green tea catechins; qNMR; qHNMR; ^{1}H NMR fingerprints; HiFSA; LC-MS/MS.

Abbreviations:

ACA: automated consistency analysis;

HiFSA: [1]H iterative full spin analysis;

QMTLS: quantum-mechanical total line shape.