Comprehensive 2D GC coupled to rapid triple quadrupole mass spectrometry for the simultaneous untargeted (MS database matching & LRI-filtering) and targeted (MRM transitions) analysis of essential oils

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Comprehensive two-dimensional gas chromatography (GC×GC) has been widely used in combination with mass spectrometry (MS), only throughout the last decade. With regards to the mass-spectrometric instrumentation type used, low-resolution high-speed time-of-flight (ToF) systems have been the most popular choice, followed by rapid-scanning low resolution single quadrupole instruments. The main objectives of most such GC×GC-MS applications have been the quantitative and/or qualitative determination of untargeted analytes. There has been only a low number of publications describing the use of other MS types, a fact related to slow spectral production rates. The requirement for high-speed MS systems is related to the very fast second-dimension separations. The present investigation is focused on the exploitation of a novel high-speed triple quadrupole (QqQ) mass spectrometer, in flow-modulated GC×GC applications. The QqQMS is capable of operation in the simultaneous full-scan/MRM (multiple reaction monitoring) mode, under the high-speed spectral production conditions required for GC×GC identification and quantification. It will be shown that, in the same GC×GC-QqQ MS analysis, both full-scan spectra relative to untargeted compounds, and MS-MS spectra relative to targeted ones, can be attained. Obviously, the use of the MRM mode enables a great increase both in sensitivity and selectivity. An untargeted/targeted GC×GC-QqQ MS application on an essential oil, containing trace-amount contaminants, will be illustrated.