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Chromatography–Quadrupole–Time of Flight Mass Spectrometry (LC–Q–TOF MS) Study for Analyzing 35 Corticosteroid Compounds: Elucidation of MS/MS Fragmentation Pathways

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Abstract

Corticosteroids have been often found to be added to a dietary supplement for the purpose of illegally improving the effect of their products. Thus, it is imperative to develop or improve a method that enables one to rapidly and reliably analyze corticosteroids in health or dietary supplements, for the safety management purpose. In the present study, results from liquid chromatography–quadrupole time-of-flight mass spectrometry (LC–Q–TOF–MS) experiments for the selected 35 corticosteroid compounds are presented, which can be useful for the qualitative screening of corticosteroids in health or dietary supplements. Specifically, retention times, accurate mass data of the protonated steroids, m/z values of major fragment ions are given for the 35 corticosteroids. Further, fragmentation pathways for the selected steroids are also suggested. Based on the suggested fragmentation pathways, it was shown that an unknown steroid compound can be readily identified using the knowledge of a group of unique and specific common skeletal fragments. The high selectivity and sensitivity of the LC–Q–TOF–MS/MS results combined with the knowledge of the fragmentation pathways can offer a new opportunity for rapid and accurate screening of corticosteroids, thus preventing health-related incidents involving adulterated products and clamping down on illegally circulated health products.

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