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LC-ESI-MS/MS Screening and Confirmation Methods for β_2 -Agonists in Human or Equine Urine

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Abstract

ESI-mass spectra of 19 common β_2 -agonists were investigated in terms of fragmentation pattern and dissociation behavior of the analytes, proving origin of fragment ions and indicating mechanisms of charge-driven as well as charge-remote fragmentation. Based on these data, LC-ESI-MS/MS screening and confirmation methods were developed for doping control purposes. These procedures employ established sample preparation steps including either acidic or enzymatic hydrolysis, alkaline extraction, and, in case of equine urine specimens, acidic re-extraction of the analytes. In addition, a degradation product of formoterol caused by acidic hydrolysis during sample preparation, could be identified and utilized as target compound in screening and also confirmation methods. The screening procedures cover 18 or 19 β_2 -agonists, the estimated LODs of which for equine or human urine samples vary between 2-100ng/mL and 2 - 50ng/mL, respectively. A single LC-MS/MS analysis can be performed within 9 minutes.

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