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Mass Spectrometric Identification and Characterization of a New Long-Term Metabolite of Metandienone

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Abstract

Anabolic-androgenic steroids have been one of the most frequently detected drugs in amateur and professional sport. Doping control laboratories have developed numerous assays enabling the determination of administered drugs and/or their metabolic products that allow retrospectives with respect to pharmacokinetics and excretion profiles of steroids and their metabolites. A new metabolite generated from metandienone has been identified as 18-nor- 17β -hydroxymethyl, 17α -methyl-androst-1,4,13-trien-3-one in excretion study urine samples providing a valuable tool for the long-term detection of metandienone abuse by athletes in sports drug testing. The metabolite was characterized using gas chromatography - (tandem) mass spectrometry, liquid chromatography - tandem mass spectrometry and liquid chromatography - high resolution/high accuracy (tandem) mass spectrometry by characteristic fragmentation patterns representing the intact 3-keto-1,4-diene structure in combination with typical fragment ions substantiating the proposed C/D-ring structure of the steroid metabolite. In addition, structure confirmation was obtained by the analysis of excretion study urine specimens obtained after administration of 17-CD₃-labeled Metandienone providing the deuterated analogue to the newly identified metabolite. 18-Nor- 17β -hydroxymethyl, 17α -methyl-androst-1, 4, 13-trien-3-one was determined in metandienone administration study urine specimens up to 19 days after application of a single dose of 5 mg, hence providing a detection period extended by more than one week compared to commonly employed strategies.

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