Elucidation of the metabolites of the novel psychoactive substance 4-methyl-N-ethyl-cathinone (4-MEC) in human urine and pooled liver microsomes by GC-MS & LC-HR-MS/MS techniques and of its detectability by GC-MS or LC-MS(n) standard screening approaches

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Résumé en anglais	4-methyl-N-ethcathinone (4-MEC), the N-ethyl homologue of mephedrone, is a novel psychoactive substance of the beta-keto amphetamine (cathinone) group. The aim of the present work was to study the phase I and phase II metabolism of 4-MEC in human urine as well as in pooled human liver microsome (pHLM) incubations. The urine samples were worked up with and without enzymatic cleavage, the pHLM incubations by simple deproteinization. The metabolites were separated and identified by gas chromatography-mass spectrometry (GC-MS) and liquid chromatography-high resolution-tandem mass spectrometry (LC-HR-MS/MS). Based on the metabolites identified in urine and/or pHLM, the following metabolic pathways could be proposed: reduction of the keto group, N-deethylation, hydroxylation of the 4-methyl group followed by further oxidation to the corresponding 4-carboxy metabolite, and combinations of these steps. Glucuronidation could only be observed for the hydroxy metabolite. These pathways were similar to those described for the N-methyl homologue mephedrone and other related drugs. In pHLM, all phase I metabolites with the exception of the N-deethyl-dihydro isomers and the 4-carboxy-dihydro metabolite could be confirmed. Glucuronides could not be formed under the applied conditions. Although the taken dose was not clear, an intake of 4-MEC should be detectable in urine by the GC-MS and LC-MS(n) standard urine screening approaches at least after overdose.
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