Ketamine-derived designer drug methoxetamine: metabolism including isoenzyme kinetics and toxicological detectability using GC-MS and LC-(HR-)MS n

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Résumé en anglais	Methoxetamine (MXE; 2-(3-methoxyphenyl)-2-(N-ethylamino)-cyclohexanone), a ketamine analog, is a new designer drug and synthesized for its longer lasting and favorable pharmacological effects over ketamine. The aims of the presented study were to identify the phases I and II metabolites of MXE in rat and human urine by GC-MS and LC-high-resolution (HR)-MS n and to evaluate their detectability by GC-MS and LC-MS^n using authors' standard urine screening approaches (SUSAs). Furthermore, human cytochrome P450 (CYP) enzymes were identified to be involved in the initial metabolic steps of MXE in vitro, and respective enzyme kinetic studies using the metabolite formation and substrate depletion approach were conducted. Finally, human urine samples from forensic cases, where the ingestion of MXE was suspected, were analyzed. Eight metabolites were identified in rat and different human urines allowing postulation of the following metabolic pathways: N-deethylation, O-demethylation, hydroxylation, and combinations as well as glucuronidation or sulfation. The enzyme kinetic studies showed that the initial metabolic step in humans, the N-deethylation, was catalyzed by CYP2B6 and CYP3A4. Both SUSAs using GC-MS or LC-MS^n allowed monitoring an MXE intake in urine.
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