Human phase I metabolism of the novel synthetic cannabinoid 5F-CUMYL-PEGACLONE

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Background

5F-CUMYL-PEGACLONE
Molecular Formula: C25H27FN2O3
Monotopic Mass: 390.2107
Binding Affinities:
K<sub>i</sub> (hCB2) = 0.1 ± 0.07 nM
K<sub>i</sub> (hCB1) = 1.56 ± 0.66 nM
[own unpublished data]

• Street name: 5F-SGT
• ‘Research chemical’ purchased online Dec. 2017
• Notified Dec. 2017 by the EMCDDA

In human phase I metabolism, the 5-fluoropentyl chain and the γ-carbolinone core were the preferred moieties for biotransformations. The parent compound was not detected in any of the authentic urine samples. In total, 12 out of 15 in vivo phase I metabolites could be confirmed by corresponding signals in the M06 wastewater, which was the most abundant metabolite in each of the analyzed urine samples but could not be detected in vitro.

In vitro metabolite characterization

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Discussion

Comparing the results to the human phase I metabolism data of the non fluorinated analog CUMYL-PEGACLONE 14, identical metabolites may occur for both compounds. Analysing six urine samples positive for CUMYL-PEGACLONE only, six identical metabolites (M01, M02, M04, M06, M08, M10) were detected (see Fig. 5). Thus, the main in vivo metabolite M06 can be used in monochromated at the core system with an unlabeled 5-fluoropentyl chain, will facilitate a selective detection of 5F-CUMYL-PEGACLONE (see Fig. 6).

Conclusions

• 5F-CUMYL-PEGACLONE is subject to extensive metabolism in humans.
• A characteristic CID pathway of γ-carbolinone derivatives was confirmed.
• M06 is a sensitive marker metabolite for 5F-CUMYL-PEGACLONE uptake but can also be formed when CUMYL-PEGACLONE was the drug of abuse.
• M13 facilitates a selective detection of 5F-CUMYL-PEGACLONE uptake.
• The degradation pathway of the 5-fluoropentyl chain to a propionic acid metabolite remains subject to further metabolism studies.

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Literature


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