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In vitro metabolism of BOD by human liver microsomes using liquid chromatography-high resolution mass spectrometry

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The appearance of new designer drugs in the illicit market poses a serious health risk because they have unknown safety profiles, a high potential for abuse, high potency and can lead to devastating health consequences. 4-methyl-2,5,beta-trimethoxyphenethylamine (BOD) as a beta-methoxy analog of 2C-D is a new amphetamine designer drug. BOD produces strongly distorted open-eye visuals and some closed-eye visuals. It also has an entheogenic effect and produces a humor. Very little data exists about the pharmacological properties, metabolism and toxicity of BOD. In this study, we identified BOD metabolites after incubation of BOD with human liver microsomes (HLM) using liquid chromatography-high resolution mass spectrometry (LC-HRMS). Formation of 3 metabolites (M1-M3) was yielded with incubating BOD in HLM. The metabolites were structurally characterized on the basis of accurate mass analyses by LC-QTOF/MS. The retention times of BOD, M1, M2 and M3 showed approximately 3.8, 3.0, 3.1 and 3.3 min, respectively. The MS spectra of metabolites M1, M2 and M3 showed a protonated molecular ion [M+H]+ at *m/z* 242.1370, 224.1263 and 212.1296, respectively. Also, the MS/MS spectra of protonated M1, M2 and M3 were observed at *m/z* 210.1118, 192.1017 and 180.1019, respectively. Based on these results, M1, M2 and M3 were identified as hydroxylation, desaturation and demethylation, respectively. The major metabolic route for BOD was hydroxylation (M1). The results will aid in the development of a screening method to determine BOD intake.

Biography

Kyoung-Moon Han has his expertise in identification of unknown compounds using the LC-MS/MS. He has worked for Ministry of Food and Drug Safety in South Korea. He has identified tentative BOD metabolites after incubation of BOD with human liver microsomes (HLM) using liquid chromatography-high resolution mass spectrometry (LC-HRMS).

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