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PII: S0039-9140(17)30867-6
DOI: http://dx.doi.org/10.1016/j.talanta.2017.08.047
Reference: TAL17843

To appear in: *Talanta*

Received date: 14 February 2017
Revised date: 9 August 2017
Accepted date: 12 August 2017

Cite this article as: Kerstin Henkel, Markus J. Altenburger, Volker Auwärter and Merja A. Neukamm, Full validation of a method for the determination of drugs of abuse in non-mineralized dental biofilm using liquid chromatography-tandem mass spectrometry and application to postmortem samples, *Talanta,* http://dx.doi.org/10.1016/j.talanta.2017.08.047

Full validation of a method for the determination of drugs of abuse in non-mineralized dental biofilm using liquid chromatography-tandem mass spectrometry and application to postmortem samples

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Abstract

Alternative matrices play a major role in postmortem forensic toxicology, especially if common matrices (like body fluids or hair) are not available. Incorporation of illicit and medicinal drugs into non-mineralized dental biofilm (plaque) seems likely but has not been investigated so far. Analysis of plaque could therefore extend the spectrum of potentially used matrices in postmortem toxicology. For this reason, a rapid, simple and sensitive method for the extraction, determination and quantification of ten drugs of abuse from plaque using liquid chromatography-tandem mass spectrometry (LC-MS/MS) was developed and fully validated. Amphetamine, methamphetamine, 3,4-methylenedioxymethamphetamine (MDMA), 3,4-methylenedioxy-N-ethylamphetamine (MDEA), 3,4-methylenedioxyamphetamine (MDA), cocaine, benzoylecgonine, morphine, codeine and 6-acetylmorphine were extracted from 2 mg of dried and powdered plaque via ultrasonication with acetonitrile. The extracts were analyzed on a triple-quadrupole linear ion trap mass spectrometer in scheduled multiple reaction monitoring mode (sMRM). The method was fully validated and proved accurate, precise, selective and specific with satisfactory linearity within the calibrated ranges. The lower limit of quantification was 10 to 15 pg mg^{-1} for all compounds except for MDA (100 pg mg^{-1}) and amphetamine (200 pg mg^{-1}). The method has been successfully applied to three authentic postmortem samples with known drug history. Amphetamine, MDMA, cocaine, benzoylecgonine, morphine and codeine could be detected in these cases in concentrations ranging from 18 pg mg^{-1} for cocaine to 1,400 pg mg^{-1} for amphetamine.[1]

Abbreviations: LC-MS/MS, liquid chromatography-tandem mass spectrometry; MDMA, 3,4-methylenedioxymethamphetamine; MDEA, 3,4-methylenedioxy-N-ethylamphetamine; MDA, 3,4-methylenedioxyamphetamine; sMRM, scheduled multiple reaction monitoring; CLSM, Confocal Laser Scanning Microscopy; EPS, extracellular polymeric substances; ACN, acetonitrile; HPLC, high performance liquid chromatography; TSB, Tryptic Soy Broth; LOD, limit of detection; LLOQ, lower limit of quantification; RSD, relative standard deviation