

USE OF MASS SPECTROMETRY FOR IDENTIFICATION OF BIOMARKERS OF
EXPOSURE TO THE FLAME RETARDANT DI(2-ETHYLHEXYL)-2,3,4,5-
TETRABROMOPHTHALATE

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Abstract

Di-(2-ethylhexyl)-2,3,4,5-tetrabromophthalate (TBPH) is one component in the technical formulation of Firemaster 550, a fire retardant used after phasing out certain polybrominated diphenyl ethers. Firemaster 550 is used widely and its use may result in human exposure to TBPH. To identify potential biomarkers of exposure to TBPH, we administered Uniplex FRP-45 (Unitex Corporation, 99% TBPH) to eight adult female Sprague-Dawley rats (500 mg/Kg bw) by gavage. We used mass spectrometry to identify potential metabolites of TBPH in the 24-h urine samples of rats collected 24-h and 48-h after dosing and in serum collected at necropsy 48-h

post-exposure. Using authentic standards, we positively identified tetrabromo benzoic acid (TBBA) and tetrabromo phthalic acid (TBPA) in both urine and serum of the dosed rats. Although TBPH is structurally similar to di-(2-ethylhexyl)phthalate (DEHP), a compound known to form numerous metabolites by oxidation of its 2-ethylhexyl alkyl chain, we did not detect TBPH oxidative metabolites similar to those formed by DEHP. We used HPLC-tandem mass spectrometry for quantification of TBBA and TBPA. The levels of TBBA present in rat urine and serum were much higher than the levels of TBPA. TBBA is also a metabolite of 2-ethylhexyl-2,3,4,5-tetrabromobenzoate (TBB). Because the FRP-45 administered to the rats was technical grade we could not conclusively rule out the presence of TBB as a contaminant which may also have contributed to urinary TBBA. Based on the above results, TBBA and TBPA may serve as potential biomarkers of exposure to the flame retardant Firemaster 550.