Facile synthesis of deuterium-labeled denatonium cation and its application in the quantitative analysis of Bitrex by liquid chromatography-mass spectrometry.

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Streszczenie

Quantitative analysis by liquid chromatographymass spectrometry (LC-MS) is frequently based on the application of isotopically labeled standards which usually have to be specially synthesized. Although the synthesis of deuterated isotopologues is relatively inexpensive, they are not considered as good internal standards due to the possible deuterium effect on the retention time during LC-MS analysis. We developed a method of deuterium labeling of denatonium benzoate (Bitrex) via H/D exchange of its α-carbon hydrogen atoms in CH2 group situated between carbonyl and quaternary ammonium groups. The proposed strategy is rapid, cost-efficient, and does not require derivatization reagents or further purification. The LC-MS analysis of isotopologues revealed that the introduced deuterons do not undergo back exchange under acidic conditions, and the co-elution of deuterated and non-deuterated forms is observed. The obtained deuterated standard was applied in the quantitative LC-MS analysis of Bitrex in commercially available household products.

Słowa kluczowe

Bitrex, Hydrogen deuterium exchange, Isotope dilution, Quantitative analysis, Liquid chromatography-mass spectrometry

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