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Title: Micellar liquid chromatographic green enantioseparation of racemic amino alcohols and

determination of elution order

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Abstract:

A micellar liquid chromatographic method was developed for the green enantioseparation of racemic amino alcohols using an aqueous solution of the mixed surfactants as an alternative for organic solvents. In this study, the derivatives of the amino alcohols were synthesized using highly reactive chiral esters of (S)-levofloxacin (Lfx) under microwave conditions, and an aqueous solution of the surfactants (Brij-35 and SDS) was used for the enantioseparation of the synthesized diastereomeric derivatives (DDs) of amino alcohols using reversed-phase HPLC. The activated ester of Lfx was synthesized by reacting with N-hydroxybenzotriazole and characterized using UV, IR, 1H NMR, high-resolution mass spectrometry, and elemental analysis. The DDs of racemic amino alcohols were separated on a C18 column using micellar LC. Chromatographic conditions were optimized by varying the concentration of the surfactants in aqueous solution and by varying the concentration and pH of the buffer. The green assessment score was calculated for the developed method (score: 82, an excellent green method). In addition, the density functional theory calculations were performed to develop the lowest energy-optimized structures of DDs. The method was validated according to the International Conference of Harmonization guidelines, and the retention factor (k), selectivity factor (α), resolution factor (RS), limit of detection (0.198 ng mL-1 or 0.291 pM mL-1), and limit of quantification (0.594 ng mL-1 or 0.873 pM mL-1) were calculated.

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