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Title:	A sensitive micellar liquid chromatographic method for the rectification of enantiomers of esmolol, and determination of absolute configuration and elution order	
Authors:	Alwera, V. (/jspui/browse?type=author&value=Alwera%2C+V.) Sehlangia, S. (/jspui/browse?type=author&value=Sehlangia%2C+S.) Alwera, S. (/jspui/browse?type=author&value=Alwera%2C+S.)	
Keywords:	Derivatization Esmolol Enantioseparation Green mobile phase RP-HPLC	
Issue Date:	2020	
Publisher:	Taylor and Francis Inc.	
Citation:	Journal of Liquid Chromatography and Related Technologies, 43(17-18)	
Abstract:	A green chromatographic method is proposed for the enantioseparation of Esmolol (Amino alcohol) in which aqueous solution of the mixed surfactants is used as the alternative of organic solvents. In this work, the diastereomeric derivatives of racemic esmolol were prepared, under microwave heating conditions, using highly reactive activated chiral esters of the (S)-levofloxacin, (S)-ketoprofen, and (S)-ibuprofen. The prepared diastereomeric derivatives were separated using surfactant based mobile phase on RP-HPLC. The effect of the varying concentration of surfactant (Brij-35 and SDS) in the eluting phase was investigated for separation and elution of synthesized diastereomeric derivatives. The green assessment score was calculated (obtain score points were 82) for developed method. In addition, the density functional theory calculations were performed, using Gaussian 09 rev. A.02 and hybrid density functional B3LYP with 6-31 G* basis set program, in order to develop lowest energy optimized structures of diastereomeric derivatives. The optimized structures used to predict elution order of synthesized diastereomeric derivatives. Our method was characterized by the following validation parameter: LOD (0.289 ng mL-1), LOQ (0.867 ng mL-1), calibration range (0.006–6.0 mg mL-1), correlation coefficient (0.999) and recovery (99.97 and 99.85% for intra-day assay and 99.42 and 99.75% for inter-day assay).	
URI:	https://www.tandfonline.com/doi/full/10.1080/10826076.2020.1798250 (https://www.tandfonline.com/doi/full/10.1080/10826076.2020.1798250) http://hdl.handle.net/123456789/3463)	

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