

Publication year: 2011

Source: Journal of Chromatography A, Available online 9 November 2011

Carlo Bertucci, Marco Pistolozzi, Daniele Tedesco, Riccardo Zanasi, Renzo Ruzziconi, ... Enantioselective high performance liquid chromatography (HPLC) coupled with a detection system based on the simultaneous measurement of UV absorption and electronic circular dichroism (ECD) allows a complete stereochemical characterization of chiral compounds, once the relationship between sign of the chiroptical properties and absolute configuration is determined. In the present communication, the development of enantioselective HPLC methods for the resolution of a series of fluorinated 2-phenanthrenylpropionic acids (1-6) is reported. Different chiral stationary phases (CSPs) were tested: ChiralcelOJ, ChiralcelOD, ChiralpakAD, (S,S)-Whelk-O1, Chirobiotic™ T and α 1-acid glycoprotein (AGP). The results allow the application of the methods to a reliable determination of the enantiomeric excess for all the examined compounds; the highest enantioselectivity values were obtained with the Hibar[(S,S)-Whelk-O1] column for some of the examined compounds. In the case of rac-2-(6-fluorophenanthren-1-yl)propionic acid (1), the relationship between circular dichroism and absolute configuration of the enantiomeric fractions was determined by ECD analysis and time-dependent density functional theory (TD-DFT) calculations. The experimental ECD spectrum of the second-eluted fraction of 1 on the Hibar[(S,S)-Whelk-O1] column was found to be in excellent agreement with the theoretical ECD spectrum of (S)-1; therefore, the absolute configuration of the first- and second-eluted enantiomers on the (S,S)-Whelk-O1 CSP was assessed as (R) and (S), respectively, and the elution orders of the enantiomeric forms of 1 were determined on all the different CSPs.

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