Simulation of ibuprofen racemate separation by FEMLAB

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Abstract

FEMLAB is a powerful interactive environment for modeling, solving all kinds of scientific and engineering problems based on partial differential equations (PDEs). Separation process of chiral compound in HPLC columns was simulated by FEMLAB. Target material was (R, S)-ibuprofen [(R, S)-2-(4-isobutyl phenyl) propionic acid], an anti-inflammatory agent, which resides the pharmacological activity in the (S)-(+)-enantiomer. Sample concentration was set to 0.5g/L and injection volume 20 μ L at a flow rate of 1ml/min. Simulated results were well fitted with experimental data.

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