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Abstract
A lipase-catalyzed enantioselective dynamic kinetic resolution thiotransesterification between (R,S)-naproxen 2,2,2-trifluoroethyl thioester and hydroxybutyl morpholine in organic solvents was developed for the synthesis of (S)-naproxen morpholinobutyl ester prodrug. Response Surface Methodology (RSM) base on a five-level, four-variable central composite rotatable design (CCRD) was employed for optimization with respect to four import reaction variables –the ratio of concentrations of hydroxybutyl morpholine and racemic naproxen 2,2,2-trifluoroethyl thioester, Lipase MY concentrations, temperature and time. The prodrugs yield (XT,Q) and enantiomeric excess of product (eep,Q) were considered as two product quality variables. A desirability function was applied to combine these two qualities as a single objective function. The optimum reaction conditions predicted for achieving maximum desirability (0.9032) are: hydroxybutyl morpholine/ racemic naproxen 2,2,2-trifluoroethyl thioester as 2.0, Lipase MY concentration as 77.29 Mm, temperature as 43.71 ℃ and time as 237.38 h. At these conditions, the actual desirability (D) was reached 0.8158, the prodrugs yield(XT,Q) and enantiomeric excess of product(eep,Q) were 90.69％ and 95.09％, respectively.
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