Lipase-catalyzed acylation of quercetin with cinnamic acid

ABSTRACT

Acylation of quercetin with cinnamic acid catalyzed by Candida antarctica lipase B (CAL-B) or Pseudomonas cepacia lipase C (PCL-C) was investigated. Specifically, the effects of reaction duration, incubation temperature, and molar ratio of substrates on bioconversion yield, initial rate of reaction, and regioselectivity were investigated. Three new acylated quercetin analogues were produced: quercetin 4′-cinnamate ($C_{24}H_{16}O_8$), quercetin 3′,4′-dicinnamate ($C_{33}H_{22}O_9$), and quercetin 7,3′,4′-tricinnamate ($C_{42}H_{28}O_{10}$). The effects of the lipase-catalyzed acylation conditions on the bioconversion yields varied across the conditions. The initial rate of reaction of acylation of quercetin with cinnamic acid catalyzed by CAL-B and PCL-C was similar. In the presence of CAL-B, acylation mainly took place at the C-4′-OH, generating mostly quercetin 4′-cinnamate; whereas with PCL-C, acylation mainly took place at both the 4′- and 3′-hydroxyls, generating quercetin 3′,4′-dicinnamate. Thin-layer-chromatography analysis showed that the three acylated quercetin analogues had higher lipophilicity when compared with quercetin. In silico investigation revealed that quercetin 4’-cinnamate and quercetin 3′,4′-dicinnamate are likely to be orally active pharmacological drugs.

Keyword: Biocatalysis; Enzymatic acylation; Lipase; Quercetin; Cinnamic acid