Biosynthesis of quercetin palmitate esters and evaluation of their physico-chemical properties and stability

ABSTRACT

Quercetin was acylated with palmitic acid, catalyzed by either Candida antarctica lipase B (CAL-B) or Pseudomonas cepacia lipase C (PCL-C) to produce quercetin palmitate esters. The effects of various operating factors including incubation temperature, reaction duration, and molar ratio of substrates on the bioconversion yield, initial rate of reaction, and regioselectivity of the reactions were investigated. Three new esters were identified: quercetin 40 palmitate ($C_{31}H_{40}O_8$, 540 g mol−1), quercetin 30 ,40- dipalmitate ($C_{47}H_{70}O_9$, 778 g mol−1), and quercetin 7,30 ,40- tripalmitate ($C_{63}H_{100}O_{10}$, 1016 g mol−1). The effects of incubation temperature, reaction duration, and molar ratio of substrates on bioconversion yields varied across the conditions. However, the highest bioconversion yield of 27.72 1.64% was obtained with PCL-C, at day 7, incubation temperature of 60 C, quercetin:palmitic acid molar ratio of 1:20. The initial rate of reaction was significantly higher with PCL-C. However, regioselectivity was similar for both PCL-C- and CAL-B-catalyzed reactions with acylation occurred successively at 4´-OH, 3´-OH, and 7-OH. Thin-layer chromatography analysis showed that the three quercetin palmitate esters possessed enhanced lipophilicity (134% higher than quercetin). Besides, in silico investigation showed that quercetin 40 -palmitate had a higher partition coefficient (log P) value than the parent compounds, indicating improved solubility. During gastrointestinal tract simulation, quercetin palmitate esters were recovered in the range of 71.03% to 79.36% after digestion, which were significantly higher than quercetin at 40.43 8.71%. Quercetin 40-palmitate was also found stable over 28 days of storage. Due to improved lipophilicity, solubility, and stability, quercetin 40-palmitate has the potential to be used in topical applications.

Keyword: Bioconversion; Enzymatic acylation; Palmitic acid; Lipase; In vitro digestibility