

Enzymatic Synthesis of Caffeic Acid Esters from Chlorogenic Acid by Transesterification and Condensation Reactions

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SUMMARY

Immature green coffee beans contain considerable amounts (4.8-5.8g 100g⁻¹) of 5-chlorogenic acid derivatives. The enzymatic conversion of their 5-chlorogenic acid derivatives into value-added products was investigated. A chlorogenate hydrolase (EC 3.1.1.42) was found to synthesize from 5-chlorogenic acid and 2-phenylethyl alcohol into 2-phenylethyl caffeate (by transesterification) and from caffeic acid and 2-phenylethyl alcohol into 2-phenylethyl caffeate (by condensation) as well as hydrolysis of 5-chlorogenic acid. Some reaction conditions including pH, temperature, substrate and solvent concentrates, and reaction time were optimized for the production of 2-phenylethyl caffeate. A maximal molar yield of 53% was achieved by transesterification and 13% by condensation. Among the parameters studied for optimization, the pH of the buffer solution and concentration of solvent affected the production of 2-phenylethyl caffeate. The optimum pH for the hydrolysis reaction was within the neutral range (pH 6.5), whereas the residual two reactions were only catalyzed within the acidic range (pH 3.0-4.0). The optimum concentration of 2-phenylethyl alcohol for two reactions were 5-70 vol.% and no 2-phenylethyl caffeate was produced in the anhydrous solvents.