Abstract

Cyclodextrins are a group of macrocyclic compounds, they are natural polysaccharides which are formed of 6, 7, or 8 α,D-glucopyranosides units joined with α-1,4-glycoside bonds. Their structure resembles a truncated cone. The outer surface of the cyclodextrins is hydrophilic and the cavity of the macrocycle is hydrophobic. This structure allows to include nonpolar molecules (ligands) or their functional groups inside them. Cyclodextrins show no cytotoxicity, therefore they are interesting carriers of active substances. They improve the solubility of the incorporated molecules and also extend the duration of their activity in the body.

The aim of the study was physicochemical research aimed at thermodynamic characteristics of the interactions of α- and β-cyclodextrin with cinnamic acid and its derivatives (p-coumaric acid, caffeic acid, ferulic acid, and sinapinic acid) in the water environment.

Spectroscopic measurements of the solubility of cinnamic acid and its derivatives in aqueous solutions of the tested cyclodextrins with increasing concentration allowed to determine the effectiveness of α- and β-cyclodextrin in increasing the solubility of cinnamic acid and its derivatives and to calculate the constant of formation of the resulting complexes.

The interactions between cinnamic acids and their derivatives and α- cyclodextrin and β-cyclodextrin in aqueous solutions were investigated using the method of isothermal titration calorimetry (ITC). The obtained results made it possible to determine the stoichiometry and calculate the constants for the formation of α and β-cyclodextrin complexes with the included molecules of the studied acids, as well as to calculate the values of standard thermodynamic functions of forming their complexes with cyclodextrins.

The characteristics of ligand-cyclodextrin systems were supplemented by studies of the properties of aqueous ligand solutions, including measurements of dissolution of sodium salts of phenolic acids in water as well as dissolution of these salts in aqueous urea solutions, selected as a model compound that well differentiates the hydrophilic-hydrophobic properties of compounds interacting with it. The obtained values of standard molar enthalpy of dissolution of sodium salts in water and in urea solutions allowed to determine heterogeneous enthalpy coefficients of interaction hxy of dissolved salt pairs with urea molecule in the water environment.

The last part of the research was densimetric measurements of aqueous solutions of sodium salts of selected phenolic acids in a wide temperature range from 288.15 to 318.15 K. Based on the experimentally obtained values of the density of aqueous solutions of sodium salts

of selected phenolic acids, the values of the apparent molar volume and the apparent partial molar volume of the tested compounds were determined.