INTERACTIONS BETWEEN SERTRALINE HYDROCHLORIDE AND SOME B-CYCLODEXTRINS

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Sertraline hydrochloride is an antidepressant with low solubility in water. To increase the bioavailability of this oral-taken drug it is worth to check influence of the cyclodextrins on this substance. Cyclodextrins are able to improve solubility of the guest drug inserted into their cavities and make the drug absorption in the gastro-intestinal tract more effective.

One of the methods to examine the complex formation between drugs and cyclodextrins is the isothermal titration calorimetry (ITC). The set of parameters of interaction given by this experimental method brings information about the strength and the energetic aspects of complex formation between guest and host molecules.

In this work the interaction parameters from ITC measurements like binding constant, enthalpy, entropy and Gibbs energy of binding β -cyclodextrin and their derivatives like heptakis(2,6-di-O-methyl)- β -cyclodextrin and 2-hydroxy-propyl- β -cyclodextrin with sertraline hydrochloride in water at 298.15 K are presented. The parameters of complex formation are compared with each other and with available literature and the conclusions are made.

INTERACTIONS BETWEEN SEVERAL AMINOPHOSPHONIC ACIDS AND UREA IN WATER AT 298.15 K

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Aminophosphonic acids are an important class of simple mimetics of natural aminoacids. These compounds differ in carboxylic and phosphonic group. The core of aminophosphonate molecule contains a constant NH₂-CH₂-PO₃H₂ group and the core of amino acids is NH₂-CH-COOH. Side substituent –R shows various affinities to water and is partly responsible for hydrofobic –hydrofilic properties.

As a result of the structural analogy of these two classes of amino acids, aminophosphonates exhibit significant biochemical activity, displayed spectacularly in agrochemistry and pharmacology field. Their variety applications include enzyme inhibitors, antibiotics, herbicydes, and also antitumor agents.

Thus it is interesting to research interaction between these compounds and constituent organisms fluids, for example urea. In these studies solution enthalpies of series aminophosphonic acids (phosphonophenylglycine, phosphonovaline and phosphononorvaline) in water and aqueous urea in 298.15 K have been measured. (Modified McMillan-Mayer theory allows use these data to calculate enthalpic heterogenous pair interaction coefficients of aminophosphonic acids – urea.)

The obtained results let us to calculate the heterogeneous enthalpic pair interaction coefficients between aminophosphonic acids and urea molecule based on McMillan Mayer theory. The enthalpic pair interaction coefficients describe the energetic effects of interactions between aminophosphonic acids molecules and urea molecule what happen in the presence of the competitive participation of water molecules. These values were interpreted in the terms of the hydrophobic effect of the side chains of aminophosphonic acids on their interactions with a molecule of urea in water.