

## Abstract:

***Application of isothermal titration calorimetry technique to thermodynamic investigation of biologically active compounds***

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In recent years, an intensive development of knowledge about biologically active compounds has been observed. Both, properties and the mechanism of their action on the living organisms are studied. The progress in research this type of substance is particularly noticeable in pharmacy, where new drugs or already used compound derivatives are synthesized. Thermodynamic data of the biologically active compound interactions can provide interesting information. Isothermal titration calorimetry (ITC) technique allows to measure the thermodynamic parameters of interactions i.e.: change of standard enthalpy  $\Delta H^\circ$ , equilibrium constant  $K_a$  and stoichiometry  $n$ .

In the thesis, the drug - carrier and inhibitor - cofactor interactions were discussed. Drugs were represented by three biologically active compounds: fluorescein isothiocyanate (FITC), doxorubicin (DOX) and methotrexate (MTX), while the innovative star-shaped copolymers represented a group of drug carriers. In the second part, thermodynamic analysis of the interaction of potential glycosyltransferases inhibitors and divalent manganese ion, which is a cofactor in the enzymatic reaction, was performed. The aim of the research was to understand the mechanisms of studied phenomenon, the selection of substances exhibiting desirable properties and discussion of the application of the selected compounds.

It has been proved ITC usefulness to study a number of interactions of biologically active compounds. The influence of choice of measurement conditions was shown, as well as problems which can be encountered during the thermodynamic analysis of various interactions were discussed. The reaction mechanism effect on the thermodynamic parameters of studied phenomena and their importance during the interpretation of the data on the molecular level was emphasized.