1. Abstract

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Title of Diploma Thesis: *Physico-Chemical properties of drugs*

To test physico-chemical properties of new molecules is necessary during drug development. It could be helpful to understand or predict the pharmacokinetic parametres of a new drug in vivo/in vitro experiments.

One of this parameters is a dissociation constant (pK). Dissociation constant is defined as „ Number on pH scale, wherein is just fifty percent of molecule in a ionization condition“. In real case this number can help us to know where in the gastro-intestinal tract (GIT) the drug will be absorbed. In GIT only molecules exhibiting pK from 3 to 11 could be absorbed. Out of this range it is not possible.

In this work I would like to introduce the ways of experimental measurement of pK values. I was working with two methods to measure the pK values of water-soluble compounds. The spectrophotometric method and the potentiometric one. I had to find out, that potentiometric titration is primary method which gets us good and accurate results. Based on my measurement I evaluated the spectrophotometric method as the secondary method. Spectrophotometric method gave us good results only for 2-aminobenzimidazole compound. The spectrophotometric method did not work with the pyrazines compounds with variety of functional groups. Potentiometric titration gave us good results.

The dissociation constant is affected by functional groups in the molecule. So I also tried to compare a variety of functional groups on pyrazine heterocyclic to show how a pK value is changed by introduction of various functional groups. Whereas it was the pyrazine nucleus was the pK values of compounds aminopyrazine, carboxypyrazine and

3-amino-2-carboxypyrazine affected in small range. All of these three compounds have the pK value in the acidic range of pH scale. This is due to the electron shift to the pyrazine ring.