INVESTIGATION OF THE CORRELATION BETWEEN VALUES OF *pKa* AND DEPROTONATION ENERGY FOR A MODEL NUMBER OF AMINO ACIDS

Kutzhanova K.Zh., Kurmanova A.F., Pustolaikina I.A., Aldangurova A.U., Makybas M.G., Bakytbekova A.Zh.

Academician Ye.A. Buketov Karaganda State University, Karaganda, Kazakhstan
kutzhanovak@mail.ru

An investigation of the acid-base properties of amino acids is considerable interest, since the values of pKa and the patterns of change in the protolytic properties of these compounds are extremely important for predicting reactivity and evaluating the pharmaceutical potential.

It was shown earlier [1] that nonempirical ab initio UHF calculations taking into account the influence of the medium on the basis of the continuum solvation model IEFPCM (solvent-water) give the most satisfactory results for this purpose.

It was carried out a quantum-chemical estimation of the deprotonization energy for the series of 15 amino acids by the nonempirical method UHF ab initio with considering solvation within the framework of the CPCM polarized continuum model with solvent water using the Gaussian-2009 program. The values of pKa were taken from the reference book [2].

The obtained graph of the dependence of the reference value of the pKa value on the deprotonation energy ΔEdeprotonation for the studied 15 amino acid series showed the presence of a direct proportional relationship between these quantities. The value of the Pearson correlation coefficient index $R = 0.94$ indicates a close relationship between these two quantities. A linear approximation equation $y = 0.0351x + 1.8691$ was found, which characterizes the relationship between the input ΔEdeprotonation. And output pKa parameters of the model sample.

References:

1. KUTZHANOVA, K. Zh., KURMANOVA, A.F. et al. 2016. Science: Scientific and Production Journal, 1, pp.269-271.
2. LURYE, U.U. 1984. *Handbook of Analytical Chemistry*