# DISTRIBUTION RATIO AT A NUMBER OF FUNCTIONAL DERIVATIVES N-R-AMINE, AND THEIR QUANTITATIVE CORELATION

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**Introduction.** The ability to predict biological properties of compounds through their lipophilicity allows to optimize the search for new drugs and is often included in equations for calculations of the quantitative structure – activity relationships (QSAR). However, experimental methods to determine logP are time-consuming and expensive, and the values obtained often differ due to the influence of many factors.

**Aim.** The aim of this work is to determine the mutual correlation of the values of the partition coefficients in the series of some functional derivatives of N-R-amines calculated by different algorithms.

**Materials and methods.** Taking into account the data we used the available free on-line methods xlogP3, AlogPs for calculations of the partition coefficients, and the ChemBioOffice2014 software package, in particular ChemBioDrawUltra 14.0 (CBDU14) and ChemBio3DUltra 14.0 (CB3DU14), for calculations of logP and ClogP. Calculations of correlations of the values of the partition coefficients calculated for compounds were performed using the STATISTIKA 8 software. According to the requirements of mathematical statistics the correlation coefficient indicates the close relationship between the values: at values less than 0.3– relationship is absent, in the range of 0.3–0.7 it is medium, more than 0.7– it is strong.

**Results and discussion.** Almost all compounds are characterized by negative values of the partition coefficients; probably it is due to the presence of the polar moiety – substituted Nitrogen atom in their structure. Increase of numeric values, and hence lipophilicity, is observed in the case of increase in the number of non-polar substituents (alkyl substituents or the phenyl nucleus in compounds). Glycine, for which the calculated values (excluding logP) agree with the experimental ones, and its alkyl substituents are characterized by the maximum values of hydrophilicity. It can be also explained by the considerations previously mentioned.

**Conclusions.** Therefore, the results of our study allow to propose the values AlogPs obtained for further application when determining QSAR, as well as the degree of its manifestation among N-R-amine derivatives for planning a targeted search biologically active substances in this series.