Nowadays, a significant part of scientific research focuses on the discovery and synthesis of biologically active compounds, studying their action, efficacy, physicochemical properties, environmental toxicity and potential use in various areas of life.

The use of various mathematical models make it possible to establish qualitative and quantitative relationships between the structure and activity of the newly synthesised compounds. The most commonly used molecular descriptor to predict the potential of a compound to be biologically active is lipophilicity.

Lipophilicity helps determine the behaviour of a drug in the body - permeability across biological membranes, ability to interact with proteins or pass through the blood-brain barrier. It also allows prediction of the ADMET profile, i.e. absorption, distribution, metabolism, secretion and toxicity.

The aim of this study was to determine the lipophilicity of 20 newly synthesised substances, i.e. eight derivatives and analogues of 2-thioxo-1,3-thiazolidin-4-one and twelve derivatives of 5-pyridylmethylidene-3-rodanine carboxylic acid. All of these compounds contain a thiazolidine ring in their structure. Reports can be found in the literature that this class of compounds exhibit high biological activity after oral administration. In addition, there are preparations containing substances with a similar chemical structure available in the general medical practice in Poland. It was investigated whether the analysed substances exhibit biological activity and, consequently, whether they could be used as new drugs in the future.

Determination of lipophilicity of the analysed substances was performed using experimental and computer methods. The experimental method used the reversed-phase thin-layer chromatography technique. Binary mixtures consisting of water and an organic modifier were used as mobile phases. In the *in-silico* method, up to nine databases and programmes were used to calculate the logarithm value of the partition coefficient of the analysed substances and their other physico-chemical and biological properties.

The results obtained experimentally and by computer were compared with each other. Statistical analysis was carried out to determine whether there was any significant correlation between determined and calculated values.

Keywords: analytical chemistry, medicinal chemistry, chemoinformatics, lipophilicity, logP, thin-layer chromatography, TLC, computational methods, *in-silico*, thiazolidine derivatives and analogues.