Liakh V., Konechna R., Novikov V.

Prediction of acute toxicity of biologically active substances *Caltha palusris*

National University «Lviv Polytechnic», Lviv, Ukraine

Relevance: Pre-experimental analysis of biologically active substances can be obtained using in silico methods. GUSAR Acute Rat Toxicity makes it possible to predict acute toxic effects on rats by the in silico method, which is more humane than the classical method.

Objective: To determine the acute toxic effect of biologically active substances of the medicinal plant *Caltha palusris* by the in silico method.

Materials and methods of research: In silico prediction of LD50 values for rats with four types of administration (oral, intravenous, intraperitoneal, subcutaneous, inhalation) by GUSAR software. The following biologically active substances of the medicinal plant *Caltha palusris* were selected for the study: protoanemonin, anemonin, pamurolid, caltolide, sitosterol, scopoletin, umbelliferone.

Results: GUSAR Acute Rat Toxicity contains information from the SYMYX MDL toxicity database. After computer screening, the following information was received:

1. Protoanemonin: intraperitoneal route of administration to rats (IP) LD50 = 275.2mg / kg; intravenous route of administration to rats (IV) LD50 = 49.34 mg / kg; oral route of administration to rats (Oral) LD50 = 2100 mg / kg; subcutaneous route of administration to rats (SC) LD50 = 404.9mg / kg.
2. Anemonine: IP - LD50 = 163 mg / kg; IV - LD50 = 11.3mg / kg; Oral - LD50 = 804.6mg / kg; SC -LD50 = 807,2mg / kg.
3. Palustrolid: IP - LD50 = 784 mg / kg; IV - LD50 = 12.31 mg / kg; Oral - LD50 = 1247mg / kg; SC - LD50 = 55.05 mg / kg.
4. Caltolide: IP - LD50 = 633.7 mg / kg; IV - LD50 = 13.38 mg / kg; Oral - LD50 = 1427 mg / kg; SC - LD50 = 106.3mg / kg.
5. Sitosterol: IP - LD50 = 1644 mg / kg; IV - LD50 = 6.026 mg / kg; Oral - LD50 = 1562 mg / kg; SC - LD50 = 332,7mg / kg.
6. Scopoletin: IP - LD50 = 329.1 mg / kg; IV - LD50 = 45,85mg / kg; Oral - LD50 = 1468mg / kg; SC - LD50 = 835.4 mg / kg.
7. Umbelliferone: IP - LD50 = 902.2mg / kg; IV - LD50 = 47,63mg / kg; Oral - LD50 = 861 mg / kg; SC - LD50 = 1434 mg / kg.

Conclusion: Acute toxicity data were obtained on rats by using the in silico method, whose application is more appropriate economically, more environmentally friendly and more humane than the use of the classical method. The resulting LD50 rat values will later be used to create new medicines and cosmetics.