

Prediction of biological activity for *Ficaria verna* compounds

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Today, compounds of natural origin are becoming increasingly popular. Their advantage over synthetic compounds is due to safety, because they do not cause allergic reactions.

The object of our study is *Ficaria verna* – representative of the family *Ranunculaceae*. *Ficaria verna* has diuretic, expectorant, laxative, anti-inflammatory, wound healing and purifying properties. However, as a medicinal plant, it is insufficiently studied. Therefore, a detailed examination and research of *Ficaria verna* for the purpose of introduction into medicinal medicine has a potential interest. The plant contains biologically active compounds, in particular saponins, protoanemonin, anemonin, ascorbic acid, carotene were found in the leaf. Phytochemical studies of flowers and leaves have identified four phenolic compounds that are of potential interest for study. Phenolic compounds are represented by the following series of compounds: nicotiflorin, vitexin, orientin, flavosativazide.

Aim. The use of *in silico methods*, including predictive screening, has made a significant impact on the search and study of biologically active compounds.

Materials and methods. Prediction of biological activity of compounds using the compensatory program PASS (Prediction of Activity Spectra for Substances). The chemical structure is represented in PASS in the form MNA descriptors (Multilevel Neighbourhoods of Atoms). The results of the forecast are obtained in the form of estimation of the probabilities of presence (P_a) and the absence of each activity (P_i), having values from 0 to 1.

Results. **Nicotiflorin** is predicted to show hemostatic ($P_a=0,992$), membrane permeability inhibitor ($P_a=0,989$), cardioprotectant ($P_a=0,990$), free radical scavenger ($P_a=0,984$), membrane integrity agonist ($P_a=0,984$), CYP1A inducer ($P_a=0,979$), vasoprotector ($P_a=0,979$) action. **Vitexin** — a potential TP53 expression enhancer ($P_a=0,973$), membrane integrity agonist ($P_a=0,966$), cardioprotectant ($P_a=0,950$), HIF1A expression inhibitor ($P_a=0,940$), free radical scavenger ($P_a=0,901$), membrane permeability inhibitor ($P_a=0,891$), anaphylatoxin receptor antagonist ($P_a=0,890$) action. **Orientin** — a potential TP53 expression enhancer ($P_a=0,974$), membrane integrity agonist ($P_a=0,961$), free radical scavenger ($P_a=0,955$), cardioprotectant ($P_a=0,952$), HIF1A expression inhibitor ($P_a=0,940$), hepatoprotectant ($P_a=0,927$), membrane permeability inhibitor ($P_a=0,927$), UGT1A9 substrate ($P_a=0,892$) action. **Flavosativaside** — a potential free radical scavenger ($P_a=0,970$), membrane integrity agonist ($P_a=0,970$), TP53 expression

enhancer ($P_a=0,966$), hepatoprotectant ($P_a=0,958$), cardioprotectant ($P_a=0,955$), membrane permeability inhibitor ($P_a=0,933$), chemopreventive ($P_a=0,932$), anaphylatoxin receptor antagonist ($P_a=0,928$) and monophenol monooxygenase inhibitor ($P_a=0,919$) action.

Conclusions. According to the results of predicting the activity of biologically active substances, *Ficaria verna* is a prospect to develop hemostatic and antioxidant agents and as a means to enhance the expression of TP53 based on the presented plant.