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MOLECULAR DIAGNOSTICS OF TOXIC AND PROTECTIVE PROPERTIES OF SUBSTANCES BY DOCKING

Background/Aim. Environmental pollution with toxic substances, in particular perchlorates and pesticides, is a factor in the development of many pathologies. Toxins enter drinking water and food through groundwater and cause disorders in the human body through endocrine and inflammatory mechanisms [1, 2]. The flavonoid quercetin is considered as a protective agent against the toxic effects of perchlorates and pesticides [3]. Therefore, it is advisable to study the molecular mechanisms of action of perchlorates, pesticides and quercetin using software. **Methods.** With the use of platforms ProTox 3.0, based on machine learning algorithms, software provision Schrödinger Maestro Glide, AutoDock, and AutoDockVina, pkCSM, admetSAR and SwissADME platforms carried out forecasting properties of perchlorate potassium, pesticide α -cypermethrin and quercetin [1, 2]. **Results.** The use of the ProTox 3.0 predicts potential interaction of potassium perchlorate with estrogen receptors. Molecular docking analysis using the aforementioned programs showed the potential antagonistic effect of α -cypermethrin on the ER. Molecular docking of quercetin, performed in for the same programs demonstrated lower binding energies with ER structures compared to α -cypermethrin and perchlorate, which may indicate a higher affinity of quercetin for ER and a potential ability to compete with these compounds for receptor binding. The parameters obtained using pkCSM, admetSAR and SwissADME predict high intestinal absorption, absence of AMES toxicity, and compliance of quercetin with the criteria of drug-likeness according to Lipinski's rule of five. **Conclusions.** In silico analysis suggests that potassium perchlorate and α -cypermethrin may interact with estrogen receptors and disrupt endocrine function. Quercetin showed higher predicted ER affinity and favorable pharmacokinetics, suggesting protective potential. Further in vitro and in vivo studies are needed to confirm these findings.

Keywords molecular docking, estrogen receptor, quercetin, cypermethrin, perchlorate.

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