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Prediction of biological activity for *Phlomis Pungens* Willd compounds

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The use of *in silico* methods, including predictive screening, has made a significant impact on the search and study of biologically active compounds. Effective methods are the use of prediction of biological activity of compounds using the compensatory program PASS (Prediction of Activity Spectra for Substances). The use of computer prediction of biological activity for compounds using the PASS program allows to estimate the overall biological potential of investigated objects. Properties of structures, discovered by these methods, are further optimized by their separation, analysis and synthesis of analogues.

The chemical structure is represented in PASS in the form of original 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.

Particularly interesting are biologically active compounds of natural origin, especially, of plant origin. The object of our study is *Phlomis pungens* Willd. – representative of the family *Lamiaceae*, characteristic for the flora of the central and southern regions of Ukraine. Since ancient times it has been used in ethnomedicine as astringent, scratched, tonic, immunostimulant, sedative remedy. However, *Phlomis pungens* is an insufficiently studied medicinal plant, and therefore it is a potential interest for detailed examination and research with a view to introducing into use in officinal medicine. Grass of *Phlomis pungens* is used as medicinal raw material. The grass is rich in essential oils (α-pinene, (E)-β-farnesene, germacrene-D, bicyclogermacrene, n-hexadecanoic acid), phenolic compounds (protocatechuic, p-hydroxybenzoic, chlorogenic, caffeic, rosmarinic acids and (+)-catechin), flavonoids.

Perspective for the study of the group of compounds are iridoids, which are represented by the following series of compounds: lamiide, forsythoside B, alyssonoside, leucosceptoside A, hattushoside [1].

We have performed the prediction of the spectrum of biological activity of iridoid compounds of *Phlomis pungens* Willd. using the PASS program. The following results are obtained: **lamiide** is predicted to show hepatoprotectant (P_a=0,924), antiprotozoal (P_a=0,773), antiinflammatory (P_a=0,765), antifungal (P_a=0,75), antineoplastic (P_a=0,76) and immunostimulant (P_a=0,702) actions; **forsythoside B –** a potential chemopreventive (P_a=0,945), hepatoprotectant (P_a=0,934), anticarcinogenic (P_a=0,934), antineoplastic (P_a=0,860), immunostimulant (P_a=0,843), antifungal (P_a=0,822), antibacterial (P_a=0,733) and antioxidant (P_a=0,702) actions; **alyssonoside –** a potential chemopreventive (P_a=0,959), has hepatoprotectant (P_a=0,950), anticarcinogenic (P_a=0,943), antineoplastic (P_a=0,858), antifungal (P_a=0,815), immunostimulant (P_a=0,792) and antibacterial (P_a=0,723) actions; **leucosceptoside A –** potential chemopreventive, obtains hepatoprotectant (P_a=0,956), anticarcinogenic (P_a=0,934), antineoplastic (P_a=0,816) and antifungal (P_a=0,786) actions; **hattushoside** has hepatoprotective (P_a=0,796), anticarcinogenic (P_a=0,789) and antineoplastic (P_a=0,782) actions.

Conclusions. According to the results of the prediction of the activity of biologically active substances of *Phlomis pungens* Willd. there is a prospect to develop anticarcinogenic, wound healing and antibacterial remedies, based on the presented plant.