MOLECULAR TARGET PREDICTION AND PHARMACOLOGICAL POTENTIAL OF ETHYL 2-[(2-CHLOROETHOXY)(PHENYL)PHOSPHORYL]ACETATE

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In recent years, *in silico* methods for predicting the biological activity of small molecules have become an integral part of the early stages of drug development. The use of computational approaches can significantly reduce the time and cost associated with experimental screening, as well as increase the probability of successful identification of promising candidates.

One of the most popular tools in this field is the SwissTargetPrediction platform [1], developed on the basis of the principle of structural similarity between the studied compound and known bioactive ligands. A number of studies have shown that the combined use of 2D and 3D descriptors provides high accuracy in predicting molecular targets, especially for compounds with already known pharmacophore fragments. The accuracy of correctly identifying at least one target among the first five predictions reaches 70–80 % for most small molecules.

Current research emphasizes that many biologically active compounds have a multi-purpose mechanism of action (polypharmacology). This approach is especially relevant in the development of antitumor and anti-inflammatory drugs, where simultaneous action on several signaling pathways can increase therapeutic efficacy. consistent with this concept.

This paper presents *an in silico* analysis of potential biological targets of the studied ethyl 2-[(2-chloroethoxy)(phenyl)phosphoryl]acetate

The method is based on a comparison of the 2D and 3D structures of the compound with a library of known ligands. The results obtained made it possible to identify a number of enzymes and proteins, mainly belonging to the classes of lyases, proteases and esterases, which indicates a possible broad pharmacological profile of the compound [2].

SwissTargetPrediction takes a combined approach based on:

- 2D structural similarity;
- 3D pharmacophore similarity;
- comparison with the ChEMBL and UniProt databases.

Each target is assigned a *Probability*, which reflects the degree of confidence of the prediction [3].

As a result of the analysis, 100 potential biological targets were identified. The most significant of them are presented in Table 1.

Table 1. Main predicted biological targets

Target protein	UniProt ID	Target Class	Probability
Carbonic anhydrase XII	O43570	Liaza	0,0536
Carbonic anhydrase IX	Q16790	Liaza	0,0536
Leukocyte elastase	P08246	Protease	0,0536
Carboxylesterase 1	P23141	Enzyme	0,0536
Carboxylesterase 2	O00748	Enzyme	0,0536

Current studies highlight the key role of these enzymes in regulating the tumor microenvironment and maintaining the hypoxic phenotype of tumor cells. Therefore, the identification of these targets suggests a potential antitumor orientation of the studied compound or its prospects as a basis for further structural optimization.

The presence of proteases such as leukocyte elastase among the predicted targets may indicate a possible effect of the compound on inflammatory processes. In the context of current research, such a profile is seen as an advantage, as the combination of anti-inflammatory and metabolic activity may extend the therapeutic use of the compound.

The predicted interaction with carboxyl esterases CES1 and CES2 deserves special attention. These enzymes play a key role in the metabolism of drugs, and their involvement may be associated with both the activation of prodrug forms and rapid metabolic clearance. From a drug development perspective, this highlights the need for further pharmacokinetic analysis (Fig. 1).

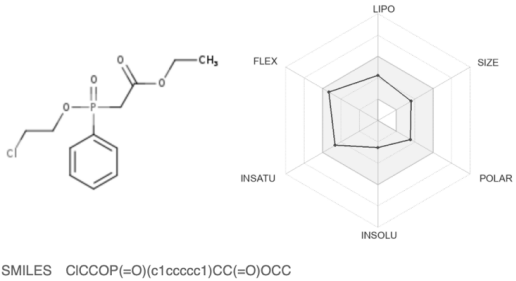

Fig. 1. SwissAdme profile of ethyl 2-[(2-chloroethoxy)(phenyl)phosphoryl]acetate

It should be noted that the probability values obtained in SwissTargetPrediction are of an estimated nature and are not direct evidence of biological activity. However, as shown in modern reviews on *in silico* prediction, such methods have a high predictive value in the early stages of the study and serve as an effective tool for forming hypotheses that are subject to experimental verification

The results obtained suggest a possible multi-purpose pharmacological profile of the compound with a predominance of interactions with enzymes, including carbonic anhydrases, proteases and esterases.

The identification of carbonic anhydrases CA IX and CA XII among the predicted targets allows us to consider the studied compound as potentially promising for further research in the field of antitumor therapy. At the same time, the predicted interaction with metabolic enzymes emphasizes the need for a comprehensive assessment of pharmacokinetic properties.

Thus, *the in silico* analysis confirms the feasibility of further in vitro and in vivo studies, as well as the use of additional computational methods (molecular docking, molecular dynamics) for an in-depth assessment of the mechanisms of action of the studied compound. The data obtained can serve as a basis for subsequent optimization of the structure and development of new pharmacologically active molecules.

References

1. Gfeller D., Grosdidier A., Wirth M. *et al.* SwissTargetPrediction: a web server for target prediction of bioactive small molecules. Nucleic Acids Research, 2014, 42(W1), W32–W38.

2. Bento A. P., Gaulton A., Hersey A. *et al.* The ChEMBL bioactivity database: an update. Nucleic Acids Research, 2014, 42(D1), D1083–D1090.

3. He T.**,** Caba K.**,** Ballester P. J.A precise comparison of molecular target prediction methods. *Drug Discovery Today: Disease Models*, 2025**.** This paper systematically compares current methods for predicting biological targets, including MolTarPred, PPB2, TargetNet, etc., with an analysis of their efficacy on a set of approved drugs.