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USING ARTIFICIAL INTELLIGENCE IN STUDYING THE MECHANISMS OF ACTION OF ORGANOPHOSPHORUS COMPOUNDS

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Abstract
The article examines the theoretical foundations of applying artificial intelligence in the study of organophosphorus compounds. The mechanisms of their toxic action, associated with the inhibition of acetylcholinesterase, are described, as well as approaches to predicting biological activity based on QSAR models. The capabilities of machine learning methods, molecular docking, and molecular dynamics for studying the interaction of compounds with biological targets and the development of antidotes are demonstrated. The importance of integrating AI into medicinal chemistry and toxicology is noted, as well as the need to take into account the ethical aspects of research.

Keywords: Organophosphorus compounds, artificial intelligence, QSAR, acetylcholinesterase, toxicity.

Introduction

Organophosphorus compounds (OPCs) are a broad class of chemicals widely used in agriculture, industry, and medicine [1]. Despite their practical importance, these compounds are characterized by high biological activity and potential toxicity, due to their ability to inhibit acetylcholinesterase , a key enzyme in the cholinergic system. Disruption of this enzyme leads to the accumulation of acetylcholine in the synaptic cleft and the development of severe pathological conditions, making the study of OPCs a priority in toxicology and medicinal chemistry.

Traditional methods for studying organophosphorus compounds, including experimental biochemical and pharmacological approaches, are highly informative, but are labor-intensive, time-consuming, and expensive. Furthermore, conducting certain experiments poses health risks to researchers and requires strict safety measures [12]. Therefore, the introduction of modern computational methods capable of significantly accelerating and optimizing the process of studying the properties of these compounds is particularly relevant.

In recent years, artificial intelligence methods have rapidly developed, finding increasing application in chemistry, pharmacology, and toxicology. The use of machine learning algorithms, molecular modeling, and data analysis allows for the prediction of the biological activity of compounds,

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assessment of their toxicity, and modeling of interactions with biotargets at the molecular level. Particularly promising are approaches based on the structure–activity relationship (QSAR) concept , which enable the establishment of quantitative relationships between a molecule's structure and its biological effects [12].

The aim of this study is to analyze the theoretical foundations and modern approaches to the application of artificial intelligence in the study of organophosphorus compounds, as well as to assess the potential for using these methods to predict their properties and develop detoxification agents . To achieve this goal, the following objectives were formulated: to examine the biochemical mechanisms of organophosphorus action, to analyze the principles of QSAR modeling and machine learning methods, and to determine the role of molecular modeling in studying the interactions of these compounds with biological targets.

The biological action of organophosphorus compounds is due to their ability to inhibit acetylcholinesterase, an enzyme that plays a key role in the regulation of cholinergic transmission. Normally, acetylcholinesterase ensures the rapid hydrolysis of acetylcholine in the synaptic cleft, which is necessary to terminate the transmission of nerve impulses [2].

Organophosphorus compounds interact with the enzyme's active site, which contains a serine residue, forming a covalent bond with its hydroxyl group. This process involves several sequential steps: the initial formation of a reversible enzyme-inhibitor complex, subsequent phosphorylation of the active site, and stabilization of the resulting complex.

Of particular importance is the so-called "aging" of the phosphorylated enzyme, which involves the cleavage of alkyl or alkoxyl groups from the phosphoryl residue. This results in the formation of a more stable chemical structure that is resistant to nucleophilic attack by reactivators , making inhibition virtually irreversible [2]. The rate of this process depends on the chemical structure of the organophosphorus compound and is a critical factor determining the effectiveness of therapy.

Inhibition of acetylcholinesterase leads to the accumulation of acetylcholine in synapses and, consequently, to hyperstimulation of both muscarinic and nicotinic cholinergic receptors. This is accompanied by the development of a characteristic cholinergic syndrome, including bronchospasm, glandular hypersecretion, seizures, and central nervous system disorders. Thus, the molecular mechanisms of organophosphate action are directly related to their toxicological effects and determine the direction of therapeutic interventions [4].

The application of artificial intelligence (AI) in the study of this work is based on the step-by-step processing and analysis of chemical information in order to predict their biological activity and toxicity [7].

The first stage involves representing molecules digitally using SMILES formats, molecular graphs, and a set of descriptors (hydrophobicity, electronic, and steric parameters). This allows the chemical structure to be converted into a numerical form suitable for analysis [13].

The second stage involves data preparation, which includes selection of relevant descriptors, normalization, and formation of training samples based on experimental data (e.g., the degree of acetylcholinesterase inhibition).

The third stage involves building machine learning models. Regression algorithms are used for quantitative prediction, and classification methods are used for toxicity assessment. For more

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complex tasks, neural networks are used, including graph models that take molecular topology into account [15].

At the fourth stage, model validation is carried out [13] , which includes checking the accuracy, robustness, and range of applicability. This is critical to ensuring the reliability of predictions [13].

The final stage is the application of models, including prediction of the properties of new compounds, virtual screening and selection of promising structures for further molecular modeling (docking , molecular dynamics) and development of antidotes.

Our next step in this mechanism involves molecular modulation, which is key in the study of organophosphorus compounds, providing a transition from statistical prediction to a detailed analysis of interaction mechanisms at the molecular level. Unlike traditional approaches, modern computational methods allow us not only to assess the probability of binding of compounds to biological targets but also to interpret the nature of these interactions [6].

The modeling process involves sequentially determining the spatial configuration of the ligand – enzyme complex, assessing the energetic characteristics of the interaction, and analyzing the system's stability over time. During the molecular docking stage , the most probable orientation of the organophosphorus compound in the active site of acetylcholinesterase is determined , after which the binding energy, reflecting the stability of the complex, is calculated. Further clarification of the mechanism is achieved using molecular dynamics, which allows for the consideration of conformational changes in the protein and ligand under conditions close to physiological ones [9].

Integrating artificial intelligence methods with molecular modeling significantly improves computational accuracy and efficiency. Machine learning algorithms are used to optimize scoring functions, select the most probable conformations, and reduce the search space. Contemporary research demonstrates a shift from static models to dynamic systems, in which AI is capable of accounting for temporal aspects of interactions [8].

The development of effective antidotes to organophosphorus compounds is a complex interdisciplinary task requiring consideration of both chemical and biological factors [5]. Traditional methods for searching for reactivators Acetylcholinesterase tests are based on experimental screening, which significantly limits the speed of obtaining results. The introduction of artificial intelligence methods allows for a more rational and targeted approach [5].

In addressing the topic of organophosphate poisoning therapy, we will examine the modern antidote development process. This includes the creation of digital compound libraries, their preliminary analysis using QSAR models and machine learning algorithms, and the selection of the most promising structures based on predicted biological activity values. Next, pharmacokinetic and toxicological parameters are assessed, after which the selected compounds are subjected to molecular modeling to confirm the mechanism of interaction with acetylcholine [14].

The use of generative models, which enable the creation of new molecules with desired properties, is particularly important. Unlike classical approaches based on the modification of known structures, this method utilizes the principle of inverse design, with the desired biological effect as the starting point. This significantly expands the search space and increases the likelihood of discovering effective and selective reactivators.

Modern research in the field of organophosphorus compounds demonstrates a shift in emphasis from experimentally-oriented toxicology to computational prediction methods based on artificial

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intelligence and the integration of ADMET parameters. This approach is particularly important for organophosphorus compounds , as these compounds are characterized by high biological activity, pronounced reactivity with acetylcholinesterase , and a significant range of toxicological profiles depending on their structural modifications.

Modern research has established that [11] the toxicity of organophosphorus compounds is directly determined by their ability to phosphorylate the active site of acetylcholinesterase , as well as the stability of the resulting complex and the rate of the aging process. These parameters, being difficult to reproduce experimentally, are increasingly becoming the subject of computational modeling using machine learning methods [11].

The toxicity assessment process in modern studies is implemented through a sequential analysis: generating structural descriptors of organophosphorus compounds, constructing training sets based on known LD_{50} and IC_{50} values, and using machine learning algorithms to predict biological activity. Ensemble methods and neural network architectures, capable of accounting for nonlinear relationships between the electronic characteristics of the phosphoryl group and the degree of enzyme inhibition, are considered the most effective.

Of particular importance is the integration of QSAR models with ADMET analysis [10], which allows for the simultaneous assessment of the toxicity and pharmacokinetic behavior of compounds. This is critical for organophosphorus compounds, as their penetration through biological membranes, tissue distribution, and metabolic stability significantly influence the severity of their toxic effects. Current research shows that hybrid models combining quantum chemical calculations and machine learning methods provide a more accurate description of the reactivity of the phosphoryl center and the processes of interaction with biological targets [10].

An additional important area of research is identifying the structural fragments responsible for the toxicity of organophosphorus compounds. Modern interpretable machine learning models allow us to isolate the contribution of individual substituents in the organophosphorus structure, facilitating a deeper understanding of the structure-toxicity mechanism. This forms the basis for the targeted design of less hazardous analogs and potential antidotes.

In the field of organophosphorus compound detection, there is active development of intelligent sensor systems, biochemical detection methods, and artificial intelligence algorithms for signal processing. Traditional analytical methods, such as gas and liquid chromatography, mass spectrometry, and electrochemical sensors, are being supplemented in modern research with machine learning methods, significantly increasing the accuracy and speed of analysis [10].

acetylcholinesterase- based biosensors, where the degree of enzyme inhibition serves as the analytical signal [3].

Modern research demonstrates that the use of classification algorithms can significantly improve the interpretation of received signals, especially in conditions of low concentrations of toxic substances and high noise levels. Particular attention is paid to the analysis of spectral data (IR spectroscopy, mass spectrometry), where machine learning methods are used to reveal hidden patterns and automatically identify compounds. Modern models are capable of not only recognizing known organophosphorus compounds but also classifying previously uncharacterized substances based on their spectral properties, reflecting the transition to next-generation intelligent detection systems [15].

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Recent research is also actively developing the concept of distributed sensor networks, in which data from multiple sensors is processed in real time using AI algorithms. This approach makes it possible to create early warning systems capable of detecting even minimal concentrations of toxic substances in the environment.

The study of organophosphorus compounds is being significantly transformed today by the introduction of artificial intelligence methods. While analysis was previously based primarily on experimental toxicology and biochemistry, today there is a shift toward predictive computational models.

The high toxicity of these compounds is associated with their ability to phosphorylate acetylcholinesterase and the subsequent process of "aging" of the complex, which makes inhibition virtually irreversible. The complexity of these mechanisms necessitates the use of AI for the analysis of structure-activity-toxicity relationships [4].

The scientific novelty lies in the integration of QSAR, machine learning, ADMET analysis, and molecular modeling into a unified system for studying organophosphorus toxicants . AI serves not only as a predictive tool but also as a means of identifying hidden patterns of their action [7].

Thus, the combination of classical approaches with AI creates a new research paradigm that improves the accuracy of predictions and the efficiency of antidote searches.

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