Tulepbayeva Gaukhar Kudabayevna – Master, Department of languages and literature, Central Asian Innovation University, Republic of Kazakhstan, 160031, Shymkent, tel.: +77025588294, e-mail: tulepbaevagauhar25@gmail.com.

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APPLICATION OF ADMETlab-3.0 FOR PREDICTION OF PHARMACOKINETICS AND TOXICITY OF CHEMICAL COMPOUNDS IN THE EDUCATIONAL PROCESS

Yergaliyeva E.M. – PhD, Assistant Professor of the Department of natural science disciplines, Akhmet Baitursynuly Kostanay Regional University, Kostanay, Republic of Kazakhstan.*

Khamit A.Zh. – 2nd year Master's student of the Department of natural science disciplines, Akhmet Baitursynuly Kostanay Regional University, Kostanay, Republic of Kazakhstan.

Zakiriyanova G.Zh. – 2nd year Master's student of the Department of natural science disciplines, Akhmet Baitursynuly Kostanay Regional University, Kostanay, Republic of Kazakhstan.

Kolbayeva Zh.Zh. – 2nd year Master's student of the Department of natural science disciplines, Akhmet Baitursynuly Kostanay Regional University, Kostanay, Republic of Kazakhstan.

In the modern conditions of development of pharmaceutical chemistry and computer modeling, the most important task is to assess the pharmacokinetic and toxicological properties of chemical compounds at the early stages of their development. This article discusses the use of the ADMETlab-3.0 tool in the educational process of bachelor's and master's chemistry students to predict the key ADME parameters (absorption, distribution, metabolism, excretion) and toxicity of potential drug molecules.

The aim of the study is to analyze the effectiveness of using ADMETlab-3.0 in teaching bachelor's and master's students, as well as to assess its role in the formation of practical skills in working with computer modeling tools. The objectives include developing a practical guide for students on the use of the platform, testing its capabilities and analyzing the impact on the educational process.

Research methods include computer modeling, analysis of predicted ADME/Tox parameters, student surveys and studying their satisfaction with training. A step-by-step guide to working with the platform, sample tasks, and recommendations for integrating ADMETlab-3.0 into educational programs are presented.

The results showed that the use of ADMETlab-3.0 contributes to the development of analytical skills, data interpretation, and critical thinking in students. The questionnaire confirmed a high level of satisfaction, but revealed the need for additional structured materials.

The theoretical significance of the study lies in demonstrating the capabilities of digital tools in education, and the practical significance lies in developing a methodology for integrating them into the educational process. ADMETlab-3.0 is a powerful tool that simplifies the assessment of the pharmacokinetic properties of compounds and facilitates the training of specialists in the field of computational chemistry.

Key words: *ADMETlab-3.0, pharmacokinetics, toxicity, ADME, computational chemistry.*

БІЛІМ БЕРУ ПРОЦЕСІНДЕ ХИМИЯЛЫҚ ҚОСЫЛЫСТАРДЫҢ ФАРМАКОКИНЕТИКАСЫ МЕН УЫТТЫЛЫҒЫН БОЛЖАУ ҮШІН ADMETlab-3.0 ҚОЛДАНУ

Ергалиева Э.М. – PhD, жаратылыстану-ғылыми пәндері кафедрасы профессорының ассистенті, Ахмет Байтұрсынұлы атындағы ҚӨУ Қостанай қ, Қазақстан Республикасы.*

Хамит А.Ж. – Ахмет Байтұрсынұлы атындағы ҚӨУ жаратылыстану-ғылыми пәндері кафедрасының 2-курс магистранты, Қостанай қ, Қазақстан Республикасы.

Закириянова Г.З. – Ахмет Байтұрсынұлы атындағы ҚӨУ жаратылыстану-ғылыми пәндері кафедрасының 2-курс магистранты, Қостанай қ, Қазақстан Республикасы.

Көлбаева Ж.Ж. – Ахмет Байтұрсынұлы атындағы ҚӨУ жаратылыстану-ғылыми пәндері кафедрасының 2-курс магистранты, Қостанай қ, Қазақстан Республикасы.

Фармацевтикалық химия мен компьютерлік моделдеуді дамытудың қазіргі жағдайларында химиялық қосылыстарды әзірлеудің бастапқы кезеңдерінде олардың фармакокинетикалық және токсикологиялық қасиеттерін бағалау аса маңызды міндет болып табылады. Бұл мақалада ADME негізгі параметрлерін (абсорбция, бөлу, метаболизм, экскреция) және дәрілік молекулалардың уыттылығын болжау үшін студенттер мен магистрант-химиктердің білім беру процесінде ADMETlab-3.0 құралын қолдану қарастырылады.

Зерттеудің мақсаты студенттер мен магистранттарды оқытуда ADMETlab-3.0 пайдалану тиімділігін талдау, сондай-ақ оның компьютерлік модельдеу құралдарымен жұмыс істеудің

практикалық дағдыларын қалыптастырудағы рөлін бағалау болып табылады. Міндеттерге студенттер үшін платформаны пайдалану бойынша практикалық нұсқаулықты әзірлеу, оның мүмкіндіктерін тестілеу және білім беру процесіне әсерін талдау кіреді.

Зерттеу әдістері компьютерлік моделдеуді, ADME/Tox болжамды параметрлерін талдауды, студенттердің сауалнамаларын және олардың оқуға қанағаттанушылығын зерделеуді қамтиды. Платформамен жұмыс істеу бойынша қадамдық нұсқаулық, ADMETlab-3.0 білім беру бағдарламаларына ықпалдастыру бойынша тапсырмалар мен ұсынымдардың үлгілері ұсынылды.

Нәтижелер ADMETlab-3.0 пайдалану студенттердің аналитикалық дағдыларын дамытуға, деректерді түсіндіруге және сыни ойлауды дамытуға ықпал ететінін көрсетті. Сауалнама қанағаттанудың жоғары деңгейін растады, бірақ қосымша құрылымдалған материалдарға қажеттілікті анықтады.

Зерттеудің теориялық маңыздылығы білім беруде цифрлық құралдардың мүмкіндіктерін көрсетуден, ал практикалық маңыздылығы – оларды оқу процесіне ықпалдастыру әдістемесін әзірлеуден тұрады. ADMETlab-3.0 қосылыстардың фармакокинетикалық қасиеттерін бағалауды жеңілдететін және компьютерлік химия саласындағы мамандарды даярлауға ықпал ететін қуатты құрал болып табылады.

Түйінді сөздер: *ADMETlab-3.0, фармакокинетика, уыттылық, ADME, компьютерлік химия.*

ПРИМЕНЕНИЕ ADMETlab-3.0 ДЛЯ ПРОГНОЗИРОВАНИЯ ФАРМАКОКИНЕТИКИ И ТОКСИЧНОСТИ ХИМИЧЕСКИХ СОЕДИНЕНИЙ В ОБРАЗОВАТЕЛЬНОМ ПРОЦЕССЕ

Ергалиева Э.М. – PhD, ассистент профессора кафедры естественно-научных дисциплин, НАО «КРУ имени Ахмет Байтұрсынұлы», г. Костанай, Республика Казахстан.*

Хамит А.Ж. – магистрант 2 курса кафедры естественно-научных дисциплин, НАО «КРУ имени Ахмет Байтұрсынұлы», г. Костанай, Республика Казахстан.

Закириянова Г.З. – магистрант 2 курса кафедры естественно-научных дисциплин, НАО «КРУ имени Ахмет Байтұрсынұлы», г. Костанай, Республика Казахстан.

Кольбаева Ж.Ж. – магистрант 2 курса кафедры естественно-научных дисциплин, НАО «КРУ имени Ахмет Байтұрсынұлы», г. Костанай, Республика Казахстан.

В современных условиях развития фармацевтической химии и компьютерного моделирования важнейшей задачей является оценка фармакокинетических и токсикологических свойств химических соединений на ранних этапах их разработки. В данной статье рассматривается применение инструмента ADMETlab-3.0 в образовательном процессе студентов и магистрантов-химиков для прогнозирования ключевых параметров ADME (абсорбция, распределение, метаболизм, экскреция) и токсичности потенциальных лекарственных молекул.

Целью исследования является анализ эффективности использования ADMETlab-3.0 в обучении студентов и магистрантов, а также оценка его роли в формировании практических навыков работы с инструментами компьютерного моделирования. Задачи включают разработку практического руководства для студентов по использованию платформы, тестирование ее возможностей и анализ влияния на образовательный процесс.

Методы исследования включают компьютерное моделирование, анализ прогнозируемых параметров ADME/Tox, анкетирование студентов и изучение их удовлетворенности обучением. Представлено пошаговое руководство по работе с платформой, примеры заданий и рекомендации по интеграции ADMETlab-3.0 в учебные программы.

Результаты показали, что применение ADMETlab-3.0 способствует развитию аналитических навыков, интерпретации данных и развитию критического мышления у студентов. Анкетирование подтвердило высокий уровень удовлетворенности, но выявило потребность в дополнительных структурированных материалах.

Теоретическая значимость исследования заключается в демонстрации возможностей цифровых инструментов в образовании, а практическая значимость – в разработке методики их интеграции в учебный процесс. ADMETlab-3.0 является мощным инструментом, который упрощает оценку фармакокинетических свойств соединений и способствует подготовке специалистов в области компьютерной химии.

Ключевые слова: *ADMETlab-3.0, фармакокинетика, токсичность, ADME, компьютерная химия.*

Introduction. The search for new compounds with medicinal properties is a complex, multi-stage process that requires a deep understanding of the interaction of chemical compounds with biological systems. One of the key aspects of this process is the study of the pharmacokinetic properties of substances that determine their behavior in the body. Pharmacokinetics describes four main stages of the drug life cycle:

absorption, distribution, metabolism, and excretion, united by the acronym ADME [1, p. 1; 2, p. 1]. These processes directly affect the efficacy, safety, and ease of use of drugs.

Contemporary computational techniques in chemistry and molecular design enable precise evaluation and prediction of pharmacokinetic characteristics at the initial stages of drug development. *In silico* methods enable students to study ADME properties of potential drug compounds, avoiding expensive and time-consuming experiments [3, p. 2; 4, p. 1760; 5, p. 6477].

Modern computer modeling tools, such as ADMETlab-3.0 [6], significantly simplify the study of pharmacokinetic properties and make it accessible to bachelor's and master's students. ADMETlab-3.0 is an advanced online platform that allows predicting ADME properties and toxicological characteristics (T – Toxicity) of chemical compounds based on machine learning data and large databases of experimental studies. This tool provides users with the ability to assess bioavailability, permeability through the blood-brain barrier, potential hepatotoxicity and other key parameters necessary for early assessment of the prospects of new molecules.

For bachelor's and master's students, working with ADMETlab-3.0 becomes an important step in mastering modern approaches to drug development, facilitating the practical application of their theoretical expertise and prepare for real tasks when performing scientific research. Such skills allow future specialists not only to better understand the mechanisms of action of biologically active compounds, but also to actively participate in the creation of innovative solutions.

The aim of this article is to demonstrate the possibilities of using the ADMETlab-3.0 online platform in the educational process for bachelor's and master's students in chemistry. Special emphasis is placed on teaching methods for evaluating ADME and toxicological properties, as well as incorporating this tool into project-based and research-oriented learning.

The objectives of the study include:

1. Developing a step-by-step guide to using ADMETlab-3.0 to analyze chemical compounds.
2. Creating practical tasks aimed at mastering the methods of predicting ADME/Tox parameters.
3. Evaluating the effectiveness of using ADMETlab-3.0 in the educational and project activities of students through a questionnaire.
4. Formulating recommendations for teachers and students to improve teaching methods using the platform.

Below is a brief overview of the platform and examples of its use in the scientific literature. ADMETlab-3.0 is a tool developed using advanced machine learning and big data methods and is an important resource for researchers involved in drug development [7, p. 424]. It allows for prediction of ADME properties, including: Absorption (oral bioavailability, intestinal permeability); Distribution (plasma protein binding, blood-brain barrier permeability); Metabolism (participation of cytochrome P450 isoenzymes); Excretion (renal or hepatic clearance).

The tool calculates key physicochemical parameters such as lipophilicity and solubility, which helps to assess the compliance of compounds with Lipinsky's "rule of five" [8, p. 3]. Toxicological analysis using this service includes prediction of toxicity (hepatotoxicity, cardiotoxicity, mutagenicity and other parameters), as well as assessment of the risks of drug interactions and side effects.

The user interface provides the ability to load SMILES formulas or SDF files for simultaneous analysis of multiple molecules. The platform allows users to visualize results in tables and diagrams, which can be further processed using external software if needed.

The advantages of ADMETlab-3.0 include: high accuracy of predictions due to the use of machine learning and a database containing millions of experimental values; a comprehensive approach: which covers all key aspects of ADME and toxicology, which allows for a complete understanding of the properties of the molecule; ease of use, which makes the service accessible to bachelor's, master's students and professionals; the ability to analyze both individual molecules and large data sets (high-throughput screening) and, finally, free access: the platform is available online without the need to install software.

The accuracy of predictions depends on the presence of similar structures in the database, which may reduce reliability for new or atypical molecules [9, p. 5]. Like other *in silico* tools, ADMETlab-3.0 provides only preliminary predictions that require confirmation by *in vitro* or *in vivo* studies.

One of the key stages of drug development is the selection of promising compounds with a high probability of successfully passing clinical trials, which is performed using early assessment of the “drug-likeness” of molecules. ADMETlab-3.0 is widely used for evaluating drug potential and for the initial screening of compounds, as confirmed by studies [10, p. 220; 11, p. 3; 12, p. 152]. The platform is also effective for optimizing pharmacokinetic parameters [13, p. 19]. An important function is the early detection of toxicological risks, as demonstrated in studies [14, p. 5; 15, p. 4], in which the predictions made it possible to identify the safest candidates and minimize risks in the preclinical stages.

ADMETlab-3.0 proves to be a versatile tool for early-stage drug discovery, offering reliable predictions that save time and resources while reducing clinical trial risks. By providing rapid and accurate predictions, this tool streamlines the drug discovery process. Its use contributes to a more efficient selection of promising compounds and a reduction in the risk of clinical failure. Compared to other freely available ADME prediction

tools such as SwissADME and pkCSM, ADMETlab-3.0 provides a broader range of parameters and a more intuitive interface suitable for educational purposes. While SwissADME focuses primarily on physicochemical and drug-likeness evaluation, and pkCSM predicts toxicity using graph-based signatures, ADMETlab-3.0 combines both approaches, making it more comprehensive for student research projects.

Some studies acknowledge that free online tools like ADMET-lab-3.0, SwissADME, and similar platforms are available and potentially useful for teaching medicinal chemistry, allowing students to predict ADMET properties without expensive software [16, p. 776, Section 2.2]. However, there is a gap in the literature regarding the systematic evaluation of these tools in pedagogical studies measuring learning outcomes, student engagement, or pedagogical effectiveness. This opens significant opportunities for future research.

Materials and methods. The study materials include the use of the ADMETlab-3.0 online platform for predicting ADME properties of chemical compounds based on machine learning data. The ChemSketch chemical editor [17] was used to prepare molecular structures, as well as the PubChem [18] and ChemSpider [19] databases to select the molecules to be studied. Well-known medicinal compounds such as caffeine, aspirin, and ibuprofen were considered as examples of analysis, which allowed students to work with real problems and interpret the obtained parameters.

The research methods included the development of tasks for students, including the preparation of molecular structures, loading data into ADMETlab-3.0, interpreting and analyzing the prediction results. The effectiveness of the platform was assessed using a questionnaire among 15 bachelor's and master's students of the “6B01504–Chemistry” and “7M01503–Chemistry” educational programs, where their satisfaction with project activities, the level of mastering the program, and suggestions for improving the teaching methods were analyzed.

GraphPad Prism 8 and MS Excel were used to calculate descriptive statistics (means and standard deviations). Correlation analysis was performed using the Pearson correlation coefficient with a 95% confidence interval. Statistical significance was established at $p < 0.05$.

Results. Step-by-step guide to working with ADMETlab-3.0. The first step is to select the molecules to be studied and prepare their molecular structures in a suitable format. The choice of molecules depends on the specific task – for example, these can be compounds isolated from natural sources, synthesized in the laboratory, or taken from chemical databases such as PubChem or ChemSpider. It is important to consider that the molecules must be representative of the class of compounds being studied and have enough data for correct prediction.

After selecting the molecules, it is necessary to prepare their molecular structures in a format supported by ADMETlab-3.0. The most common formats are SMILES (Simplified Molecular Input Line Entry System) and SDF (Structure Data File). SMILES are textual representations of molecular structures that can be easily created using chemical editors such as ChemSketch or online tools. SDF files contain more detailed information, including atomic coordinates and bonds, and can be exported from molecular modeling programs such as PyMOL [20] or Avogadro [21, p. 17]. Before uploading, make sure that the files are correctly formatted and free of errors, as this may affect the accuracy of the predictions.

At the second step you need to go to the official website of the platform (https://admetlab3.scbdd.com/). Registration is not required to perform the analysis and receive the results. In the *Services* menu, you need to select *ADMET Evaluation* or *ADMET Screening*. The *ADMET Evaluation* item is intended for the analysis of individual molecules, while *ADMET Screening* is used for high-throughput screening of large data sets, which allows you to evaluate many compounds simultaneously.

Upload prepared files with molecular structures in SMILES or SDF format via the upload window (Figure 1). To load a molecule as a file, select *Draw Molecule*, then the *Properties* icon and *Open from File* icon. After downloading, click *Submit*.

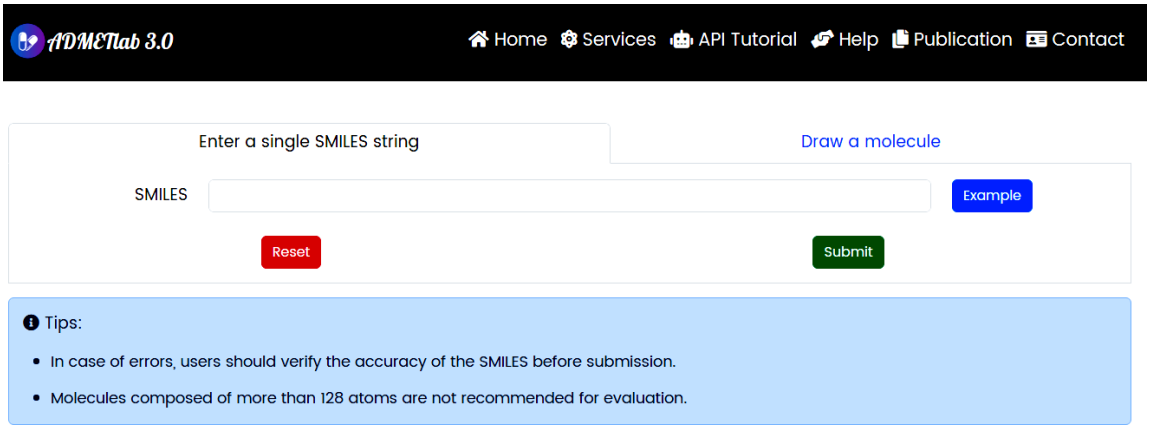

Figure 1 – Screenshot of the ADMETlab-3.0 structure loading window

The platform will process the information and provide the results in the form of tables that can be used for further study and interpretation.

The prediction results window in ADMETlab-3.0 provides detailed information about the properties of the loaded molecules, including bioavailability, toxicity, and other ADME parameters (Figure 2). Users can export the results in various formats (e.g., CSV or PDF) for further study or reporting. The description of the presented characteristics and units of measurement pop up in a tooltip when hovering over the information symbol.

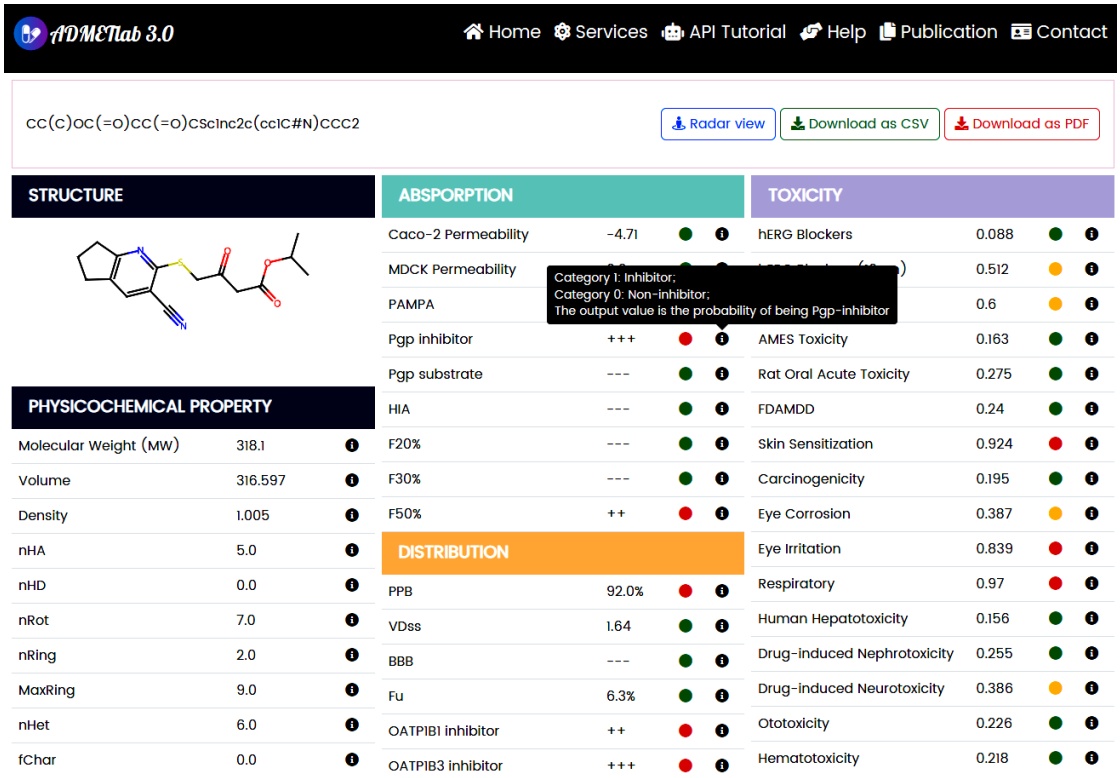

Figure 2 – ADMETlab-3.0 forecasting results

The results of the compound bioavailability prediction can also be presented as a radar diagram (Figure 3). In this diagram, the upper limits of the property values empirically determined for drug compounds are shown as blue dots, the lower limits are green, and the properties of the compound under study are yellow. Thus, if all the dots lie within the purple highlighted area, the compound can be determined as drug-like. To get the radar diagram, click *Radar View.*

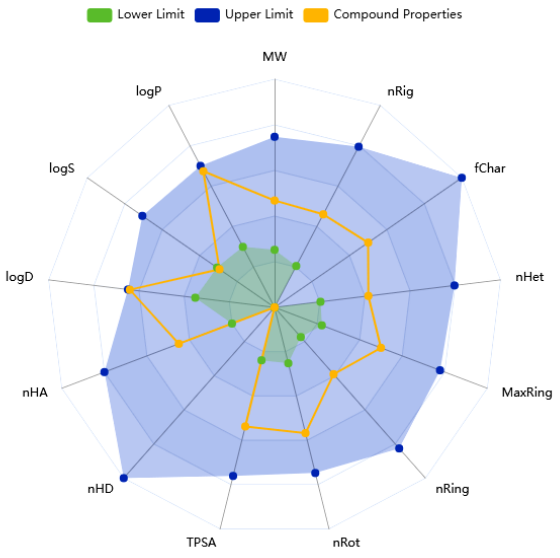

Figure 3 – Radar diagram of the bioavailability of the predicted compound

The next important step in prediction is the interpretation of the results. ADMETlab-3.0 evaluates key pharmacokinetic and toxicological parameters such as lipophilicity (the ability of a compound to dissolve in lipids, which affects absorption and distribution in the body), water solubility (determines oral bioavailability), blood-brain barrier permeability (important for drugs intended to affect the central nervous system), as well as metabolic stability and potential toxicity.

To interpret the results, it is necessary to compare the obtained values with the acceptable ranges established for therapeutic compounds: for example, high lipophilicity can improve penetration through cell membranes, but increases the risk of accumulation in adipose tissue and toxicity. Solubility is analyzed in the context of the route of administration – low solubility can limit absorption in the gastrointestinal tract, which is critical for oral drugs. Permeability through the blood–brain barrier (BBB) is assessed on a scale where values above a certain threshold indicate the ability of the substance to reach the CNS, which is necessary for neurotropic drugs, but undesirable for agents acting peripherally [22, p. 18].

It is important to consider the interrelationships between parameters during the analysis: for example, good solubility and moderate lipophilicity can compensate for low permeability, while high plasma protein binding affects distribution and efficacy.

The results of ADMETlab-3.0 are compared with data from reference drugs or compounds with known properties to determine whether the molecule meets the requirements for further optimization or clinical trials. A key step is to identify parameters that fall outside the acceptable range, which requires modification of the chemical structure to improve the safety and efficacy profile.

The analysis of the results involves selecting the necessary data (if only certain parameters are analyzed), compiling summary tables (when the properties of several compounds are compared), interpreting key properties and their values. It is also necessary to pay attention to the units of measurement of the values presented.

ADMETlab-3.0 analyzes physicochemical and pharmacokinetic parameters using specific units of measurement, which requires detailed interpretation. For example, lipophilicity (logP) is measured in logarithmic units: logP = 1.35-1.8 is considered optimal for oral absorption and intestinal absorption. If logP exceeds 5.5, it may cause accumulation in adipose tissue, increasing the risk of toxicity [23].

Metabolic stability can be expressed through plasma clearance (CL_{plasma}, ml/min/kg), which determines the overall exposure of the drug and allows for the calculation of the required dosage. Empirical ranges of clearance: >15 ml/min/kg – high; 5–15 ml/min/kg – moderate; <5 ml/min/kg – low. High clearance indicates rapid elimination, which may limit the therapeutic effect without increasing the dose.

The half-life ($T_{1/2}$, hours) depends on clearance and volume of distribution. A short T1/2 (<1 hour) indicates rapid elimination, while a long $T_{1/2}$ (>8 hours) indicates slow elimination. These parameters help to evaluate the pharmacokinetics and optimize the dosage of the drug [24].

Acute toxicity is estimated by LD_{50} (mg/kg). In the program, LD_{50} is converted to a logarithmic scale: for example, LD_{50} = 500 mg/kg → $\log_{10} \approx 2.7$ (units: $-\log_{10}$[(mg/L)/(1000*MW)]). High toxicity requires caution, while moderate toxicity (LD_{50} = 300 mg/kg → $\log_{10} \approx 2.48$) is considered acceptable for many drugs [25].

Plasma protein binding (PPB, %) also affects pharmacokinetics: 90% binding means that only 10% of the molecules remain active in the blood, which may require an increase in dosage. For example, with 95% binding and low solubility (10 μg/ml), the drug may only be effective in high doses, which increases the risk of side effects [26].

Below are examples of tasks created for the purpose of teaching and using ADMETlab 3.0 in the classroom with chemistry students:

Task 1. Preparing molecules for analysis

Objective: Learn how to prepare molecular structures for loading into ADMETlab 3.0.

1. Using the chemistry editor, draw the structure of ibuprofen, caffeine, and aspirin.
2. Save the molecule in SMILES and SDF formats.
3. Check the structure for errors (e.g., incorrect valences).

Task 2. Loading data and analyzing prediction results.

Objective: To analyze physicochemical properties.

1. Load the molecules into ADMETlab 3.0.
2. Select parameters for analysis from the prediction results: lipophilicity, water solubility, BBB permeability. Interpret and conclude on the pharmacokinetic profile of the compounds.

Questions: Is caffeine suitable for oral use? Compare the solubility of caffeine with the solubility of ibuprofen and aspirin. How does this affect bioavailability?

Task 3. Interpretation of toxicological parameters

Objective: To assess the safety of the compound.

1. Load the aspirin molecule (SMILES: CC(=O)OC1=CC=CC=C1C(O)=O).
2. Analyze the prediction results: LD_{50}, hepatotoxicity, cardiotoxicity (hERG inhibition) and other toxicities.

Questions: What is the relationship between the structure of aspirin and its toxicity? Suggest a modification of the molecule to reduce toxicity

Task 4. ADMET-based structure optimization

Goal: Improve the pharmacokinetic profile.

1. Select a molecule with low solubility (e.g. LogP = 5.0, solubility = 5 μg/mL).

2. Modify the structure:

a) Add a hydroxyl group (-OH);

b) Replace the alkyl substituent with an amino group ($-NH_2$).

3. Reload the modified molecule in ADMETlab 3.0 and compare the parameters.

Question: How did the solubility and lipophilicity change? Why?

These tasks can be varied using different chemical structures from databases. Also, when completing tasks, students are divided into groups and present the results in the form of projects. Group discussions are organized during the defense of the projects.

Recommendations for the use of ADMETlab-3.0 in teaching bachelor's and master's students in chemistry.

The integration of ADMETlab-3.0 into the educational process is based on combining theoretical knowledge with practical tasks. Effective mastery of the tool begins with an exploration of theoretical concepts that explain the foundational principles of ADMET forecasting and parameter interpretation. For instance, during class or as part of independent study, students can be assigned tasks to examine key metrics such as logP, solubility, and blood-brain barrier (BBB) permeability using real-world examples of drug molecules like paracetamol and ibuprofen. Emphasis should be placed on the relationship between the chemical properties of compounds and their bioavailability, toxicity, or metabolism.

Project examples and research tasks can range from simple to advanced. A basic project might involve analyzing known drugs from databases such as ChemPub, followed by comparing the calculated ADMET parameters with literature data. More complex assignments could include optimizing hypothetical molecules, such as modifying the structure of a neurotropic drug to enhance BBB permeability or reduce hepatotoxicity. Master's students can investigate the impact of substituents on metabolic stability by examining a series of derivatives of a single compound. For advanced research projects, tasks related to computer-aided drug design can be proposed, with ADMETlab-3.0 serving as a virtual screening stage prior to molecular docking.

By incorporating these approaches, students gain hands-on experience while deepening their understanding of the interplay between chemical properties and biological effects. This methodological framework ensures a comprehensive learning experience that bridges theory and practice.

Examples of master's theses topics where ADMET analysis was used:

1. Application of molecular docking to search for promising compounds – GSK-3 inhibitors.

2. Quantum-chemical calculations of the electronic structure and theoretical study of the properties of new compounds based on N-benzoylpiperidine.

3. Modeling of the electronic structure and computer prediction of the pharmacological properties of new compounds based on 1,3,5-triazines and their complex salts.

4. Quantum-chemical study of the electronic structure and computer prediction of the spectrum of biological activity of di- and tetraazabicyclononan-9-ones.

The results of the completed project work are being prepared for publication and will become part of master's theses.

The assessment criteria for the results include the ability to work with different data formats and interpret graphical reports. Another assessment criterion may be the creativity of solutions when optimizing structures, for example, adding polar groups to reduce toxicity. For projects, it is useful to use peer assessment: students present their findings and ask each other questions. Bachelor's and master's students must relate numerical values of parameters to biological effects: for example, explain why high lipophilicity worsens solubility but increases membrane penetration., conducting a discussion. At the same time, it develops critical thinking and argumentation skills.

In order to analyze the effectiveness of using ADMETlab-3.0 in students' project work, a survey was conducted, in which 15 bachelor's and master's students took part. Table 1 contains the results of statistical processing of students' responses.

Table 1 – Statistical indicators of the survey results to assess the use of ADMETlab-3.0 (N=15)

№	Evaluation Parameter	Mean (M)	Standard Deviation (SD)
1	Satisfaction with project work	3.80	1.15
2	Ease of mastering functions	3.67	0.82
3	Help in understanding tasks	3.73	1.16
4	Level of teacher support	3.67	1.05
5	Contribution to skills development	3.93	0.70
6	Usefulness of the interface	3.47	0.99

Continuation of Table 1

7	Quality of educational materials	3.53	0.99
8	Alignment with research needs	3.67	0.98
9	Presence of technical issues*	3.33	0.72

* For item 9, the scale is inverted

Survey results indicate high student satisfaction (over 80%), confirming the platform's ease of use and educational potential. The highest average scores were obtained for questions regarding the platform's contribution to skill development (M=3.93) and satisfaction with project work (M=3.80). The lowest average score, as expected, was obtained for the question regarding technical problems (M=3.33). Low standard deviations (mostly below 1.0) indicate a relatively homogeneous group of opinions; that is, students were generally unanimous in their assessments.

To identify relationships between various aspects of ADMETlab-3.0 use, a correlation analysis was conducted using the Pearson correlation coefficient (r). The results are presented in Table 2.

Table 2 – Correlation matrix between key parameters of the questionnaire

Item	Satisfaction (1)	Ease of mastering functions (2)	Level of teacher support (4)	Quality of educational materials (7)
Satisfaction (1)	1	0.84 ***	0.95 ***	0.92 ***
Ease of mastering functions (2)	0.84 ***	1	0.86 ***	0.94 ***
Level of teacher support (4)	0.95 ***	0.86 ***	1	0.94 ***
Quality of educational materials (7)	0.92 ***	0.94 ***	0.94 ***	1

*Note: ***$p < 0.001$

Correlation analysis revealed multiple statistically significant relationships between various aspects of ADMETlab-3.0 use. The strongest positive correlations were observed between satisfaction with project work and assistance in understanding tasks ($r = 0.975$, $p < 0.001$), as well as between interface usefulness and the quality of training materials ($r = 0.966$, $p < 0.001$).

The responses to the open-ended question (What would you change or add in the methodological materials offered to you on the use of ADMETlab-3.0 in project activities?) were summarized and presented below:

1. Add more examples of use for specific chemical problems.
2. Develop step-by-step instructions for completing projects so that students could master the program independently.
3. Develop additional materials for independent study of the program, such as video tutorials or interactive guides.

Discussion. The study aimed to analyze the effectiveness of the ADMETlab-3.0 platform in the educational process of chemistry students. The survey results (Table 1) indicate high student satisfaction with the platform's use in project-based activities. The highest average score (M = 3.93) was assigned to the "Contribution to skills development" parameter, which directly aligns with the primary goal of the study—the development of practical competencies in computer modeling.

The relatively low score assigned to the "Presence of technical issues" parameter (M = 3.33) confirms the stability and reliability of the platform, which is a key factor for its successful use in the classroom. Relatively low standard deviations (mostly < 1.0) indicate consensus among respondents, reinforcing the reliability of these findings. Correlation analysis (Table 2) revealed statistically significant strong relationships between key learning aspects. The strongest correlations were found between "Satisfaction with project work" (1) and "Level of teacher support" (4) ($r = 0.95$, $p < 0.001$), as well as between "Quality of learning materials" (7) and "Ease of learning" (2) ($r = 0.94$, $p < 0.001$). Successful implementation depends on two key factors: 1) the active role of the teacher and 2) the availability of high-quality, structured teaching materials that, taken together, help students connect the tool's functionality to the solution of specific educational and research problems.

This conclusion is fully supported by the students' qualitative responses to the open-ended question. Requests for step-by-step instructions, additional examples, and video tutorials directly indicate the need for more in-depth methodological development of the course.

As noted above, there is a gap in the systematic pedagogical evaluation of free ADMET tools in education. This study makes a direct contribution to filling this gap.

The main limitations of this study are the relatively small sample size (N=15) and its location within a single university. It would be advisable to expand the scope of the study by including students from other

universities. A promising direction is also the development and testing of the same set of structured materials (video tutorials, interactive assignments), the need for which was identified during the survey. Furthermore, a comparative pedagogical study would be of interest, in which students would use not only ADMETlab-3.0 but also other platforms, such as SwissADME or pkCSM, to develop a more comprehensive understanding of the capabilities and limitations of modern in silico tools.

Thus, this study not only confirmed the high educational value of ADMETlab-3.0 but also allowed us to develop specific recommendations for its effective use, laying the foundation for further improvements in computational chemistry teaching methods.

Conclusion. The article explores the application of the ADMETlab-3.0 tool for studying the pharmacokinetic and toxicological properties of chemical compounds within the context of training bachelor's and master's students in chemistry. By integrating ADMETlab-3.0 into the educational process, students gain a unique opportunity to apply theoretical knowledge in practice, address contemporary scientific challenges, and prepare for real-world research. The platform's user-friendly interface, support for various data formats (SMILES, SDF), and visualization capabilities in the form of diagrams significantly simplify the analysis process.

A review of the literature highlights the necessity of structured materials, such as step-by-step instructions, task-specific examples, and video tutorials, to ensure successful mastery of the platform. These resources would enable students to quickly adapt to working with ADMETlab-3.0 and maximize its potential. Integrating the platform into curricula represents a crucial step in training highly qualified specialists capable of working at the intersection of chemistry, biology, and computer science. For master's students, incorporating ADMETlab-3.0 into research activities opens up opportunities for in-depth exploration of the pharmacokinetic properties of new compounds and optimization of their structures.

The practical tasks and example scenarios proposed in the article demonstrate how ADMETlab-3.0 can be effectively integrated into the educational process to solve real-world problems. Survey results indicate that most participants positively assessed the platform's use in project activities. However, students emphasized the need for additional educational materials and practical assignments to facilitate more effective learning. These findings underscore the importance of developing comprehensive resources to support students' mastery of the tool.

In conclusion, ADMETlab-3.0 plays a vital role in helping students understand the mechanisms of interaction between chemical compounds and biological systems. This understanding is a critical step in preparing specialists equipped with knowledge of computational chemistry tools. Future research should focus on developing pedagogical strategies for integrating ADMETlab-3.0 alongside other *in silico* tools such as SwissADME or pkCSM, enabling comparative learning experiences for students.

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Information about the authors:

Yergaliyeva Elmira Murzabayevna – PhD, Professor Assistant of the Department of natural science disciplines, Akhmet Baitursynuly Kostanay Regional University, Republic of Kazakhstan, 110000, Kostanay, 47 Baitursynov Str., tel.: +77478796175, e-mail: erg_el@mail.ru.*

Khamit Aizat Zhumabekkyzy – 2nd year Master's student, "7M01503-Chemistry" educational program, Akhmet Baitursynuly Kostanay Regional University, Republic of Kazakhstan, 110000, Kostanay, 47 Baitursynov Str., tel.: +77029961319, e-mail: aizat.khamit2003@mail.ru.

Zakiriyanova Guldana Bolatbekovna – 2nd year Master's student, "7M01503-Chemistry" educational program, Akhmet Baitursynuly Kostanay Regional University, Republic of Kazakhstan, 110000, Kostanay, 47 Baitursynov Str., tel.: +77075591780, e-mail: bolatbekovna76@gmail.com.

Kolbayeva Zhaina Zhanibekkyzy – 2nd year Master's student, "7M01503-Chemistry" educational program, Akhmet Baitursynuly Kostanay Regional University, Republic of Kazakhstan, 110000, Kostanay, 47 Baitursynov Str., tel.: +77775776656, e-mail: zhainakolbaeva@gmail.com.

Ергалиева Эльмира Мурзабаевна – PhD, жаратылыстану-ғылыми пәндері кафедрасы профессорының ассистенті, Ахмет Байтұрсынұлы атындағы Қостанай өңірлік университеті, Қазақстан Республикасы, 110000, Қостанай қ., Байтұрсынов көш. 47, тел.: +77478796175, e-mail: erg_el@mail.ru.*

Хамит Айзат Жумабеккызы – «7М01503-Химия» ББ-ның 2-курс магистранты, Ахмет Байтұрсынұлы атындағы Қостанай өңірлік университеті, Қазақстан Республикасы, 110000, Қостанай қ., Байтұрсынов көш. 47, тел.: +77029961319, e-mail: aizat.khamit2003@mail.ru.

Закириянова Гульдана Болатбековна – «7М01503-Химия» ББ-ның 2-курс магистранты, Ахмет Байтұрсынұлы атындағы Қостанай өңірлік университеті, Қазақстан Республикасы, 110000, Қостанай қ., Байтұрсынов көш. 47, тел.: +77075591780, e-mail: bolatbekovna76@gmail.com.

Кольбаева Жайна Жанибекқызы – «7М01503-Химия» ББ-ның 2-курс магистранты, Ахмет Байтұрсынұлы атындағы Қостанай өңірлік университеті, Қазақстан Республикасы, 110000, Қостанай қ., Байтұрсынов көш. 47, тел.: +77775776656, e-mail: zhainakolbaeva@gmail.com.

Ергалиева Эльмира Мурзабаевна – PhD, ассистент профессора кафедры естественно-научных дисциплин, Костанайский региональный университет имени Ахмет Байтұрсынұлы, Республика Казахстан, 110000, г. Костанай, ул. Байтурсынова 47, тел.: +77478796175, e-mail: erg_el@mail.ru.*

Хамит Айзат Жұмабекқызы – магистрант 2-го курса ОП «7М01503 – Химия», Костанайский региональный университет имени Ахмет Байтұрсынұлы, Республика Казахстан, 110000, г. Костанай, ул. Байтурсынова 47, тел.: +77029961319, e-mail: aizat.khamit2003@mail.ru.

Закириянова Гульдана Болатбековна – магистрант 2-го курса по ОП «7М01503 – Химия», Костанайский региональный университет имени Ахмет Байтұрсынұлы, Республика Казахстан, 110000, г. Костанай, ул. Байтурсынова 47, тел.: +77075591780, e-mail: bolatbekovna76@gmail.com.

Кольбаева Жайна Жанибекқызы – магистрант 2-го курса ОП «7М01503 – Химия», Костанайский региональный университет имени Ахмет Байтұрсынұлы, Республика Казахстан, 110000, г. Костанай, ул. Байтурсынова 47, тел.: +77775776656, e-mail: zhainakolbaeva@gmail.com.

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ИНФОРМАТИКА МҰҒАЛІМДЕРІН ДАЯРЛАУ ҮДЕРІСІНДЕ ЛОГИКАЛЫҚ ОЙЛАУДЫ ДАМЫТУ ҮШІН БЛОКТЫҚ БАҒДАРЛАМАЛАУДЫ ҚОЛДАНУДЫҢ ПЕДАГОГИКАЛЫҚ НЕГІЗДЕРІ

Есейқызы А. – PhD докторы, оқытушы-дәріскер, І.Жансүгіров атындағы Жетісу университеті, Талдықорған қ., Қазақстан Республикасы.

Кыдырбаева Г.Т. – педагогика ғылымдарының кандидаты, оқытушы-дәріскер, І.Жансүгіров атындағы Жетісу университеті, Талдықорған қ., Қазақстан Республикасы.*

Ермекова Н.С. – оқытушы-дәріскер, І.Жансүгіров атындағы Жетісу университеті, Талдықорған қ., Қазақстан Республикасы.

Есейқызы Ұ. – PhD докторанты, І.Жансүгіров атындағы Жетісу университеті, Талдықорған қ., Қазақстан Республикасы.

Бұл ғылыми мақала болашақ информатика мұғалімдерін даярлау контекстінде логикалық ойлау қабілетін дамытудың әдістемелік және педагогикалық негіздерін зерттеуге арналған. Зерттеудің өзектілігі ақпараттық-коммуникациялық технологиялардың (АКТ) қарқынды дамуы жағдайында мамандардың жүйелі және сыни ойлау дағдыларына қойылатын талаптардың артуымен негізделген, бұл өз кезегінде білім беру сапасын арттыруды талап етеді. Зерттеу барысында болашақ информатика мамандарын кәсіби даярлау үдерісінде блоктық бағдарламалауды (мысалы, Scratch, Blockly сияқты визуалды орталар) қолдану арқылы логикалық ойлауды қалыптастырудың тиімді механизмдері мен дидактикалық шарттары қарастырылады. Авторлар блоктық бағдарламалаудың күрделі алгоритмдік және абстрактілі ұғымдарды визуалды, интуитивті түрде меңгеруге мүмкіндік беретін жоғары дидактикалық әлеуетке ие құрал ретіндегі рөлін талдайды. Осы әдістемені қолдану оқытуды жекелендіруге және студенттердің оқуға деген ішкі уәжін арттыруға қосымша мүмкіндіктер беретіні көрсетілген. Нәтижелер блоктық бағдарламалау орталарын мақсатты түрде пайдалану болашақ мұғалімдердің алгоритмдік және дедуктивті ойлау қабілеттерін арттыруда, сондай-ақ пәндік біліктіліктерін нығайтуда айтарлықтай оң әсер ететінін көрсетеді. Сондай-ақ, бұл тәсіл олардың болашақ кәсіби қызметінде күрделі ақпараттық міндеттерді шешуге дайындығын қамтамасыз етеді. Ұсынылған педагогикалық негіздер информатика пәні бойынша жоғары оқу орындарындағы оқытудың мазмұнын жетілдіруге теориялық және практикалық үлес қосады. Мақала ғылыми-педагогикалық қауымдастыққа, докторанттарға және білім беруді цифрландыру мәселелерімен айналысатын мамандарға арналған.

Түйінді сөздер: *білім беру, оқыту, инновациялық технологиялар, блоктық бағдарламалау, логикалық ойлау.*

ПЕДАГОГИЧЕСКИЕ ОСНОВЫ ИСПОЛЬЗОВАНИЯ БЛОКОВОГО ПРОГРАММИРОВАНИЯ ДЛЯ РАЗВИТИЯ ЛОГИЧЕСКОГО МЫШЛЕНИЯ В ПРОЦЕССЕ ПОДГОТОВКИ УЧИТЕЛЕЙ ИНФОРМАТИКИ

Есейқызы А. – доктор PhD, преподаватель-лектор, Жетысуский университет имени И.Жансугурова, г. Талдыкорган, Республика Казахстан.

Кыдырбаева Г.Т. – кандидат педагогических наук, преподаватель-лектор, Жетысуский университет имени И. Жансугурова, г. Талдыкорган, Республика Казахстан.*

Ермекова Н.С. – преподаватель-лектор, Жетысуский университет имени И. Жансугурова,