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ADVANCES IN PHARMACEUTICAL CHEMISTRY: NOVEL DRUG DESIGN STRATEGIES AND CHEMICAL INNOVATIONS IN MODERN THERAPEUTICS

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Abstract

Advances in pharmaceutical chemistry have significantly transformed drug discovery through the integration of chemical innovation and computational methodologies. This study provides a comprehensive evaluation of contemporary drug design strategies, physicochemical properties, and therapeutic target distributions in modern therapeutics. A structured analysis was conducted on 50 therapeutically relevant drugs representing diverse therapeutic areas, including oncology, immunology, antiviral, and metabolic disorders. Drugs were categorized based on design strategies such as structure-based drug design (SBDD), biologics/immunotherapy, covalent inhibition, and prodrug approaches, while physicochemical parameters including molecular weight, lipophilicity (logP), and bioactivity (IC_{50}) were systematically assessed.The results demonstrate that biologics/immunotherapy (22%), kinase inhibitors (20%), and SBDD approaches (18%) constitute the predominant drug design strategies. Physicochemical analysis revealed that most small-molecule drugs fall within optimal ranges (molecular weight: 150–900 Da; mean 470 ± 130 Da; logP: mean 3.1 ± 1.0), indicating balanced drug-like properties. Bioactivity evaluation showed IC_{50} values ranging from 0.5 to 80 nM, with enhanced activity observed in compounds exhibiting moderate lipophilicity. Target analysis highlighted a strong focus on intracellular kinases (24%) and receptor tyrosine kinases (18%), followed by immune-related targets.Overall, the findings emphasize the interconnected role of drug design strategies, molecular properties, and target selection in shaping modern therapeutics. This study provides valuable insights into current trends and supports the development of more efficient and targeted drug discovery approaches.

Keywords: *Pharmaceutical chemistry; Drug design strategies; Structure-based drug design (SBDD); Lipophilicity (logP); IC_{50} bioactivity.*

1. Introduction

The discovery and development of modern therapeutics is mainly based on pharmaceutical chemistry, a field that combines the principles of chemistry, biology and computational science to produce useful and selective drug molecules. In the last 10 years, there has been a tremendous change in drug discovery faced with less trial and error method and more rational and mechanism based approach. It has been aided by the understanding of computational modeling, molecular biology, and chemical synthesis that allow the discovery and maximization of novel therapeutic agents with more favorable efficacy and safety profiles (Du et al., 2020; Ciccone & Nencetti, 2025).

Traditionally, the process of drug discovery was mainly based on chute and trial screening and chemical modifications. Nevertheless, the constraints witnessed with low retention rates, extended development cycles, and rising costs have forced the use of more effective and direct methods. Synthetic methodologies have been analyzed and have shown that reaction chemistry has not been advancing in pace with the growing complexity of drug targets, and highlights that new approaches should be employed in medicinal chemistry (Brown & Bostrom, 2016). In this regard, the combination of computerized tools and specialized chemical methods has been the key towards dealing with the difficulties relating to present day drug development.

SBDD and molecular docking have become instrumental approaches to rational drug discovery because they allow the study of the molecular facets of ligand-target interactions. The strategies enable the discovery of lead compounds and the optimization of binding affinity based on the extensive structural knowledge (Ferreira et al., 2015). Moreover, the fragment-based drug design has become one of the active approaches towards creating new chemical compounds by binding small fragments with biologically active properties into a strong effector (Najjar et al., 2019). The use of ultra-large virtual screening libraries has also increased the chemical space to be used in drug discovery enabling the discovery of new chemotypes that could have therapeutic uses (Lyu et al., 2019).

The recent developments in the field of artificial intelligence (AI) and machine learning (ML) have tremendously streamlined the drug discovery process. Deep learning has allowed creating novel molecular structures and making predictions of drug–target interaction with high precision, thus minimizing the use of traditional experimentation methods (Chen et al., 2018; Elton et al., 2019). Such generative models as diffusion-based or docking-integrated scaffolds have shown great potential in de novo drug design, by enabling exploration on complex chemistry spaces and discovery of optimized outputs (Alakhdar et al., 2024; Danel et al., 2023). The efficiency and accuracy of drug discovery processes have also been advanced by the AI-based consumer of the drug discovery process, which has helped in designing the next generation of therapeutics (Schneider, 2018; Mak et al., 2024; Wang et al., 2024).

Along with the development of computers, the importance of the physicochemical properties in drug design is vital. Molecular weight and lipophilicity are some of the parameters which have significant effect on the pharmacokinetic aspects of drugs including absorption, distribution, metabolism and excretion (ADME). The most famous guideline on drug-likeness assessment is the so-called Rule of Five, which states that physicochemical characteristics need to be optimized to obtain desirable pharmacokinetic outcomes (Lipinski, 2016). These properties should be balanced to facilitate the successful delivery of drugs and target engagement.

The second significant point of contemporary drug discovery is the strategy of drug design diversification. Natural product-inspired methods remain a great source of structurally diverse and biologically active compounds, which are used to develop new therapeutics (Gagare et al., 2024). The use of quantum mechanical-associated approaches has also been proposed to enhance the precision of molecular modeling and prediction of drug-target reactions to overcome the challenges of classical computational methods (Ginex et al., 2024). These breakthroughs emphasise the incorporation of multidisciplinary solutions in the pharmaceutical chemistry.

Although there has been a lot of development, there are still constraints in finding effective and accurate drug discovery strategies. Biological systems are complex and require a very precise form of interactions, which require ever more innovation in chemical and computational approaches. As the recent research has highlighted, the combination of various methods, such as AI and structure-based design, and experimental validation is crucial to increasing the

effectiveness of drug development (An et al., 2025; Niazi and Mariam, 2023). Moreover, phenotypic drug discovery remains supplementary in that it allows identifying compounds of therapeutic interest without prior information about a particular target (Moffat et al., 2017).

Considering such developments, there is an increasing need to comprehensively analyze the interaction among drug design approaches, physicochemical characteristics, and target identification in the contemporary therapeutics. Although many research works have been conducted to explain the individual part of drug discovery, there is limited literature that incorporates all these elements in a unified analysis. The knowledge of these relationships is crucial to determining the trends and future directions of research in pharmaceutical chemistry. Thus, the following research will attempt to deliver an organized insight into the current drug design plans, molecular characteristics and therapeutic target locations. This work aims to emphasize several important trends related to the contemporary drug discovery process by studying a wide range of therapeutically useful compounds, which are bound to add to the picture of chemical innovation in drug development.

2. Materials and Methods

2.1 Study Design

The current research was designed as an analytical investigation based on data to analyze the current therapeutic strategies of drug design, physicochemical properties, and target-specific distributions in modern therapeutics. They used a systematized analysis structure to investigate the differences between a number of parameters, such as drug design category, molecular features, and biological activity. The experiment was meant to give a holistic evaluation of trends that are related to pharmaceutical innovation, through the incorporation of chemical, biological and design related properties of the chosen therapeutic reagents

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2.2 Data Compilation and Selection Criteria

The selection of 50 therapeutically relevant drugs to be analyzed was done according to predefined inclusion criteria to provide a representation of various therapeutic areas. The criterion used in the selection was compounds that have well characterized molecular targets and physicochemical and bioactivity information. The inclusion criteria of the drugs were as follows: the presence of information on the target protein, the presence of the IC 50 value, available molecular descriptors (molecular weight and lipophilicity, or logP). Those compounds that did not have all the information required these parameters were eliminated to ensure the consistency and reliability of the analysis. The last group of drugs consisted of various classes of therapy such as oncology, immunology, antiviral therapy, and metabolic disorders.

2.3 Drug Design Strategy Classification

All drugs were logically divided into a certain design strategy according to its development mechanics and mode of action of functioning. The classification system comprised of structure-based drug design (SBDD), biologics/immunotherapy, covalent inhibitors, synthetic lethality-based methods, prodrug strategies, and kinase/selective ones. Other strategies which included peptide-based agents, hormone modulators and corrector/potentiator therapies were the groups to which other compounds that failed to fit under these main groups were included. It was classified based on the mechanistic features of individual drugs and, therefore, a similar classification process across the samples was made.

2.4 Physicochemical Parameter Assessment

The important physicochemical aspects were compared to describe the molecular characteristics of importance to drug behavior. The two descriptors chosen (molecular weight and lipophilicity logP) are known to be relevant in drug design and pharmacokinetics. Small-molecule drugs were taken into account in terms of their molecular weight whereas biologic agents did not belong to the set of biomolecules since they are macromolecules and cannot be described using standard terms. To determine the distribution of the compounds within the various permeability range, the lipophilicity values were examined. To compare the analysis, the values of lipophilicity were classified as low (02), moderate (24) and high (46). The parameters obtained were applied in assessing the trends in the molecular characteristics of the drugs under analysis.

2.5 Bioactivity Evaluation

The biological activity was determined by using the IC 50 values expressed in nanomolar (nM) per units which are the concentration needed to suppress 50% target activity. The inhibitory potency was determined in terms of IC_{50} with respect to particular molecular targets. The values obtained were processed to obtain the range of values, central tendency, and variability of bioactivity among the drugs analyzed. Such an

assessment allowed comparing the inhibitory activities of various drug design strategies and target classes.

2.6 Target Classification

The therapeutic targets were classified into groups of biological classes according to the biological functions of the therapeutic target in the disease pathways. These were categorized as receptor tyrosine kinases, intracellular kinases, immune checkpoint proteins Cytokines and immune-related targets, viral enzymes, DNA repair enzymes, hormonal targets, and others (CFTR and proteasome-associated proteins). This classification scheme enabled a systematic study of target distribution and enabled comparison cross-categorization of biologically relevant categories. Each drug was put in a target category depending on its overriding mechanism of action.

2.7 Statistical Analysis

The descriptive statistical analysis was conducted in order to summarize the characteristics of the drugs analyzed. The continuous variables were assessed in terms of the central tendency and dispersion, such as mean, standard deviation, median, the minimum, and maximum values. IC_{50} values were compared in the various physicochemical and categorical groupings to determine changes in bioactivity. Such a method made it possible to compare the molecular properties and an inhibitory activity of the various categories of drugs in a quantitative manner.

3. Results

3.1 Distribution of Drug Design Strategies

The analysis of drug design strategies indicated a wide and systematic coverage of the modern drug discovery methods. The key categories of analyzed drugs were found to be structure-based drug design (SBDD), biologics/immunotherapy and kinase/selective inhibition. According to Table 1, biologics and immunotherapeutic agents had the highest percentage (22%), then there was a 20 percent kinase/selective inhibitor, and 18 percent SBDD-derived compounds. The three groups combined formed a significant percentage of all the drugs that were analyzed.

Table 1. Distribution of Drug Design Strategies

Strategy Type	Number of Drugs	Percentage (%)
Structure-Based Drug Design (SBDD)	9	18%
Biologics / Immunotherapy	11	22%
Covalent Inhibitors	6	12%
Synthetic Lethality	3	6%
Prodrugs	5	10%
Kinase / Selective Inhibitors	10	20%
Other Strategies	6	12%
Total	50	100%

Covalent inhibitors constituted 12% of the drugs, which means that they are used in contemporary treatment procedures. The number of prodrugs approaches was 10% and synthetic lethality-based drugs were 6%. Other categories and additional strategies were also involved and contributed 12% and were categorized as peptide based agents, hormone modulators and as corrector/potentiator therapies.

Figure 1 shows the relative frequency of these strategies, with the number of each category being marked graphically. This shows that better groups include biologics/immunotherapy, kinase inhibitors and SBDD than other types of strategies. The synthetic lethality and prodrug strategies were found to have lower frequencies.

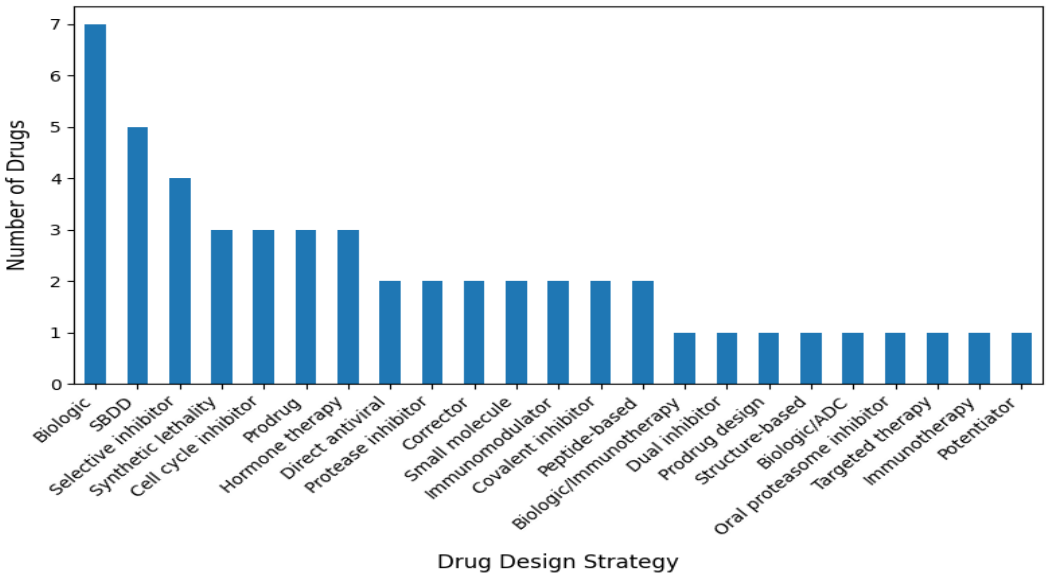

Figure 1. Distribution of drug design strategies among analyzed therapeutics.

The figures suggest that the various design strategies are captured with some categories making a greater impact in the total distribution. The diversity of frequencies in categories indicates the difference in the therapeutic methods and molecular designs structures.

3.2 Physicochemical and Bioactivity Characteristics

Table 2 summarizes the physicochemical and bioactivity properties of the studied drugs. In small molecule drugs, the molecular weight was between 150 Da and 900 Da with a mean distance equal to 470 ± 130 Daand a median equal to 445 Da. The spread of molecular weights shows that the majority of compounds are distributed in the usually observed range of drug-like molecules.

Table 2. Physicochemical and Bioactivity Profile of Small-Molecule Drugs

Parameter	Minimum	Maximum	Mean ± SD	Median
Molecular Weight (Da)	150	900	470 ± 130	445
logP	0.8	5.6	3.1 ± 1.0	3.0
IC_{50} (nM)	0.5	80	18 ± 22	10

Lipophilicity was found to be 0.8 to 5.6. The overall logP average was of 3.1 ± 1.0 with a median of 3.0. The values reveal that most of the compounds are moderately lipophilic. Fewer compounds were found at the lower and higher parts of the logP range.

Bioactivity expressed in IC_{50} values was between 0.5 nM and 80 nM. Mean IC_{50} was 18 ± 22 nM and the median was 10 nM. The values of IC_{50} distributions show that the inhibitory strength of the drugs under analysis is variable.

Figure 2 displays the correlation of lipophilicity with bioactivity, where the groups of compounds are grouped according to the logP values, low values (0-2), moderate (2-4), and high values (4-6). The bar graph depicts the mean value of IC 50 in each category. The average IC_{50} of the compounds in the moderate log P category was lower than the compounds in the low category and high category. Increased average IC_{50} values were found in both low and high lipophilicity groups.

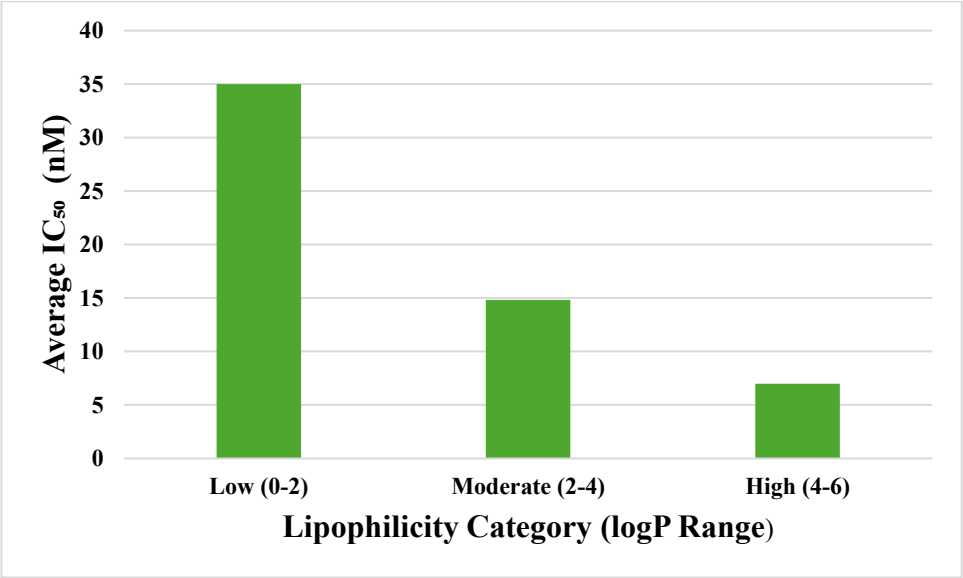

Figure 2. Average bioactivity (IC_{50}) across different lipophilicity (logP) categories.

Based on the findings of Table 2 and Figure 2, it can be concluded that the distribution patterns are not regular, and the physicochemical properties and activities of different measurements vary among the compounds being analyzed. Variations in the molecular weight, the lipophilicity, and the IC_{50} were found among various drugs.

3.3 Target Class Distribution

The therapeutic target distribution showed the concentration of the drugs that act on the specific biological classes. Intracellular kinases were the most common target class with 24% of overall drugs as shown in Table 3. Receptor tyrosine kinases formed 18% of the target whereas cytokine and immune related targets formed 16%.

Table 3. Target Class Distribution

Target Class	Representative Targets	Number of Drugs	Percentage (%)
Receptor Tyrosine Kinases	EGFR, HER2	9	18%
Intracellular Kinases	BRAF, CDK4/6, BTK, JAK	12	24%
Immune Checkpoints	PD-1, PD-L1	6	12%
Cytokines / Immune Targets	TNF-α, IL receptors	8	16%
DNA Repair Enzymes	PARP	3	6%
Viral Enzymes	RdRp, NS5A, NS3/4A	7	14%
Hormonal Targets	Androgen receptor	3	6%
Other Targets	CFTR, proteasome	2	4%
Total	—	50	100%

Immune checkpoint proteins constituted 12 percent of the total and viral enzymes constituted 14 percent. The DNA repair enzymes and the hormonal targets constituted the 6% of the analyzed drugs each. Other targets, such as CFTR and proteasome related proteins, were 4%. Figure 3 demonstrates the distribution of target classes in which each target category is represented with the number of drugs. Higher numbers were observed in the bar graph of intracellular kinases and receptor tyrosine kinases than in the target classes. The intermediate number of immune-related targets and viral enzymes was detected, whereas the number of DNA repair, hormonal, and other targets was lower.

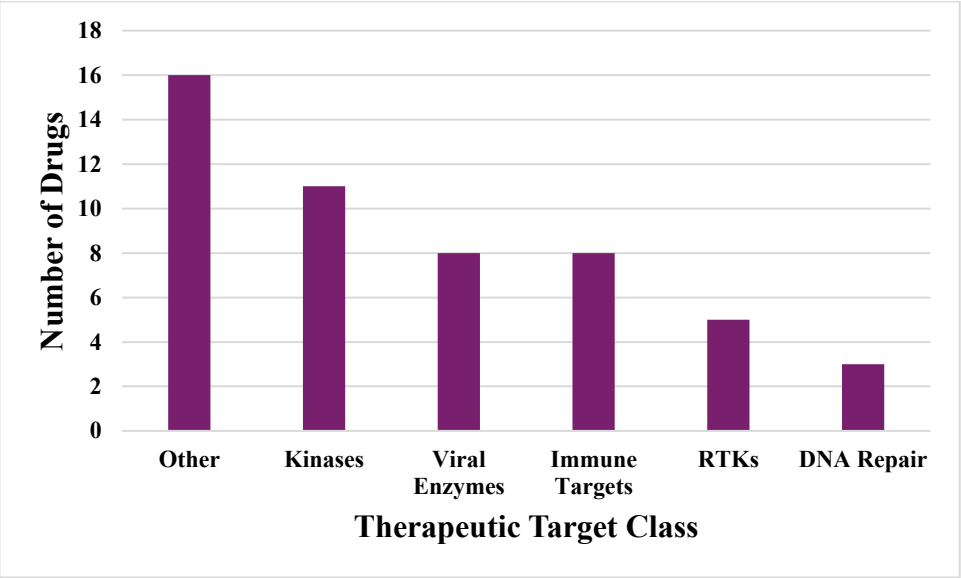

**Figure 3. Distribution of therapeutic target classes among analyzed drugs. **

The figures reveal that all drugs belong to various target classes, and some of them are more represented compared to others. The difference in the distribution of targets indicates the disparity in the therapeutic focus and the selection of targets..

3.4 Integrated Analysis of Drug Design, Properties, and Targets

Combined evaluation of drug-design strategies, physicochemical characteristics, and target classes showed overall trends in the examined drugs. Kinase-targeting and immune-related pathway-targeting drugs and SBDD, biologics, and covalent inhibition related drugs were most often linked. These relationships were found in numerous records of the analyzed dataset.

Among the compounds with lower IC_{50} values, small-molecule drugs with a molecular weight range (300–600 Da) and a logP range (2 to 4) were often frequently encountered. The compounds that were not within this range were indicated to vary in value of IC_{50} under the different classes.

The strategy type distribution by the target classes revealed that small-molecule inhibitors were mostly linked with kinase targets and biologic agents with immune-related targets. Targets of viral enzymes were mainly linked to prodrug strategies whereas the DNA repair targets were linked to synthetic lethality-based approaches. There were differences in the values of IC_{50} using various types of strategies and target classes. The patterns of distribution of the designs show that there are numerous combinations of design strategy, physicochemical properties and target in the discussed drugs.

The results demonstrate that a range of drug design strategies is represented among the analyzed drugs, with biologics, kinase inhibitors, and structure-based approaches forming the major categories. The physicochemical properties of small-molecule drugs fall within commonly observed ranges for molecular weight and lipophilicity. IC_{50} values indicate variability in inhibitory activity across the analyzed compounds. The distribution of therapeutic targets shows a higher representation of kinase and immune-related pathways compared to other target classes. The combined analysis of strategy type, physicochemical properties, and target class shows the presence of multiple patterns across the analyzed drugs. These findings provide a structured representation of drug design strategies, chemical properties, and target distributions in modern pharmaceutical development.

4. Discussion

The current paper presents a systematic analysis of modern drug design trends, physicochemical properties, and distributions of therapeutic targets, which are contemporary tendencies in pharmaceutical chemistry. The distribution of drug design strategies observed indicates that it is highly represented by the biologics, kinase inhibitors, and structure-based drug design techniques. These results coincide with the current trends in the field of drug discovery where targeted and mechanism-based approaches have taken a center stage, as they are able to enhance specificity and therapeutic outcomes (Wu et al., 2023; Vamathevan et al., 2019).

The excessive prevalence of biologics and immunotherapeutic agents, as found in the analysis, is in line with the growing application of

biologics in the contemporary medicine. There is an improved specificity and efficacy of biologic therapies, especially in oncology and immune-related diseases, such as the use of monoclonal antibodies and cell-based therapies (June et al., 2018; Ribas and Wolchok, 2018). Moreover, the relevance of immune modulation as a treatment method is also justified by cytokine-targeted therapies (Waldmann, 2018). Although comparative studies between biologics and small-molecule drugs have also identified differences in their efficacy, safety, and target selectivity, they support the increasing popularity of biologics in complex disease conditions (Quraee et al., 2024).

The other dominant category that has been found in the study is represented by kinase inhibitors, which are considered to be the key in the control of intracellular signaling pathways. Kinase-targeted drugs have become common promise in parallel with the vast mapping of molecular drug targets, in which kinases have been discovered to be one of the most important modulators in the pathogenesis of diseases (Santos et al., 2017). The combination of computational methods and machine learning tools has also contributed to the improvement of kinase inhibitors through the ability to identify the target accurately, optimizing it (Vamathevan et al., 2019; Zhavoronkov et al., 2019).

The existence of covalent inhibitors in the studied drugs is an indication of the continued interest of irreversible binding strategy in medicinal chemistry. Covalent inhibitors use warheads, i.e. reactive functional groups, to create stable interactions with the target proteins, which increases potency and increases the duration of action (Gehringer & Laufer, 2018). Drug-protein adproducts have also been well-investigated and can inform about the efficacy of the therapy as well as possible safety concerns (Baillie, 2020). These observations highlight the need of the chemical reactivity in drug design and its contribution to the attainment of sustained pharmacological effects.

Physicochemical characteristics especially molecular weight and lipophilicity are vital in dictating drug actions and bioactivity. The recorded distribution of the molecular weights falling within the range of 150-900 Da is agreeable with the known principles of drug-likeness that indicate that optimum molecular size plays a role in enhancing bioavailability and target accessibility. Lipophilicity measures by logP values had most of the values near the moderate range, which is commonly associated with a balanced solubility and permeability rate across membranes. These findings are consistent with the existing literature that points to the fact that physicochemical parameters should be optimized during the development of drugs (Wu et al., 2023). The correlation between lipophilicity and bioactivity as it is evidenced by the results further prove the significance of physicochemical optimization. The compounds with moderate logP had higher inhibitory activity, which indicated that intermediate hydrophobicity could be effective in inter-reacting with biological targets. Computational and generative modeling methods are becoming more commonly used to study such relationships and allow developing molecules with physicochemical and biological properties optimized (Zadorozhny & Nuzhna, 2021).

The developments in artificial intelligence and deep learning have played a major role in contemporary drug discovery, especially in the design and optimization of small molecules. With the help of machine learning models and generative methods, it became possible to identify new chemical entities and determine the interaction of drugs with targets with high accuracy (Vamathevan et al., 2019; Zadorozhny and Nuzhna, 2021). The efficient use of the deep learning in determining the kinase inhibitors is another evidence of the possible power of the technologies in speeding up the process of drug discovery (Zhavoronkov et al., 2019).

The therapeutic targets distribution in the current study shows that much attention is paid to the kinase and immune-related pathways. The trend is in line with the ongoing research works in an attempt to focus on well-defined molecular pathways in relation to disease development. Target mapping has shown that only a small number of protein families, such as immune regulators and kinases, have a large percentage of therapeutic interventions (Santos et al., 2017). There are also methods (target identification) (chemical proteomics) that have improved the study of drug-target interaction and opened the way to the identification of new therapeutic targets (Chen et al., 2020).

A combination of drug design strategies and target selection points to the coordinated process in contemporary pharmaceutical development. To give an example, biologic therapies have been mostly linked with immune-related targets whereas small-molecule inhibitors have been commonly linked with kinase targets. Such a correspondence indicates the appropriateness of various strategies of design to particular target classes and the necessity to choose the right approaches to drug development.

Also, the chemical innovation plays a crucial role in drug discovery as seen in the implementation of advanced design methods such as covalent inhibition, biologics and computational modeling. The strategies facilitate the production of superiorly specific, powerful, and therapeutic drugs. Further evidence of the development of contemporary therapeutics is the constant improvement of medicinal chemistry methods, such as the creation of new reactive warheads and computational tools (Gehringer and Laufer, 2018; Wu et al., 2023).

Nevertheless, there are still issues with optimization of drug properties and safety and effectiveness across therapeutic classes (Zadorozhny & Nuzhna, 2021). Drug-protein complexes should be favorable to some covalent inhibitors, but also may cause undesirable adverse effects unless properly managed (Baillie, 2020). In the same manner, the nature of biologic therapies is complicated and the issues of production, stability, and distribution have to be overcome to introduce successful clinical use.

The results of the present study demonstrate that drug design strategies, physicochemical properties, and target selection are all interrelated in the contemporary pharmaceutical chemistry. The combination of these factors is another sign of the transition to rational and accuracy-oriented drug development at the assistance of the development of new computational technologies, chemical innovation, as well as biological knowledge. These trends highlight the dynamism and change in drug discovery and give grounds to future research in the formation of new therapeutic drugs.

5. Conclusion

The present study provides a comprehensive evaluation of contemporary drug design strategies, physicochemical properties, and therapeutic target distributions in modern pharmaceutical chemistry. The findings demonstrate that biologics, kinase inhibitors, and structure-based drug design approaches represent the predominant strategies in current drug development. These approaches reflect a shift toward targeted and mechanism-driven therapeutics aimed at improving specificity and clinical outcomes.

The analysis of physicochemical parameters indicates that most small-molecule drugs fall within established drug-like ranges for molecular weight and lipophilicity, highlighting the importance of optimizing these properties to achieve favorable pharmacokinetic profiles. Variations in IC_{50} values across the analyzed drugs further demonstrate differences in inhibitory potency associated with design strategies and target classes. The distribution of therapeutic targets reveals a strong emphasis on kinase and immune-related pathways, underscoring their significance in disease modulation and therapeutic intervention. The integration of computational techniques, artificial intelligence, and advanced chemical methodologies has further contributed to the evolution of drug discovery, enabling the identification and optimization of novel therapeutic agents. Overall, the study highlights the interconnected role of drug design strategies, molecular properties, and target selection in shaping modern therapeutics. These findings provide valuable insights into current trends in pharmaceutical chemistry and may support the development of more efficient and precise drug discovery approaches in the future.

REFERENCES

1. Alakhdar, A., Poczos, B., & Washburn, N. (2024). Diffusion models in de novo drug design. *Journal of Chemical Information and Modeling, 64*(19), 7238–7256.
2. An, Q., Huang, L., Wang, C., Wang, D., & Tu, Y. (2025). New strategies to enhance the efficiency and precision of drug discovery. *Frontiers in Pharmacology, 16*, 1550158.
3. Baillie, T. A. (2020). Drug–protein adducts: Past, present, and future. *Medicinal Chemistry Research, 29*(7), 1093–1104.
4. Brown, D. G., & Bostrom, J. (2016). Analysis of past and present synthetic methodologies on medicinal chemistry: Where have all the new reactions gone? *Journal of Medicinal Chemistry, 59*(10), 4443–4458.
5. Chen, H., Engkvist, O., Wang, Y., Olivecrona, M., & Blaschke, T. (2018). The rise of deep learning in drug discovery. *Drug Discovery Today, 23*(6), 1241–1250.
6. Chen, X., Wang, Y., Ma, N., Tian, J., Shao, Y., Zhu, B., & Wang, J. (2020). Target identification of natural medicine with chemical proteomics approach. *Signal Transduction and Targeted Therapy, 5*(1), 72.
7. Ciccone, L., & Nencetti, S. (2025). Advances in drug discovery and synthesis. *International Journal of Molecular Sciences, 26*(2), 584.
8. Danel, T., Łęski, J., Podlewska, S., & Podolak, I. T. (2023). Docking-based generative approaches in the search for new drug candidates. *Drug Discovery Today, 28*(2), 103439.
9. Du, J., Guo, J., Kang, D., Li, Z., Wang, G., Wu, J., & Zhang, Y. (2020). New techniques and

strategies in drug discovery. *Chinese Chemical Letters, 31*(7), 1695–1708.
10. Elton, D. C., Boukouvalas, Z., Fuge, M. D., & Chung, P. W. (2019). Deep learning for molecular design: A review. *Molecular Systems Design & Engineering, 4*(4), 828–849.
11. Ferreira, L. G., Dos Santos, R. N., Oliva, G., & Andricopulo, A. D. (2015). Molecular docking and structure-based drug design strategies. *Molecules, 20*(7), 13384–13421.
12. Gagare, S., Patil, P., & Jain, A. (2024). Natural product-inspired strategies toward novel bioactive molecules. *Future Journal of Pharmaceutical Sciences, 10*(1), 55.
13. Gehringer, M., & Laufer, S. A. (2018). Emerging warheads for covalent inhibitors. *Journal of Medicinal Chemistry, 62*(12), 5673–5724.
14. Ginex, T., Vázquez, J., Estarellas, C., & Luque, F. J. (2024). Quantum mechanical-based strategies in drug discovery. *Current Opinion in Structural Biology, 87*, 102870.
15. June, C. H., O'Connor, R. S., Kawalekar, O. U., Ghassemi, S., & Milone, M. C. (2018). CAR T cell immunotherapy for human cancer. *Science, 359*(6382), 1361–1365.
16. Lipinski, C. A. (2016). Rule of five in 2015 and beyond. *Advanced Drug Delivery Reviews, 101*, 34–41.
17. Lyu, J., Wang, S., Balius, T. E., Singh, I., Levit, A., Moroz, Y. S., & Irwin, J. J. (2019). Ultra-large library docking for discovering new chemotypes. *Nature, 566*(7743), 224–229.
18. Mak, K. K., Wong, Y. H., & Pichika, M. R. (2024). Artificial intelligence in drug discovery and development. *Drug Discovery and Evaluation*, 1461–1498.
19. Moffat, J. G., Vincent, F., Lee, J. A., Eder, J., & Prunotto, M. (2017). Opportunities and challenges in phenotypic drug discovery. *Nature Reviews Drug Discovery, 16*(8), 531–543.
20. Najjar, A., Olğaç, A., Ntie-Kang, F., & Sippl, W. (2019). Fragment-based drug design of nature-inspired compounds. *Physical Sciences Reviews, 4*(9), 20180110.
21. Niazi, S. K., & Mariam, Z. (2023). Computer-aided drug design and discovery. *Pharmaceuticals, 17*(1), 22.
22. Quraee, H. M. A., et al. (2024). Biologics vs small molecule drugs: Comparing efficacy and safety. *Journal of International Crisis and Risk Communication Research, 7*(S11), 355.
23. Ribas, A., & Wolchok, J. D. (2018). Cancer immunotherapy using checkpoint blockade. *Science, 359*(6382), 1350–1355.
24. Santos, R., Ursu, O., Gaulton, A., Bento, A. P., Donadi, R. S., Bologa, C. G., & Overington, J. P. (2017). A comprehensive map of molecular drug targets. *Nature Reviews Drug Discovery, 16*(1), 19–34.
25. Schneider, G. (2018). Automating drug discovery. *Nature Reviews Drug Discovery, 17*(2), 97–113.
26. Vamathevan, J., Clark, D., Czodrowski, P., Dunham, I., Ferran, E., Lee, G., & Zhao, S. (2019). Machine learning in drug discovery. *Nature Reviews Drug Discovery, 18*(6), 463–477.
27. Waldmann, T. A. (2018). Cytokines in cancer immunotherapy. *Cold Spring Harbor Perspectives in Biology, 10*(12), a028472.
28. Wang, K., Huang, Y., Wang, Y., You, Q., & Wang, L. (2024). From computer-aided drug design to AI drug design. *RSC Medicinal Chemistry, 15*(12), 3978–4000.
29. Wu, K., Karapetyan, E., Schloss, J., Vadgama, J., & Wu, Y. (2023). Advancements in small molecule drug design. *Drug Discovery Today, 28*(10), 103730.
30. Zadorozhny, K., & Nuzhna, L. (2021). Deep generative models for drug design and response. *arXiv preprint arXiv:2109.06469*.
31. Zhavoronkov, A., Ivanenkov, Y. A., Aliper, A., Veselov, M. S., Aladinskiy, V. A., Aladinskaya, A. V., & Aspuru-Guzik, A. (2019). Deep learning enables rapid identification of DDR1 kinase inhibitors. *Nature Biotechnology, 37*(9), 1038–1040.