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Quantum Machine Learning for Molecular Design and Drug Discovery: A Qualitative Study

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ABSTRACT

Quantum machine learning (QML) has become a key research field on the interface between quantum computing, artificial intelligence, chemistry and pharmaceutical science. By enhancing the molecular representation, predictive modeling, generative chemistry, and quantum-assisted simulations workflows, researchers are increasingly arguing that QML can aid work in molecular design and drug discovery. Meanwhile, this field is still in its new frontiers with much of the published literature only comprising reviews, simulations, proof-of-concept applications, and hybrid quantum-classical demonstrations as opposed to large-scale pharmaceutical application. In this qualitative study, the literature emerging is reviewed to determine how QML is being conceptualized, areas of application seem the most promising, and what obstacles remain that hamper its practical implementation in actual drug discovery pipelines. The paper presents five large themes segmented into a thematic analysis of recent reviews and representative

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studies and includes relevant themes as QML as a representational innovation, QML in predictive tasks, e.g., drug-target interaction and ADMET modeling, QML in generative molecular design, hybrid quantum-classical workflows as the most plausible approach in the near term, and the continuation of restrictions in terms of hardware, trainability, data This research paper concludes that the idea of QML must be seen at present as a field not as an alternative to the classical machine learning in drug discovery, but it is an opportunity with strategic and scientific potential whose future realization may be found in the subproblems carefully chosen where the influence of molecular quantum effects, the complexity of learning, and the hybrid implementations converge.

Keywords: quantum machine learning, molecular design, drug discovery, qualitative study, quantum computing, generative chemistry, ADMET, drug-target interaction

1. Introduction

Drug discovery has continued to be one of the most costly, uncertain and time-consuming processes in contemporary science and business. It can take years and go through high failure rates in experiments, attrition rates in experiments and significant risk of capital to develop a biological target all the way to an approved medicine. Although biotechnology, medicinal chemistry, and computational modeling have advanced, the likelihood that an early candidate can be a success therapeutic product is very low. This has led to the increasingly important role of computational approaches that are capable of enhancing the early prioritization, anticipate failure earlier, or sample chemical space more productively in drug innovation (Zhou et al., 2026; Smaldone et al., 2024; Quantum Intelligence in Drug Discovery, 2025).

There are already several aspects of the drug discovery pipeline that have already been altered by classical machine learning. Hit discovery, lead optimization, toxicity estimation, and compound prioritization are all now aided by deep learning, graph neural networks, virtual screening systems, molecular property predictors and generative chemistry models. Such methods have enhanced speed and scalability particularly in data-filled environments where massive molecular libraries and results of assays are accessible. They nonetheless have a fundamental drawback,

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namely that molecules are quantum-mechanical systems, whereas most machine learning models describe them as graphs, strings, fingerprints, or engineered descriptors, instead of using any direct quantum description of their behavior (Smaldone et al., 2024; Quantum Mechanical-Based Strategies in Drug Discovery, 2024).

With this limitation, quantum computing, and especially quantum machine learning, has sparked recent interest as a potential new framework of molecular science. In a broader sense, QML can be defined as learning systems that make use of quantum algorithms, quantum circuits or hybrid quantum-classical artificial intelligence to perform prediction and classification optimisation, as well as generation. QML has been suggested in the context of molecular design and drug discovery as a means to encode molecular information into more expressive feature spaces, enable more expressive learning systems, execute more useful quantum chemistry computations in specified quantum chemistry computational resource requirements, and increase search in large chemical spaces (Smaldone et al., 2024; Zhou et al., 2026).

Meanwhile, the sphere is still characterized by doubts and controversy. A few scientists have termed QML as a long-term breakthrough that may transform pharmaceutical computing, whereas others point to the fact that current assertions of benefit tend to be premature, restricted to toy problems, or founded on simulated demonstrations, as opposed to demonstrations at hardware level. Several concerns have yet to be answered regarding scalability, trainability, benchmarking, noise tolerance, and the ability of quantum methods to solve realistic drug discovery problems better than strong machine learning classification methods do on classes (Pitfalls and Prospects of Quantum Machine Learning, 2025; Smaldone et al., 2024).

Due to the heterogeneous and developing nature of the field, a qualitative review would particularly come in handy. In place of the testing of one benchmark or model, this paper will look at how the literature as a body of work characterizes the role of QML in molecular design and drug discovery. It raises 3 primary questions: How does QML conceptualize with respect to molecular science? What are the most promising applications? What are the obstacles to routine practice in

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pharmaceutics? To answer these questions, the paper will attempt to present a fair depiction of a subject that is emerging and has since been viewed either too optimistically or too pessimistically (Timulak, 2017; Zhou et al., 2026).

2. Research Design and Methodology

The paper uses the qualitative thematic review method due to the conceptual and methodological dissimilarity in the literature on QML in drug discovery. The field covers among others theoretical ideas, perspective articles, review articles, proof-of-concept models, simulation-based work, hybrid workflow proposal, and fewer application oriented demonstrations. The range of data contained in these studies, model formulations, computational hypotheses, assessment metrics, and real-life assertions is quite broad, which is why a very focused quantitative synthesis is not suitable in this section (Timulak, 2017; Smaldone et al., 2024).

A qualitative design can be applied in a new area especially where conceptual framing is standing out as a significant portion of the research landscape itself. In QML in molecular design, numerous publications do not merely report outcomes; they also debate on what problems should be tackled with quantum techniques, how well-being ought to be determined and what realistic expectations ought to appear over various durations of time. This is what thematic synthesis can do to detect recurring patterns, assumptions, and tensions in the literature (Pitfalls and Prospects of Quantum Machine Learning, 2025; Zhou et al., 2026).

The source base of the present study is oriented towards recent literature, particularly the period of 2023-2026, so as to capture the up-to-date situation in the field. Since they assist in defining the position of QML in drug discovery discourse, review and perspective articles were given priority. Also representative application studies, particularly in drug-target interaction prediction, ADMET modeling, generative chemistry, and quantum-refined molecular workflows, were incorporated so that broader conceptual assertions could be traced to specific use cases (Smaldone et al., 2024; Kao et al., 2023; Pallavi et al., 2025; Yan et al., 2024).

The three-stage analysis was done. First, the literature was analyzed concerning recurrent assertions concerning why QML could be of importance in molecular design and pharmaceutical research. Second, these arguments were

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combined into larger sets including representation, prediction, generation, hybridization and barriers. Third, the categories have been compared across sources to describe areas of agreement and disagreement, specifically on the aspects of feasibility, practical value, and scientific maturity (Quantum Intelligence in Drug Discovery, 2025; Pitfalls and Prospects of Quantum Machine Learning, 2025).

The study is not meant to be a statistical meta-analysis of the model performance. Rather, it provides an ordered understanding of the key themes, assumptions and unloading questions that characterize the field. That is a right ambition of a field where narrative positioning and strategic expectation is key to the development of the field.

3. Background: Why QML Matters for Molecular Design and Drug Discovery

The background of QML in molecular design The first step in the attractiveness of QML in molecular design is a simple fact: molecules are themselves quantum systems, and most machine learning processes in chemistry are still classical abstractions of those systems. The end results of quantum-mechanical interactions are molecular properties like binding affinity, reactivity, stability, electronic behavior and conformational dynamics. The classical computational chemistry has already yielded numerous useful approximate methods of studying these processes, and the problem of calculating them exactly is growing less and less solvable with system size (Quantum Mechanical-Based Strategies in Drug Discovery, 2024; Zhou et al., 2026).

By learning on a large scale of experimental and computed data, machine learning has generalized classical chemistry, which explicitly resolves every physical equation. This has significantly improved the speed of prediction of properties and molecular prioritization, yet has not removed the representational gap between quantum phenomena and classical encodings. Graphs, fingerprints, SMILES strings or learned embeddings are all useful but incomplete abstractions used to depict molecules. It can be used to explain why researchers are investigating the problem of whether quantum encodings or quantum-enhanced learning systems can more easily encode some chemical relationships (Smaldone et al., 2024; Quantum Intelligence in Drug Discovery, 2025).

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The other reason why QML is important is the size of the chemical space. The volume of potentially drug-like molecules is astronomically huge, which is why the only very small portion of them may ever be synthesized or even experimentally screened. Discovery of drugs thus puts a lot of reliance on the computational platforms capable of ranking, filtering, predicting and producing compounds effectively. Assuming that QML can assist with the embedding, comparison, optimization, or generation of compounds, it could provide researchers with the opportunity to explore chemical space more intelligently than can be achieved at present (Zhou et al., 2026; Smaldone et al., 2024).

Nevertheless, conceptual appeal does not mean performed performance. The major reviews do consistently mention that QML is yet to demonstrate solid and generalizable outperformance in many actual drug discovery problems over strong classical baselines. This introduces the overarching tension of the subject: the idea of quantum machine learning is still attractive because the underlying science of molecules is quantum, but the bridge between this knowledge and useful pharmaceutical benefit has not yet been made (Pitfalls and Prospects of Quantum Machine Learning, 2025; Quantum Intelligence in Drug Discovery, 2025).

4. Findings

4.1 QML as a Representational Innovation

It is one of the most powerful points in the literature that QML is typically not presented primarily as a faster calculator, but a novel way of how chemical information is represented. The issue of representation is very important when it comes to the discovery of drugs since predictive performance is sensitive to the manner in which molecular structure and behavior are coded prior to the initiation of learning. Traditional cheminformatics uses descriptors, fingerprints, graph representations and coded strings that all reduce the complexity of actual molecules. According to the researchers of quantum machine learning, quantum feature spaces and quantum kernels can provide more effective methods to encode subtle molecular relationships, especially when a classical description is able to reductionally encode an important structural variation (Smaldone et al., 2024; Quantum Intelligence in Drug Discovery, 2025).

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This framing changes the value proposition of QML. Alternatively to supposedly inference that quantum systems will merely run typical machine learning tasks with greater relief, most studies propose that quantum techniques can modify the geometry of the learning process by mapping data on surfaces where useful classes are simpler to dissect or convoluted interactions are simpler to represent. This, in theory, would enhance generalization during tasks like prediction of molecular activities, comparison of scaffolds, or estimation of properties.

Nevertheless, the literature is still reserved. A more detailed space in theoretical features can only add value when encodings can be done in an efficient manner, and the resulting model can be trained and evaluated in a stable manner. Moreover, most classical approaches already generate highly expressive learned embeddings with the help of graph neural networks and transformer-based architectures. It is not whether quantum representations are different into important tasks under realistic constraints, the real question, though, is whether they are meaningfully better (Pitfalls and Prospects of Quantum Machine Learning, 2025; Smaldone et al., 2024).

4.2 Predictive Tasks as the Best Near-Term Application Area.

The most stable area of application of QML in drug discovery described in the literature is supervised predictive tasks. These applications are molecular prediction of property, drug-target interaction, toxicity modeling, and ADMET. Their appeal lies in the fact that they already fit existing machine learning models, can be assessed using existing datasets, and can be potentially useful even with small predictive performance boosts (Pallavi et al., 2025; Quantum Machine Learning Predicting ADME-Tox Properties in Drug Discovery, 2023).

The prediction of drug-target interactions is the most crucial, as it assists the determination of the likelihood of a candidate compound to bind to a biological target of interest. More accurate prediction of interactions can be used to minimize unsuccessful experiments and to prioritize compounds so that they can be progressed in the early discovery stage. One such direction is the QKDTI model, which a quantum kernel approach to prediction can be used to capture the prediction of interactions and contends that feature mapping of quantum features can be used

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well to predict the association between compounds and their targets (Pallavi et al., 2025).

Other valuable areas are ADMET modeling, as absorption, distribution, metabolism, excretion, and toxicity failures are frequent causes of eventual failures of promising candidates in development. The current research indicates that quantum-enhanced or hybrid models have the capability to play competitively on a handful of benchmarking datasets, particularly when operating on a small scale or on a small-scale simulator. Such findings are significant as predicting ADMET is commercially valuable and scientifically challenging even in drug discovery (Quantum Machine Learning Predicting ADME-Tox Properties in Drug Discovery, 2023; Smaldone et al., 2024).

Simultaneously, the literature indicates that the majority of predictive QML outcomes are somehow provisional. There is a great amount of literature involving limited data sets, restricted assessment configurations or insufficient comparisons of baseline. Consequently, predictive QML is potential and testable, but not currently superior enough to be applied to industrial operations (Pitfalls and Prospects of Quantum Machine Learning, 2025; Quantum Intelligence in Drug Discovery, 2025).

4.3 Generative Molecular Design as an Ambitious but Immature Area

Generative molecular design is one of the most ambitious objectives in QML in drug discovery. Here, we are not merely interested in modelling the properties of already known molecules but we are interested in generating new candidate structures which fulfill a broad range of desired properties. Given that drug discovery remains a search problem in the vast chemical space, the use of generative models is an enticing solution in the search of new ones in a more efficient manner than a brute-force treatment or random search (Kao et al., 2023; Zhou et al., 2026).

Already, variational autoencoders, adversarial networks, reinforcement learning, and sequence-based models are some of the methods that have enabled classical generative chemistry to advance notable improvements. QML makes forays into this space with proposals that quantum-enhanced generative systems or hybrid systems could also be trained to represent molecular distributions differently, or they could also search in new ways. According to initial success of quantum

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generative adversarial network in quantum hybrid generation, encouraging results were achieved on the generation of valid chemical structures and small scale generative models (Kao et al., 2023; Hybrid Quantum-Classical Machine Learning for Generative Chemistry and Drug Design, 2023).

And yet this is the point too at which the distance between vision and application is particularly large. In medicinal chemistry, a generated molecule should be not only valid or novel. It should also be in vivo synthetically amenable, biologically workable, needs to be project-goal-relevant, patent-conscious and compliant with diverse optimization prerequisites, such as potency, safety, selectivity and developability. Most of the existing studies on QML generativeness do not already accomplish this. They can more be interpreted as frontier demonstration than a production-level design drug tool (Smaldone et al., 2024; Zhou et al., 2026).

4.4 The Hybrid Quantum-Classical Workflows: The Most Realistic Future.

Hybrid quantum-classical workflows are one of the few aspects that are well agreed upon in the literature as the most realist model of implementing QML in drug discovery in the immediate term. Actual drug research is based on huge classical structures, including information systems, bioinformatics technologies, molecular simulation technologies, medicinal chemistry technologies and experimental feedback circuits. The existing quantum devices cannot substitute these systems. The most common rationale in the support of QML, therefore, is that quantum elements could be controlled to be included in specific points of greater classical pipes, rather than being used as alternatives (Smaldone et al., 2024; Quantum Intelligence in Drug Discovery, 2025).

It is in practice a quantum circuit as a feature map to the input of a classical classifier, quantum kernel to a similarity-learning problem, quantum part to a generative subroutine and the rest of the work handed over to classical tools to do the preprocessing, pruning and global coordination. Simulation-based research is another use where machine learning can be used to expedite or inform multiscale quantum refinement as opposed to supplanting the rest of the classical workflow (Yan et al., 2024).

This is a major aspect of bio-polar framing because it offers an intermediate

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ground between hype and dismissal. It is opposed to the most insane speculations of quantum methods replacing all medications AI, but also the misguidedness of thinking that a type of technology will need to completely replace a pipeline so that this can be beneficial. Often, directed augmentation can be a viable choice also in factories, which may be more accessible to acceptance than total replacement. It is thanks to that that hybrid QML is not only technically viable, but also organizationally possible (Zhou et al., 2026; Smaldone et al., 2024).

4.5 Barriers and Unresolved Tensions

The last significant theme in the literature is that QML in drug discovery is still limited by a number of continuing technical and translational obstacles. Hardware limitation is the most obvious among them. The particular devices used in noisy intermediate-scale quantum computing currently are limited in the number of qubits, coherence time, circuit depth, and error rates, all of which render chemically significant large-scale computation challenging. These restrictions are decisive on the existence of what can be accomplished beyond modest experiments and simulated examples (Pitfalls and Prospects of Quantum Machine Learning, 2025; Zhou et al., 2026).

The second greatest challenge is trainability. Variational quantum circuit based methods that are the focus of numerous QML methods are susceptible to optimization issues like barren plateaus, where gradients become zero and learning cannot occur. It is of great concern regarding scalability and whether more expressive quantum models can be trained in practice (Pitfalls and Prospects of Quantum Machine Learning, 2025).

The third problem is the encoding of data. The vast majority of pharmaceutical data are classical in nature, such as molecular structures, descriptors, assay results and clinical observations. Measurement of these data can be computationally costly, not to mention that in certain instances it is the loading cost of the data that can nullify the downstream benefit. It is particularly significant due to the fact that it is one of the fundamental pillars of every argument that presents quantum benefit (Smaldone et al., 2024; Pitfalls and Prospects of Quantum Machine Learning, 2025).

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Fourth impediment is inconsistent benchmarking. Various QML publications tend to be based on disparate datasets, preprocessing, simulation models, circuit models, and classical baseline meaning that it is hard to directly compare them. It is difficult to evaluate the extent to which any given success is the result of a sound methodological advantage or merely a favourable experimental design unless more rigorous standards of benchmarking are in place (Quantum Intelligence in Drug Discovery, 2025; Smaldone et al., 2024).

Lastly, an algorithmic research has only a translational distance to actual pharmaceutical practice. In addition to being a challenging computational task, drug discovery is also a scientific, regulatory, organizational, and economic endeavor. Models need to be accommodating of medicinal chemistry decision-making, assay cycles, strategy in intellectual property, manufacturing feasibilities, and portfolio constraints. This level of integration is not yet incorporated in most QML studies. This does not render the study insignificant, however, it indicates that operational readiness must not be confused with scientific promising (Zhou et al., 2026; Smaldone et al., 2024).

5. Discussion

According to the literature, QML has three key roles in molecular design and drug discovery at the moment. To begin with, it serves to introduce a conceptual intermediation between machine learning and the fact that living matter is quantum-mechanical. It is significant since it questions the idea that future computational drug discovery should be purely classical in its representation and learning strategy (Quantum Mechanical-Based Strategies in Drug Discovery, 2024; Smaldone et al., 2024).

Second, QML acts as a methodological testable area of hybrid innovation. It provides researchers with a tool to investigate how quantum kernels, variational circuits or quantum-enhanced generative modules can provide value to certain aspects of existing workflows. Not necessarily providing complete quantum advantage, such efforts nevertheless serve to keep the question of quantum approaches to realistic pharmaceutical computing in focus (Smaldone et al., 2024; Yan et al., 2024).

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Third, QML is a strategy horizon-based technology. It could have a role in organizations because it is not yet better than classical AI, but organizations might find it interesting to explore it as it might gain significance in the future in case hardening becomes better, and in case some chemically based use cases are refined. This long-term vision is what can justify the serious presence of the field although its current restrictions are still apparent (Zhou et al., 2026; Smaldone et al., 2024).

Simultaneously, the literature is solidly in favor of caution. At this point, there is no evidence to support that QML is soon to have a wide-ranging revolution in pharmaceutical research. A less justifiable stance is reduced: QML can be applicable to the reduced subproblems where representation complexity, quantum relevance in chemistry, or hybrid workflow design can present a good environment. It means that further advancement will rely on the trained benchmarking, more realistic classical comparisons, more realistic medicinal chemistry problems, and more accurate measurement of the decision-making value, and not on the abstract predictive accuracy in isolation (Pitfalls and Prospects of Quantum Machine Learning, 2025; Quantum Intelligence in Drug Discovery, 2025; Zhou et al., 2026).

6. Conclusion

The article was about qualitative research in which a thematic synthesis of the current literature was done on the use of quantum machine learning in molecular design and drug discovery. The review found five common themes, the most evident of which are that QML is introduced as a form of representational innovation, predictive tasks are the most viable, and the field remains immature, hybrid quantum-classical workflows are the most viable way to proceed, and the field continues to be shaped by persistent challenges (Smaldone et al., 2024; Quant<|human|>The review identified five common themes, with predictive

It is the most logical conclusion that QML is not yet able to be called a replacement of standard machine learning in the pharmaceutical field research. Classical AI is more mature, more scalable, and more built in to industrial processes. However, neither can QML be credited to hype. It has already brought conceptual and methodological enhancements useful in terms of molecular representation, hybrid modeling, and quantum-informed chemical computation in particular

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(Smaldone et al., 2024; Yan et al., 2024).

It is likely to only be useful in selective hybrid training such as drug-target interaction modeling, predicting ADMET and machine-learning-assisted quantum refining but not be used in wholesale in the entire discovery pipeline. The future significance will depend on the hardware development, the improvement of the algorithms, the increase of the benchmarking capabilities, the ability to demonstrate its value on the real-life pharmaceutical projects. At that, QML may be characterized as a rather prospective but hypothetical frontier: scientifically relevant, strategically useful, and potentially transformative, but as of yet, not clearly shown to bring any sort of practical value (Pitfalls and Prospects of Quantum Machine Learning, 2025; Zhou et al., 2026) to it.

References

1. Gircha, A. I., Boev, A. S., Avchaciov, K., Fedichev, P. O., & Fedorov, A. K. (2023). Hybrid quantum-classical machine learning for generative chemistry and drug design. *Scientific Reports*, *13*, Article 8250.
2. Kao, P.-Y., et al. (2023). Exploring the advantages of quantum generative adversarial networks in generative chemistry. *Journal of Chemical Information and Modeling*.
3. Pallavi, G., et al. (2025). QKDTI: A quantum kernel based machine learning model for drug target interaction prediction. *Scientific Reports*.
4. Li, W., Ma, Y., & Deng, D.-L. (2025). Pitfalls and prospects of quantum machine learning. *Nature Computational Science*.
5. Quantum intelligence in drug discovery: Advancing insights with quantum machine learning. (2025). *Drug Discovery Today*.
6. Quantum machine learning predicting ADME-Tox properties in drug discovery. (2023). *Journal of Chemical Information and Modeling*.
7. Quantum mechanical-based strategies in drug discovery: Finding the pace of QM and ML integration. (2024). *Current Opinion in Structural Biology*.
8. Smaldone, A. M., Shee, Y., Kyro, G. W., Xu, C., Vu, N. P., Dutta, R., Farag, M. H., Galda, A., Kumar, S., Kyoseva, E., & Batista, V. S. (2024). *Quantum machine learning in drug discovery: Applications in academia and pharmaceutical industries.*

Online ISSN 3007-3197
Print ISSN 3007-3189

arXiv.

9. Timulak, L. (2017). Metasynthesis: An original method to synthesize qualitative literature in psychiatry. *Frontiers in Psychiatry, 8*, Article 269.
10. Yan, Z., et al. (2024). Accelerating reliable multiscale quantum refinement of protein-drug systems enabled by machine learning. *Nature Communications, 15*, Article 4128.
11. Zhou, Y., Chen, J., Cheng, J., Cao, X., Zhang, Y., Karemore, G., Zitnik, M., Chong, F. T., Liu, J., Fu, T., & Liang, Z. (2026). Quantum-machine-assisted drug discovery. *npj Drug Discovery, 3*, Article 1.
12. Kovyrshin, A., Tornberg, L., Crain, J., Mensa, S., et al. (2025). Prioritizing quantum computing use cases in the drug discovery and development pipeline. *Drug Discovery Today, 30*(3), Article 104323.
13. What is the future role of quantum computation in drug discovery? (2025). *Computational Biochemistry and Chemistry.*
14. Synergizing quantum techniques with machine learning for advancing drug discovery. (2024). *Scientific Reports.*
15. Harnessing AI and quantum computing for revolutionizing drug discovery and development. (2025). *Exploratory Research and Hypothesis in Medicine.*
16. Computer-aided drug discovery: From traditional simulation methods to AI and quantum computing approaches. (2024). *Journal of Molecular Modeling.*
17. Quantum computing and the implementation of precision medicine. (2025). *npj Precision Oncology.*
18. AQuaRef: Machine learning accelerated quantum refinement of protein structures. (2025). *Nature Communications.*
19. How exascale computing can shape drug design: A perspective from rigorous molecular simulation. (2024). *Current Opinion in Structural Biology.*
20. Quantum-machine-assisted drug discovery. (2024). *arXiv preprint* arXiv:2408.13479.