CODEN [USA]: IAJPBB ISSN : 2349-7750

INDO AMERICAN JOURNAL OF
PHARMACEUTICAL SCIENCES
SJIF Impact Factor: 7.187
https://doi.org/10.5281/zenodo.24443408

Available online at: http://www.iajps.com Review Article

AN OVERVIEW ON APPLICATIONS OF QUANTUM COMPUTING AND QUANTUM MACHINE LEARNING IN PHARMACEUTICAL SCIENCES

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Abstract:

Finding new medications is a crucial but difficult, costly, and time-consuming procedure. The quality of the predictions provided by computer-aided drug design tools, which usually rely on empirically generated functions, might be greatly enhanced by electronic structure approaches. With potential uses in healthcare and medicine, quantum machine learning is a new subject that combines artificial intelligence and quantum computing. Preclinical drug development and healthcare could be completely transformed by combining quantum computing with conventional high-performance platforms. In the end, this combination can result in more effective and efficient drug development procedures by enhancing data processing capabilities, speeding up research timelines, and optimizing the analysis of complicated biological data. The creation of novel treatments, medication design, and the simulation of intricate chemical interactions—including customized medicine approaches—can all be accelerated with the help of quantum computing. Quantum developments have the potential to reduce the time and expenses associated with the drug development process by streamlining it. The potential uses of quantum computing and quantum machine learning in the pharmaceutical sciences are discussed in this article.

Keywords: *artificial intelligence, quantum computing, computer-aided drug design, quantum machine learning*

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Please cite this article in press ***Asma A. Mokashi*** *et al.,* ***An Overview On Applications Of Quantum Computing And Quantum Machine Learning In Pharmaceutical Sciences.,****. Indo Am. J. P. Sci, 2026; 13(11).*

INTRODUCTION:

Pharmaceutical sciences are among the numerous sectors that have shown a great deal of interest in artificial intelligence (AI) and machine learning in particular. The quantity of data generated daily, including pharmacological data, has significantly increased. The phrase "big data" is becoming more and more popular in many fields of study. In pharmaceutical sciences, "big data" can therefore be seen as both a challenge and an opportunity. The possibility of employing big data in pharmaceutical sciences has increased with the development of AI, especially machine learning technologies that allow computers to "learn" and perform jobs [1].

Machine learning (ML)

A common AI technology is machine learning (ML) (Fig. 1), which enables computers to precisely adjust or change their activities (e.g., generating predictions). Supervised learning and unsupervised learning are the two main types of machine learning algorithms. The algorithm in supervised learning makes use of generalizations to react correctly to a collection of training samples. The input-output data included in the dataset to be learned are known as training examples. The output data are referred to as "targets" because they are known to be the right answers. In the end, the machine learning model seeks to forecast a result that is more in line with the goal. Regression analysis, support vector machines (SVMs), random forests (RF), and artificial neural networks (ANNs) are a few examples of supervised machine learning techniques. Principal component analysis (PCA) and other feature extraction techniques without examples are the foundation of unsupervised learning [2].

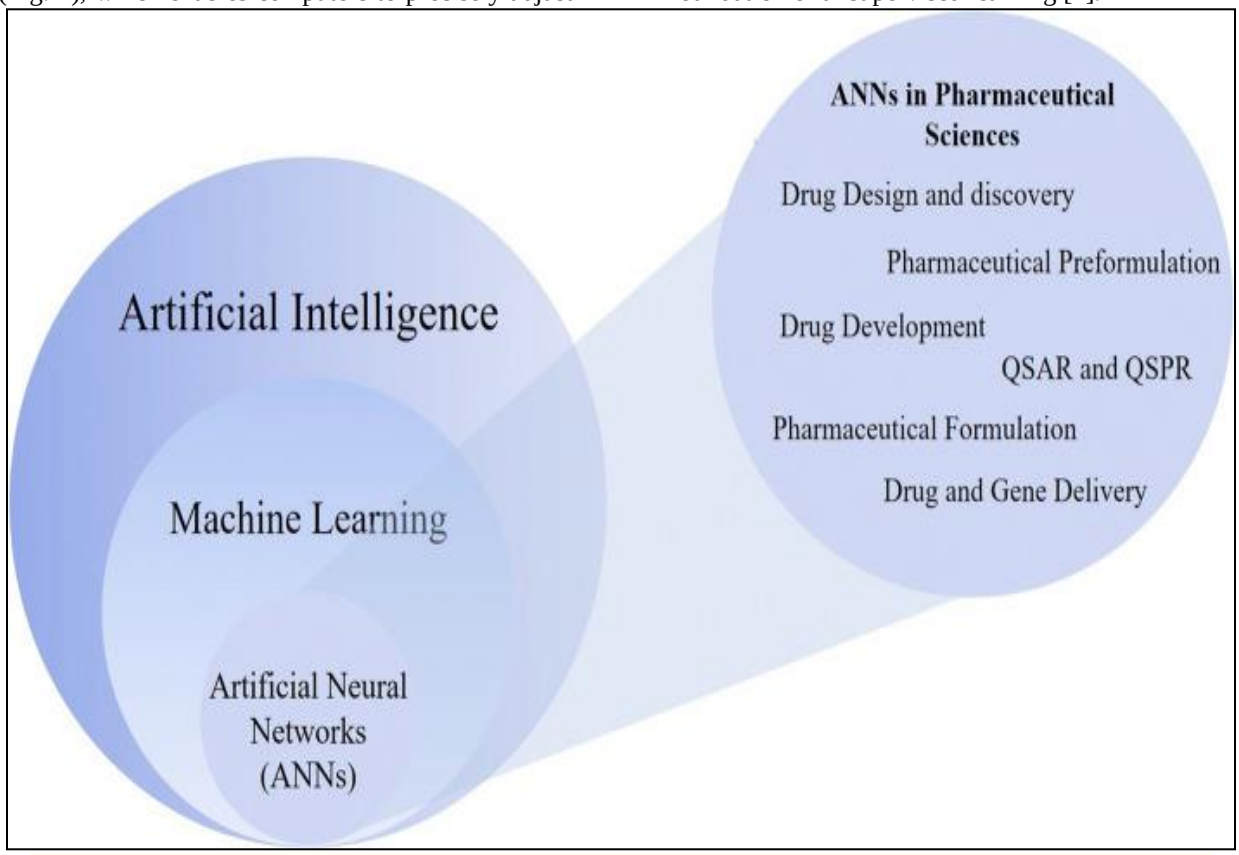

Fig. 1: Schematic showing the relationship between AI, machine learning, and artificial neural networks (left), and a number of applications of artificial neural networks in pharmaceutical sciences (right)

Unsupervised machine learning models like SVMs and ANNs may be supported by some supervised models [3]. Pharmaceutical sciences frequently employ machine learning techniques such as linear regression, ANNs, KNN, SVM, DT, and RF; PCA is regarded as an unsupervised dimensionality reduction technique that is typically integrated into computational manipulation of unlabeled data to identify a lower-dimensional collection of axes [4]. PCA is typically employed as a preprocessing tool in machine learning, even though it may be thought of as a statistical method for analyzing multidimensional data [5]. Table 1 includes summary of machine learning models.

Machine learning method	Learning algorithm	Machine learning model	Learning problem	Dataset size	Advantages	Disadvantages/ limitations
Linear regression	Supervised	Parametric	Regression	Varies	Easy implementation	Applicable only for linear modeling
Artificial Neural Networks (ANNs)	Supervised and unsupervised	Parametric	Classification and regression	Large	Modeling complex nonlinear relationships	Overfitting/ underfitting Relatively slow training time
K-Nearest Neighbor (KNN)	Supervised	Nonparametric	Classification and regression	Large (dependent on noise level in data)	Simple and easy to implement with single pre-defined parameter (*i.e.*, the number of nearest neighbors)	Intolerant of noise
Linear regression	Supervised	Parametric	Regression	Varies	Easy implementation	Applicable only for linear modeling
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K-Nearest Neighbor (KNN)	Supervised	Nonparametric	Classification and regression	Large (dependent on noise level in data)	Simple and easy to implement with single pre-defined parameter (*i.e.*, the number of nearest neighbors)	Intolerant of noise
Support vector machine (SVM)	Supervised and unsupervised	Nonparametric	Classification and regression	Small	Able to represent complex functions Offer resistant to overfitting	Relatively slow training time High complexity of the model Long computing time
Decision tree (DT)	Supervised	Nonparametric	Classification and regression	small	Easier than RF Can deal with noisy and missing data Fast	Unstable. Its performance can be affected by slight variations in the training data
Random forest (RF)	Supervised	Nonparametric	Classification and regression	large	Similar to decision trees in addition to its capability to overcome overfitting	Complex
Principal Component Analysis (PCA)	Unsupervised	Feature extraction	Classification and regression	Large	Reduces the dimensionality of multivariate data while maintaining the relevant information in the original dataset	It assumes Gaussian distribution of data which might limit their use if data are not normally distributed such as gene expression data
LightGBM**	Supervised	Nonparametric	Classification and regression	Large	Fast training speed High efficiency and accuracy	Sensitive to overall

Table 1: Summary of machine learning models

Quantum computing (QC)

In the pharmaceutical sector, computational chemistry is a crucial instrument. By making calculations that are currently unattainable conceivable, quantum computing (QC), a rapidly developing technology, has the potential to drastically alter computational capabilities in many fields of chemical research [6]. Drug design is a complicated process that combines wet-lab techniques with computers to find new medications. Although the majority of computer-aided drug design (CADD) techniques rely on statistical fitting techniques or classical mechanics, it has been suggested that more precise quantum mechanical techniques have a significant impact on a number of CADD aspects [7,8,9]. Quantum mechanics (QM) techniques offer a detailed description of chemical reactions and receptor-ligand interactions. Their application in drug discovery and design is growing, particularly for complex systems with metal ions in the binding sites, the creation of highly selective inhibitors, the optimization of bi-specific compounds, the comprehension of enzymatic reactions, and the investigation of covalent ligands and prodrugs. Additionally, they are employed in the parameterization of force fields and the generation of molecular descriptors for predictive QSAR/QSPR models. QM techniques are starting to be included in the conventional tools used in CADD because of the GPUs' constant improvement in processing capacity and the advancement of complex algorithms [10]. Since quantum computers are quantum systems in and of themselves, they are ideally suited to simulating quantum mechanical problems without experiencing exponential memory depletion. Accurate quantum approaches are anticipated to assist several areas of chemical research, including the pharmaceutical sector [11, 12]. QC offers special capabilities for solving complicated problems that are impractical for traditional computers, signifying a paradigm change in computational capacity. Advances in drug development, molecular modeling, genomics, and medical diagnostics have all been influenced by QC. Furthermore, important quantum methods are described, emphasizing their applicability in healthcare, including quantum algorithms, quantum machine learning (QML), and quantum-enhanced imaging. The article also discusses issues in the sector, such as integration in clinical settings, scalability, and hardware constraints [13].

Quantum Machine Learning (QML)

The new combination of QC and AI, known as QML, holds the potential to address computational issues that traditional systems are unable to handle. QML offers exponential speedups and new paradigms for data processing in machine learning tasks by utilizing quantum concepts including superposition, entanglement, and interference [14]. The pharmaceutical business has experienced significant change in the last few decades due to the incorporation of machine learning into different phases of the drug discovery process. Despite the fact that machine learning has expedited drug development and molecular screening, it still confronts significant obstacles such reliance on vast, high-quality datasets, limited interpretability, and increased computational complexity for huge systems. In order to overcome these constraints, QML has become a potent substitute that combines QC with artificial intelligence. QML offers increased accuracy and scalability by utilizing quantum systems' capacity to process high-dimensional data effectively. With an emphasis on molecular property prediction, docking simulations, de novo design, constraints, ethics, and future approaches, this study examines the contributions of QML to drug discovery [15].

The use of sophisticated computer techniques has significantly changed drug development and design in the current pandemic context. These approaches speed up the drug development process, improve accuracy, and save costs by utilizing advanced algorithms, machine learning, artificial intelligence, and high-performance computing. Predictive modeling, virtual screening, and de novo drug discovery have all been transformed by machine learning and artificial intelligence, making it possible to find and optimize new compounds with desired qualities. Understanding therapeutic efficacy at the atomic level is made easier by molecular dynamics simulations, which offer a thorough understanding of protein-ligand interactions and conformational changes. While structure-based drug design uses docking studies and fragment-based design to increase drug-receptor binding affinities, quantum mechanics/molecular mechanics (QM/MM) approaches provide accurate predictions of binding energies and reaction processes. To find new drug targets and comprehend intricate connections, network pharmacology and systems biology techniques examine polypharmacology and biological networks. Cheminformatics uses data mining to identify patterns in massive datasets while exploring enormous chemical landscapes. By anticipating negative consequences early in development, computational toxicology lessens the need for animal testing. To find biomarkers and comprehend how genetic variants impact drug response, bioinformatics combines genomic, proteomic, and metabolomics data. Finally, high-throughput screening and thorough data analysis are made possible by cloud computing and big data technology. When taken as a whole, these computational advancements are causing a paradigm

shift in drug design and discovery, making it more precise, efficient, and economical [16].

High drug failure rates during development, the need for larger and more complex clinical trials, a shift toward biologics and more complex small molecules, and an emphasis on complex and poorly understood drugs are all contributing factors to the declining R&D productivity in the life sciences sector, particularly pharmaceuticals. Innovative technology solutions, such as more accurate modeling tools, are desperately needed [17]. At present, the combination of quantum computation and machine learning has garnered significant interest in nearly every industry, including biology, chemistry, and various engineering specialties. By cutting development costs and time associated with the drug discovery process, quantum computers have the ability to increase high-throughput experimental procedures and screen billions of compounds [18].

APPLICATIONS of QC and QML

In Biomolecular dynamics simulation

The practicality of biomolecular dynamics modeling, a crucial tool for life sciences research, depends on its accuracy and efficiency [19]. When it comes to supporting large macromolecules, quantum chemistry methods such as density functional theory and conventional molecular dynamics simulation have limited precision and scalability [20, 21].

Wang et al. presented AI2BMD, an artificial intelligence-based dynamics simulation tool that effectively and precisely models the folding and unfolding of large proteins using protein fragmentation and a machine learning force field. Surrounded by an explicit solvent represented by a polarizable force field, AI2BMD is a generalizable solution that effectively simulates a variety of full-atom proteins with ab initio accuracy (Fig. 2). Proteins are divided into overlapping protein units using a generalizable protein fragmentation technique. The AI2BMD simulation system runs simulations. The AI2BMD potential, which is based on ViSNet7, accurately computes the protein's energy and atomic forces at each simulation step. AI2BMD shows good agreement with wet-lab experimental results after thorough investigation from the perspectives of kinetics and thermodynamics [22].

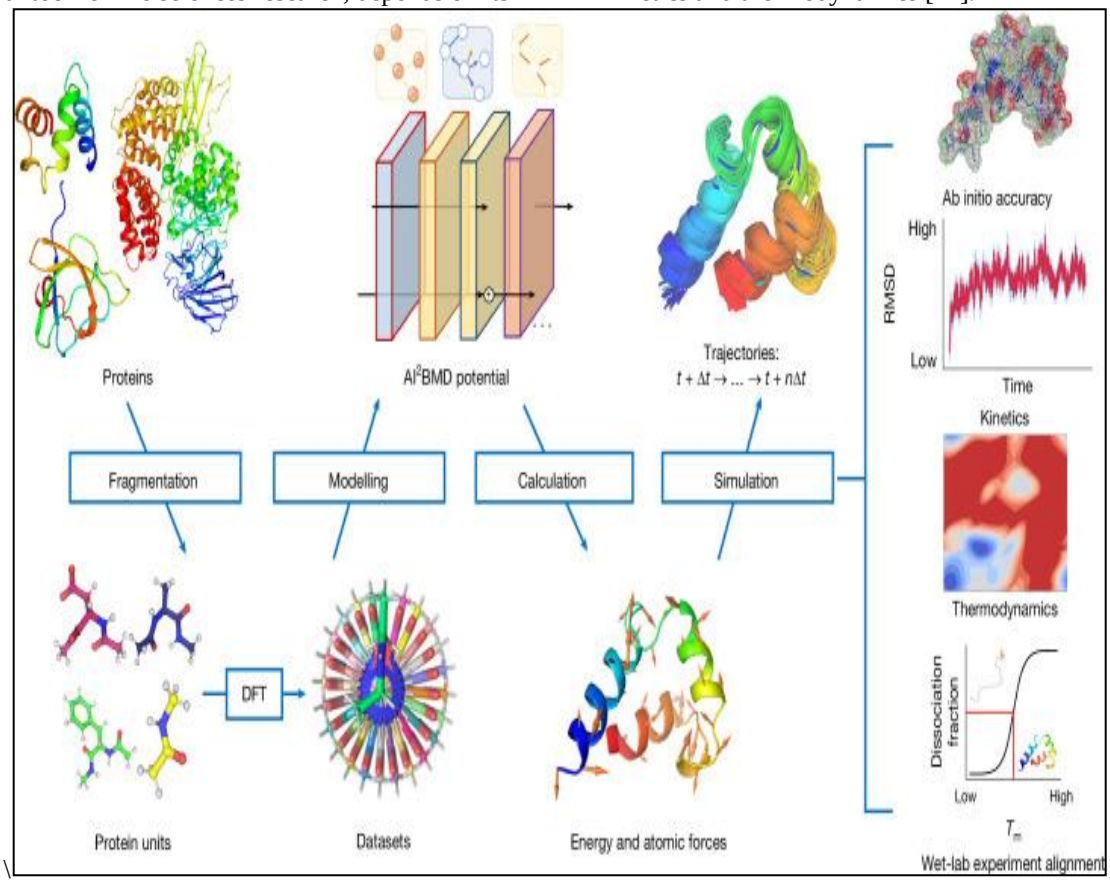

Fig. 2: The overall pipeline of AI^{2}BMD

Conformational flexibility (dynamics and induced fit upon binding), entropic considerations, inaccuracies in the deposited structural data (incorrect atom types due to missing hydrogen atoms, incorrect evaluation of functional group flexibility, inconsistent geometry restraints, fitting errors), chemical complexity (such as non-obvious protonation states), overly simplified atomic properties, and highly complex energy landscapes in molecular recognition by their targets are some of the factors that seriously impede biomolecule structure analysis and quantum chemistry. Currently, attempts to train AI models necessitate implicit inference of this missing data. This inference fails due to the small amount of protein–ligand structures (~20,000) that are publically available and the absence of thermodynamic data. Because of this, structure-based models are unable to yield innovative outcomes. Based on experimental protein-ligand structures, MISATO (molecular interactions are structurally optimized) is a protein-ligand structural database. MISATO is a structure-based drug discovery database that integrates molecular dynamics simulations on about 20,000 protein-ligand structures with QM data. The machine learning and drug discovery groups can easily access the artificial intelligence models that are included. According to Siebenmorgen et al., the database aids in improving model training in domains other than drug discovery. This covers bioinformatics, general structural biology, and quantum chemistry. It offered structural curation and refinement based on quantum chemistry, including ligand geometry regularization. It added missing dynamic and chemical data to this database, such as molecular dynamics (MD) on a timescale that enables the identification of transitory and mysterious states for specific systems. For drug design to be successful, the latter are crucial. As a result, it added as many physical factors as possible to experimental data. This makes it easier for AI models to learn all of this knowledge implicitly, freeing them up to concentrate on the primary learning task. An easy-to-use format that may be loaded straight into ML codes is offered by the MISATO database. Additionally, it offered a number of preprocessing scripts for dataset filtering and visualization. To facilitate adoption, example AI baseline models are provided for the computation of quantum chemical parameters (such as chemical hardness and electron affinity), the computation of binding affinity, and the prediction of protein flexibility or induced-fit features. The baseline models for QM, MD, and AI are thoroughly tested using experimental data. Our goal is to make MISATO an ambitious community initiative that will have a significant impact on the entire drug development industry [23].

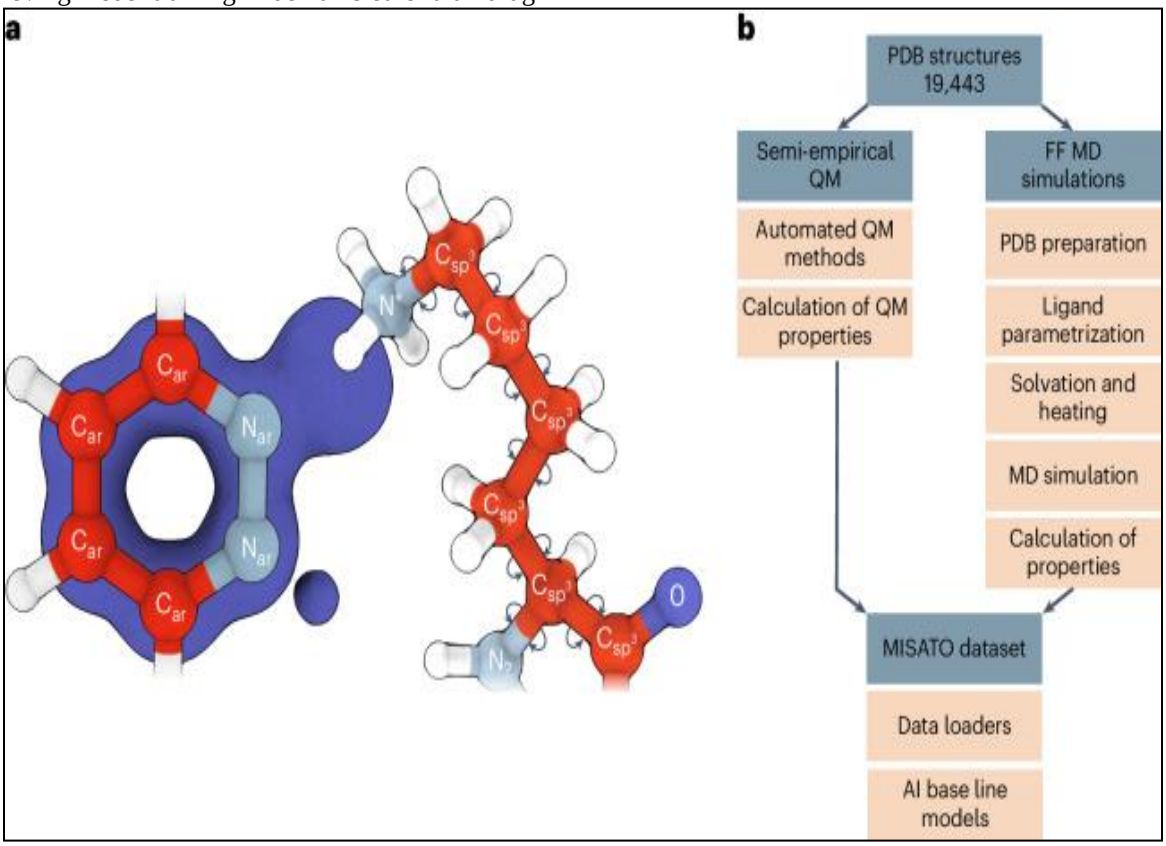

Fig. 3: MISATO combines QM data with MD-derived protein–ligand dynamics.

Leveraging antimalarial datasets, Dorsey et al. applied machine learning to create quantum Quantitative Structure Activity Relationship (qQSAR) models. By developing a Latent Bernoulli Autoencoder (LBAE) machine learning model to compress bit-vector descriptors to a size that can be computed with quantum computers for classification tasks with minimal loss of embedded information, it demonstrated a classical-quantum hybrid computational technique. They also extended their feature map reduction technique to quantum classification algorithms, such as the Classifier, an entirely new machine learning algorithm that has no equivalent in conventional computers. Using quantum simulation software, these approaches were applied to create quantum machine learning models for small molecule antimalarials, which were then compared to classical machine learning techniques [24].

In the realm of molecular modeling, machine learning potentials (MLPs) have become a significant topic of study. New MLP architectures that are intended to increase their accuracy, speed, transferability, and data efficiency have proliferated in recent years. One of the fastest-growing atomistic molecular simulation engines, OpenMM is a popular program for molecular modeling, particularly biological macromolecules. This flexibility is extended to MLPs by OpenMM 8. Two objectives are the focus of the new features listed below. They first give researchers creating new MLPs or simulation protocols a strong environment. It is simple to incorporate arbitrary PyTorch models into a simulation and use them to calculate forces and energy. Second, by enabling end users to choose from a collection of verified general-purpose MLPs and execute simulations with them, they close the distance to production simulations. These new features make it just as easy to set up and run an ML or ML/MM simulation as it is to use a traditional force field. In their research, Eastman et al. noted that OpenMM 8 adds new tools to facilitate the application of machine learning potentials in molecular simulations. For researchers creating novel pretrained potentials, OpenMM's tools offer a potent environment. Users who want to run simulations with those future potentials can then have easy access to them [25].

Additionally, a large number of quantum chemistry datasets have been released; however, their generality is typically substantially lower. It is improbable that a model will function in scenarios that are very different from the data used to train it. Any dataset will inevitably have a limited range of uses due to the almost unlimited nature of chemical and conformational space. For instance, there are extremely few chemical elements in some of the most widely used datasets. Some are limited in their ability to train potential functions that can be used in molecular dynamics because they only contain energy-minimized conformations. Some are only made up of neutral molecules, which make them less helpful for learning how to mimic charged substances. More datasets that can be utilized for different purposes are therefore constantly needed. A quantum chemistry dataset called SPICE was created to train machine learning potentials. It focuses especially on simulating the interactions of tiny compounds that resemble drugs with proteins. The original version includes forces and energies for 1.1 million molecular conformations that span a broad variety of chemical space, such as solvated amino acids, dipeptides, and pharmacological compounds. There are several covalent and non-covalent interactions, charged and uncharged molecules, low and high energy conformations, and a total of fifteen elements. Eastman et al. employed an updated version of SPICE that covers more than 20,000 additional compounds in chemical space. Additionally, it adds two extra elements (silicon and boron) and enhances sampling of non-covalent interactions. They used it to train Nutmeg, a collection of machine learning potentials. The TensorNet architecture serves as their foundation. To increase precision on charged and polar compounds, they employ a new technique. The model receives static, pre-calculated atomic partial charges as inputs, providing it with comprehensive data regarding the average charge distribution. In order to mitigate the instabilities present in many machine learning potentials, they also include a short-range repulsive term. They demonstrate the models' capacity to generate precise energy and steady simulation trajectories by validating them on a range of tasks [26].

The MD program GENeralized-Ensemble Simulation System (GENESIS) was created to model the conformational dynamics of a single biomolecule as well as molecular interactions between many biomolecules in cellular settings and in large biomolecular assemblies. In their description of GENESIS 2.1, Jung et al. emphasized aspects of atomistic, CG, and QM/MM MD computations. Additionally, we provided an overview of the recently released GENESIS data-driven simulations, trajectory analysis software, improved sampling techniques, and free-energy perturbations (FEPs). Additionally displayed are the computational results of the FEPs and atomistic, coarse-grained, QM/MM MD

simulations. Lastly, we talk about current developments that our teams and partners want to incorporate into upcoming iterations of GENESIS. With almost 50 tutorials spread over 16 sections, users may easily perform MD simulations using sophisticated approaches and create new functions and molecular models within the GENESIS framework because all implementations and algorithms are clear to them [27].

In evaluation of drug ADME-Tox properties

Combinatorial chemistry and high throughput screening in the 1980s and 1990s provided a significant increase in the number of compounds available that required testing after academia and industry had spent years developing in vitro methods for absorption, distribution, metabolism, excretion, and toxicity (ADME/Tox). At the same time, there was mounting pressure due to rising drug development costs and ADME/Tox attrition failure rates. It was then suggested that several kinds of computational models or filters may be used to overcome the issue of determining the ADME/Tox characteristics. Recent efforts have also been made to use a variety of computer models to predict drug-drug interactions using 3D pharmacophores and different molecular descriptors. We can confidently state that in silico ADME/Tox models have advanced significantly from their modest origins and tiny training sets in just over 20 years. The latest advancements in algorithms, software for de novo design of new compounds, and a move to larger molecules like PROTACS present potential to update the models' capabilities, even though there is still room for significant improvements. The quantity of data produced will thus be greatly impacted. It's possible that in vitro ADME/Tox data creation has already peaked and reached a tipping point when it becomes more focused. The need for generative molecule design integrated with these ADME/Tox models will now have to be given top priority by commercial software tools. As these programs create synthesizable molecules with optimal bioactivity and ADME/Tox properties, these predicted properties may eventually become undetectable to drug designers [28].

Bhatia et al. presented a QML system that combines a kernel-based quantum classifier with a traditional support vector classifier approach. The evaluation of chemical/drug ADME-Tox characteristics is done using a quantum support vector classifier and the simplified molecular input line entry system (SMILES) notation-based string kernel to show the viability of the proposed QML framework. Large-scale simulations are used to validate and evaluate the proposed quantum machine learning framework. According to our numerical simulation results, the quantum model outperformed its classical counterparts in terms of the area under the receiver operating characteristic curve (AUC ROC; 0.80-0.95) for predicting outcomes on ADME-Tox data sets for small molecules with varying feature counts. Making the best choices feasible would be greatly aided by the implementation of the suggested framework in the pharmaceutical sector [18].

Because medications with comparable features are more likely to share interaction targets and so influence each other's pathways, a common method for using machine learning (ML) in drug-drug interaction prediction has been to calculate similarity metrics between a drug's properties. In order to predict changes in drug exposure brought on by pharmacokinetic drug-drug interactions (PK DDIs), Gill et al. looked into the application of regression-based machine learning. From 120 clinical medication-drug interaction studies that were taken from the SimCYP compound library files and the Washington medication Interaction Database, fold changes in exposure compared to substrate drug monotherapy were gathered. Features of the drug, including its structure, physicochemical characteristics, in vitro pharmacokinetic parameters, cytochrome P450 metabolic activity, and demographic characteristics, were gathered. The prediction task was then subjected to three distinct regression-based supervised machine-learning models: support vector regressor, elastic net, and random forest. Fivefold cross-validation was used to assess the model's performance. Support vector regression performed the best, with 78% of predictions falling within two times the observed changes in exposure. The findings demonstrate that regression-based machine learning models trained on data available early in drug development may reasonably anticipate changes in drug exposure. This study has demonstrated that using features accessible early in the drug-discovery process, regression-based machine learning may be utilized to predict changes in substrate AUC due to PK DDIs produced by time-dependent inhibition/induction. Drug candidates' early DDI risk can be informed by predictive algorithms as explained here [29].

In Genomics and Personalized Medicine

In order to deliver individualized therapy suggestions, quantum algorithms can use a variety of data sources, including a patient's genome, medical history, and lifestyle factors [30]. By processing data in a fundamentally new way, quantum computing uses the

concepts of quantum mechanics to give previously unheard-of computer power. Quantum computing has the potential to improve patient outcomes and treatment quality. It promises better surgical accuracy, better patient outcomes, and individualized medical treatment due to its innate accuracy and sensitivity [31]. These intricate relationships can be more effectively modeled by quantum computers, which can spot trends and genetic abnormalities that lead to illnesses like cancer, Alzheimer's, and heart disease. In the field of personalized medicine, quantum models have the capacity to optimize treatment regimens by analyzing large datasets, including a patient's genetic information, medical history, and environmental factors, in order to customize treatments that are unique to each patient's genetic composition. By guaranteeing that treatments are both focused and flexible enough to accommodate each patient's own genetic profile, this customized strategy enhances treatment outcomes [32]. Genomic, transcriptomic, proteomic, and metabolomic profiles are examples of high-dimensional, multi-omics datasets that quantum-enhanced machine learning can analyze more quickly and accurately than conventional systems. Quantum computing has the potential to transform healthcare from a reactive to a fully predictive and preventive model by enabling the development of tailored therapeutic approaches in neurology, cancer, and uncommon genetic disorders by capturing the entire range of biological complexity [33].

In Medical Imaging and Diagnostics

A potent tool for improving diagnostic imaging methods is quantum machine learning (QML). Quantum algorithms are especially well-suited for pattern recognition, which can be used to find minute details in complicated medical images that traditional algorithms can miss. The goal of ongoing research on QML models is to increase the precision and speed of medical diagnoses using imaging data, with possible uses in automated diagnostic systems and early illness detection. In diseases like cancer and neurological disorders, where early detection is essential for effective treatment outcomes, this skill is particularly helpful [34]. Technically speaking, advanced picture denoising and dimensionality reduction can be accomplished using quantum methods like the quantum Fourier transform and quantum-enhanced principal component analysis (qPCA). Compared to their classical equivalents, these allow for quicker and more accurate analysis of high-resolution photos with fewer computer resources [33].

In Precision Medicine

Precision medical applications of quantum computing technology have the potential to revolutionize approaches to diagnosis, treatment, and data interpretation. Precision medicine and quantum computing indicate that QC uses different strategies to address precision medicine. Based on genetic and molecular data, QML aids in precision medicine by providing the appropriate medication to the appropriate patient. As a result, treatment efficacy increases, side effects are decreased, trial-and-error prescribing is avoided, early illness prognosis is aided, etc. For feature selection on genomic data, QA reformulates combinatorial problems into Quadratic Unconstrained Binary Optimization (QUBO) models [35]. Quantum Walks (QW) employ quantum interference to propagate networks for disease-gene prioritization on protein-protein interaction networks [36]. Hybrid quantum methods mix quantum subroutines with classical pipelines for molecular applications. The Variational Quantum Eigensolver (VQE) is used to calculate ground state energies for tiny molecules and drug-target interaction simulations. Quantum Approximate Optimization (QAO) handles molecular docking by reframing protein-ligand binding as combinatorial optimization that can be resolved by counter-diabatic driving [37]. These algorithms facilitate genetic analysis, ailment prioritization, and molecular modeling in precision medicine.

In Biomarker Discovery

Biomarkers play a major role in the gradual progress of medicine toward proactive, customized precision diagnosis and treatments. The identification of biomarkers may be considerably aided by the advanced information processing and methods for identifying complex connections that quantum computing offers. A biomarker is a particular characteristic that is measured as an indication of biological processes that are either healthy or ill, or as a response to an exposure or intervention. Biomarkers are biological molecules and other indicators of illnesses, as opposed to symptoms and more general medical results. Biomarkers might be based on physiological, histological, molecular, and radiographic characteristics. They might also be aggregate high-dimensional features [38].

CONCLUSION:

The application of quantum computing in conjunction with current computational techniques holds great promise for boosting success rates and speeding up drug discovery procedures. The versatility of quantum computing in pharmaceutical research is demonstrated by applications spanning from drug repurposing to

structure-based drug design. These technologies facilitate more effective screening of possible drug candidates and offer more precise predictions for drug design and drug discovery. Additionally, they are essential to the advancement of precision medicine, biomarker discovery, medical imaging and diagnostics, genomics, and personalized medicine. Prominent partnerships between quantum computing businesses and pharmaceutical corporations have already started to produce useful applications in drug discovery processes. Ongoing technological advancements and growing industry usage point to a promising future, despite present difficulties with hardware, algorithmic development, and worker competence.

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