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Artificial Intelligence and Machine Learning in Health Science Technology from the Perspective of Quantum Biology and Biomedical Engineering: Using CHOP protocol from DNA to Aging

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Abstract: This work highlights the transformative synergy between artificial intelligence (AI) and quantum biology in advancing the detection and treatment of breast cancer. Recent clinical research in chemotherapy underscores the expanding role of AI-driven deep learning (DL) frameworks and machine learning (ML) applications in omics-based precision diagnostics, rational drug design, and personalized therapeutic strategies enabled through biomarker discovery. The integration of intelligent medical engineering with quantum biological principles and deep learning methodologies offers significant advancements in targeted drug delivery, minimizes the adverse effects and toxicity associated with chemotherapeutic agents, and enables robust real-time monitoring of treatment responses. Collectively, these innovations demonstrate substantial potential to enhance therapeutic efficacy and improve clinical outcomes in breast cancer management. One well-known method is the CHOP protocol, which combines cyclophosphamide, doxorubicin, vincristine, and prednisone. Therefore, we simulated a series of anti-breast cancer agents, including cyclophosphamide, 5-fluorouracil, and methotrexate, combined via a PEG linker using QM/MM methods. This approach aims to improve therapeutic effectiveness while reducing side effects, guided by deep learning and AI-based optimization strategies. Finally, this study provides an overview of current trends in AI-based healthcare nanotechnologies and concludes that integrating AI into healthcare offers significant benefits, paving the way for a more advanced and effective future in medicine. Finally, in a short, quantum biology here is the study of "life at the quantum scale," and AI is the tool that can decode and harness these effects for health and cognition. Finally, since AI optimization claims refer to assertions that artificial intelligence systems can improve efficiency, accuracy, performance, or outcomes in complex biological, medical, or engineering processes, such claims often involve enhanced biomarker detection, improved predictive modeling, such as biological aging clocks, accelerated drug discovery, personalized treatment optimization, or system-level integration of multi-omics data.

Keywords: breast cancer; artificial intelligence (AI); cyclophosphamide; 5-fluorouracil; methotrexate; machine learning (ML); deep learning (DL); molecular mechanics and docking simulation; QM/MM methods.

1. Introduction

Nowadays, Chemotherapeutic drugs exert their antitumor effects primarily by interfering with cellular replication mechanisms and inducing irreversible genetic damage in malignant cells. By impairing DNA synthesis and cell division, these agents suppress cancer progression and reduce uncontrolled tumor expansion. Several major categories of anticancer compounds are commonly used in oncology. Alkylating agents include altretamine, bendamustine, busulfan, carboquone, and carmustine. Another important group is the anthracycline family, which comprises drugs including daunorubicin, doxorubicin, epirubicin, idarubicin, aclarubicin, and mitoxantrone. Taxane-derived agents, such as paclitaxel, docetaxel, cabazitaxel, larotaxel, tesetaxel, and albumin-bound paclitaxel (Abraxane), are also widely used because they disrupt microtubule dynamics during mitosis. Additional therapeutic classes include topoisomerase- and histone-targeting agents, including camptothecins (e.g., camptothecin, irinotecan, topotecan, exatecan, and gimatecan). Molecularly targeted kinase inhibitors, including erlotinib, gefitinib, imatinib, vemurafenib, vismodegib, and bortezomib, are designed to block signaling pathways essential for cancer cell survival and proliferation.

In clinical oncology, multiple anticancer agents are frequently administered together in multidrug regimens, commonly referred to as combination chemotherapy or polychemotherapy. This strategy is intended to improve therapeutic response while minimizing resistance development. One well-known example is the CHOP protocol, which combines cyclophosphamide, doxorubicin, vincristine, and prednisone. Other frequently applied combinations involve cyclophosphamide (CP), 5-fluorouracil (5-FU), and methotrexate. Beyond conventional cytotoxic chemotherapy, cancer pharmacotherapy also includes endocrine-based therapies and biologically targeted treatments. These noncytotoxic modalities act by selectively interfering with hormonal activity or specific molecular signaling pathways involved in tumor development and progression. In contrast, therapeutic agents that interfere with hormone-mediated growth signaling pathways, particularly estrogen signaling in breast cancer and androgen signaling in prostate cancer, are categorized as hormonal therapies. Furthermore, compounds designed to inhibit receptor tyrosine kinases and other growth-signaling pathways are classified as targeted therapies. Collectively, chemotherapy, hormonal therapy, and targeted therapy are referred to as systemic therapies because they are delivered through the bloodstream and can exert therapeutic effects throughout the body. These systemic approaches are frequently integrated with local treatment modalities such as surgery, radiotherapy, and hyperthermia, which act specifically at the treatment site. This study is organized into four principal sections. The first section examines the applications of AI, ML, and DL within the biosciences. The second section focuses on cancer biomarkers and their diagnosis using AI-driven methodologies. The third section presents the design of a novel therapeutic candidate developed through quantum biology modeling, employing QM/MM simulations of cyclophosphamide, 5-fluorouracil, and methotrexate conjugated via PEG linkages. The fourth section provides the experimental and computational findings, followed by a comprehensive discussion evaluating the therapeutic effectiveness of the proposed drug against breast cancer using AI- and deep learning–based analytical models. The primary aim of this research is to investigate the contribution of AI and ML to advancing healthcare technologies through the integrated frameworks of quantum biology and biomedical engineering, encompassing biological mechanisms from DNA-level interactions to systemic

aging processes. The specific objectives of the study are as follows:To develop and assess deep learning models capable of identifying aging-associated biomarkers from multi-omics datasets, including genomic, epigenomic, proteomic, and metabolomic data. To design and optimize AI-driven biological aging clocks that integrate molecular, physiological, and clinical indicators. To investigate the application of generative AI systems for the development of dual-targeting therapeutic candidates aimed at modulating both aging pathways and age-related diseases. To explore the computational modeling of quantum biological mechanisms, including electron transfer, mitochondrial dynamics, and DNA stability, using AI-based methodologies. To evaluate the translational potential of AI-enabled biomedical engineering technologies, such as biosensors, imaging systems, and wearable devices, for real-time aging assessment and personalized therapeutic interventions. The hypotheses proposed in this study are outlined below: H_1: Deep learning architectures integrating multi-omics datasets will achieve significantly greater predictive accuracy in estimating biological age compared with conventional machine learning approaches.

H_2: AI-based biomarker discovery methods will identify novel molecular signatures associated with aging that remain undetectable using traditional statistical techniques. H_3: Generative AI models will facilitate the design of dual-targeting therapeutic compounds capable of simultaneously modulating aging pathways and disease-specific mechanisms more efficiently than conventional drug discovery methods. H_4: Incorporating quantum biology-informed parameters into AI frameworks will enhance the mechanistic interpretability and predictive performance of computational aging models. H_5: AI-integrated biomedical engineering technologies, including intelligent biosensors and advanced imaging systems, will improve the early detection and longitudinal monitoring of physiological changes associated with aging.

2. AI and related components

2.1. Biological concepts of ML and DL.

Nowadays, ML has become a powerful tool in the fields of biomedical engineering and health science technology, leading to a transformation in the way information is examined, understood, and used in clinical and research settings. Popular computational approaches often struggle to meet the analytical requirements as biological data becomes increasingly complex and precise due to advancements in DNA sequencing, imaging technologies, MRI, and OMICS platforms. Additionally, AI, particularly ML, deep learning (DL), Reinforcement Learning (RL), and natural language processing (NLP), offer advanced and quantifiable methods for processing and comprehending biological data, accelerating progress in medical engineering and improving biological outcomes. During the investigation of computational methods in the early 1990s, AI was first applied to the study of DNA and protein sequences, marking its beginnings in biomolecular research. The volume of bioinformatics data, such as genomic information, has increased significantly with next-generation sequencing (NGS), necessitating more advanced and flexible computational systems. Since then, AI has progressed from focusing on primary sequences in RNA and DNA to predicting protein structures, diagnosing mutations, detecting biomarkers associated with diseases, and aiding in real-time, accurate medical decision-making, and has earned Libbrecht a Nobel Prize in 2015 [1]. Using AI in health science technology, biomedical engineering, and biology goes beyond automation. In other words, AI makes predictive and prescriptive simulation possible, enabling the mimicry of biological phenomena and revealing hidden aspects in intricate datasets. In 2015, scientists

at Harvard and MIT investigated deep learning based on a deep mind algorithm [2]. This pattern discerns RNA-binding enzyme sites and reveals previously unknown regulatory nucleotides in the genome. Researchers are progressively using this groundbreaking technology to address biological phenomena, from predicting protein folding to identifying disease-causing mutations [3,4]. For instance, DeepMind's AlphaFold uses advanced neural networks to accurately identify the 3D structures of enzymes, leading to new insights in quantum biology. These advancements have significantly impacted genomics, medical engineering, medicinal plant discovery, and drug design. Nowadays, utilizing AI and ML in quantum biology has improved genomics approaches, disease detection, and drug delivery methods [4]. AI is capable of accurate analysis of genomic data and DNA mutations, and it supports disease treatments and cancer therapy [5, 6]. Furthermore, it predicts the effective mechanisms of drugs through identifying cellular targets, consequently reducing trial-and-error experiments. By analyzing DNA genetics, RNA translation in ribosomes, and other biological phenomena, DL uncovers subtle algorithms that are beyond our current understanding of biological mechanisms [7, 8]. It is notable that AI and DL patterns require high-quality databases that are insufficient in some biological aspects [8, 9]. The foundations of machine learning (Table 1) were established in 1986 and subsequently expanded in 2000 by Igor Aizenberg and his collaborators through the integration of artificial neural network methodologies based on Boolean threshold neurons [10]. The emergence of large-scale biological databases, together with significant advances in computational capacity, has accelerated the development of deep learning approaches, demonstrating their substantial influence on modern biological and biomedical concepts.

Table 1. Convolutional neural networks, recurrent neural networks, as well as transformers in DNA, genomics, protein folding, and OMICS for evaluating single cells.

Category	DL Algorithm	Using in quantum and computational Biology	References
supervised by deep learning	Deep Survival investigation	Cancer recognition	[5]
	CNNs or Convolutional Neural Network	Gene expression evaluation and Histopathology image investigation	[11-13]
	Reversible Neural Network (RNNs)	DNA sequence detection and prediction of Protein folding, including gene co-regulation	[13-15]
	Short/long Memory (SLTM)	RNA analysis prediction	[16]
	Convolutional Recurrent Neural Network (CRNN)	Analysis of the Chromatin situation	[17]
	Deep Neural Network (DNN)	Meta-genomic investigation	[18]
	Deep Transfer Educating and Learning (DTE)	Drug sensitivity detection	[19]
	Deep Clustering	Cell and tissue samples recognition	[20]
Unsupervised DL but generative	Inimical Generative Networks	artificial biology, artificial protein folding and designing, artificial data generation, and artificial gene synthesis	[21-23]
	Auto encoders variables	Metabolism information and single-cell genomics, including prioritization of gene-disease associations	[24-26]
	Autoencoders	Disease prediction and detection, using single-cell epi-genomics evaluation, including DNA motif exploration	[27,28]
	Deep self-reliance Networks	diverse Genetic categories, Recognition of drug side effects, Structure detection for proteins	[29,30]
	Inimical autoencoders	phenotypic screening according to Image-based and Gene expression information	[31,32]
	Deep learning of the Boltzmann Machines	Epigenetic data investigation	[33]
	Deep Generative machines	genetic sequence produced in DNA	[34]

Category	DL Algorithm	Using in quantum and computational Biology	References
The latest designs and architectures	Transducer Networks	RNA detection and transcription, investigating, including protein contact recognition	[11,21,35,36]
	Mesh working charts for Neural Networks	Diagnosis of Protein–protein interaction and drug targeting; Cell type classification from the viewpoint of single-cell transcription	[25,37,38]
	Convolutional Mesh charts for networks	Predictions of Drug–goal interaction; Drug action and targeting network evaluation	[39- 41]
	DL and RL activities	Drug exploration and Drug target recognition, including Protein folding as well as prediction of Protein–ligand interaction affinity; Antibiotic resistance detection and genome sequence designing	[40- 43]
	Capsule Networks	Protein structure categorization, Function of Protein–protein interaction, and cancer subunit grouping	[44,45]

Figure 1 illustrates the central objective of AI, which is to integrate concepts from mathematics, quantum science, and biology into a unified interdisciplinary framework capable of influencing a wide range of scientific and technological domains. Within this framework, deep learning (DL) and ML represent fundamental branches of AI that continuously learn by extracting information and patterns from diverse direct and indirect data sources within intelligent systems. Advanced DL and ML architectures enable the processing of complex multidimensional datasets, thereby supporting the development of increasingly sophisticated AI technologies. Such progress may ultimately lead to the emergence of highly autonomous, potentially self-aware artificial systems.

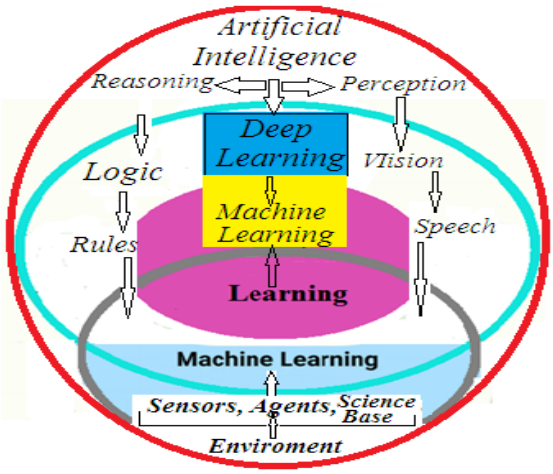

Figure 1. Schematic representation of the major components of artificial intelligence.

2.2. Cancer-treatment via AI.

Statistical analysis combined with the Monte Carlo randomization method was employed as a predictive modeling approach to evaluate the prognosis of follicular lymphoma. Stochastic number generation was utilized to construct multiple neural network models capable of identifying pathogenic marker genes associated with disease progression [46]. Egwom *et al*. [47] also investigated an LDA-SVM-based machine learning model for categorizing various types of oncologists' diseases, with a particular focus on breast cancer. They utilized linear discriminant analysis (LDA) to detect cancer features, which resulted in increased prediction accuracy. A DL model named Sturgeon was trained on methylation profiles of Central Nervous System (CNS) tumors. It is capable of categorizing the tumors' sub-genome with a scanning time between 50 and 100 minutes [48]. Additionally, a detectable model was shown to predict Caspase-8 in B-cell lymphoma using the algorithm suggested by the expression of other genes

[49]. The CanProSite [50] and MutBLESS [51] web servers were adapted to detect potential cancer sites using deep learning models. CanProSite [50] was used to identify DNA mutations in lung cancer, while MutBLESS [51] was used to detect mutations in 20 cancer types, classified into five cancer categories: breast cancer, endometrial carcinoma, acute myeloid leukemia, stomach cancer, and skin cancer. Recently, *GBMDriver* [52] represents a machine learning–based platform specifically designed for brain tumor analysis. This system employs predicted amino acid secondary structure. In addition, a variety of computational approaches have been introduced to evaluate the functional consequences of genetic mutations, including AlphaMissense [53], *FATHMM* [54], Mutation Assessor [55], *SIFT* [56], *PROVEAN* [57], and *CADD* [58]. These predictive frameworks demonstrate strong accuracy in identifying genomic regions associated with cancer susceptibility, thereby supporting the discovery and development of targeted therapeutic strategies.

2.3. Application of "AI" in biomedical engineering.

AI is an expanding discipline within computer science that integrates data science techniques to develop and analyze intelligent computational systems. Its ability to process and interpret large-scale datasets makes it a valuable tool across multiple domains, particularly in biomedical engineering and medical sciences. In public health and epidemiology, AI supports disease detection, surveillance, and early intervention strategies [59]. Moreover, AI incorporates geospatial analytics to examine environmental and spatial factors influencing disease transmission and monitoring, thereby enhancing epidemiological understanding [60]. In healthcare administration, AI offers significant operational advantages, including optimization of pharmaceutical supply chains, workforce scheduling, and hospital resource allocation [61]. Several organizations, such as IBM Watson Health, have developed AI-driven platforms that assist clinicians in delivering personalized medical care based on individual patient histories and genomic information. Such approaches improve diagnostic confidence and may reduce healthcare costs by minimizing unnecessary diagnostic procedures [62]. AI also extends healthcare accessibility, particularly for elderly populations, by enabling portable and remote monitoring technologies. These systems enable continuous health tracking outside clinical environments and support telemedicine applications [63]. In addition, AI-enabled technologies are increasingly applied in sports and wellness domains under the concept of "smart fitness," allowing long-term monitoring of physiological and performance-related metrics during physical activity [64]. Figure 2 illustrates key applications of biomedical engineering within healthcare systems. Artificial intelligence was designed as a cornerstone of biomedical engineering to enhance detection abilities, develop AI biosensors for cancer treatment, improve the efficiency of biomedical devices in hospital instruments, and enhance the quality of healthcare systems [65]. For example, in MRI and medical imaging, it improves resolution, leading to clearer image details and reducing mistakes that could occur when viewed by human eyes.

A novel AI created by Google Health, based on a large dataset of mammograms, was analyzed in real clinical data and outperformed human radiologists by making fewer false positives and false negatives. This model was modified and improved by radiologists to interpret breast cancer from mammograms [66]. Furthermore, physicians using these systems and AI tools should be aware of how they operate and be able to analyze predictions, assess efficiency, and compare results to determine the best-fit outcome for their clinical applications [67].

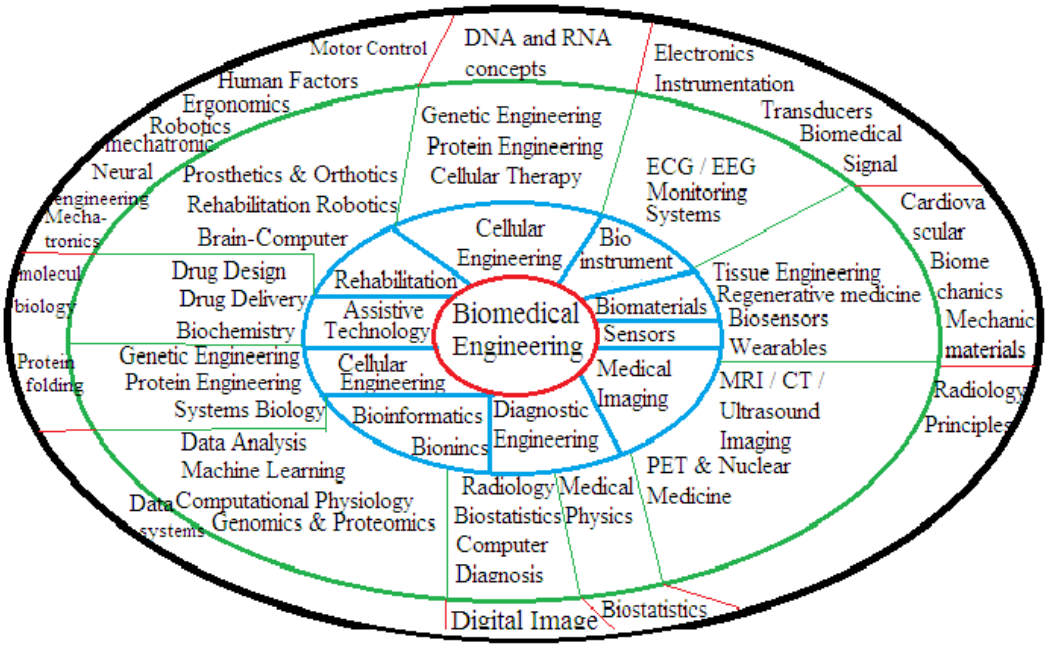

Figure 2. Biomedical engineering scheme: This diagram exhibits a multidisciplinary field of biomedical engineering related to an AI model, consisting of engineering, biology, medicine, quantum physics, and several other sciences. Its aim is to develop innovative solutions for healthcare and medical treatment based on AI.

Another system, known as Class Activation Mapping (CAM), enhances MRI imaging by providing clear visual insights into AI decisions by focusing on key regions affected by AI outcomes [68]. Therefore, AI's collaboration with biomedical engineering enables comprehensive biomedical research, shaping the future of healthcare and improving treatment outcomes in the digital world. The use of AI in medical care is progressing over time. For example, AI is being used to discover 3-D macromolecules such as DNA, RNA, enzymes, and membranes in the nanobiotechnology industry. The synthesis of drugs and biomaterials is becoming more efficient thanks to AI's role in developing drug and chemical products. AI enables assistance in drug design and discovery, with a focus on developing biochemical products in metabolic engineering, immunology, and pharmacology [69]. AI has benefits in pathogen analysis and in the clustering of pathogen resistance patterns among antimicrobial bacteria, which is a key area for global health [70]. AI basically involves replicating human intelligence within machine systems, enabling us to achieve tasks that typically require human understanding and make informed decisions. Biomedical engineering is advancing thanks to AI concepts that can solve many complex healthcare problems. However, integrating AI into interdisciplinary features requires accurate details and focus in order to increase its contribution to related issues. AI in biomedical engineering spans several fields, including medical imaging, disease detection, and disease treatment. It has become a vibrant field where advanced algorithms are improving the precision of patient results and treatment planning.

2.4. Quantum biology progresses under artificial intelligence

This subject encompasses subfields of AI, including automated planning, machine learning, deep learning, computer vision, natural language processing, and operating systems. It is notable that AI quantum biology involves using computational methods to solve biological phenomena. One dimension of quantum AI refers to the application of quantum computing for solving computational problems in AI. Approaches for AI include ML and deep learning (DL)

methods that support the entire mechanism of quantum patterns, theatrical design, parameter optimization, the design of quantum circuits, error removal during execution, and the calibration of quantum devices (Figure 3). These components form the foundation of AI in the field of biological sciences. Although the design and execution of quantum patterns are usually carried out manually by human experts, there are various ML and deep learning (DL) approaches that support AI for both experimental and theoretical design and protocol development. Therefore, most approaches to protocol design suggest using reinforcement learning to minimize the impact of human operators [71]. Therefore, the method MELVIN proposes using ML models to discover novel biological methods for experimental data to create and manipulate complex quantum states. Therefore, the method MELVIN proposes using ML models to discover novel biological methods for experimental data to create and manipulate complex quantum states. In other words, creating experimental information can be achieved through optical components, random control of quantum states, calculation and analysis, and simplified structures defined by the user. It is notable that the MELVIN method demonstrated correct and useful but unfamiliar, asymmetric techniques that are difficult to analyze.

According to the methods developed by Melnikov and his coworkers [72,73], they use the ML-based projective simulation approach based on Reinforcement Learning (RL) to design experimental information. For example, Melnikov employed projective modeling to investigate a photonic quantum system using data from biological experiments that involved multi-photon states entangled in high dimensions. Consequently, these insights emerge through highly experimental techniques, especially by interacting with a set of optical elements to design experiments. These elements evaluate the quantum states' information and receive rewards according to the given state before iterating the process. In [73], a similar method was applied to discover and optimize protocols for long-distance quantum bioscience. The results showed that reinforcement learning enabled quick identification of solutions that outperformed those designed by humans for long-distance communication challenges.

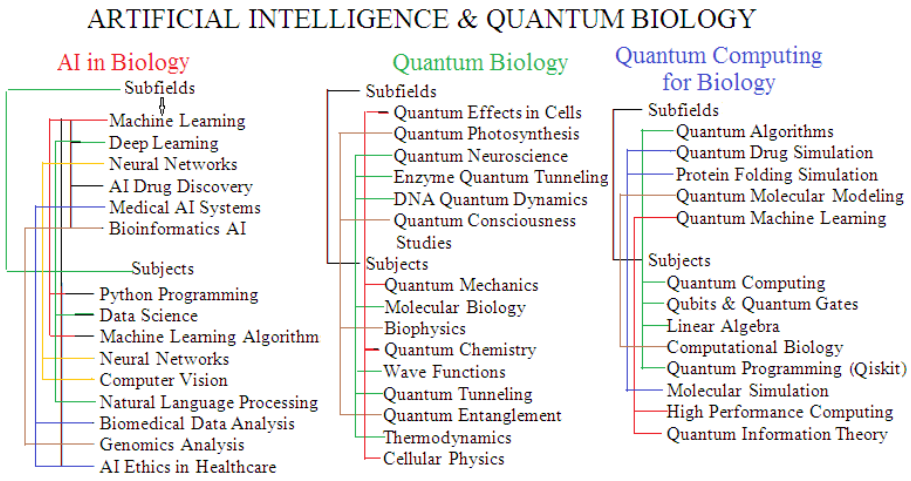

Figure 3. A collection of tasks in the structures of quantum biology computing devices, combined with AI techniques.

3. Biomarkers

3.1. Biomarker detection through quantum techniques and artificial intelligence

By utilizing quantum techniques, we can detect DNA mutations, RNA patterns, proteins, and metabolites. For example, quantum control involves fine-tuning the quantum

states of spin-spin coupling in biological systems. Quantum mechanics offers significant potential for enhancing cancer biomarker detection [74] through precise manipulation of quantum approaches and the quantum states of biological probes [75-77], such as chemical tags or labels, antibodies, and contrast agents (refer to Figure 4 and Table 2). This improves the sensitivity of biological probes [78-80]. These techniques enhance optical measurements by increasing binding specificity, improving imaging quality, and enabling early cancer diagnosis. In the field of quantum nanomolecules, quantum dots (QDs) have been widely recognized as essential tools for biomarker detection [80]. These semiconductor materials enable ultrasensitive detection [81] and simultaneous detection of multiple cancer biomarkers, thereby increasing diagnostic speed as much as possible. Quantum dots (QDs) that have been enhanced through quantum control [82,83] exhibit special optical and unique electrical properties. This makes them ideal as fluorescent tags, particularly for antibodies, aptamers, oligonucleotides, or peptides, enabling precise targeting [84-86]. In addition to quantum dots (QDs), nitrogen-vacancy (NV) atoms in diamond nanoparticles also play a critical role in diagnosing biomarkers [87, 88]. These quantum Nano-probes, such as QDs or NV diamonds, detect specific cancer biomarkers using related Nano-sensor instruments and provide highly sensitive evaluation performance. They also facilitate the extracellular delivery of detection agents through quantum tunneling [89, 90]. Furthermore, QDs function as nanoreporters, providing information on the presence of biomarkers through their fluorescence signals. QDs play a crucial role in cancer analytical systems, such as microarrays, by enabling PCR measurements across various temperatures and DNA lengths.

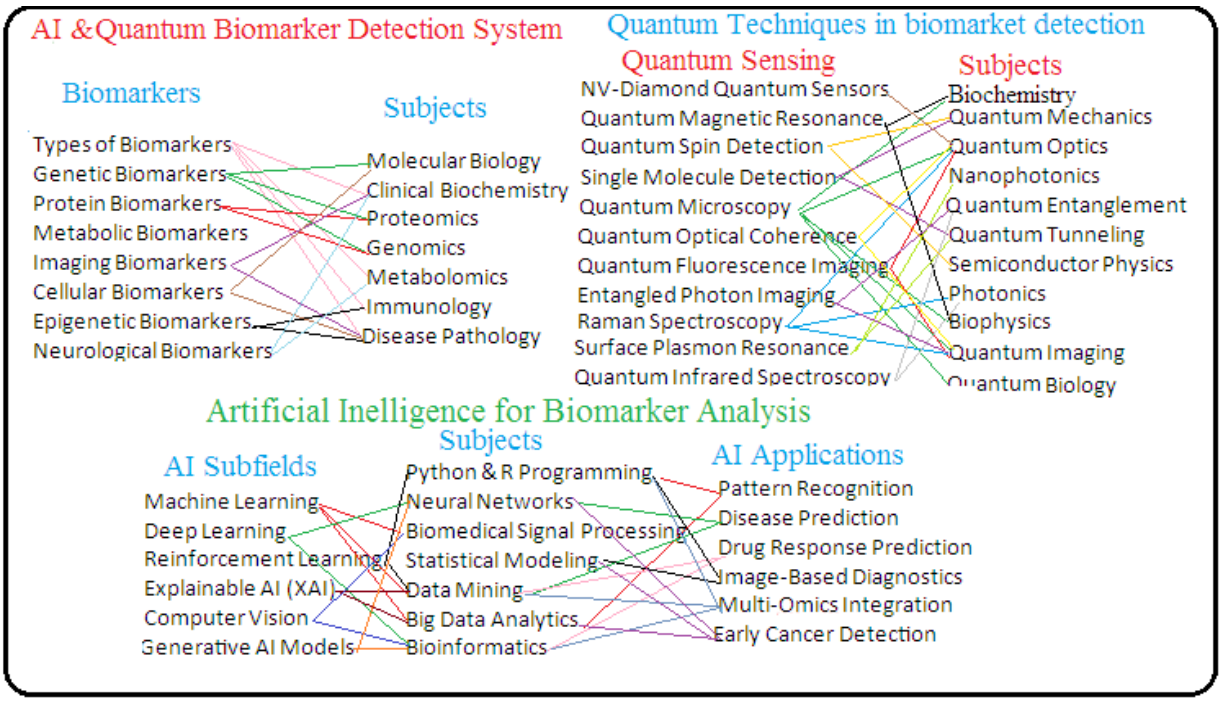

Figure 4. Scheme diagram of AI-Quantum biology applications in biomarker detection and cancer therapy.

They are also used in nanoscale electrical sensors according to their superior photo stability, high fluorescence signal, decreased spectral blue shift, and optimized blinking. For instance, those methods were applied to detect specific biomarkers, such as CA-125 from pancreatic cancer, that are derived from miRNAs. These advancements lead to more accurate biomarker diagnosis and improved discrimination between normal and various mutated sequences. This is crucial for identifying unique mutations such as EGFR [91] in breast cancer

or KRAS [92], which is common in lung and colon cancer, enhancing sensitivity for diagnosing minor variants.

Table 2. Various quantum technologies.

Bio system	Methode	Technology	Running a quantum application	Advantages
RNA	Sequencing and NGS technique	DNA or NA extraction and PCR	Quantum calculations [93–96]; quantum bio markers, including: antibodies improving [97, 98]; enzymology [99–102]; quantum foundation and basic [103,104]; single molecular genetic sequencing [105, 106]; using quantum thermometry [107,108]; increasing gaussian amplitude [109,110]	Quick conversion, saving material loss, improved properties, brighter in resolution, increasing accuracy, huge reading, quick analysis, and decreasing sequencing errors
	Single sequencing in RNA	Microfluidic instrument including NGS; PCR	Similar to the above row techniques, in addition, quantum microfluidics integrated with quantum sensors [111,112]	Advanced single-cell isolation; accurate in RNA extraction; proper transcriptome characterization [113–115]
	Ribo-seq	Ribosome trace isolation NGS	Quantum application of free enzyme; quantum sensors; quantum microfluidics [111,112]; quantum computers	enhancing sensitivity, reducing bias, increasing resolution, and faster data processing
Protein	Testing and Immunology Protein/Protein interaction	properties Interactions for Y2H and Co-IP; for antibody Western blotting	Quantum of biomarkers [116,117]; quantum sensors [118]; quantum computers [119-121]	increasing accuracy of multiplexed bioprobes [122,123], minimizing enzymology, enhanced sensitivity, improved background noise [122,123]
	Proximity Labeling	Enzyme-based tags: purification and identification of proteins	labeling of quantum microfluidics [111,112]	Accurate controlling, improving sensitivity, and perfect analysis
Metabolic	Mass Spectrometry	Ionization; mass spectroscopy analysis and recognition	chemical quantum mass spectrometry (QC-MS) [124–126]; superconducting qubits and trapped ions by quantum sensors	Improved signal versus noise sensitivity, multiplexing potential, and quick analysis [124]
	NMR Spectroscopy	strong field magnetism; IR pulses; signal detection	Quantum-based resonance; quantum-based magnetometry [126]	Facilitating analysis, improving performance, and recognizing low-amount metabolites recognition
Cells/Tissues	Confocal Microscopy	Laser and fluorescence light emission	Quantum control of biomarkers; High-resolution of entangled photons [127,128]	Improved sensitivity ratio of signal-to-noise, increased resolution imaging
	Electron Microscopy	TEM, SEM, and vacuum systems	Quantum-based electron light emission; quantum-based vacuum pumps; quantum qubits and trapped ions	selective spectrophotometry; nanoscale resolution, improved coherence, and quicker processing, lower noise
	Flow Cytometry	Microfluidics; opto-acoustic forcing, sorting, or recognition [129, 130]	Quantum fluidic approach, quantum microscopy opto-acoustics [129]	Quick analysis, increased sensitivity (improved signal-to-noise ratio), super resolution, single subcellular analysis

3.2. Various biomarkers in human saliva for breast cancer detection.

Breast cancer (BC) remains one of the leading causes of cancer-related mortality among women worldwide [131]. The rapidly increasing incidence of BC underscores the critical importance of early diagnosis, which not only improves therapeutic efficacy but also mitigates the psychological, economic, and social burdens associated with the disease [132-136]. Nevertheless, early detection is frequently impeded by economic constraints and sociocultural barriers, particularly in low- and middle-income settings [137,138]. Consequently, considerable research effort has been directed toward identifying reliable liquid biomarkers and assessing their diagnostic utility [139,140]. Liquid biopsy approaches, particularly those

targeting tumor-derived biomarkers in blood and saliva, have attracted growing interest for cancer detection and prognostic evaluation [141,142]. Among these biofluids, saliva has emerged as a promising diagnostic medium due to its potential to detect cancer before the manifestation of clinical, histological, or radiological abnormalities, thereby supporting the advancement of personalized medicine strategies [143–145]. Saliva reflects systemic physiological and pathological conditions and has been increasingly explored for the screening, diagnosis, and monitoring of BC [146,147]. Recent studies have reported a diverse spectrum of salivary biomarkers, encompassing proteomic, metabolomic, transcriptomic, and reagent-free biophotonic signatures [148–163], collectively referred to as "salivaomics" [164]. Saliva-based diagnostics offer several practical advantages, including non-invasive, straightforward sample collection; minimal training requirements for personnel; rapid processing; ease of storage and transportation; reduced susceptibility to clotting; and lower occupational risk for healthcare workers [165–167]. However, biomarker composition and concentration in saliva may differ substantially from those in other biological fluids [168-170], underscoring the need to rigorously validate salivary biomarkers with adequate sensitivity and specificity for BC detection. Notably, accumulating evidence indicates that salivary and mammary gland cells share functional and pathological similarities [171–174]. Moreover, salivary gland cells release exosome-like microvesicles containing proteins and mRNAs, which can be detected in saliva and may serve as valuable molecular indicators of breast cancer. Multiple studies have investigated alterations in salivary protein profiles in breast cancer (BC) patients using diverse analytical approaches [175–177].

Additionally, the diagnostic potential of salivary C-erb-B2 (HER2) has been evaluated, with evidence suggesting its possible utility as a noninvasive biomarker for BC detection [178,179]. Salivary sialic acid (SA) has also been examined, including the influence of disease stage and chemotherapeutic interventions on SA levels and the salivary sialo-glycomic profile of BC patients [180]. Furthermore, salivary concentrations of lectins, polyamines, and N-acetylated compounds have been assessed across multiple investigations [181,182]. Notably, Porto-Mascarenhas *et al*. reported that salivary biomarkers may be more detectable in advanced stages of BC than in early-stage disease [183]. In parallel, recent salivary metabolomic analyses have demonstrated the capacity of specific metabolite signatures to discriminate BC patients from healthy controls [154]. Moreover, emerging evidence indicates that certain salivary mRNAs may possess high diagnostic accuracy, underscoring their potential role in BC screening and early detection [147,150]. Despite the growing body of salivaomics research and the consistently promising findings supporting salivary-based diagnostics, substantial heterogeneity exists among published studies. Variations in sample size, saliva type, collection protocols, biomarker classes, analytical platforms, and detection methodologies may significantly influence reported diagnostic performance. Consequently, a comprehensive systematic evaluation of salivary biomarkers as reliable diagnostic tools for BC is critically warranted. To the best of our knowledge, no systematic review has yet synthesized the available evidence in this domain. In this work, we simulated A PEG and 5-Fu, including the CP system, according to our previous data [184-201].

4. CHOP protocol

4.1. CP and 5-FU Conjugated via PEG Linkages

One well-known example is the CHOP protocol, which combines cyclophosphamide, doxorubicin, vincristine, and prednisone. Other frequently applied combinations involve cyclophosphamide (CP), 5-fluorouracil (5-FU), and methotrexate. Cyclophosphamide (CP), also known as cytophosphane (Figure 5-a), is a chemotherapeutic agent widely used to suppress the immune system, primarily in the treatment of breast cancer. It is also applied as an immunosuppressive therapy in conditions such as nephrotic syndrome and ANCA-associated vasculitis [202,203]. Because this drug is administered either orally or intravenously, many patients experience side effects, including leukopenia, loss of appetite, nausea and vomiting, alopecia, and hemorrhagic cystitis. Moreover, there are other serious adverse effects, such as an increased long-term risk of cancer, infertility, allergic reactions, and pulmonary fibrosis in some patients. Cyclophosphamide belongs to the alkylating agent class and the nitrogen mustard family of drugs, which exert their effects by interfering with DNA replication and RNA synthesis [203,204]. Although cyclophosphamide, when used in combination with thalidomide or lenalidomide and dexamethasone, has demonstrated documented efficacy as an off-label treatment for AL amyloidosis, in this study, we demonstrate that cyclophosphamide and 5-fluorouracil (5-FU) conjugated via PEG linkages show superior performance in breast cancer chemotherapy [204,205]. This conjugate appears to represent a promising alternative to traditional melphalan-based therapy, particularly for patients who are not suitable candidates for autologous stem cell transplantation.

4.2. Poly (ethylene glycol) spacer and linker for conjugate drugs.

Poly (ethylene glycol) is among the most effective polymers employed in drug design, particularly in anticancer drug delivery for chemotherapy. PEGylation, the covalent attachment of PEG to peptides, proteins, or small-molecule drugs, has been widely demonstrated to improve the aqueous solubility of hydrophobic therapeutic agents. In addition, PEGylation prolongs systemic circulation, minimizes nonspecific cellular uptake, and enhances tumor-selective accumulation via the enhanced permeability and retention (EPR) effect. To date, numerous PEG-based therapeutic formulations have been developed, several of which have obtained regulatory approval. Substantial clinical experience with PEGylated systems has enabled the rational design of PEG prodrug conjugates that exhibit enhanced therapeutic efficacy and reduced systemic toxicity. Despite these advances, continued optimization of PEG-based pro-drug conjugation strategies remains essential to improve clinical outcomes further. In this context, we propose the design of PEG-linked pro-drug conjugates incorporating cyclophosphamide (Figure 5-a) and a carbon-based spacer for conjugation to 5-fluorouracil derivatives. The proposed structures, Figures 5(a–d), represent promising candidates for subsequent evaluation in gynecological malignancies. Based on their distinct structural and physicochemical properties, these conjugates may also be extended to broader oncological applications. Advances in PEG–pro-drug conjugation methodologies that integrate clinically relevant bioactive agents offer significant potential for translational development, including regulatory approval and progression into clinical trial formulations.

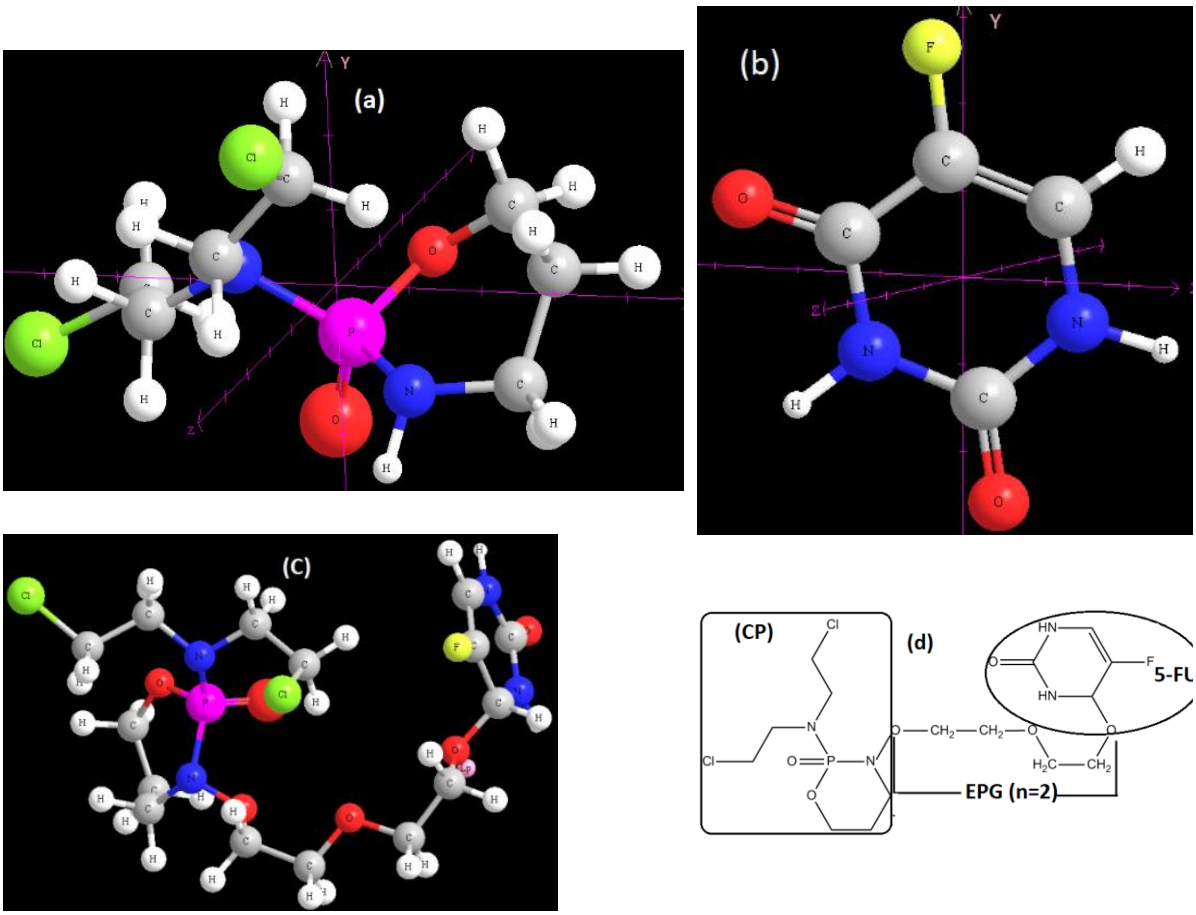

Figure 5. (a) Optimized Structure of CP by B3LYP/cc-PVTZ; **(b)** Optimized of Structure 5-FU by B3LYP/cc-PVTZ; **(c)** Optimized Structure of CP-[PEG(n=2)]-5-FU, by B3LYP/cc-PVTZ; **(d)** A schematic image of CP-[PEG(n=2)]-5-FU.

5. Results and Discussion

5.1. Optimization and abinito calculation of CHOP protocol for HPV16 E2 protein

In clinical oncology, multiple anticancer agents are frequently administered together in multidrug regimens, commonly referred to as combination chemotherapy or polychemotherapy. This strategy is intended to improve therapeutic response while minimizing resistance development. One well-known example is the CHOP protocol (Figure 6), which combines cyclophosphamide, doxorubicin, vincristine, and prednisone via a PEG linker (6-b). CHOP is a combination chemotherapy regimen primarily used for treating certain types of lymphomas. The acronym stands for the drugs involved: Cyclophosphamide, an alkylating agent that interferes with DNA replication; Hydroxydaunorubicin (also called doxorubicin) – an anthracycline that damages DNA and inhibits topoisomerase II, Oncovin (vincristine) – a vinca alkaloid that blocks microtubule formation, preventing cell division; Prednisone – a corticosteroid that induces cancer cell apoptosis and reduces inflammation. PEGylation is the attachment of PEG chains to a molecule (like a drug or protein). Benefits include increased solubility, longer circulation time, and reduced immune recognition. Some experimental approaches involve PEGylating one or more CHOP drugs, or conjugating them to PEG carriers, to improve pharmacokinetics and reduce toxicity. For instance, PEGylated doxorubicin (such as liposomal doxorubicin) circulates longer in the blood and accumulates more in tumor tissue, thereby improving the therapeutic index. The “through PEG linkage” phrase usually refers to chemically attaching CHOP drugs to PEG molecules, forming a prodrug or nanoformulation

that gradually releases active agents. The CHOP protocol via PEG linkage is a modified chemotherapy strategy in which CHOP drugs are chemically linked to PEG molecules to enhance stability, circulation time, and tumor targeting while reducing systemic side effects. Here, we used the CHOP protocol to dock the HPV16 E2 protein using docking methods, and the results are listed in Table 3. The E2C region of HPV16 E2 protein is a truncated form of the E2 regulatory protein that retains the C-terminal DNA-binding and dimerization domain while lacking the N-terminal transactivation region. Because E2 normally functions as a dimer when recognizing specific viral DNA sequences, researchers sometimes engineer modified E2C constructs to alter oligomerization behavior and investigate DNA-binding mechanisms, viral replication control, or protein–protein interactions. A short peptide linker of approximately 12 residues may be introduced between protein segments or fused domains to: 1-Increase structural flexibility; 2-Reduce steric interference between adjacent protein regions; 3-Control intermolecular associations; 4-Facilitate the design of constructs that favor a predominantly monomeric state rather than spontaneous dimer formation. The exact amino-acid composition is often as important as the length. Flexible linkers are often enriched in residues such as glycine and serine because they introduce mobility while minimizing unwanted secondary structure. In engineered E2C variants, monomerization is generally achieved by modifying residues involved in the native dimer interface and/or by introducing linker-based designs that disrupt favorable dimer contacts. Biophysical techniques such as size-exclusion chromatography, analytical ultracentrifugation, dynamic light scattering, or crystallography are commonly used to verify whether the engineered protein behaves as a monomer in solution. Monomerized HPV16 E2C derivatives have been explored for studying sequence-specific viral DNA recognition, Mapping dimerization interfaces, developing dominant-negative inhibitors of E2 function, and structural biology experiments where homogeneous monomeric protein preparations are advantageous. A HPV16 E2C construct containing a 12-amino-acid linker for monomerization is typically an engineered research tool designed to disrupt the natural dimerization of the E2 DNA-binding domain while maintaining sufficient structural integrity for biochemical and functional studies. The linker serves as a molecular spacer that helps optimize folding and conformational behavior in the modified protein.

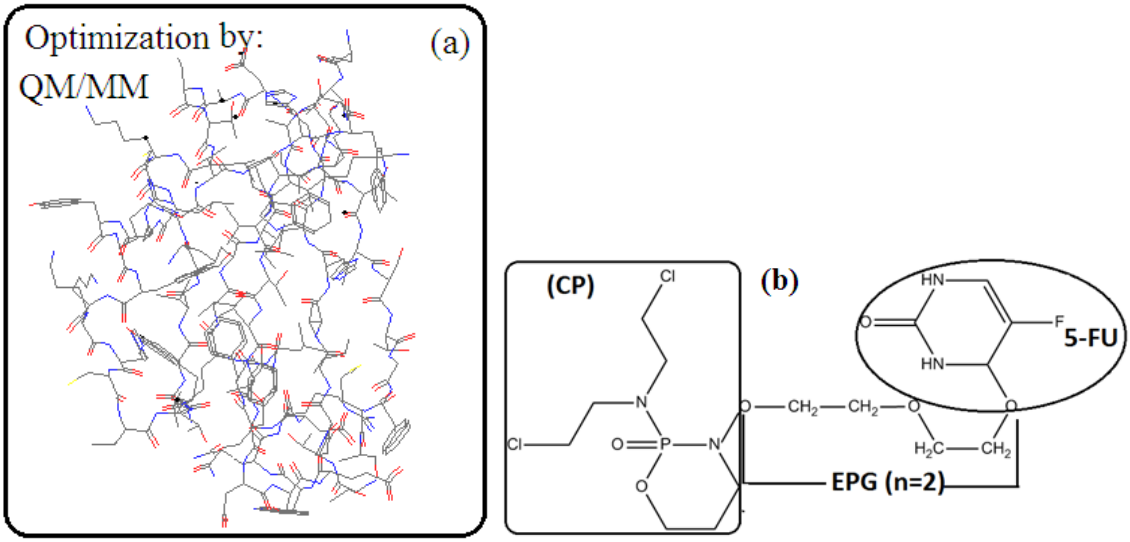

Figure 6. (a) Structure of single chain E2C from HPV16 with a 12aa linker for monomerization.(b) A schematic image of CP-[PEG(n=2)]-5-FU.

Table 3. Total Energy, VDW, H-Bond, Electrostatic energy of {CP–[PEG(n)]–5-FU (n=2-18)} ligands docked to 2Q79.pdb *(HPV16 E2 protein)*.

Number	Composed with {CP–[PEG(n)]–5-FU (n=2-8)}	Energy Kcal/mol	VDW Kcal/mol	H-Bond Kcal/mol	Electrostatic energy Kcal/mol	Monomer Number in PEG
1	2Q79	-91.55	-61.01	-33.43	-17.42	n=2
2	2Q79	-90.44	-64.20	-32.19	-18.14	n=4
3	2Q79	-93.85	-63.40	-31.14	-19.84	n=6
4	2Q79	-92.33	-65.10	-28.97	-18.49	n=8
5	2Q79	-97.44	-68.90	-29.42	-18.73	n=10
6	2Q79	-102.34	-62.53	-33.33	-17.92	n=12
7	2Q79	-101.44	-63.43	-34.11	-18.02	n=14
8	2Q79	-105.66	-60.33	-36.24	-18.10	n=16
9	2Q79	-104.43	-51.46	-33.31	-17.69	n=18

5.2. Optimization and abinito calculation of CP-{[PEG (H − (O−CH2−CH2)$_n$−OH)2] ,(n=1-to 10)]-5-FU,systems by B3LYP/cc-PVTZ.

QM/MM is a hybrid computational approach used in computational chemistry to study large molecular systems, especially enzymes, proteins, and solvated reactions, where treating the entire system quantum mechanically would be computationally too expensive.

It combines Quantum Mechanics (QM) with an accurate treatment of bond-breaking/forming, electronic structure, and charge transfer. Molecular Mechanics (MM): Efficient classical treatment of large environments (proteins, solvent, membranes). The quantum mechanical (QM) component was used to perform quantum biology calculations on CP–[PEG (n = 2–18)]–5-FU conjugates. The resulting *ab initio* data were subsequently integrated into simulations of the crystal structure of 1N8Z.pdb [206], 1JNX.pdb [207], and 3HB5.pdb [208] which represent the extracellular domain of the human HER2 receptor in complex with the Herceptin Fab fragment, Crystal structure of the BRCT repeat region from the breast cancer associated protein, BRCA1, and Binary and ternary crystal structure analyses of a novel inhibitor with 17beta-HSD type 1: a lead compound for breast cancer therapy, respectively (Figure 7). Overexpression of HER2 in breast tissue is associated with tumor development and aggressive disease progression, and current clinical treatments include monoclonal antibodies such as trastuzumab and pertuzumab. However, the therapeutic efficacy of these agents is often limited by poor pharmacokinetic profiles and inadequate tumor penetration. To address these limitations, PEG conjugation with CP and 5-FU (Figure 6-b) was investigated as a strategy to prolong systemic circulation. A multi-scale computational framework was employed to evaluate the impact of PEGylation using molecular dynamics and docking simulations conducted in GROMACS, representing the molecular mechanics (MM) component. The integration of *ab initio* QM calculations with MM simulations enabled a more accurate and comprehensive characterization of the system through the QM/MM approach. Amplification or overexpression of HER2 occurs in approximately 10–15% of breast tumors and is associated with higher recurrence rates and reduced overall survival [209,210]. PEG conjugation in CP–[PEG(n)]–5-FU conjugates represents a strategy to extend circulation time and reduce immunogenicity by increasing hydrodynamic size and shielding epitopes from immune surveillance.

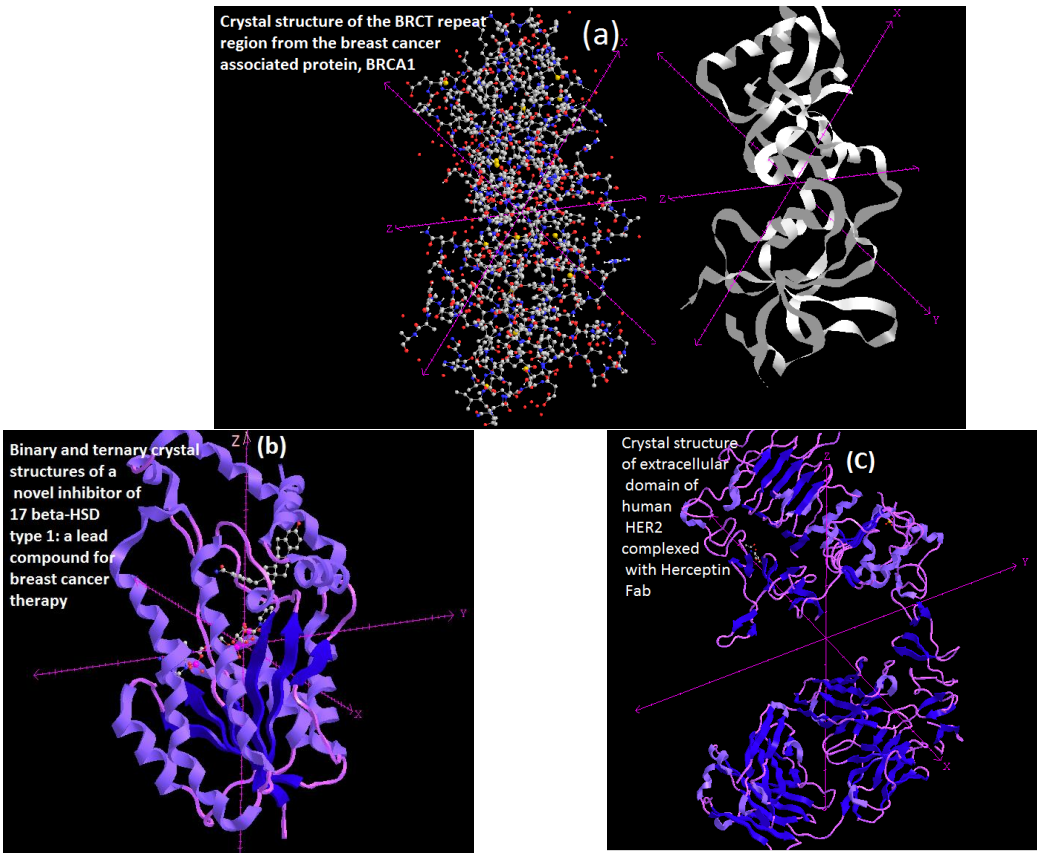

Figure 7. (a) Crystal structure of BRCT region from breast cancer (1JNX.pdb); **(b)** Crystal structure of 17-beta –HSD from breast cancer(3HB5.pdb); **(c)** Crystal structure of human HER2 complexed with Herceptin (1N8Z.pdb).

5.3. Ligand and protein preparation and docking simulation.

Chemical structures were drawn using ChemDraw (version 19.0.1.8, PerkinElmer) and imported into Chem3D Ultra (version 19.0.1.8, PerkinElmer). Initial geometry optimization was performed using the MM2 and MMFF9 force fields to obtain reliable three-dimensional conformations, which were saved in Z-matrix (Zmt) format. Final geometry optimization was carried out using Gaussian 2016 at the B3LYP/6-31G* level of theory. Two gynecological cancer-related protein targets, one corresponding to each cancer cell line (1N8Z.pdb [206], 1JNX.pdb [207], and 3HB5.pdb [208]), were selected for molecular docking studies (Figure 7). The docking protocol was validated by re-docking the co-crystallized ligands {CP–[PEG (n)]–5-FU (n=2-18)}, yielding RMSD values of 1.79 Å and 1.20 Å, respectively. As shown in Figures 8 and 9, the amino acids from the ligand {CP–[PEG(n)]–5-FU (n = 2–18)} that interact with 3HB5 are Ser11 and Ser12 in the H–S interaction, Arg37 in the H–S interaction, and also Arg37 in the H–M interaction. In addition, V–M interactions involve Gly9, Ser11, and Gly92, while V–S interactions involve Ser11 and Arg37. All of these residues are completely located within the active site of 3HB5, which corresponds to the crystal structure of 17β-HSD from breast cancer (Figure 7). Similarly, the amino acids from the ligand {CP–[PEG(n)]–5-FU (n = 2–18)} that interact with 1JNX are Cys1697, Arg1699, and Asp1739 in the H–M interaction, Asp1692 and Cys1692 in the V–M interaction, Glu1698 and Val1740 in the V–S interaction, and finally only one residue (Glu1698) in the H–S interaction. These residues are also completely located within the active site of 1JNX, which represents the crystal structure of the BRCT region associated with breast cancer (Figure 7). Therefore, these ligands may play an

important role in controlling and treating breast cancer through their specific interactions with these active sites.

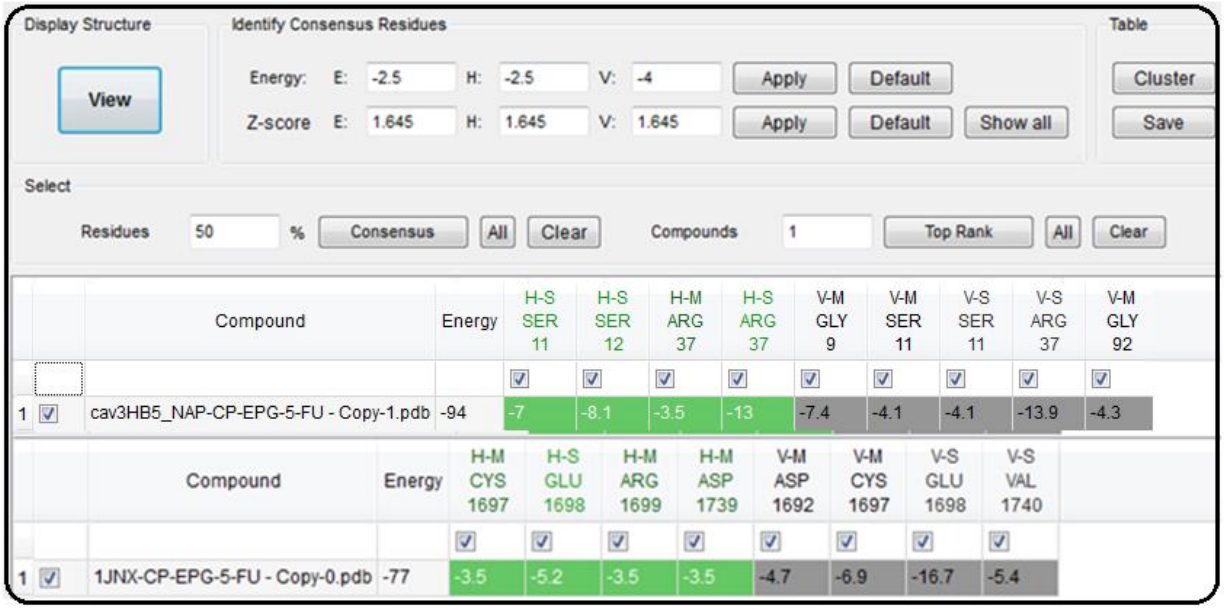

Figure 8. The amino acids from the ligand {CP–[PEG(n)]–5-FU (n = 2–18)} that interact with 3HB5 and 1JNX.pdb.

The simulations were performed based on our previously reported methodology. Favorable interactions with key active-site residues were visualized through binding-mode analysis.

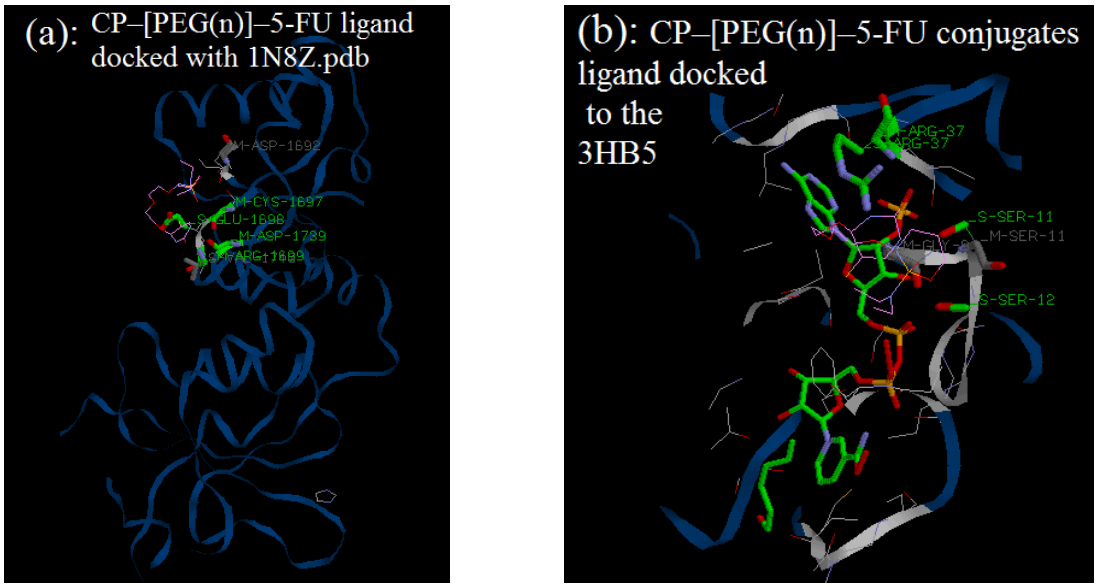

Figure 9. {CP–[PEG(n)]–5-FU (n=2-18)} docked with **(a)** 1JNX.pdb; **(b)** 3HB5.pdb.

Molecular docking was conducted using the Molegro Virtual Docker (MVD) for {CP–[PEG(n)]–5-FU (n=2-18)} compounds against multiple cancer-related protein targets obtained from the Protein Data Bank, including (1N8Z.pdb [206], 1JNX.pdb [207], and 3HB5.pdb [208]). Docking score thresholds were established by comparing the binding scores of the test compounds with those of the reference drug gemcitabine and compounds 1-8 (Figures 10 and 11).

Docking simulations were performed using [specify software, e.g., AutoDock Vina or Glide], with active sites defined according to the co-crystallized ligand positions. The grid box parameters were carefully set: Grid center: centroid of the co-crystallized ligand in the binding

pocket, Grid size: large enough to encompass all key residues within the active site, Grid spacing: 0.375 Å for high-resolution sampling. All ligands were docked into their respective protein targets, and ten poses per ligand were generated. Binding affinities were evaluated using the scoring function embedded in the docking software, which accounts for van der Waals, hydrogen-bonding, and electrostatic interactions. To validate the docking protocol, co-crystallized ligands were re-docked into each protein structure. The root mean square deviation (RMSD) between the predicted poses and the experimental crystallographic conformations was calculated: 3HB5: RMSD = 1.79 Å, 1JNX: RMSD = 1.20 Å, RMSD values below 2 Å indicate that the docking protocol reliably reproduces the experimental ligand positions, confirming the accuracy and robustness of the docking setup.

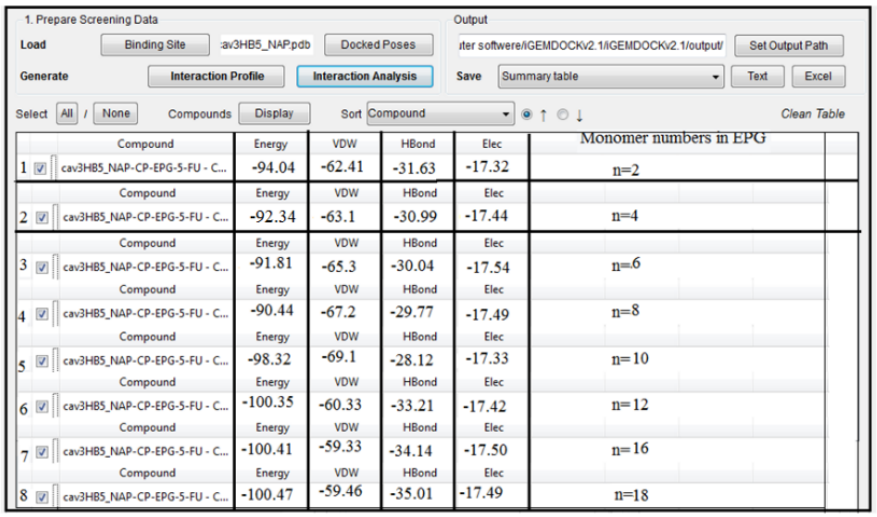

Figure 10. Total Energy, VDW, H-Bond, Electrostatic energy of {CP–[PEG(n)]–5-FU (n=2-18)} ligands docked to 3HB5.pdb

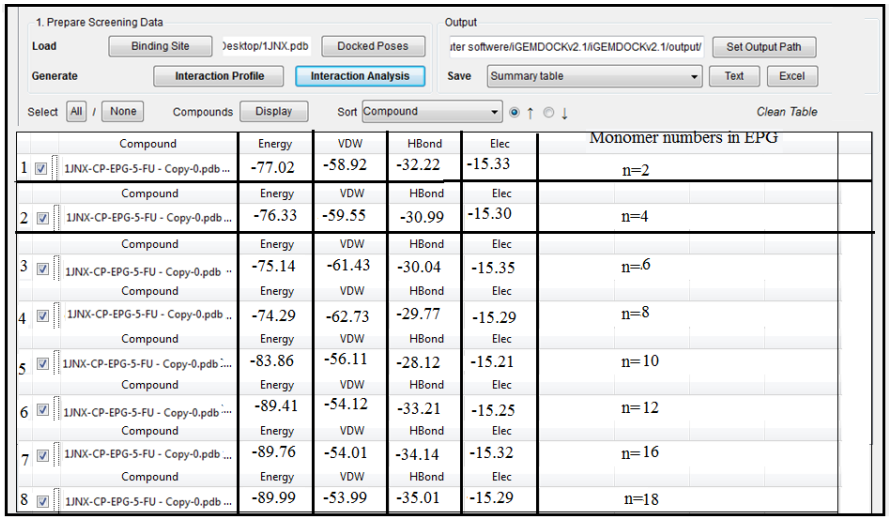

Figure 11. Total Energy, VDW, H-Bond, Electrostatic energy of {CP–[PEG(n)]–5-FU (n=2-18)} ligands docked to 1JNX.pdb.

5.4. AI-assisted optimization of monomer numbers in {CP–[PEG (n)]–5-FU (n = 2–18)} ligands.

To date, biotechnology in medical science has made significant progress in drug design, drug delivery, and the treatment of cancer. AI has immense potential for various applications in the pharmaceutical industry. AI enables the design of novel drugs for delivery to tissue and

cellular targets by enabling the discovery of specific chemical structures. A subfield of AI, machine learning, is commonly used in disease analysis and detection. Obviously, the results of predicting experimental help improve the precision of the testing output significantly. AI enables scientists to manage complex subjects, including qualitative and quantitative epidemiological prediction, accurate drug development, and host-pathogen relationships. The broad scope of AI, combined with the insights of DL and ML, helps improve disease treatment by providing more accurate results with fewer errors and faster decision-making. The use of AI-based techniques has significantly increased due to the numerous tissue biomarkers and their evaluations. AI-based biomarkers help physicians quickly control diseases after diagnosis by monitoring patients' responses to treatment, ultimately improving patient health. Additionally, accurate simulations from the sociology-biological field enhance reasoning modeling. As an example, the data from Figures 10 and 11 were plotted in Figure 12. The variation in total energy shows an inverse relationship with the van der Waals (VDW) and hydrogen-bond (H-bond) energies. Both the total energy and H-bond energy exhibit a minimum at n = 10, and beyond n = 12, they follow an approximately linear trend. In contrast, the VDW energy reaches a maximum at n = 8 and exhibits approximately linear behavior beyond n = 12. These energy characteristics depend on multiple variables related to thermodynamic, kinetic, and physical chemistry aspects. Due to the large volume and complexity of the data, it was difficult to determine optimal parameters using conventional analysis methods. However, AI and deep learning (DL) techniques enable efficient extraction of meaningful patterns from such datasets. Based on machine learning analysis, the systems {CP–[PEG(n)]–5-FU (n = 2–18)} were identified as the most favorable candidates for these simulations. Therefore, we recommend that experimental researchers synthesize these ligands and evaluate their properties experimentally. The calculated energies of PEG oligomers with monomer numbers ranging from n = 1 to 6 were analyzed to assess the effect of chain length on energetic stability. While a slight increase/decrease in total energy was observed with increasing monomer number, the differences among the oligomers were within the range of computational variability. Statistical analysis using one-way ANOVA indicated that these variations were not statistically significant ($p > 0.05$). Therefore, no reliable trend in energy as a function of PEG chain length could be established under the conditions studied. The results suggest that oligomerization up to six monomers does not substantially affect the overall energetic stability of the PEG chains.

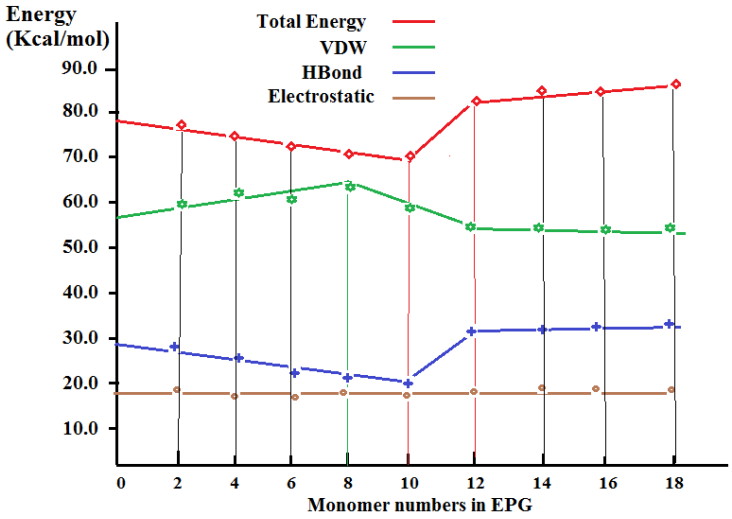

Figure 12. The energy changes according to the number of monomers in EPG.

6. AI, DL, and Aging

DL and GenAIcan be used to detect biomarkers, predict the aging clock, and generate dual-targeting drugs for both aging and patient use. Although a few works have examined the impact of AI on aging research, none have focused exclusively on GenAI and DL. Marino *et al*. investigated the use of AI in aging within specific hallmarks of aging [211]. Czaja *et al*. focused on the mechanisms of AI integration into daily life, such as health monitoring, quality of life, and nutrition for older adults [212]. Bernal *et al*. studied a classification of literature on the application of AI to aging physical changes, geographical living, without concentrating on clinical applications [213]. Meng *et al.* [214] focused on their research on biological phenomena related to age estimation, while Wang *et al*. interpreted the effects of biomarkers on aging clocks [215]. However, neither of them provided a detailed explanation focused on GenAI, DL, and AI. Steurer *et al*. presented a review of multi-system transformers, a type of GenAI, in the context of aging concepts [216], while Lyu *et al*. explored aspects of this review beyond DL and GenAI [217]. Since Zhavoronkov *et al*. took an in-depth approach to AI, ML, and DL in the aging phenomenon [218], rapid progress has been made in AI models. This has highlighted the need for further essential studies. As a result of these advancements, research on the concepts of DL and GenAI in aging research, specifically aiming to achieve healthy longevity, has been ongoing from 2016 to the present. In this regard, ML and deep learning (DL) have significantly advanced AI models through computer devices by accessing vast databases [219]. In contrast to several traditional ML models that use approaches such as decision trees and support vector machines, DL distinguishes itself by employing Deep Neural Networks (DNNs) with multiple layers, allowing for automatic learning and pattern prediction across different types of data [220]. In aging studies, twins are considered particularly valuable because they share identical environments and thus provide a powerful means to evaluate longitudinal data, such as the genome, saliva biomarkers, and typical physical activity. This allows scientists to investigate and estimate indicators of the aging process [221]. In widely used DNNs, specific structures have been investigated to utilize different sequences of data and functions in Convolutional Neural Networks (CNNs) that recognize algorithms in grid-like data, such as images, across multiple layers [222,223].

In conclusion, Deep Learning (DL) and Generative Artificial Intelligence (GenAI) represent a transformative shift in aging research by enabling the integration, analysis, and generation of complex biological data at an unprecedented scale. Unlike traditional machine learning approaches, DL architectures—such as deep neural networks and convolutional neural networks provide automated feature extraction and high-dimensional pattern recognition, which are essential for decoding multifactorial aging processes. Meanwhile, GenAI extends these capabilities beyond prediction by generating novel biomarkers, refining biological aging clocks, and proposing candidate compounds that may simultaneously target aging pathways and disease-specific mechanisms. Although previous studies have explored artificial intelligence within aging-related contexts, a focused examination of DL and GenAI highlights their unique capacity to bridge computational modeling with translational applications. As multi-omics datasets, longitudinal cohort studies, and multimodal clinical data continue to expand, these advanced AI frameworks are positioned to accelerate precision geroscience. Ultimately, leveraging DL and GenAI in aging research not only enhances our understanding of biological aging mechanisms but also supports the development of personalized interventions to extend healthspan and promote healthy longevity.

7. Summary

This study explores the integration of AI, quantum biology, and computational chemistry for the design and optimization of novel breast cancer therapeutics. We focused on cyclophosphamide (CP) and 5-fluorouracil (5-FU) conjugated via PEG linkages as potential chemotherapeutic agents with enhanced stability, solubility, and tumor-targeting capabilities. A hybrid QM/MM approach was employed to perform *ab initio* calculations on CP–[PEG(n)]–5-FU conjugates, evaluating their interactions with key breast cancer-related protein targets, including HER2, BRCA1, and 17β-HSD. Molecular docking simulations identified the active site residues involved in hydrogen bonding and van der Waals interactions, highlighting the potential efficacy of these conjugates in inhibiting tumor-associated proteins. The study also explored AI-assisted optimization to evaluate the influence of PEG chain length (n) on molecular stability and binding. Preliminary analyses of energy profiles, hydrogen bonding, van der Waals interactions, and docking data suggest that PEG chain lengths of n = 30–35 may provide optimal physicochemical and pharmacological properties. In addition, the work emphasizes the broader impact of AI and ML in biomedical research, including the analysis of genomic and proteomic datasets, the design of novel drug molecules, and the identification of salivary biomarkers for early cancer detection. Integrating AI with quantum biology and computational modeling enables predictive, data-driven drug design, potentially accelerating breast cancer therapy development while minimizing trial-and-error experimentation. Overall, this interdisciplinary approach demonstrates the synergy between AI, quantum biology, and biomedical engineering, offering a promising framework for the rational design of next-generation chemotherapeutics and personalized medicine strategies.

8. Conclusion

One of the most important scientific achievements in this century, the era of Industry, is the potential to design a machine that can interact with living human tissues, particularly the brain, enhancing human intelligence. Improving humans' ability to detect biological issues and make quick decisions for treating diseases is a key focus of biological and biochemical engineering. Recently, AI has emerged as a valuable tool in achieving this goal by utilizing the cognitive and perceptual abilities of living organisms. AI can be used in the biological world, particularly in quantum biology, which includes medical science, medicinal plants, pharmacology, brain diseases, cancer treatment, and the development of bio-based instruments for our sustainable life. This important task for medical doctors, which involves using AI in their patient treatment, would not only save millions of lives but also reduce costs. Moreover, AI-based models with performance patterns are currently being developed to ensure effective inputs and outputs in drug delivery and drug design. In addition, combining AI with quantum biology could revolutionize cognitive and brain biology in this new era. It is clear that quantum biology is a novel interdisciplinary field with contributions from several disciplines, including quantum mechanics, biological chemistry, chemical biology, biophysical chemistry, chemical biophysics, mathematicians, computational engineers, and spectroscopy scientists. As explained here, significant advances have been made in well-established fields such as microtubules, consciousness, Alzheimer's disease, photosynthesis, enzyme catalysis, life and entropy, and tunneling effects, as well as in lesser-known areas such as fluorescent proteins, ion channels, protein folding, NMR protein areas, MRI, and proton tunneling in DNA. Future experimental validation should include *in vitro* studies: cytotoxicity assays on breast cancer

cell lines, binding assays (SPR, ITC), and enzyme inhibition studies. In vivo studies: Xenograft tumor models, biodistribution, and toxicity assessment. Pharmacokinetic evaluation: Plasma half-life, clearance, and tissue accumulation to verify the advantages of PEGylation. These studies are essential for confirming the predictive insights from AI-assisted computational analyses and translating these findings into clinically relevant therapeutics. In conclusion, integrating artificial intelligence with quantum biological principles can enhance human cognitive function and improve the detection, treatment, and prevention of complex diseases by enabling precise modeling of molecular and neural processes, thereby creating a new paradigm for personalized and efficient biomedical interventions.

Author Contributions

Conceptualization, MM; methodology, MM; software, FM and AHS; validation, MM, AHS, FM and MK; investigation, MM and AHS; resources, FM and AHS; data curation, MM; writing—original draft preparation, MM and FM; writing—review and editing, MM, AHS, FM and MK; visualization, FM and AHS; supervision, MM; project administration, MM. All authors have read and agreed to the published version of the manuscript.

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Informed Consent Statement

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Data Availability Statement

Data supporting the findings of this study are available upon reasonable request from the corresponding author.

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Conflict of Interest

The authors declare no conflict of interest.

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