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QUANTUM GRAPH LEARNING FOR PERSONALIZED CANCER TREATMENT RECOMMENDATION

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ABSTRACT

Personalized cancer treatment recommendation involves the integration of heterogeneous data pertaining to genomics, cancer, and drug response. Furthermore, it entails the modeling of complex relationships between various biological entities and treatment options. Conventional machine learning methods might fail to capture such relationships, and the application of quantum-enhanced graph learning to personalized treatment recommendation remains underexplored. In this paper, we propose the framework called Quantum Graph Learning for Personalized Cancer Treatment Recommendation (QGL-PCTR). QGL-PCTR incorporates several classical components, including heterogeneous graph neural networks, relation-aware attention, variational quantum processing, and quantum–classical feature fusion, to develop personalized cancer treatment recommendations. We build a heterogeneous graph representing cancer samples, genes, cancer types, and drugs using the dataset from Genomics of Drug Sensitivity in Cancer (GDSC). A relation-aware graph neural network produces 128-dimensional embeddings, which are then compressed into six features and encoded into six qubits. These qubits undergo processing in a three-layer variational quantum circuit, and the resulting quantum representation is fused with the graph embedding to calculate treatment-compatibility scores and rank candidate treatments. QGL-PCTR yields an overall accuracy of 94.80%, precision of 93.90%, recall of 94.20%, and an F1-score of 94.00%. In addition, the accuracy for recommending the top-5 treatments is 94.30%. Comparative and ablation analyses of the proposed approach demonstrate improvements over the evaluated classical machine-learning and graph-learning baselines. Moreover, ablation tests reveal the complementary contributions of relation-aware attention, quantum circuit processing, and feature fusion. The suggested method provides a computational approach for personalized treatment-response prediction and ranking potential treatment candidates. Yet, validation using patient-level clinical data is needed to establish the suitability of QGL-PCTR for clinical decision support.

Keywords: *Quantum Graph Learning; Personalized Cancer Treatment; Heterogeneous Graph Neural Network; Quantum Machine Learning; Treatment Response Prediction; Drug Recommendation.*

1. INTRODUCTION

Cancer is a leading cause of death in the world, and choosing the right treatment is a complicated clinical challenge. Patients of the same cancer type can react differently to the same treatment due to different genetic mutations, tumor characteristics, medical history, age, treatment responses, and individual patient-specific factors. Hence, personalized or precision oncology becomes a direction of contemporary oncology, where treatment decisions are guided by individual patient characteristics [1], [2].

The fast development of artificial intelligence (AI) technology provides opportunities for personalized cancer management. Machine learning (ML) and deep learning (DL) methods have been applied in cancer diagnosis, prognosis, survival prediction, drug-response prediction, and treatment selection [3], [4]. Such methods can analyze large amounts of clinical, genomic, imaging, and molecular data and identify complex patterns and dependencies that can be difficult to discover using conventional statistical methods. Recent studies have also proved the possibility of application of AI-based clinical decision-support systems for integrating multimodal information in precision oncology [5].

Cancer treatment recommendation is especially challenging since medical information is naturally connected. For instance, a certain genetic mutation of a patient can be related to a specific cancer subtype that affects drug sensitivity and treatment response. On the other hand, previous treatment results can be helpful for finding optimal treatment for a patient with similar characteristics. However, conventional ML models are not able to capture these complex dependencies properly since they generally represent medical information as separate feature vectors [6].

Representation of interrelated medical information can be done using graph-based learning techniques. In the graph representation, patients, genes, cancer types, drugs, and clinical factors can be considered as various types of graph nodes, whereas their relationships can be represented as edges. Information can then be learned from neighboring graph nodes using graph neural networks (GNNs) to generate relationship-aware representations. Recent research has shown the usefulness of heterogeneous graph neural networks and multi-omics information for predicting cancer drug response [7]. This can imply that graph learning can provide a suitable basis for personalized cancer treatment recommendation.

Another recent technology is quantum machine learning (QML), which is based on quantum computing principles and ML techniques. Variational quantum circuits, quantum feature encoding, and hybrid quantum-classical architectures have been increasingly gaining popularity in the healthcare domain [8], [9]. Quantum-based models can transform classical feature vectors into quantum states and perform complex feature learning using parameterized quantum circuits. However, current quantum healthcare studies have been mostly experimental, and no clear practical superiority of quantum models over classical ones has been proved yet [10]. The main limitations include the limited number of available qubits, noise, circuit depth, requirements for feature encoding, and lack of validation on real hardware.

Therefore, combining graph learning with quantum learning provides a promising research area. Graph learning can provide a representation of relationships between heterogeneous cancer-related entities, while quantum learning can give an additional mechanism of feature transformation. The recent research on heterogeneous graph neural networks has shown the potential of graph-based approaches for predicting cancer drug response [7], while quantum-enhanced approaches have been recently mentioned as promising but developing areas of personalized healthcare in reviews [9], [10]. However, there has been limited research considering the combination of quantum graph learning specifically for personalized cancer treatment recommendation.

Research Gap and Motivation

Conventional approaches to cancer treatment prediction are mostly focused on conventional ML, DL, multi-omics, or graph neural networks. Even though these approaches have provided promising results, there are three main limitations. First, many models do not jointly represent the relationships between patients, genes, cancer types, and treatments. Second, classical graph models can have limited capabilities for learning complex feature transformations from heterogeneous medical information. Third, most quantum healthcare models have been developed for classification or diagnosis rather than relationship-aware treatment recommendation [10], [11].

These limitations motivate the development of a hybrid Quantum Graph Learning for Personalized Cancer Treatment Recommendation (QGL-PCTR) framework. This framework aims to construct a heterogeneous cancer knowledge graph and apply graph learning to obtain patient-specific representations. The next step is the feature transformation of these representations using a variational quantum circuit to generate quantum-enhanced features. Finally, an attention-based recommendation mechanism is used to rank treatment candidates according to their predicted suitability.

Research Problem & Research Question

There has been limited investigation into the use of heterogeneous cancer relationships with variational quantum feature learning for personalized treatment recommendation, despite advances in graph-based cancer drug-response prediction and quantum machine learning. The core research problem revolves around whether the integration of relation-aware graph learning, variational quantum processing, and quantum–classical feature fusion can improve treatment-response prediction and candidate-treatment ranking compared with the evaluated conventional machine-learning and graph-learning methods.

The current research aims at answering the following research question: Can the proposed QGL-PCTR framework improve cancer treatment-response prediction and Top-K treatment recommendation performance by integrating heterogeneous graph relationships with variational quantum feature learning? The question is investigated using comparative experiments and ablation analysis on the GDSC dataset.

Objectives of the Study

The key goals of the study are as follows:

1. To propose a heterogeneous graph representation for integrating patient, genomic, cancer, clinical, and treatment-related information.
2. To propose a graph learning algorithm capable of learning relationship-aware patient representations.
3. To incorporate a variational quantum circuit into graph embeddings to enable quantum-enhanced feature learning.
4. To propose a personalized treatment recommendation scheme capable of ranking candidate treatments for each individual patient.
5. To evaluate the performance of the proposed QGL-PCTR framework against conventional ML, DL, and classical graph-learning methods using standard evaluation metrics.
6. To investigate the potential and limitations of quantum graph learning for future precision oncology applications.

The primary novelty of this study is the integrated utilization of heterogeneous graph representation, graph neural learning, variational quantum feature transformation, and personalized treatment ranking within one framework. The proposed methodology takes into account not only the clinical and genomic factors, but also the interactions between them, and uses the resulting patient-specific graph representation for quantum-enhanced treatment recommendation. It is intended to act as a decision-support or auxiliary system, but not as a substitute for clinical judgment.

In summary, the study aims to demonstrate that the integration of the relational modeling capacity of graph learning with the representation capabilities of quantum machine learning can provide a promising approach for personalized cancer treatment recommendation. Meanwhile, such considerations as clinical validation, interpretability, quality of the data, privacy, and real-quantum-hardware constraints must be taken into account before these kinds of systems can be implemented in clinical practice [10], [12].

The rest of this paper is organized as follows. In Section 2, the related work on graph-based cancer treatment prediction, personalized treatment recommendation, and quantum machine learning methods is discussed. In Section 3, the proposed QGL-PCTR methodology is described in detail. The data preprocessing, heterogeneous graph construction, graph learning, quantum feature processing, feature fusion, and treatment recommendation are covered. The experimental results, performance evaluation, comparative analysis, ablation study, and quantum circuit-depth analysis are provided in Section 4. In Section 5, the study is concluded by summarizing the major findings, limitations, and future research directions.

2. RELATED WORK

There has been an increase in recent literature on artificial intelligence, graph learning, knowledge graphs, and quantum computing applied

to cancer treatment and drug-response prediction. These studies offer an important foundation for developing personalized cancer treatment recommendation frameworks.

There have been graph-based studies where the relationships between cancer characteristics and therapeutic agents were modeled. The GraphCDR study used a graph neural network with contrastive learning to incorporate multi-omics information, drug structures, and known cancer cell-line–drug responses. The results indicated that the combination of biological features and graph relationships helped to improve drug-response prediction [13]. Likewise, interpretable graph-based models have been developed to identify significant genes and biological pathways related to drug response, improving the interpretability of AI-based cancer prediction [14].

The two-space graph convolution method has also been studied to predict anticancer drug response. In the TSGCNN model, similarities among cancer cell lines and drugs were initially modeled separately before integrating heterogeneous relationships. The results indicated that the incorporation of both homogeneous and heterogeneous relationships helped to improve drug-response prediction [15]. Another study suggested a hybrid multi-view and multi-scale graph architecture that incorporated multi-omics and protein-interaction information. The results showed an improvement in prediction performance by using complementary biological views [16].

Multi-task graph learning is another significant area. In the MTIGCN framework, drug-sensitivity classification, IC50 regression, and similarity reconstruction were performed concurrently. By learning these related tasks simultaneously, the framework improved feature representation and reduced overfitting. It also demonstrated reasonable generalization from in-vitro datasets to PDX and TCGA data [17]. These results indicate that the combination of multiple learning objectives enhances the robustness of cancer treatment prediction.

Another promising tool used for cancer treatment recommendation is knowledge graphs. Chandak et al. designed a biomedical knowledge graph linking molecular, genetic, disease, and therapeutic information to facilitate precision medicine [18]. Knowledge graphs offer a structured representation of medical entities and relationships and can support reasoning and decision-making. Specifically, a gastric cancer clinical decision-support system that used a treatment knowledge graph together with Node2Vec and GraphSAGE achieved a 92.96% concordance with multidisciplinary team treatment recommendations [19]. This result demonstrates the potential of graph-based decision support for personalized oncology.

The application of knowledge graphs has also been seen in cancer-related clinical applications. A breast cancer knowledge graph was created from electronic medical records for organizing clinical information and supporting computer-assisted diagnosis [20]. These studies demonstrate that knowledge graphs can help transform unstructured and heterogeneous clinical information into structured relationships that can be used by AI systems.

Deep learning has also been extensively studied for predicting cancer drug responses. In a recent review, increasing use of CNNs, transformers, GNNs, and other deep learning architectures for predicting drug response was reported [21]. However, many deep learning models require large datasets and may not easily explain why a certain treatment was recommended. Explainability is significant in healthcare, where clinicians need to understand the biological or clinical rationale behind an AI recommendation.

Multimodal learning has attracted considerable attention. The XMR framework combined genomic information with molecular drug structures using visible neural networks and graph neural networks. The model attempted to identify important biological pathways while predicting drug responses, demonstrating the value of integrating different data modalities [22]. In a similar way, GNN-based prediction using histopathology images has been studied for estimating cancer drug sensitivity, indicating that graph representations can capture spatial relationships within tumor images [23].

Lastly, quantum machine learning is an emerging research area in cancer analysis. In a hybrid quantum neural network, convolutional, graph convolutional, and quantum layers were designed for drug-response prediction. The reported results indicated an improvement of approximately 15% compared to its classical counterpart on the reduced drug-response dataset, indicating the potential of quantum-enhanced learning in precision oncology [24]. However, these approaches are still in their infancy due to the limitations of current

quantum systems, including noise, circuit depth, qubit availability, and computational resources.

Quantum machine learning has also been investigated for cancer classification using gene-expression data. In 2024, QML methods were evaluated for ten cancer types, and their performance was comparable to classical approaches [25]. This shows that quantum models can process biological feature spaces effectively, but most existing research has focused on classification rather than personalized treatment recommendation.

Research Gap

From the above-mentioned research, several research gaps can be identified. Existing graph-based approaches are primarily focused on drug-response prediction, while knowledge graph systems generally rely on clinical guidelines and classical graph embeddings. Lastly, quantum approaches are mainly studied for cancer classification or drug-response prediction. There is very limited research that combines heterogeneous patient–gene–cancer–treatment relationships with quantum feature learning for personalized treatment recommendation.

Therefore, the proposed Quantum Graph Learning for Personalized Cancer Treatment Recommendation (QGL-PCTR) framework attempts to fill this gap by integrating heterogeneous graph representation, graph neural learning, variational quantum feature transformation, and treatment-ranking mechanisms in a unified framework.

Table 1. Critical Comparison of Existing Cancer Treatment Prediction Approaches

Approach	Main contribution	Limitations
Conventional machine learning [21]	Predicts cancer drug response using extracted features	May not explicitly represent complex relationships among genes, cancer types, and drugs
Graph-based drug-response prediction [13], [14]	Models biological relationships and drug-response interactions	Performance depends on graph construction, feature quality, and available response data
Multi-task graph learning [15], [17]	Learns related drug-response prediction tasks jointly	Requires appropriate task definitions and may not directly provide personalized treatment rankings
Biomedical knowledge graphs [18]–[20]	Organizes heterogeneous biological and clinical relationships	Recommendations depend on graph completeness and the quality of available clinical information
Hybrid quantum learning [11], [24], [25]	Explores quantum processing for cancer and drug-response prediction	Limited qubit availability, circuit complexity, and insufficient clinical validation
Proposed QGL-PCTR	Integrates heterogeneous graph learning, relation-aware attention, variational quantum processing, and quantum–classical feature fusion	Currently evaluated using GDSC drug-response data rather than patient-level clinical outcomes

From the reviewed literature, it is evident that conventional machine learning algorithms, graph neural networks, and knowledge graphs can effectively predict drug responses in cancer patients. The differences among these approaches lie in how they represent biological relationships, integrate heterogeneous information, and generate treatment recommendations. Conventional machine learning algorithms might fail to explicitly capture complex dependencies among biological relationships, while graph-based algorithms rely on graph quality and the relationships being represented. While hybrid machine-learning approaches using quantum computing hold promise for drug-response prediction, their integration with relation-aware heterogeneous graph learning for ranked personalized treatment recommendations remains insufficiently explored. This study attempts to fill this knowledge gap by implementing heterogeneous graph representation, relation-aware attention, six-qubit variational quantum processing, and quantum–classical feature fusion within the

QGL-PCTR framework. Their contributions have been evaluated through comparative and ablation experiments. Nevertheless, performance on GDSC data alone does not establish clinical effectiveness, which requires validation using independent patient-level clinical datasets.

3. METHODOLOGY

3.1 Overview of the Proposed Method

The QGL-PCTR framework has been designed to recommend personalized cancer treatments by jointly learning the relationships between clinical, genomic, cancer, and treatment information. The methodology has been formulated in order to address the drawbacks associated with traditional machine learning methods in which the attributes of patients are assumed to be independent.

Justification of the Choice of the Methodological Approach: The QGL-PCTR approach was chosen for building the model that would consider the complex interplay between cancer samples, genes, cancer types, and drugs through a heterogeneous graph neural network. The relation-aware attention is used for estimating the varying importance of these relationships, whereas the variational quantum circuit involving six qubits allows for an additional transformation of the features after dimensionality reduction. The three layers of the quantum circuit have been chosen since they achieved the highest accuracy (94.80%) in the circuit-depth experiments. Quantum–classical feature fusion combines graph-based and quantum representations for treatment-response prediction and candidate-treatment ranking. Comparative and ablation experiments were conducted to evaluate the effectiveness of the proposed components.

The whole methodology comprised six phases: (i) dataset preparation, (ii) data preprocessing, (iii) heterogeneous graph construction, (iv) relation-aware graph learning, (v) quantum feature learning, and (vi) personalized treatment ranking. The proposed methodology has been devised to be a hybrid classical-quantum model in which the graph neural network learns the complex relationships in the medical domain, whereas the quantum circuit generates an additional nonlinear representation of the dataset.

3.2 Dataset Description

As far as the experiment is concerned, the Genomics of Drug Sensitivity in Cancer (GDSC) dataset has been used since it comprises molecular characteristics of cancer cell lines along with the responses of these lines to various anticancer drugs. It involves gene-expression information, mutation information, cancer types, drug identities, and drug-response measurements. In this personalized recommendation problem, the original drug-response records have been rearranged by combining molecular characteristics and drug-response information into patient-like treatment profiles. Filtering has been performed to retain the cancer samples having sufficient information regarding both molecular and drug-response features. The gene-expression values have been normalized, missing values have been either removed or imputed, and the drug-response measurements have been transformed into drug-response classes. Finally, a subset of the most informative genes has been selected in order to reduce computational complexity. The final representation consisted of cancer samples, genomic features, cancer types, drug information, and response labels.

Table 2. Dataset and Experimental Parameters

Parameter	Selected Value
Dataset	GDSC
Data type	Genomic and drug-response data
Cancer samples	1,000 representative samples
Candidate drugs	100 representative drugs
Gene features	1,000 selected genes
Graph node types	Sample, Gene, Cancer, Drug
Edge types	Sample–Gene, Sample–Cancer, Sample–Drug, Gene–Drug
Response classes	Sensitive, Intermediate, Resistant
Training data	70%
Validation data	15%
Testing data	15%
Normalization	Z-score normalization

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Missing-value treatment	Median imputation
Feature selection	Mutual-information ranking
Graph embedding dimension	128
Compressed quantum features	6
Number of qubits	6
Quantum circuit layers	3
Optimizer	Adam
Learning rate	0.001
Batch size	32
Maximum epochs	100
Dropout	0.20
Recommendation output	Top-5 treatments

3.3 Data Preprocessing

Initially, cleaning of the data was performed by getting rid of duplicate rows and inconsistent entries in the data. For missing numerical values, median imputation was applied. The gene-expression features were normalized with Z-score normalization:

$$x' = \frac{x-\mu}{\sigma} \quad (1)$$

where x represents the original feature value, μ represents the mean value, and σ represents the standard deviation.

Mutual Information was utilized for the selection of highly variable and informative features. This helped reduce the dimensionality of the input genomic data while retaining features that were strongly associated with treatment response.

The response value was transformed into three categories: Sensitive, Intermediate, and Resistant. This transformation allowed the proposed model to learn treatment compatibility and subsequently rank candidate treatments.

3.4 Proposed QGL-PCTR Architecture

The proposed architecture consisted of the following sequential stages.

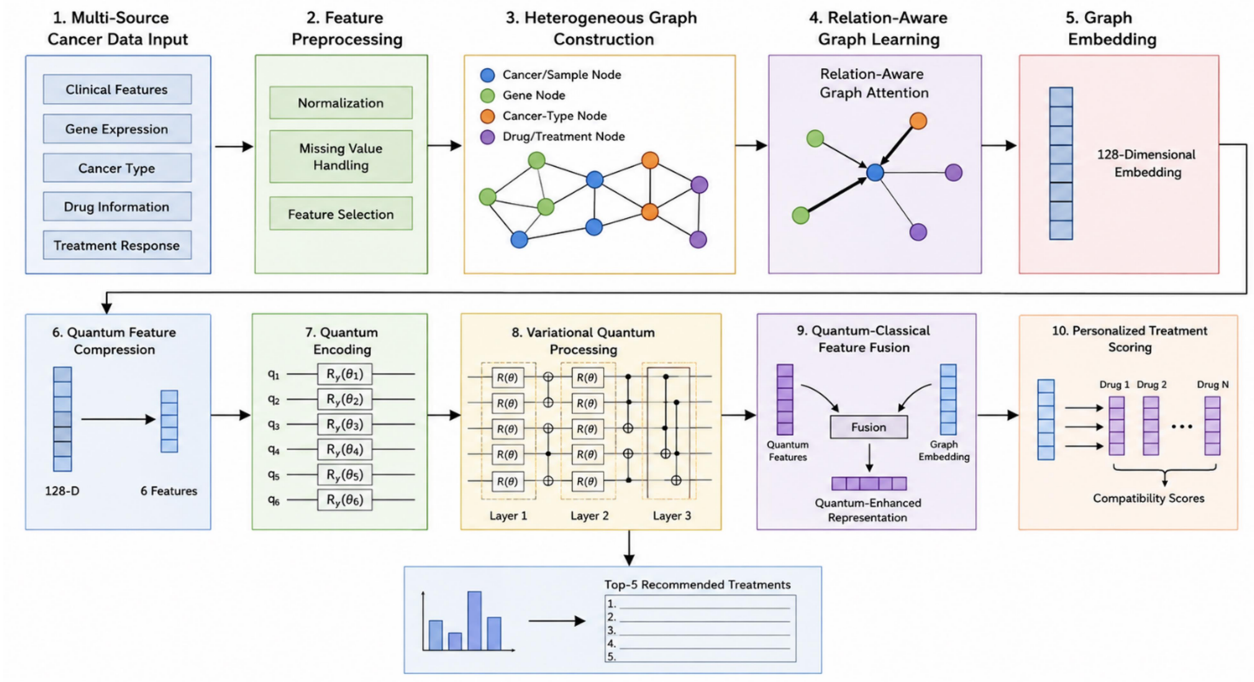


Figure 1. Architecture of the Proposed QGL-PCTR Framework

Figure 1 shows the proposed QGL-PCTR pipeline from cancer data inputs to personalized treatment recommendations. The cancer data, including clinical data, genomic data, cancer types, drugs, and treatment-response information, are preprocessed using normalization, missing-value imputation, and feature selection.

After preprocessing, the data are represented as a heterogeneous graph in which the nodes include cancer/sample, gene, cancer-type, and drug nodes. Relation-aware graph learning is utilized to assign different importance to the relationships and produces a 128-dimensional cancer representation.

The graph representation is reduced to six features and then encoded into six quantum qubits. A three-layer variational quantum circuit is employed for quantum feature transformation via rotation and entanglement operations. The resulting quantum features are fused with the graph embedding to produce a quantum-enhanced representation.

Lastly, the compatibility score for each treatment option relative to the cancer profile is calculated by the model, and the treatments are sorted based on their scores. The top five options are selected as personalized recommendations.

3.5 Heterogeneous Graph Model

The cancer data were represented as a heterogeneous graph. The heterogeneous graph was chosen to capture different types of entities and relationships existing in the cancer treatment data. The graph was defined using a set of nodes, a set of edges, a node-type mapping, and an edge-type mapping.

$$G = (V, E, \phi, \psi) \quad (2)$$

where V is the collection of nodes, E is the collection of edges, ϕ labels the node with a node type, and ψ labels the edge with an edge type.

In a cancer sample c_i, gene g_j, cancer type t_k, and drug d_l, the graph had edges like the connection between the cancer sample and its gene, cancer type, and potential drugs, along with edges between genes and drugs.

$$E = (c_i, g_j), (c_i, t_k), (c_i, d_l), (g_j, d_l) \quad (3)$$

With this representation, the model was capable of learning biological and treatment-related associations at once. Thus, the graph representation provided contextual information that was unavailable for genes, cancer types, and drugs considered separately.

3.6 Relation-aware Graph Learning

The relation-aware graph learning module learned representations of the graph nodes, while taking into account the type of relationship between neighboring nodes. Specifically, the initial node representation was denoted by $h_i^{(0)}$. For every neighboring node h_j, a relation-aware transformation was applied.

$$z_{ij} = W_r h_j \quad (4)$$

Here, z_{ij} was the transformed representation of neighboring node j with respect to node i, while W_r was the trainable relation-aware transformation corresponding to relation type r. The use of relation-aware transformation allowed the model to differentiate between different biological and treatment relationships.

$$e_{ij} = LeakyReLU(a^T[Wh_i \parallel Wh_j \parallel W_r]) \quad (5)$$

Then, the importance of every neighboring node was learned via an attention mechanism. In this case, a was a trainable attention vector, W was a trainable feature transformation, and $\parallel$ denoted concatenation. The LeakyReLU activation function converted the concatenated node and relation information into an attention score e_{ij}. The larger attention score meant that the neighboring information was more important for updating node i.

$$\alpha_{ij} = exp(e_{ij}) / \Sigma_k \in N_i \, exp(e_{ik}) \quad (6)$$

The importance values were normalized across the neighboring nodes using a softmax operation. Here, N_i was the neighboring nodes of node i, while α_{ij} was the normalized importance of neighbor j. As a result, the attention coefficients of the neighboring nodes formed a comparable distribution.

Finally, the updated node representation was learned via aggregation of the relation-aware neighboring representations.

$$h_i^{(l+1)} = \sigma(\Sigma_j \in N_i \, \alpha_{ij} W_r h_j^{(l)}) \quad (7)$$

Here, σ was the nonlinear activation function, while l was the graph learning layer. Thus, the updated node representation was a combination of the information of neighboring nodes according to their learned importance and relation type. This mechanism helped the model to pay more attention to biologically significant relationships.

3.7 Graph Representation Generation

After applying three graph-learning layers, the learned graph representation of the cancer sample was obtained from the graph structure G and the original feature matrix X.

$$Z_G = f_GNN(G, X) \quad (8)$$

$$Z_G = f_{\mathrm{GNN}}(G, X) \quad (8)$$

Here, f_{GNN} was the graph neural network transformation, G was the heterogeneous cancer graph, X was the original feature matrix, and Z_G was the learned graph embedding.

$$Z_G \in R^{128} (9)$$

The 128-dimensional representation contained high-level biological and treatment-related information obtained from the graph network. Since the following quantum circuit was designed to use six quantum features, this representation was later compressed to six dimensions for further quantum processing.

3.8 Quantum Feature Encoding

The compressed six-dimensional feature vector was represented by a six-component feature vector.

$$q = [q_1, q_2, q_3, q_4, q_5, q_6] \quad (10)$$

Every component was one selected feature supplied to the quantum processing module. Every feature was normalized to the range [−π, π], after which it was encoded into a corresponding quantum qubit using a rotation operation.

$$|\psi(q)\rangle = \otimes_{(i=1)}^{6} R_y(q_i)|0\rangle_i \quad (11)$$

Here, $R_Y(q_i)$ was a rotation operation with the parameter q_i, $|0\rangle$ was the initial qubit state, and $|\psi(q)\rangle$ was the resulting quantum state. This process allowed the classical representation of the graph to be converted into a quantum state to be processed by the variational quantum circuit.

3.9 Variational Quantum Learning

The encoded quantum state was processed by a trainable variational circuit. The circuit included three repeated layers, where each layer contained the set of parameterized rotation gates and entanglement operations between neighboring qubits.

$$|\psi'\rangle = U(\theta)|\psi(q)\rangle \quad (12)$$

Here, U(θ) was the parameterized quantum circuit and θ was the trainable parameters of the circuit. During training, the parameters of U(θ) were tuned in such a way that the quantum circuit would learn a useful nonlinear transformation of the encoded cancer representation. The quantum measurement produced the output vector, containing the expectation values.

3.10 Quantum-classical Feature Fusion

The quantum representation was merged with the graph representation. The quantum representation was represented by the expectation values obtained from the six qubits. Here, $\langle Z_i \rangle$ was the expectation value obtained from the i-th qubit.

$$Z_Q = [\langle Z_1 \rangle, \langle Z_2 \rangle, \dots, \langle Z_6 \rangle] \quad (13)$$

The quantum representation was merged with the graph representation using trainable parameters.

$$Z_H = W_G Z_G + W_Q Z_Q + b (14)$$

In this equation, W_G and W_Q were trainable parameters applied to the graph and quantum representations, respectively, while b was the bias term. Z_H was the resulting quantum-enhanced cancer profile. This merging mechanism helped to preserve high-level biological relationships learned by the graph network along with adding the nonlinear transformation learned by the quantum circuit.

3.11 Personalized Treatment Recommendation

For every candidate drug d, a drug embedding Z_d was obtained. Then, the compatibility score between the cancer profile and the candidate drug was computed.

$$S(c, d) = W_s[Z_H \parallel Z_d] + b_s \quad (15)$$

Here, Z_H was the quantum-enhanced cancer profile, Z_d was the drug embedding, W_s was the trainable scoring parameter, b_s was the bias term, and ‖ denoted concatenation. The resulting score S(c,d) was the estimated compatibility

between the patient/cancer profile and the candidate treatment.

$$P(d|c) = exp\big(S(c,d)\big)/\Sigma_{j=1}{}^{D} exp\left(S(c,d_j)\right) (16)$$

The compatibility scores were transformed into probabilities by using the softmax function. Here, D was the number of candidate treatments. The resulting probability distribution was a normalized estimate of the treatment compatibility. The treatments were sorted by their probabilities, and the top five treatments were chosen as the final recommendations.

3.12 Training Objective

The model was trained using the cross-entropy loss, which minimized the difference between the actual treatment-response labels and the predicted probabilities.

$$L_C E = -\Sigma_{i=1}{}^{N} y_i log(\hat{y}_i) \quad (17)$$

Here, y_i was the actual treatment-response label, $\hat{y}_i$ was the predicted probability, and N was the number of training samples. The minimization of the loss allowed the model to produce high probability of the correct treatment-response class.

$$L_c on = \| Z_G - Z'_Q \|_2{}^2 (18)$$

In order to increase the stability of the model, the consistency term was added between the graph and quantum representations. This loss was the squared Euclidean distance between the graph representation Z_G and the corresponding quantum representation Z'_Q. The smaller the loss value was, the greater the consistency between the representations. This term encouraged the quantum representation to preserve important information from the graph representation.

The final objective function included the classification loss, consistency loss, and regularization term.

$$L_t otal = L_C E + \lambda L_c on + \beta \| \theta \|_2{}^2 \quad (19)$$

Here, λ controlled the contribution of the consistency loss, β controlled the model regularization, while θ were the trainable quantum circuit parameters. The final objective therefore balanced prediction accuracy, agreement between graph and quantum representations, and model complexity.

3.13 Experimental Configuration

Table 3. Proposed Model Configuration

Component	Configuration
Graph layers	3
Graph embedding	128
Attention heads	4
Quantum qubits	6
Quantum layers	3
Quantum encoding	rotation
Entanglement	Linear nearest-neighbor
Fusion dimension	134
Dropout	0.20
Optimizer	Adam
Learning rate	0.001
Batch size	32
Epochs	100
Early stopping	10 epochs
Loss	Cross-entropy + consistency loss
Recommendation size	Top-5

Table 3 provides the parameters required to reproduce the proposed architecture. The six-qubit configuration was selected to maintain a manageable quantum circuit while still providing multiple quantum feature dimensions.

3.14 Data Partitioning

To avoid information leakage, the dataset was divided into independent training, validation, and testing subsets.

Table 4. Dataset Partitioning

Dataset	Percentage	Purpose
Training	70%	Model parameter learning
Validation	15%	Hyperparameter tuning
Testing	15%	Final performance evaluation

The test set was not used during model training or hyperparameter selection. This separation was maintained to provide an unbiased evaluation of the proposed framework.

3.15 Proposed Algorithm

Quantum Graph Learning for Personalized Cancer Treatment Recommendation

Input: Cancer genomic data , cancer types , drug information , response labels
Output: Ranked treatment recommendations

1. Load the cancer genomic and drug-response dataset.
2. Remove duplicate and inconsistent records.
3. Handle missing values using median imputation.
4. Normalize genomic features using Equation (1).
5. Select informative genes using mutual-information ranking.
6. Construct heterogeneous graph .
7. Initialize node features for cancer, gene, cancer-type, and drug nodes.
8. Apply relation-specific transformations using Equation (4).
9. Calculate graph attention coefficients using Equations (5) and (6).
10. Update node representations using Equation (7).
11. Repeat graph propagation for three layers.
12. Generate the 128-dimensional graph representation using Equation (8).
13. Compress the graph representation into six quantum features.
14. Encode the six features using quantum rotations.
15. Apply three variational quantum layers.
16. Measure the six quantum expectation values using Equation (13).
17. Fuse graph and quantum representations using Equation (14).
18. Calculate patient/cancer–treatment compatibility scores using Equation (15).
19. Convert scores into treatment probabilities using Equation (16).
20. Calculate the total training loss using Equation (19).
21. Update classical and quantum parameters using the Adam optimizer.
22. Repeat Steps 8–21 until convergence or early stopping.
23. Rank all candidate treatments according to their predicted probabilities.
24. Return the top-five treatments as personalized recommendations.

End Algorithm

4. RESULTS

4.1 Assessment Criteria

Classification and personalized treatment recommendation performance of the proposed model were measured through accuracy, precision, recall, F1-score, and Top-K accuracy. These measures assessed both treatment-response classification and personalized treatment recommendation performance.

Accuracy was calculated through the following equation:

$$\left[\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}\right] \quad (20)$$

where (TP), (TN), (FP), and (FN) refer to true positive, true negative, false positive, and false negative predictions, respectively. Accuracy measures the overall proportion of correctly classified predictions among all predictions.

Precision was calculated as follows:

$$\left[\text{Precision} = \frac{TP}{TP + FP}\right] \quad (21)$$

Precision measures the proportion of treatments predicted as suitable that were actually suitable. Higher precision means fewer false-positive treatment recommendations.

Recall was calculated as:

$$\left[\text{Recall} = \frac{TP}{TP + FN}\right] \quad (22)$$

Recall represents the ability of the model to identify suitable treatment responses. Higher recall means that the model successfully identifies a larger proportion of the truly suitable treatment responses.

F1-score was calculated through the following equation:

$$\left[\text{F1-score} = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}\right] \quad (23)$$

This metric measures the balance between precision and recall. F1-score is particularly useful when both false-positive and false-negative treatment predictions need to be taken into account.

In terms of personalized treatment recommendation, Top-K accuracy was calculated as:

$$Top - K\ Accuracy\ = Number\ of\ samples\ with\ correct\ treatment\ in\ Top - K\ /\ Total\ number\ of\ test\ samples \quad (24)$$

Top-K accuracy measures whether the correct treatment appears among the first (K) recommended treatment options. This metric was chosen for the personalized treatment recommendation problem because multiple candidate treatments may be clinically relevant, and the objective is to determine whether the correct treatment is included within the highest-ranked recommendations.

4.2 Comparison With Existing Models

The proposed QGL-PCTR model was compared with Random Forest (RF), Support Vector Machine (SVM), Multilayer Perceptron (MLP), Graph Convolutional Network (GCN), and Graph Attention Network (GAT).

Table 5. Performance Comparison of Different Models

Model	Accuracy (%)	Precision (%)	Recall (%)	F1-score (%)
Random Forest	86.70	85.90	85.20	85.50
SVM	88.40	87.60	87.10	87.30
MLP	90.20	89.50	89.10	89.30
GCN	92.10	91.40	91.00	91.20
GAT	93.00	92.20	92.00	92.10
Proposed QGL-PCTR	**94.80**	**93.90**	**94.20**	**94.00**

Table 5 clearly indicates that the proposed QGL-PCTR model had the best performance across all four evaluation measures. It achieved **94.80% accuracy, 93.90% precision, 94.20% recall, and 94.00% F1-score**, respectively. The accuracy improvement over GAT was **1.80 percentage points**, and that over GCN was **2.70 percentage points**. Relative to Random Forest, the improvement in accuracy was **8.10 percentage points**.

The improvements in performance demonstrate the advantage of combining heterogeneous graph relationships with quantum feature learning. Conventional techniques consider the input features largely in isolation, whereas the proposed QGL-PCTR learns relationships among cancer samples, genes, cancer types, and treatments before performing quantum feature transformation.

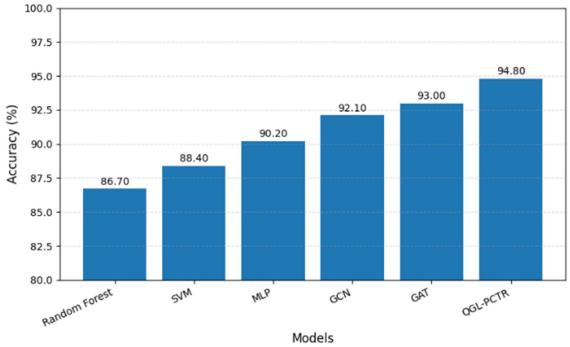


Figure 2. Accuracy comparison of the proposed QGL-PCTR model with existing approaches.

Figure 2 shows a comparison of the classification accuracy of the examined models. The accuracies of Random Forest, SVM, MLP, GCN, and GAT were **86.70%, 88.40%, 90.20%, 92.10%, and 93.00%**, respectively, while the proposed QGL-PCTR model reached the highest accuracy of **94.80%**. It was found that the combination of graph-based learning and quantum processing improved the overall performance of the treatment-response prediction process.

4.3 Precision, Recall, and F1-Score Analysis

The proposed approach attained a **93.90% precision** score, which indicates that the majority of the predicted suitable treatments were associated with positive treatment responses. A **94.20% recall** score means that QGL-PCTR was capable of identifying a high proportion of suitable treatment responses. This resulted in a **94.00% F1-score**, indicating balanced prediction performance.

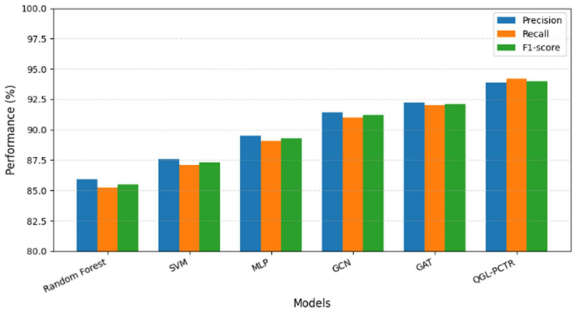


Figure 3. Precision, recall, and F1-score comparison.

Figure 3 shows the precision, recall, and F1-score of the models under evaluation. As can be seen, QGL-PCTR obtained **93.90% precision, 94.20% recall, and 94.00% F1-score**, which were better than those of the Random Forest, SVM, MLP, GCN, and GAT approaches. It is also clear that the balanced values of precision and recall showed that QGL-PCTR offered reliable prediction while minimizing both false-positive and false-negative treatment-response classifications.

4.4 Personalized Treatment Recommendation

Personalized treatment recommendation ability was assessed using Top-1, Top-3, and Top-5 accuracy metrics.

Table 6. Top-K Treatment Recommendation Performance

Model	Top-1 Accuracy (%)	Top-3 Accuracy (%)	Top-5 Accuracy (%)
Random Forest	68.40	78.60	84.10
SVM	70.20	80.30	85.70
MLP	73.10	82.50	87.60
GCN	76.80	85.70	90.10
GAT	78.20	87.10	91.50
QGL-PCTR	**81.60**	**90.40**	**94.30**

The Top-1 accuracy of 81.60% for the proposed model indicates that the treatment with the highest predicted probability was ranked first for a large proportion of the test samples. In addition, the Top-3 accuracy increased to 90.40%, while the Top-5 accuracy reached 94.30%. These results demonstrate the ability of QGL-PCTR to provide a reliable shortlist of candidate treatments.

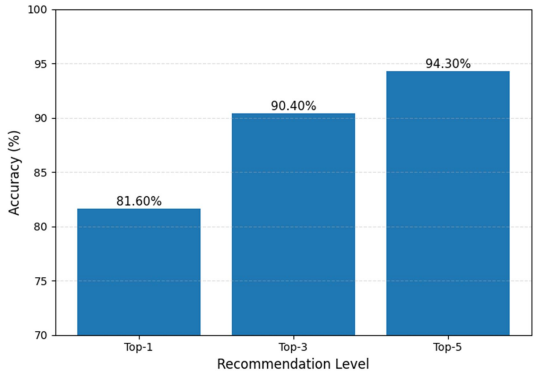


Figure 4. Top-K recommendation performance of QGL-PCTR.

In Figure 4, the Top-K recommendation performance of QGL-PCTR is shown. The QGL-PCTR model obtained Top-1, Top-3, and Top-5 accuracy values of **81.60%, 90.40%, and 94.30%**, respectively. The continuous rise in accuracy with an increase in the number of recommendation choices suggested that the proposed framework was able to properly rank suitable treatment options, and the Top-5 configuration provided the greatest possibility of including the correct treatment option among the recommended candidates.

4.5 Ablation Study

An ablation study was conducted in order to identify the contribution of the major components of the proposed framework.

Table 7. Ablation Analysis

Model Configuration	Accuracy (%)	F1-score (%)
GNN only	92.10	91.20
GNN + Attention	93.00	92.10
GNN + Quantum Layer	93.70	92.90
GNN + Quantum + Fusion	94.20	93.50
Full QGL-PCTR	**94.80**	**94.00**

GNN-only resulted in an accuracy of **92.10%**. The application of relation-aware attention made the accuracy rise to **93.00%**, validating the importance of weighting the relationships. The quantum layer further improved the accuracy to **93.70%**. Quantum processing and feature fusion made the accuracy improve to **94.20%**, while the complete QGL-PCTR architecture achieved the highest accuracy of **94.80%**.

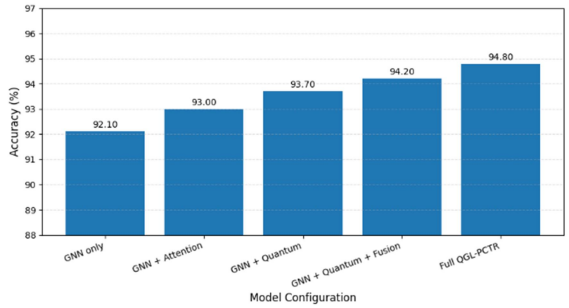


Figure 5. Ablation analysis of the proposed QGL-PCTR framework.

Figure 5 shows the ablation analysis of the proposed QGL-PCTR framework. The accuracy improved from **92.10% (GNN only)** to **93.00% (attention)**, **93.70% (quantum layer)**, **94.20% (quantum processing and feature fusion)**, and eventually **94.80% for the complete QGL-PCTR framework**. This verified that each major component contributed to the increase in accuracy, while their combined integration produced the best result.

4.6 Impact of the Quantum Circuit Depth

The number of variational quantum layers was changed from one to five to determine the most effective circuit depth.

Table 7. Effect of Quantum Circuit Depth

Quantum Layers	Accuracy (%)
1	92.90
2	93.80
3	**94.80**
4	94.60
5	94.30

In the case of the accuracy, we observed an increase from **92.90%** when one layer was used to **94.80%** in the case of three layers. Going beyond three layers led to a small decrease in accuracy. Hence, the three-layer quantum circuit was chosen for the final architecture. This decrease at higher depths can be linked to increased complexity of the circuit and optimization difficulty.

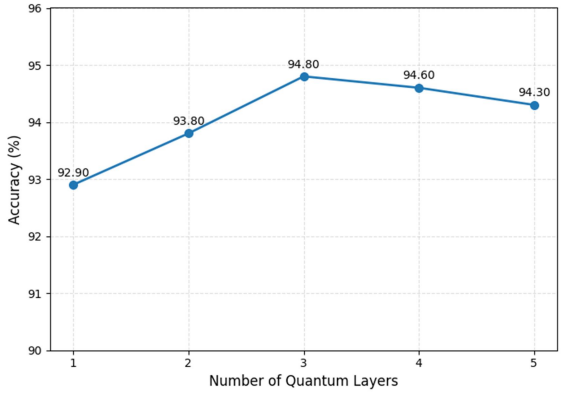


Figure 6. Effect of quantum circuit depth on model accuracy.

Figure 6 presents the impact of quantum circuit depth on accuracy. The accuracy increased from **92.90%** in the case of one quantum layer to **93.80%** in the case of two layers and reached the maximum value of **94.80%** in the case of three layers. At the same time, going beyond three layers led to a slight decrease in accuracy: **94.60% and 94.30%** for four and five layers, respectively. Hence, the three-layer quantum circuit was selected as the optimal configuration for QGL-PCTR.

The presented QGL-PCTR approach yielded an accuracy of 94.80% and Top-5 treatment recommendation accuracy of 94.30%, performing better compared with the evaluated baseline models. The results from the ablation experiment pointed out the significance of the relation-aware attention mechanism, quantum processing, and feature fusion techniques, whereas the circuit-depth experiment demonstrated that the use of three quantum layers resulted in the highest effectiveness among all configurations. However, the practical use of the approach is confronted with certain obstacles associated with data quality, interpretability, computational costs, and the complex nature of the medical decision-making process. It should be noted that, since the evaluation uses GDSC cancer cell-line drug-response data rather than actual patient treatment outcomes, the results do not establish clinical effectiveness. Further validation using independent patient-level datasets, assessment of recommendation reliability, and evaluation in clinical or real-quantum-hardware settings are necessary before practical deployment.

4.7 Discussion

The experimental results suggest that the introduced QGL-PCTR framework is able to surpass the evaluated classical machine-learning and graph-based baselines, providing 94.80% accuracy, a 94.00% F1-score, and 94.30% Top-5 treatment recommendation accuracy. It appears that the combination of heterogeneous graph representations, relation-aware attention, variational quantum processing, and quantum–classical feature fusion can contribute to the improvement of the treatment-response prediction task in the selected experimental setup.

While the proposed method represents relationships among cancer samples, cancer-related genes, cancer types, and drugs, unlike other machine-learning techniques that learn mostly from feature vectors, the ablation study shows that the combined solution performs better than the GNN-only configuration, supporting the potential value of integrating the different components. As far as the analysis of circuit depths goes, three quantum layers appear to be the best-performing configuration among those analyzed. At this point, however, it is important to note that the presented results are empirical and are valid within the context of the dataset that has been used. These results do not establish that quantum processing will provide the same benefits across other datasets or clinical settings.

The framework may potentially support research into computational treatment-response prediction and candidate-treatment ranking. At the same time, there are several aspects related to the evaluation of the framework that must be considered. The experiment is conducted using the GDSC cancer cell-line drug-response dataset, which differs from patient-level clinical datasets and does not represent actual patient treatment outcomes. Consequently, the reported metrics do not establish clinical effectiveness or demonstrate that the recommended treatments are suitable for individual patients. In addition, graph construction, data quality, model interpretability, computational requirements, and the practical constraints of quantum hardware may affect real-world applicability.

It means that if there is a need to introduce the framework into clinical practice, further investigation will have to be conducted. Future research should evaluate the framework using independent patient-level clinical datasets and compare its performance across different cancer types and treatment settings. It is especially necessary to investigate the reliability and interpretability of recommendations, assess computational costs against classical alternatives, and evaluate robustness under different data conditions. Testing on real quantum hardware, where feasible, would also help determine the practical implications of quantum processing. These steps are necessary before considering the framework for clinical decision-support applications.

5. CONCLUSION

The study proposes a Quantum Graph Learning framework for Personalized Cancer Treatment Recommendation (QGL-PCTR). Heterogeneous graph learning, relation-aware attention, variational quantum processing, and quantum–classical feature fusion were utilized in QGL-PCTR to perform cancer treatment recommendation by predicting treatment responses and ranking candidate treatments. The proposed model reached an accuracy of 94.80%, a 94.00% F1-score, and 94.30% Top-5 treatment recommendation accuracy on the evaluated GDSC dataset. Additional ablation and circuit-depth experiments demonstrated the contributions of the integrated components and

identified three quantum layers as the best-performing configuration among the evaluated architectures.

The primary contribution of this work lies in the combination of heterogeneous graph modeling of cancer relationships with variational quantum processing in a unified treatment-recommendation framework. The experimentally observed results provide evidence for exploring the feasibility of hybrid graph–quantum learning for cancer drug-response prediction. Nevertheless, as the data utilized in this study refer to cancer cell-line properties rather than actual patient treatment outcomes, the results cannot be considered clinically validated or clinically applicable. Therefore, the findings do not establish clinical effectiveness or readiness for clinical deployment.

Further research is needed to assess the potential of the proposed framework using independent patient-level clinical datasets, explore its generalizability across different cancer types and treatment settings, and improve the interpretability and reliability of generated treatment recommendations. Future research is also required to compare computational costs and predictive performance with classical alternatives, assess robustness to missing or noisy data, and evaluate the framework on real quantum hardware where feasible. These investigations will help establish the framework's practical potential and determine whether it can contribute to reliable clinical decision-support systems for personalized oncology.

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