Int. J. Sci. R. Tech., 2025 2(11)
A Multidisciplinary peer-reviewed Journal
www.ijsrtjournal.com [ISSN: 2394-7063]

Original Article

A study on Quantum Computing Could Revolutionize Drug Discovery

Yogesh C.*, Manoj S. G., S. Aruna, Dr. D. P. Sivasaktibalan

KRM Public School

ABSTRACT

The traditional drug discovery process is slow, resource-intensive, and often unsuccessful. This is mainly because regular computers find it hard to accurately model complex molecular interactions at the quantum level. This abstract suggests that Quantum Computing (QC) could change the game. It uses the principles of superposition and entanglement to transform pharmaceutical research. QC will provide a significant increase in computing power for quantum chemistry simulations. This will help researchers model the electronic structure of molecules and their exact behavior, including protein folding, binding affinities, and off-target effects, with great accuracy and speed. Algorithms like the Variational Quantum Eigensolver (VQE) are expected to uncover insights into drug-target interactions that we cannot currently obtain. This will greatly reduce the need for costly and lengthy physical experiments. Additionally, QC can improve virtual screening and support next-generation Quantum AI for faster analysis of genomic data and better optimization of drug candidates. Though the technology is still in its early stages, using QC could notably shorten development timelines and lower costs. This will enable the discovery of more targeted and effective drugs, leading to significant progress in treating complex diseases and a new era of precise, personalized medicine. The shift will require ongoing investment in reliable quantum hardware and specialized quantum algorithms.

Keywords: Quantum Computing (QC), Drug Discovery, Variational Quantum Eigensolver (VQE)

INTRODUCTION

Quantum computing is a growing field in computer science and engineering. It takes advantage of the unique aspects of quantum mechanics, the physics that deals with very small things like atoms and subatomic particles, to carry out calculations. Classical computers use bits to store information as either a 0 or a 1. In contrast, quantum computers use quantum bits, or qubits, which can be in multiple states at the same time. This capability allows them to solve specific problems much faster than even the most powerful classical supercomputers.

Hypothesis: Using quantum simulation algorithms, such as VQE, to model the electronic structure of drug candidates and their target binding sites will produce binding affinity predictions for new molecules that are at least twice as accurate. This means there will be a 50% reduction in prediction error compared to the current classical methods used in the industry, like Density Functional Theory or empirical force fields. This applies to systems with strong electron correlation.

How quantum computing helps in discovering drug discover

Molecular Simulation (Quantum Chemistry): The behavior of molecules follows the laws of quantum mechanics, which involve the movement and interaction of electrons. Classical computers find it hard to solve the Schrödinger equation for complex molecules such as proteins and potential drug compounds because the number of possible electron interactions increases rapidly. Quantum computing, based on quantum mechanics, can model these interactions with remarkable accuracy and speed. Binding Affinity Prediction: Quantum computing can calculate the binding energy between a potential drug molecule (ligand) and its biological target (protein) with precision. This is important for predicting a drug's effectiveness and is currently the biggest computational challenge in drug design. De Novo Drug Design: By simulating the properties of millions

Relevant conflicts of interest/financial disclosures: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

of possible molecules in a short time, quantum computing can quickly screen large chemical spaces. It helps researchers design new molecules with improved properties, moving beyond slow trial-and-error approaches. Protein Folding: Quantum computing has the potential to tackle the very complex problem of protein folding. This is vital for understanding many diseases such as Alzheimer's and Parkinson's and for creating targeted therapies.

He role of technology in the drug pipeline
How It Operates

The Quantum Computer
Create and model molecules.
Solves complicated chemical equations, such as the Schrödinger equation, using qubits (superposition/entanglement).

Traditional Detection
Calculate the drug content of a sample.
methods such as UV-
Vis Spectroscopy, Mass Spectrometry (MS), or High-Performance Liquid Chromatography (HPLC).

Sensors with Quantum Propertiestool for extremely sensitive analysis in the future.
Quantification of drug molecules, metabolites, or bio markers in a patient's body or in a drug formulation may become possible with the use of non-invasive, highly sensitive, and real-time devices such as Diamond Nitrogen-Vacancy (NV) centers or Optical Magnetometers, which use quantum properties to detectute magnetic or electrical signals from molecules.

METHODOLOGY:

Sample: detecting caffeine in coffee powders

The standard, proven methodology for determining caffeine concentration involves a three-step process using classical instruments:

Sample Preparation: The coffee powder must be prepared so the caffeine is soluble and can be analyzed. This typically involves extraction (e.g., using hot water or a solvent like methanol or a mixture of water/ethanol) followed by filtration to remove solid coffee particles.

Instrumental Separation/Measurement: The prepared sample is analyzed using a technique like High-Performance Liquid Chromatography (HPLC) or Spectroscopy (e.g., UV-Vis or Fourier-Transform Infrared, FTIR).

HPLC: Separates the caffeine from other compounds in the extract, and a detector measures the amount of caffeine passing through at a specific time (retention time).

Spectroscopy: Measures the absorption of light at a wavelength known to be specific to the caffeine molecule (e.g., around 270-280 nm in the UV range).

Quantification: The instrument's signal (e.g., peak area in HPLC or absorbance in Spectroscopy) is compared against a calibration curve generated from samples of known caffeine concentration to accurately calculate the concentration in the unknown coffee sample.

Proposed Quantum Computing Methodology (Computational Role)

Quantum computing would not replace the experimental measurement but would offer a significant speed-up and higher accuracy in the prediction, simulation, and interpretation phases of complex chemical analysis, particularly in:

1. Quantum Simulation of Molecular Properties

The Problem: Calculating the electronic structure and properties of molecules like caffeine is computationally intensive (scales exponentially) for classical computers, especially when considering the complex environment of a coffee extract (caffeine interacting with water, chlorogenic acids, etc.).

The Quantum Solution: Quantum algorithms, such as the Variational Quantum Eigensolver (VQE) or Quantum Phase Estimation (QPE), can efficiently solve the Schrödinger equation for the caffeine molecule and its interactions.

The Output: This simulation yields highly accurate predictions of molecular properties, such as the exact absorption spectrum (the shape of the UV/IR light absorption curve) or Nuclear Magnetic Resonance (NMR) shifts. This detailed, ab initio (from first

principles) knowledge is crucial for precisely setting up and interpreting the classical experiment.

2. Enhanced Spectroscopic Analysis

The Problem: In analytical techniques like Near-Infrared (NIR) spectroscopy for direct powder analysis, a large dataset is needed to train a statistical model (chemometrics) to correlate the complex, overlapping spectral data with the caffeine concentration.

The Quantum Solution: Quantum algorithms could be used for:

Simulating NIR Spectra: Generating highly accurate, synthetic training data for spectroscopic methods, which can significantly reduce the need for extensive real-world data collection and improve the model's robustness.

Accelerated Chemometrics: Quantum Machine Learning algorithms could potentially process the vast spectroscopic datasets and build the concentration-prediction model much faster than classical algorithms.

3. Molecular Dynamics and Environmental Effects

The Problem: The measurement of caffeine can be influenced by the surrounding molecules (the matrix effect), which slightly shifts its spectroscopic properties.

The Quantum Solution: Quantum simulation can accurately model the molecular dynamics of the caffeine-solvent or caffeine-coffee matrix system. This allows researchers to predict the exact quantum-mechanical shifts in the caffeine's spectrum due to its environment, leading to a more precise correction factor for the concentration calculation.

In summary, the role of quantum computing is not in the physical act of measurement but in providing exponential speedup for the computational chemistry that underpins and validates the most sophisticated analytical techniques.

Quantum computing could theoretically determine the amount of caffeine in coffee powder by using its abilities in molecular simulation and chemical analysis.

This application is still mostly theoretical or in early research stages, but the general approach would be as follows

1. Quantum stimulation of the caffeine molecules Schrödinger equation: quantum computers can stimulate quantum systems,a task that is too complicated for classical super computers when it comes to all but the smallest molecules. Caffeine molecule, though small, has many quantum states, required in a large number of qubits for full and accurate stimulation (estimates suggest around 160 fault – tolerant qubits)

Determining Electronic structure: Quantum algorithms like the Variational Quantum Eigensolver (VQE) could calculate the electronic structure and ground-state energy of caffeine molecule accurately.

Predicting chemical properties: This accurate simulation would enable predictions of caffeine's specific quantum chemical parameters (such as orbitals and molecular descriptors) as well as its spectroscopic signature, which describes how it absorbs or emits at different wavelengths.

2. Quantum-Enhanced spectroscopic analysis classical methods for determining caffeine (like HPLC or UV-vis/FTIR spectroscopy) depends on the molecule's unique chemical and light absorption properties. Quantum computing could improve these methods by providing unmatched accuracy in predictions:

Improved Reference Data: The accurate quantum simulations would create a perfect theoretical signature for pure caffeine. This would serve as better reference standard for comparing with experimental data from the coffee powder sample.

Stimulating complex interactions: Coffee powder is complex mixture. Quantum simulation could model the interactions between caffeine and other compounds, such as chlorogenic acids are other organic compounds, that might interfere with spectral measurements. This would allow for more accurate

separation of the experimental spectra from the coffee sample

Quantum Machine learning/optimization: Quantum algorithms could optimize chemometric calibration models used in current techniques like Fourier Transform Infrared (FTIR) or UV-vis spectroscopy. This model connect a measured spectroscopic signals (from the coffee powder extract) to the caffeine concentration. Quantum machine learning could process this complex data faster and more accurately than classical algorithms, resulting in a more precise concentration value.

CONCLUSION

Even though quantum computing is not a substitute for existing ways to measure properties in the lab, it is lifesaving in improving the precision and efficiency of analytical techniques, by way of powerful molecular simulations. Fulfilling rapid and indistinguishable chemistry analysis at the quantum scale, quantum computing can change the way we measure and interpret our understanding of things (like the caffeine content in coffee powder for an example), in a new age of computationally driven science discovery.

REFERENCE

1. Cao, Y., Romero, J., Olson, J. P., Degroote, M., Johnson, PD., Kieferová, M., & Aspuru-Guzik, A. (2019). Quantum chemistry in the age of quantum computing. Chemical Review 119(19), 10856–10915. https://doi.org/10.1021/acs.chemrev.8b00803
2. McArdle, S., Endo, S., Aspuru-Guzik, A., Benjamin, S. C., & Yuan, X. (2020). Quantum computational chemistry. Reviews of Modern Physics, 92(1), 015003. https://doi.org/10.1103/RevModPhys.92.015003
3. Reiher, M., Wiebe, N., Svore, K. M., Wecker, D., & Troyer, M. (2017). Elucidating reaction mechanisms on quantum computers. Proceedings of the National Academy of Sciences, 114(29), 7555–7560. https://doi.org/10.1073/pnas.1619152114
4. Kandala, A., Mezzacapo, A., Temme, K., Takita, M., Brink, M., Chow, J. M., & Gambetta, J. M. (2017). Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets. Nature, 549(7671), 242–246. https://doi.org/10.1038/nature23879
5. Bai, S., Ye, Y., Ma, X., & Wang, Q. (2023). Quantum generative models in drug discovery. Journal of Chemical Information and Modeling, 63(3), 653–668. https://doi.org/10.1021/acs.jcim.2c01323
6. Peruzzo, A., McClean, J., Shadbolt, P., Yung, M. H., Zhou, X. Q., Love, P. J., … & O'Brien, J. L. (2014). A variational eigenvalue solver on a photonic quantum processor. Nature Communications,5, 4213. https://doi.org/10.1038/ncomms5213
7. Tilly, J., Chen, H., Cao, S., Setia, K., Li, Y., Grant, E., … & Aspuru-Guzik, A. (2022). The Variational Quantum Eigensolver: A review of methods and best practices. Physics Reports, 986, 1–128.
8. Reiher, M., Wiebe, N., Svore, K. M., Wecker, D., & Troyer, M. (2017). Elucidating reaction mechanisms on quantum computers.
9. Proceedings of the National Academy of Sciences, 114(29), 7555–7560. https://doi.org/10.1073/pnas.1619152114
10. Cohen, A. J., Mori-Sánchez, P., & Yang, W. (2012). Challenges for Density Functional Theory. Chemical Reviews, 112(1), 289–320. https://doi.org/10.1021/cr200107z
11. Tilly, J., Chen, H., Cao, S., Setia, K., Li, Y., Grant, E., … & Aspuru-Guzik, A. (2022). The Variational Quantum Eigensolver: A review of methods and best practices.
12. Physics Reports, 986, 1–128. https://doi.org/10.1016/j.physrep.2022.08.003
13. Cao, Y., Romero, J., Olson, J. P., Degroote, M., Johnson, P. D., Kieferová, M., … & Aspuru-Guzik, A. (2019). Quantum chemistry in the age of quantum computing. Chemical Reviews, 119(19), 10856–10915. https://doi.org/10.1021/acs.chemrev.8b00803
14. O'Malley, P. J. J., et al. (2016). Scalable quantum simulation of molecular energies. Physical Review X, 6(3), 031007. https://doi.org/10.1103/PhysRevX.6.031007
15. Nielsen, M. A., & Chuang, I. L. (2010). Quantum Computation and Quantum Information: 10th Anniversary Edition. Cambridge University

Press.
https://doi.org/10.1017/CBO9780511976667.

HOW TO CITE: Yogesh C.*, Manoj S. G., S. Aruna, Dr. D. P. Sivasaktibalan, A study on Quantum Computing Could Revolutionize Drug Discovery, Int. J. Sci. R. Tech., 2025, 2 (11), 505-509. https://doi.org/10.5281/zenodo.17641580