Research Paper
Impact Factor: 7.352
Peer Reviewed Monthly Journal
www.ijmdrr.com

IJMDRR
E- ISSN –2395-1885
ISSN -2395-1877

ACCELERATING THE SUSTAINABLE DEVELOPMENT GOALS THROUGH MOLECULAR DOCKING FOR DRUG SYNTHESIS: SOME EFFORTS AND OPPORTUNITIES

Dr.M.Meenakumari
Assistant Professor, Department of HS-NFSM&D, S.A.College of Arts & Science, Chennai.

Abstract
Molecular docking is such a ground breaking computational chemistry that has been applied to accelerate the drug discovery and creation procedure within the range of objectives of the United Nations Sustainable Development (SDGs). Docking is fast to facilitate rational drug design, redundancy within experiments is minimized and the environmental impact of traditional drug development is lowered through prediction of accurate protein-ligand interactions. Its use has been able to aid SDG 3 (Good Health and Well-being) by expediting the process of therapeutics against infectious diseases, and cancers and neglected conditions SDG 9 (Industry, Innovation, and Infrastructure) through the use of pipelines of sustainable innovation. The use of advances into better scoring features, flexible docking algorithms and interoperability with artificial intelligence (AI) and machine learning (ML) has made docking-based methods more accurate, fast, and scalable. All these advancements facilitate drug re-use, natural product discovery and precision medicine, which are economical and fair healthcare interventions, particularly where the resources are limited. Moreover, molecular docking is environmentally friendly in drug development since it reduces the level of chemical wastage, resources are saved and there is open source cooperation. The future crossroad of docking and quantum computing, multi-omics data and analytics of big data promises to reach new heights in drug synthesis precision, as well as additional personalization. Despite model accuracy, validation and ethical concerns have been a thorn in the flesh, molecular docking has been a change agent of sustainable healthcare development, balancing scientific progress and equity in healthcare provision globally in the search of the SDGs.

Keywords: Molecular docking, Drug discovery, Sustainable Development Goals (SDGs), Artificial intelligence (AI), Machine learning (ML), Precision medicine, Drug repurposing, Sustainable healthcare innovation.

Introduction

The most significant computational tool of SBDD, molecular docking, has been created to predict the most preferred 3D orientation of the ligand-biological target complexes and their affinity. Docking has developed since its initial creation that is, as an extension of geometric fitting algorithms in the 1970s, into the form of highly elaborate, energy-based scoring models. The effect of these developments has been the minimization of the cost and time used in drug discovery as the compounds are prioritized before synthesis.

The SDGs implemented by the UN in 2015 (especially, SDG 3, Good Health and Well-being, and SDG 9, Industry, Innovation, and Infrastructure) have a direct relationship with the progress in pharmaceutical innovation. Computational drug design allows the healthcare innovation to be cheap and sustainable. United Nations (2015).

Advances in Molecular Docking Techniques

Contemporary docking methods include structure-based and ligand-based methods. Structure-based docking employs 3D protein structures whereas ligand-based docking employs activity patterns of known compounds. The hybrid schemes that use such with simulation using molecular dynamics are much more accurate by simulating flexibility of a receptor. The enhanced predictive accuracy and computing speed are promoted by the enhancements in the scoring mechanisms and in the optimization algorithms, i.e. genetic algorithms or multi-objective optimizations. The examples of such enhancements can be found in such tools as AutoDockVina that allows screening a large library of compounds with high-throughput efficiency (Eberhardt et al., 2021). The combination of AI and ML with docking has advanced the prediction accuracy field to the next level with the ability to estimate binding affinities and de novo drug design by using data (Jin et al., 2022).

Molecular Docking and the Sustainable Development Goals

Molecular docking has a direct contribution to SDG 3 through rapid therapeutic discovery of infectious diseases, cancer and NTDs. As an example, within the context of the COVID-19 pandemic, computational docking suprised more than one promising inhibitor of SARS-CoV-2 main protease in the records of Ton et al., 2020. Similarly, a few docking-assisted repurposing of trypsinase4 inhibitors on Trypanosomabrucei have accorded significance to the cost-effective NTD therapies as established by de Souza et al.

Molecular docking reduces the waste and wasted costs of experiments by optimizing virtual screening, therefore focusing on SDG 9 about Innovation and SDG 12 about Responsible Consumption and Production.

Natural Products and Photochemical in Docking-Based Drug Discovery

Natural products continue to be a good source of novel Chemical scaffold. Similarly, molecular docking has been used to screen petrochemicals in pathways like TCM and IMPPAT and this enables the discovery of promising antivirals and anticancer agents in a virtual manner. Wang et al., 2020
Docking combined with ADMET prediction systems, including Swiss ADME is used in enhancing the prioritization of compounds to guarantee efficacy and safety. Daina et al., 2017

Their biggest issue however is that the natural products may be computationally complicated due to their complex stereochemistry. Equally, AI-based docking algorithms have been developed; these algorithms attempt to model these structures in an even more precise manner.

AI and Machine Learning Integration

The docking workflow has been enhanced with AI, rendering the generative models and deep learning architectures efficient and more accurate than other alternatives. Equally, such less complex frameworks as Double SG-DTA, and graph isomorphism networks have modeled complex interactions between drugs and their targets, thereby enhancing their predictive ability (Huang et al., 2021).
Other generative models, including GANs and VAEs, create compound libraries of special interest on particular targets, including CDK2 and SARS-CoV-2 MPro. These integrative pipelines help in the process of open science, which will hasten the world in the sustainable discovery of drugs.

Drug Repurposing for Sustainable Therapeutics

The docking approach to drug repurposing utilizes existing pharmacokinetic and safety profiles to decipher new curative uses of existing approved drugs. This plan would reduce the cost, time, and resource input and support SDG 3 and SDG 10 (Reduced Inequalities).

The most successful cases of this are the reuse of the kinase inhibitors to treat parasitic infections and antiviral drugs to treat emerging pathogens (Pushpakom et al., 2019). Network pharmacology coupled with computational docking enhances this sustainability solution.

Challenges and Limitations

In spite of this, the protein flexibility technique coupled with a lack of structure information limits the technique of docking to increase the accuracy of docking. Scoring functions are not capable of modelling complex thermodynamics and results have to be provided experimentally.

Such biological complexities include allosteric modulation and off-target that significantly interferes with the attainment of the objectives of translating biological complexities into clinical meaning. To overcome the issues, docking and molecular dynamics coupled with artificial intelligence (AI) and network pharmacology should be taken into account to make sure that the transparency and reproducibility are not sacrificed.

Future Directions

The new technologies will require that docking techniques of drug synthesizing change: Quantum computing will exponentially enhance the accuracy and speed of docking. The multi-omics will allow the personalization of the drugs to some degree, but this movement is aligned with precision medicine.
The sustainable and inclusive innovation is the case of open-source collaboration systems that may be characterized by such a system as Open-Source Malaria.

Conclusion

Molecular docking is a complex system; this requires not only a computer and AI evolution, but also a global cooperation that is to be mentioned as the best innovation in the sustainable search of drugs. An SDG improvement approach which may involve docking can be made around the areas of health, innovation and sustainability as it can hasten the development of therapies and reduce resource and access to different technologies in a democratic way.

Such type of progress in the computations should support justifiable health results on the planet, which can be drawn by further interdisciplinary analysis, information broadcasting and socially responsible AI conduct.

References

1. Morris, G. M., et al. (2009). AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. Journal of Computational Chemistry, 30(16), 2785–2791.
2. Trott, O., & Olson, A. J. (2010). Auto DockVina: Improving the speed and accuracy of docking. Journal of Computational Chemistry, 31(2), 455–461.
3. Eberhardt, J., et al. (2021). Auto DockVina 1.2.0: New docking methods, expanded force field, and Python bindings. Journal of Chemical Information and Modeling, 61(8), 3891–3898.
4. United Nations. 2015. Transforming our world: The 2030 Agenda for Sustainable Development.
5. Daina, A., Michielin, O., &Zoete, V. (2017). SwissADME: A free web tool to evaluate pharmacokinetics and drug-likeness. Scientific Reports, 7(1), 42717.
6. Ton, A. T., et al. (2020). Rapid identification of potential inhibitors of SARS-CoV-2 main protease through docking and drug repurposing. Molecular Informatics, 39(8), 2000028.

7. de Souza, R. O. M. A., et al. (2020). Phosphodiesterase inhibitors as potential antitrypanosomal agents: Insilico and in vitro evaluation. Parasitology Research, 119(3), 923–935.
8. Wang, J., et al. (2020). Traditional Chinese medicine for COVID-19 therapy: Molecular docking and network pharmacology. Frontiers in Pharmacology, 11, 589586.
9. Jin, W., et al. (2022). AI-assisted molecular docking for drug discovery. Nature Machine Intelligence, 4(1), 43–52. Pushpakom, S., et al. (2019).
10. Drug repurposing: Progress, challenges and recommendations. Nature Reviews Drug Discovery, 18(1), 41–58. Bauer, B., et al. (2020).
11. Quantum algorithms for chemical simulations. Chemical Reviews, 120(22), 12685–12717. Hasin, Y., et al. (2017).
12. Multi-omics approaches to disease. Genome Biology, 18(1), 83. Huang, K., et al. (2021). Deep learning models for drug-target interaction prediction. Bioinformatics, 37(1), 112–118. Zhavoronkov, A., et al. (2020). Deep generative models for drug design. Nature Biotechnology, 38, 103–110. Zhou, T., et al. (2023).
13. Machine learning for natural product-based drug discovery. Chemical Society Reviews, 52, 1201–1220. Pagadala, N. S., et al. (2017).
14. Software for molecular docking: A review. Biophysical Reviews, 9(2), 91–102. Tropsha, A., &Golbraikh, A. (2021).
15. Predictive modeling of drug–target interactions using AI. Drug Discovery Today, 26(2), 316–324.

IJMDRR
E- ISSN –2395-1885
ISSN -2395-1877