INDUSTRY BRIEF

ENHANCING DRUG DISCOVERY RESEARCH WITH AI

NVIDIA

OVERVIEW

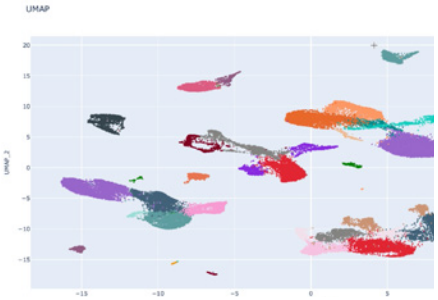
Drug discovery is the critical process of identifying new medicine. The task of researchers in drug discovery is to find novel molecules that will have positive therapeutic effects and help solve current health problems.

However, unravelling the complex interplay between the underlying genes, biochemical pathways, chemistry of the protein target, and absorption, distribution, metabolism, and excretion (ADME) processes is challenging—to say the least. Taken together, a successful drug will modulate a target in a very specific way along the disease pathway. Identifying a novel small molecule as a drug target that combats a specific pathway to improve patient outcomes, while diminishing undesirable side effects, is the goal in drug discovery.

Leveraging NVIDIA GPUs, AI-powered drug discovery efforts are enabling pharmaceutical and biotechnology companies to streamline research and development. These technologies help researchers transform vast patient datasets into digestible, tangible information, identify personalized and precision medicine opportunities, and forecast potential responses to new drugs.

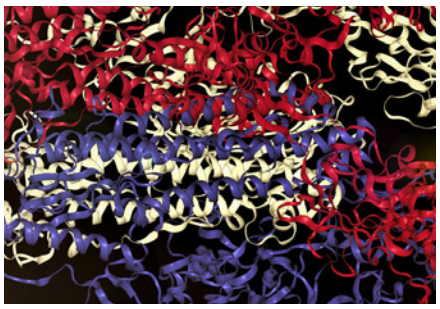
Genomics

Understanding the biology of a disease is essential for developing an effective therapeutic. One component of this is the disease pathway, which may involve thousands of proteins that interact and feedback through complicated mechanisms. Ultimately, a druggable protein target must be identified. Analysis of the human genome provides invaluable insights into the disease mechanism and can help identify new protein targets along the disease pathway.



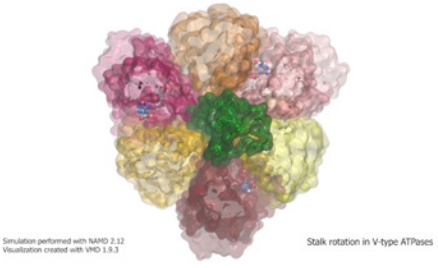
Protein Structure Determination

Protein structure determination is the assignment of a three-dimensional structure to a sequence of amino acids. The 3D structure provides physical information about the shapes and properties of small molecules that might make suitable drugs. Protein structures are typically determined by some form of electron microscopy, like cryogenic electron microscopy (cryo-EM). Increasingly, both physics-based computational methods and AI methods are able to accurately predict the 3D structure of a protein given only a sequence of amino acids and perhaps some limited data from nuclear magnetic resonance (NMR).



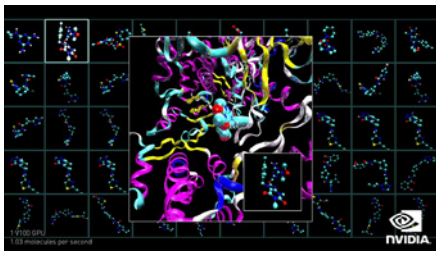
Cheminformatics

So vast is the chemical space that searching it, organizing it, and creating chemical databases has come to be known as cheminformatics. Armed with a protein target and its 3D structure, a researcher can begin an in silico search for molecules that may have just the right chemical properties to favorably bind. One way that researchers comb the chemical space is by computing a vector of physical quantities for each molecule;



this is known as a fingerprint and can be thought of as the coordinates for each molecule in a chemical space. Fingerprinting and related embedding methods make it possible to apply widely used methods from data mining and machine learning, such as clustering algorithms, molecular property prediction, and development of qualitative structure-activity relationship (QSAR) models.

Simulations in Drug Discovery



Molecular simulation provides key physics-based insights into the viability of a drug candidate molecule based on interactions between the drug and the protein target. Simulations can be performed at various levels of accuracy, based on the desired throughput. Docking, for example, provides a coarse description of the physical interactions and, due to the simplified computation, can be used to screen billions of compounds. Free energy perturbation (FEP) methods, molecular dynamics, and quantum methods provide increasingly accurate pictures of the interactions, providing essential go/no-go information to the synthetic chemists.

Advancing Drug Discovery with AI

More companies and researchers are beginning to turn to AI to enhance current methods in drug discovery. Molecular simulation like docking, FEP, and molecular dynamics requires a huge amount of computing power. At every phase of drug discovery, researchers are incorporating AI methods to accelerate the process. Predicting the folded 3D state of a protein, ligand-target binding energy, as well as pharmacokinetics like toxicity and absorption are just a few AI methods that are being developed today. The new AI methods complement existing workflows by advancing research while providing the same results as computationally expensive methods. By using AI to run simulations, researchers are saving money and discovering new potential drugs faster than before.

Accelerating Research with NVIDIA GPUs

NVIDIA is helping to accelerate research by enabling the GPU-powered compute and AI software that drive calculations for drug discovery workflows. With NVIDIA-powered platforms and software, researchers and pharmaceutical companies can develop and deploy intelligent applications that improve analysis and computations for research. With NVIDIA Clara™ Parabricks, researchers can accelerate genomics workflows. And with NVIDIA RAPIDS™, researchers can do lightning-fast, GPU-accelerated dataframe manipulations—seamlessly integrated with machine learning algorithms like clustering, dimensionality reduction, and tabular tasks—all in a Python notebook. Essentially, GPUs can accelerate virtually every key computational chemistry code, from docking and FEP to molecular dynamics and quantum electronic structure calculations.

EXPLORE NVIDIA GPU-ACCELERATED SOFTWARE

Clara Parabricks

- NVIDIA Clara Parabricks is a computational framework that supports genomics applications from DNA to RNA.

RAPIDS

- The RAPIDS suite of open-source software libraries and application programming interfaces (APIs) delivers the ability to execute end-to-end data science and analytics pipelines entirely on GPUs.

AMBER

- GPU-accelerated AMBER is a molecular dynamics application developed for the simulation of biomolecular systems.

NAMD

- NAMD is a parallel molecular dynamics code designed for high-performance simulations. With NAMD, researchers can simulate the movement of atoms within a molecular system.

GROMACS

- GROMACS is an application designed to simulate biochemical molecules like proteins, lipids, and nucleic acids. GROMACS runs up to 3X faster on systems accelerated with NVIDIA GPUs than on CPU-only systems, enabling users to run molecular dynamics simulations in hours instead of days.

BrianQC

- BrianQC is a GPU module for Q-Chem. It speeds up density functional theory and Hartree-Fock single-point, geometry optimization and frequency calculations, as well as many other methods.

To learn more about NVIDIA GPU-accelerated software, visit: **Clara Parabricks**, **RAPIDS**, **AMBER**, **NAMD**, **GROMACS**, and **BrianQC**.

Learn more about how NVIDIA is helping to advance drug discovery and research.

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