FF4EuroHPC Success Story

Advanced HPC Based Drug Discovery with Converged Deep Physics and AI

Organizations

Iktos is a French start-up SME specialising in AI applied to drug discovery. Iktos has developed a retro-synthesis algorithm and generative AI for drug design.

Qubit Pharmaceuticals is a French start-up SME specialised in physics-based simulations for drug discovery. Using advanced simulation software and AI-enhanced medicinal chemistry, the company develops novel drug candidates and identifies their modes of action against challenging targets.

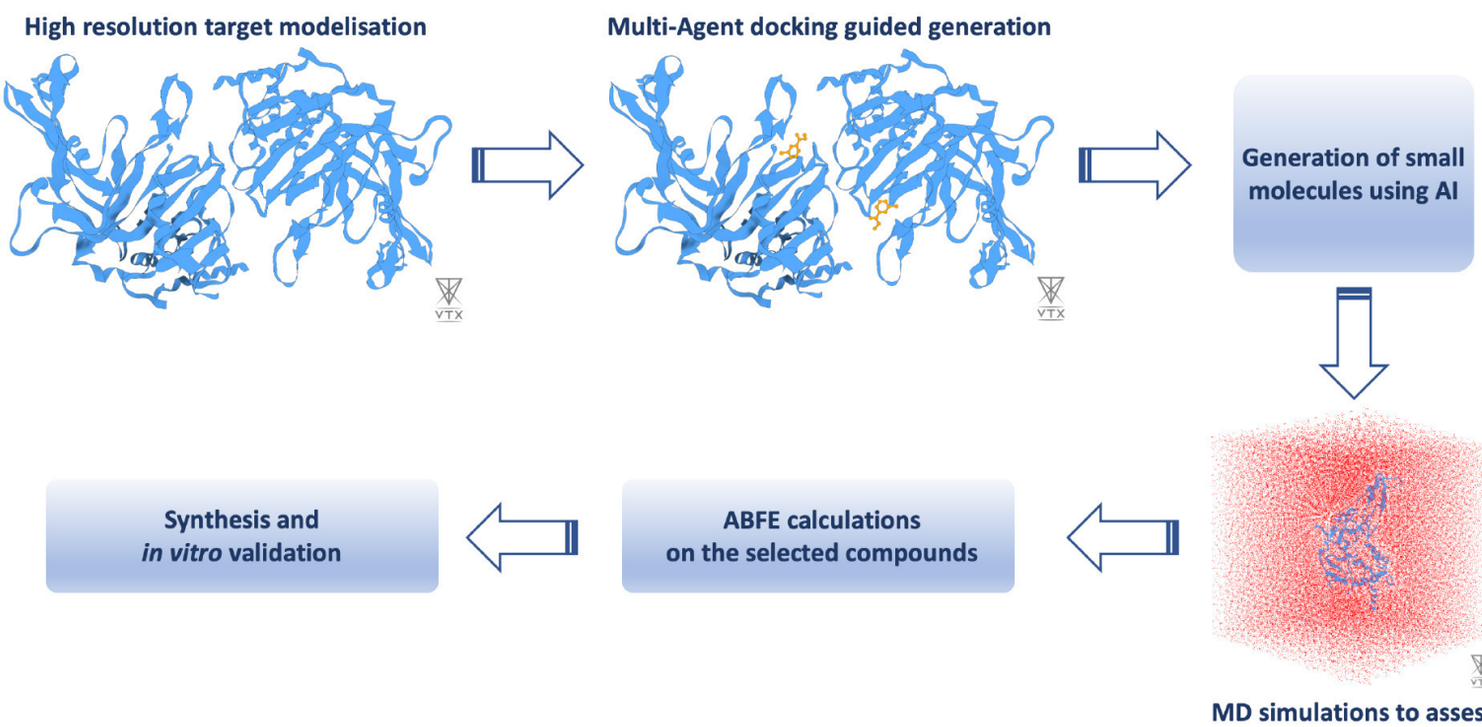
End User

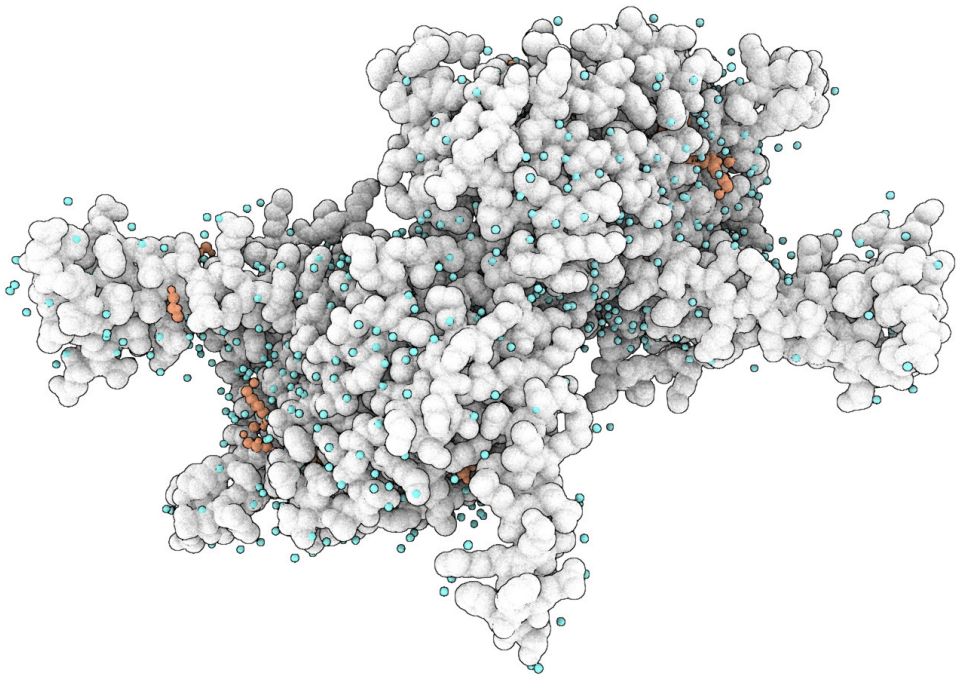
Domain Expert

The Challenge

The development of new drugs consists of two phases: discovery and development. The discovery phase can cost up to €800m, lasts around 5 years and is often covered by specialised companies. While conventional drug discovery strategies have been successfully used to deliver drugs with therapeutic applications, these strategies are costly and time-consuming. Therefore, computer-aided drug design has emerged as a new in silico method for the discovery stage and many SMEs are competing in this field. The tendency is to outsource the research effort outside of pharma companies to contract research organisations.

Both Iktos and Qubit Pharmaceuticals offer services and products for the drug discovery stage. Iktos would benefit from more powerful computing resources for their product, while an approach combining the strength of both products would create a unique offering to the customers of both SMEs. Particularly suited for hard targets, and would also considerably speed up and improve the process of internal drug discovery studies by Qubit Pharmaceuticals.





Industry Sector
Healthcare

Technology used:
HPC, ML, AI, Molecular Dynamics Simulations

The Solution

The organisations conceived a drug discovery strategy and toolchain focused on small molecules targeting novel proteins. Iktos contributed AI algorithms that generate novel molecules, and Qubit pharmaceuticals provided high-end absolute binding free energy calculations that predict how these compounds bind to challenging targets. Using HPC, the combined technology can speed up the drug design process and improves the quality of the generated compounds, thereby improving the entire drug discovery process and shortening it by 25%.

Exploiting this new capability, the combined workflow was applied to a target that has resisted pharma efforts over the last decade, the USP7, involved in cancer pathways. Progress in the drug discovery stage for this target could lead to drugs for various kinds of cancer.

The Impact

The organisations developed an in silico framework for drug discovery with the potential to cut drug discovery time by 25% and reduce overall drug development costs by 20%, which leads to savings of several million Euros. As time constraints and agility become crucial in the pharmaceutical industry, a new service offered through Iktos and based on this framework will be a competitive advantage in a challenging market, and represent an unrivalled product especially for hard-to-drug targets.

Additionally, the novel hit families of drugs targeting USP7 already discovered during the experiment will support the two SMEs' internal drug discovery pipeline. An estimated €200 Million will further be invested to bring these hit families to the pre-candidate stage. Having successfully reached that stage, the SMEs will be able to enter into a licensing agreement with pharma companies. Qubit Pharmaceuticals intends to use the new toolchain in further in-house drug discovery programs promising high profit by exploiting considerably increased success rates (40% vs 10%) enabled by the newly developed technology.

Benefits

- A unique physics-based AI-assisted workflow cuts the drug discovery time by 25% and reduces the cost of drug development by 20% (potentially saving several million Euros).
- Novel, highly profitable services to be offered by the SMEs.
- Discovered promising compounds which could lead to new cancer drugs, potentially generating substantial income for the SMEs far beyond the invested sums.