COMPANY	INDUSTRY	ISV
Nimbus Therapeutics	Pharmaceutical	Nanome

CASE STUDY

Accelerating drug discovery to create a healthier future

Nimbus Therapeutics is using VR solutions from Nanome and Oculus to help design breakthrough medicines.

BY INVESTING IN VR, NIMBUS EXPECTS TO SAVE

TENS OF THOUSANDS OF DOLLARS PER YEAR

ON PROJECT COSTS AND POTENTIALLY INCREASE EARNINGS BY GETTING COMPOUNDS TO MARKET FASTER

> **“Nanome with Oculus increases our ability to communicate and it increases our productivity. For a drug company to be running one of its chemotypes based on an idea we discovered in VR, well, there’s a lot of money being invested there.”**

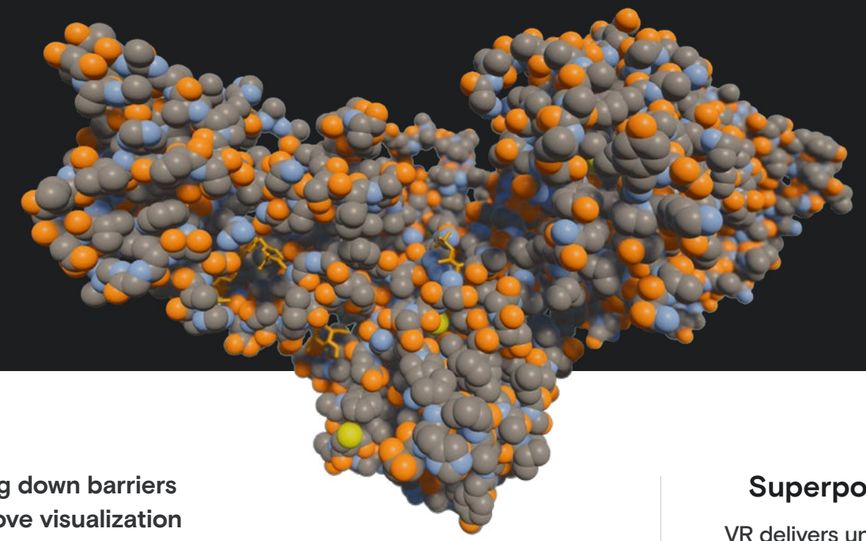
Lewis Whitehead, PhD
Director of Computational Chemistry
Nimbus Therapeutics
and Treasurer of the Computers in Chemistry Division at the American Chemistry Society

How Nimbus Therapeutics is developing tomorrow’s medicines with help from Nanome and Oculus.

Nimbus Therapeutics focuses on early-stage drug discovery and development with the goal of creating life-changing medicines. The company’s chemists design small-molecule compounds that target proteins known to drive disease. (Think of the targets as locks with many keyholes, and the compounds as keys that can potentially open the locks to alleviate illness or cure disease.) Then Nimbus biologists test those compounds in cells and animals to determine the potential effects on humans.

Until recently, computational medicinal chemists like Nimbus’s Dr. Lewis Whitehead didn’t have a good way to share their molecular structure designs with the chemists and biologists on their teams. “My head is full of 3D,” Whitehead says, “but my counterparts don’t necessarily live in 3D the way I do.” In recent years he’s tried to bridge that gap in different ways, first by creating a web-based platform for viewing and manipulating 3D molecular models, and next by having his team use a projector and 3D glasses to look at structures on a big screen.

Then, at the 2018 American Chemical Society conference, he discovered Nanome — developers of a cutting-edge virtual reality solution for molecular modeling. The Nanome team handed him an Oculus VR headset for a demo. “When I put the headset on,” he says, “I had an epiphany moment.”



Breaking down barriers to improve visualization and communication

The Nanome solution ingests structural data and simulation algorithms from computational chemists like Dr. Whitehead and turns them into 3D visualizations in VR. This allows scientists to physically interact with molecular structures, moving and rotating them to see details that are often missed using traditional 2D software and other simulations. “We create an immersive environment where chemists can build small molecules in the context of a protein’s binding site,” says Sam Hessenauer, Nanome CTO. “It’s like being able to build a key from inside a lock.”

Dr. Whitehead appreciates the ability to do immersive design. “Structural biology keeps getting bigger and bigger,” he says. “When you’re looking at complex structures on a small computer screen, it’s taxing on the eye and difficult to move around. With Nanome and the Oculus Quest controllers, I can get inside a structure for a 360-degree view — a few control instructions and I’m where I want to be.”

The VR visualizations enhance communication between the computational chemists designing the chemical structures and the synthetic chemists and biologists who take over from there. Rob Svensson, an expert oncology and metabolism biologist at Nimbus, says, “I spend a lot of time in meetings with chemists looking at slides of compounds, binding pockets, and the interactions they have at the atomic level. Chemists are so fluent in it, but for biologists it can be hard to understand.” When looking at structures in Nanome with an Oculus Quest headset, however, he says, “It’s like night and day. You can actually see the different amino acid residues the modelers are talking about and how potentially you might want to interact with them via a compound to drive selectivity. It’s very impressive.”

Superpowers of VR

VR delivers unique capabilities that give enterprises a competitive edge.

Top 3 VR superpowers for Nimbus Therapeutics:

Possible Impossible Scenarios

Big Dollar Savings

Real-time collaboration

Enhancing collaboration in the office and via remote

Before COVID-19 forced offices to close, Dr. Whitehead had begun using Nanome to share new drug target ideas with colleagues. Instead of presenting the usual 2D PowerPoint slides at a large company meeting, he put on his headset and shared his VR visualizations to colleagues' computer screens. "With Oculus Quest headsets you don't need cables and you don't need to be physically attached to a computer, so I could roam from meeting room to meeting room and rapidly deploy the system with a project team."

He also sees the potential for improved collaboration. "The vision is to use multiple headsets at team meetings, or when we're meeting with our research partners," he says. That way, everyone can view structures together and collaborate on them in real time.

Nanome's Hessenauer says that collaboration is one of the most powerful aspects of the solution. "The overwhelming majority of applications leveraged by scientists do not support real-time collaboration," he says. With Nanome, chemists can have live group design sessions, and chemists and biologists can discuss structures and share real-time feedback to accelerate their work.

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>
> Lewis Whitehead, PhD

Saving money and speeding up critical discoveries

While it takes many years and millions of dollars to bring a drug from discovery to clinical trials to pharmacy shelves, VR is beginning to help Nimbus reduce those initial timelines and some of the associated costs. Recently while evaluating the AMPKβ2 enzyme — a node that's considered a therapeutic target in metabolic diseases — Whitehead and team thought they'd determined the best strategy for drug selectivity within AMPKβ2's large macromolecular structure. However, once he put on his Oculus Quest headset and looked at a simulation of the protein moving in Nanome, he realized that strategy needed to be changed and another synthetic vector was more promising.

"Being able to inspect these structures inside VR gives us the opportunity to ask other questions, propose additional experimentation, and test our ideas to move the science forward," he says. Given that his team is trying to shorten the 12-18 month "lead optimization" cycle to get to a clinical candidate as fast as possible, Nanome and Oculus represent a significant advantage. "In the AMPKβ2 example, we were able to make our compounds more active on the target. These kinds of decisions can save tens of thousands of dollars a year."