
Welcome to Nanome

Welcome to Nanome - a Social VR Platform for Exploring Chemistry. It allows for the observation, manipulation, and building of molecules in an immersive virtual environment. Its applications extend to research scientists working in the laboratory and developing new drugs and insights from existing data.

Nanome is a startup co-founded in 2015 by engineering students at the University of California San Diego, who saw a need for 3D visualization tools to help medicinal and computational chemists and structural biologists reduce their time to market and increase the efficacy of new drugs (a process that can cost billions of dollars per drug).

Getting Started [5 minutes]

- Nanome is available on all the major VR stores such as Oculus, Steam, and Viveport. Simply, download the app from the Quest store on your headsets
- Sign into an account or sign up (a valid email address is needed)
- Follow the Nanome Basics tutorial to get familiar with the virtual environment and controllers. Once done, exit the tutorial and return to the lobby
- Join the public room “mo_puh” (or “makel99”)
    - If you do not see the room, press the refresh button at the top of the Lobby Navigation Bar Buttons
    - If you are unable to join the public room, feel free to create your own private user room and follow along with us

The Environment [4 minutes]

[adapted from the official Nanome Documentation]

- In addition to physically moving around in VR, users can teleport around the environment by pointing to a spot on the floor and pressing and holding down the trigger button with their index finger
- In order to scale the environment or molecular structures, press down on the middle finger 'grip' button on each controller. Next, bring the controllers together to scale the environment smaller or pull them apart to scale the environment larger
- In order to grab a structure, reach out and press the middle finger 'grip' button on one of the left or right controllers
- Users can also grab structures from afar by pointing their ray/laser and then pressing the 'grip' button
- Once the structure is grabbed, users can use the joystick or touchpad of their controllers to move the structure closer or farther away from them

COVID-19 Main Protease [6 minutes]

- Under the load menu, click on featured molecules and load the COVID-19 main protease
    - The COVID-19 main protease is responsible for breaking down the virus RNA into functional fragments to allow for its reproduction
    - Explore the molecule for 2 minutes
        - Select/Deselect substructures from the hierarchy menu for a better view of certain sites (such as the active site)
        - Change colors and scale
        - Change the display options for atoms, ribbons, and substructures; you can also add/remove labels
            - Can be done using the display menu under the main menu
        - Apply certain computations using the comput feature under Modify
        - Look at what other users are looking into
        - check out the whiteboard feature
        - The tools menu in general is really interesting to explore - ruler, lazer, periodic table
- If you still have some time on your hand, go to “load → workspace → 6vYB” and load the entire workspace
    - This is the spike that covers the COVID-19 virus in the open state which binds to receptor proteins on the human cell

Build Your Own Molecule [5 minutes]

[ideally, this new molecule would be designed with the COVID-19 main protease active site in mind. Such a molecule would act as an inhibitor prohibiting the replication of the virus. Because we are not chemists, feel free to build any molecule that comes to mind or just see what you come up with!] [adapted from Nanome Documentation]

- Click on the Build Menu (opens new window)Tab Button on the top right of the MedChem menu on the left hand
- Click on a structure on the Build menu (opens a new window) to select it for placement
- Overlap the structure on the right controller with an atom on the ligand
- Once a yellow outline encloses the atom(s) that you want to build on, press down trigger button on your right controller in order to place the structure
- Take a screenshot of the molecule and its properties!

Evaluation [5 minutes]

- Please take a couple of minutes to complete the evaluation form, HERE, and reflect on your experience with Nanome, its tools, and collaboration features

Academic and Enterprise Features

Here are some pretty awesome features that come with the paid versions of Nanome. These features are beyond the scope of this in-class activity but I highly recommend you explore them on your own, especially since you all just started your two weeks free trial:

- The Electron Density tab
- Load structures/molecules directly from databases such as RCSB, DrugBank, and Pubchem
- Password-protected public rooms
- Unlimited molecules you can load

References

- https://ryanschultz.com/2021/06/25/nanome-a-brief-introduction-to-a-social-vr-platform-for-exploring-chemistry/
- https://docs.nanome.ai/