- **Title:** SARS-CoV-2 Main Protease & Potential Inhibitors
- **Software:** Nanome
- **Motivations/Goals:**
    - Explore VR-based learning tools in relation to biochemistry, drug development and pandemics
    - Explore molecular visualization in VR (with a focus on the SARS-COVID-2 molecule, its different mutations, proteases and active binding sites)
    - Explore how VR enhanced our understanding of the virus, pandemic and related drugs
    - Collaborate on understanding the molecule as well as development of potential drugs
    - Evaluate existing molecular visualization softwares (beyond Nanome) and their real life applicability
    - Evaluate Nanome's user interface and features (focus on collaboration)
- **In-class activity:**
    - A brief description of Nanome and its most important features
    - Visualizing the COVID-19 main protease structure with an emphasis on the active site
    - Explore fragment-based lead drug discovery
    - Grow/combine/create fragments to produce a lead for a small molecule inhibitor that binds to the active site with a higher affinity
    - Compare our molecules and analyze their real life applicability
    - Produce screenshots of the molecules and their properties
- **Evaluation Metrics:**
    - Wave 1 - evaluate collaboration, user interface and molecule development features using surveys distributed to classmates (during in class activity)
    - Wave 2 - personal evaluation of 2D vs desktop 3D vs immersive 3D
    - Wave 3 - evaluating Nanome in relation to other popular softwares, such as UnityMo (metrics can include: speed, interactivity, resolution, flexibility ..)
- **Timeline:**
    - **2/14**
        - Setup Nanome and familiarize myself with the software (how to import molecules, controls ..)
        - Wiki contribution #1 (improving on Nanome tutorials)
    - **2/16**
        - A biochemistry refresher: protease, active sites, identifying the SARS molecule and its main protease
        - Literature review on similar exercises and related reports/documentations
        - Wiki contribution #2 (applications of VR in biochemistry in general)
    - **2/23**
        - Rehearse in class activity
        - finalize collaboration evaluation form to be distributed to classmates after the in-class activity

- **2/28**
  - In Class activity
  - Collect responses to evaluation form
  - Collect screenshots of new molecules and their properties
  - Wiki contribution #3 (screenshots and information from in-class activity)
- **3/02**
  - Synthesis outcomes from in class activity and evaluation forms
  - Compare to literature
  - 1st individual evaluation activity - comparing different modes of visualizing the SARS-COVID-19 main protease and its active site
- **3/07**
  - 2nd individual evaluation activity
  - What more can we learn about COVID-19 and similar viruses ? interesting applications in Nanome and other software
  - Wiki contributions #4 (evaluation report) and #5 (COVID related applications)
- **3/09**
  - Finalize and review all wiki contributions

Project 01 - Evaluation Rubric

The proposed project clearly identifies deliverable additions to our VR Software Wiki	**4**
The proposed project involves collaboration in VR	**5**
The proposed project involves large scientific data visualization along the lines of the "Scientific Data" wiki page and identifies the specific data type and software that it will use	**5**
The proposed project has a realistic schedule with clear and measurable milestones at least each week and mostly every class	**5**
The proposed project explicitly evaluates VR software, preferably in comparison to related software	**4**
The proposed project includes an in-class activity, which can be formative (early in the project) or evaluative (later in the project)	**5**
The proposed project has resources available with sufficient documentation	**5**

RR - Random Research

Project	Three things will do during the project	One class activity	Potential deliverables
Viral Transmission in response to stimuli (coughing, speaking, singing …)		• User chose a stimuli and observe subsequent transmission in a closed room	• Applications of AR in disaster medicine • Flow Immersive visualizations
Visualize the biomolecular structures of COVID-19 variants	• Conduct literature review of the technologies available for visualizing molecules and add to the wiki • Visualize COVID-19 molecules and different mutations in VR • Provide information that help the user understand the molecular structure and more	• User can point at protein structures/ receptors and a text box will pop up w information • Random artificial forces applied by the user	• artificial 3D environment & software for the visualization of 3D molecular structures: VMD, PyMol (NOT VR) • VR-based learning tools: NanoOne, Molecular Zoo, Peppy (not interactive) • MolDRIVE → allows interactive molecular dynamic simulations with artificial forces applied by the user • Desktop applications: Molecular Rift, UnityMo, UCSF Chi-meraX, VMD, Nanom • Web tools: VRmol, ProteinVR, apps for smartphones, • Smartphone apps: PROteinVR, Corona VRus, Coaster

Resources:

- https://blog.matryx.ai/covid19-in-vr-episode-guide-b708b0ec8ff4
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