

FAIR sharing

of molecular visualization experiences

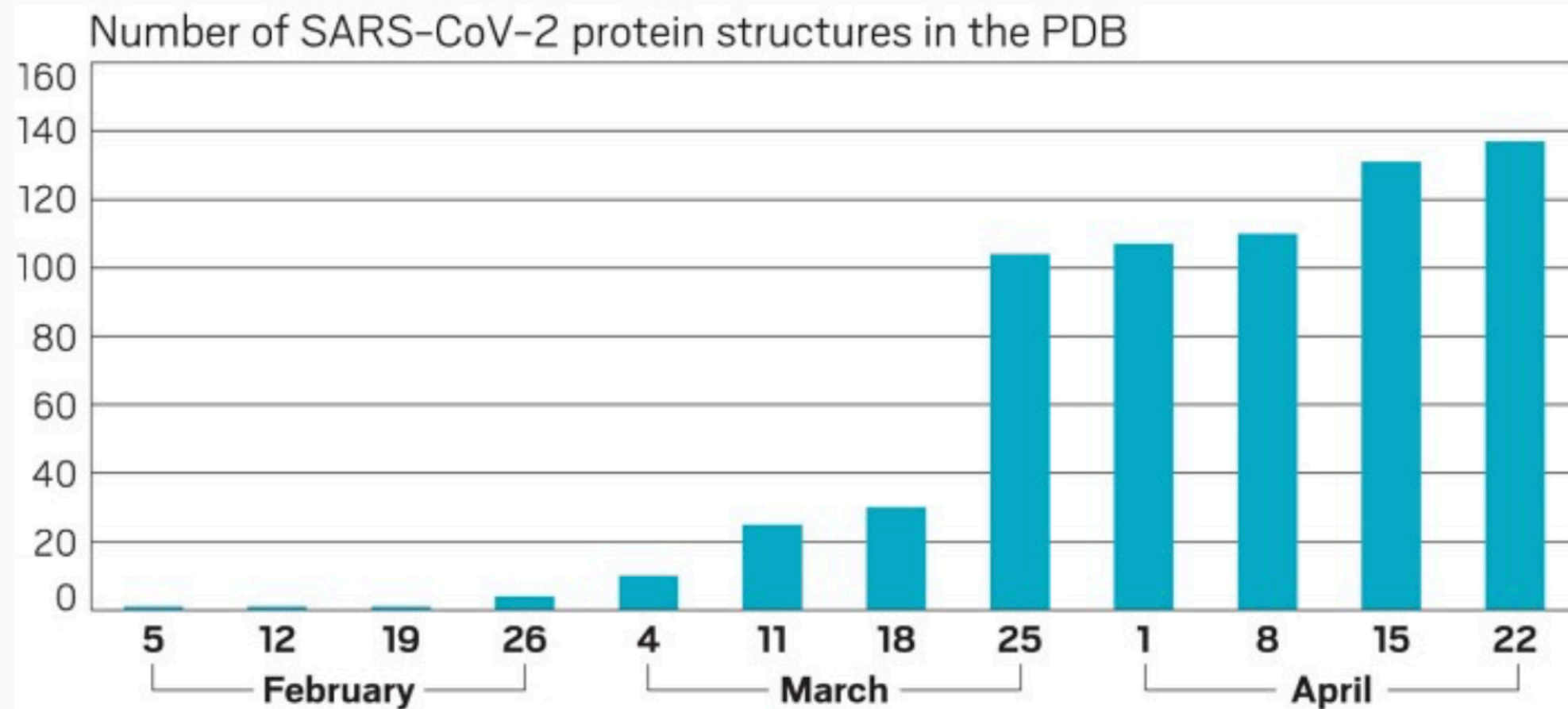


COVID19 as use case

We have structures!

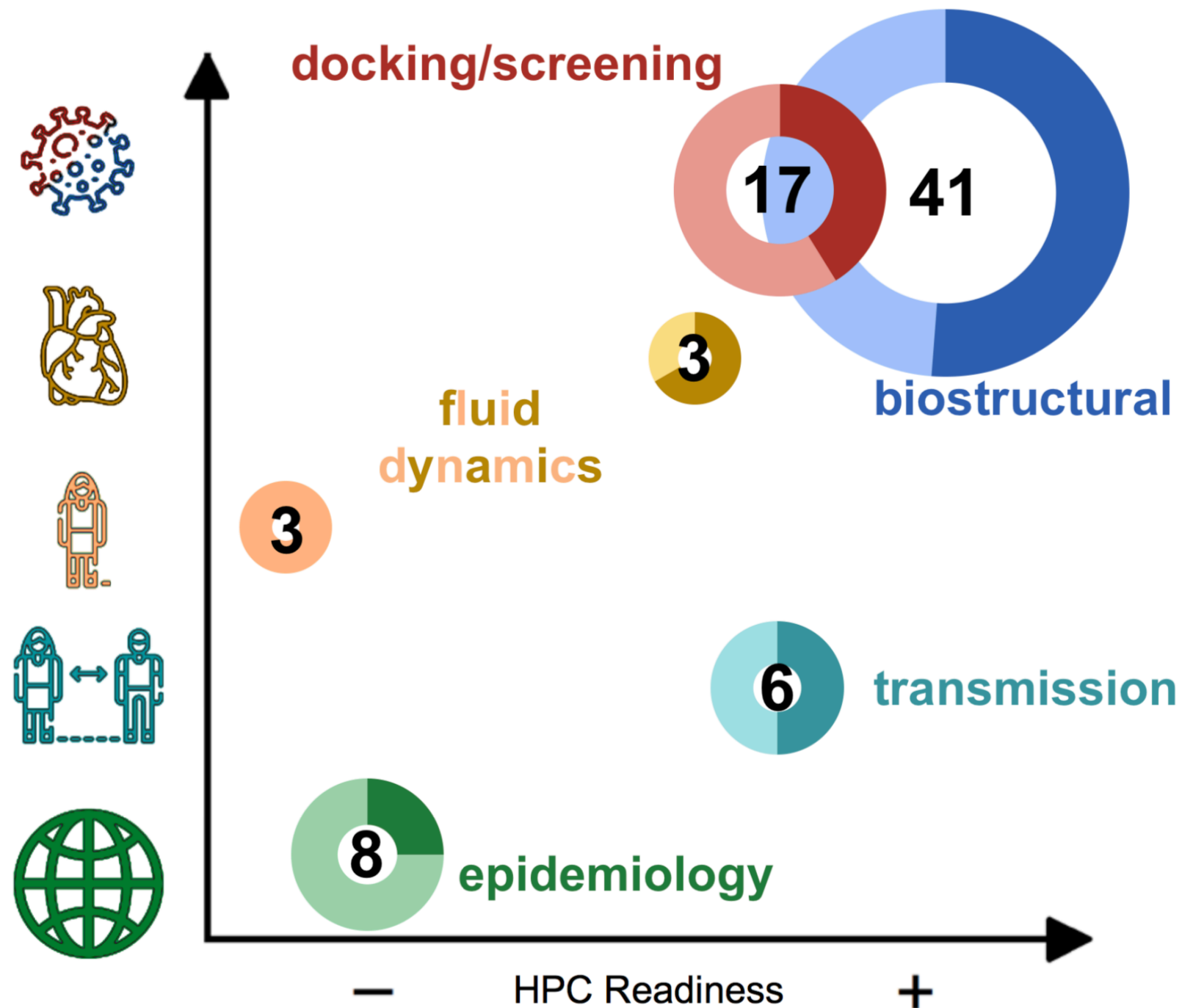
A SURGE IN STRUCTURES

Since early February, over 100 structures related to SARS-CoV-2 proteins have been released by the Protein Data Bank.



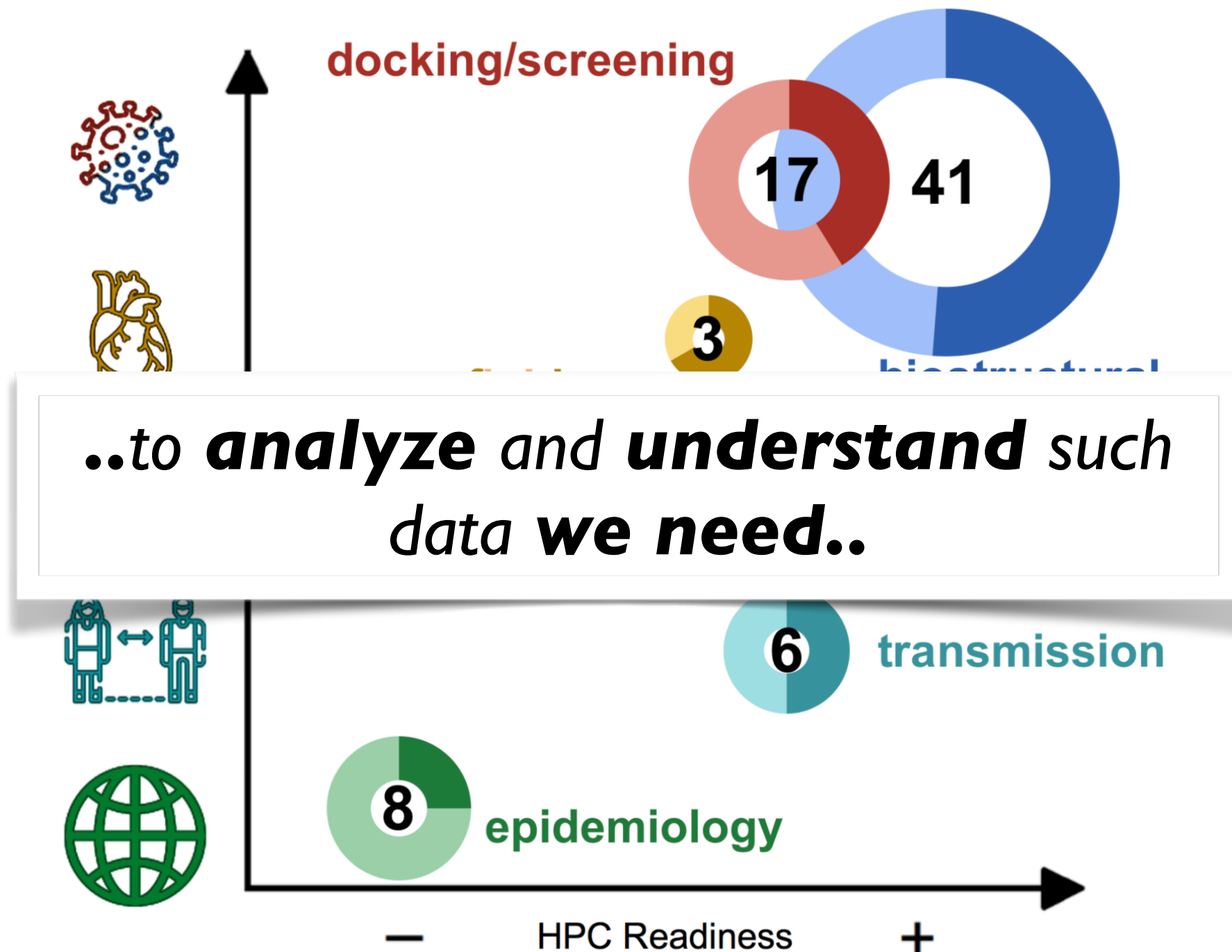
Credit: Source: Protein Data Bank.

We have simulations!



example: PRACE fast-track call at EU level, >80 projects received, >500 million CPU hours assigned

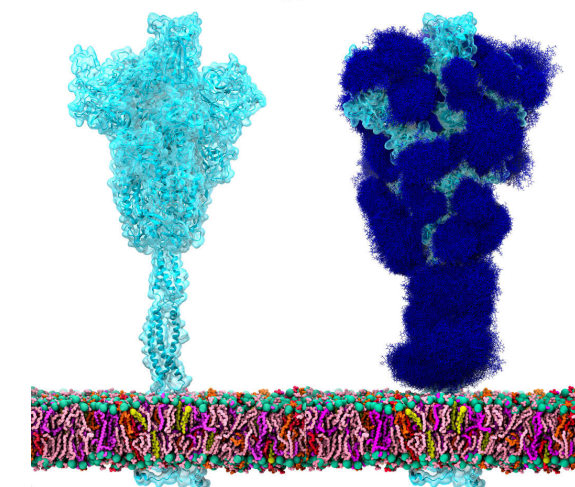
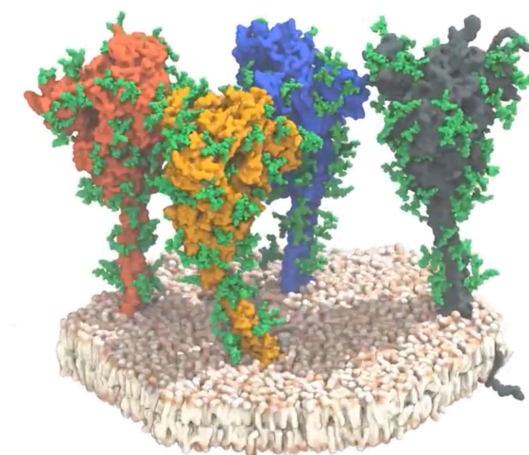
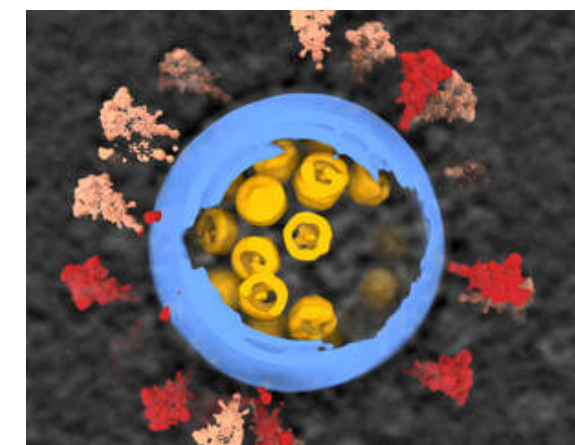
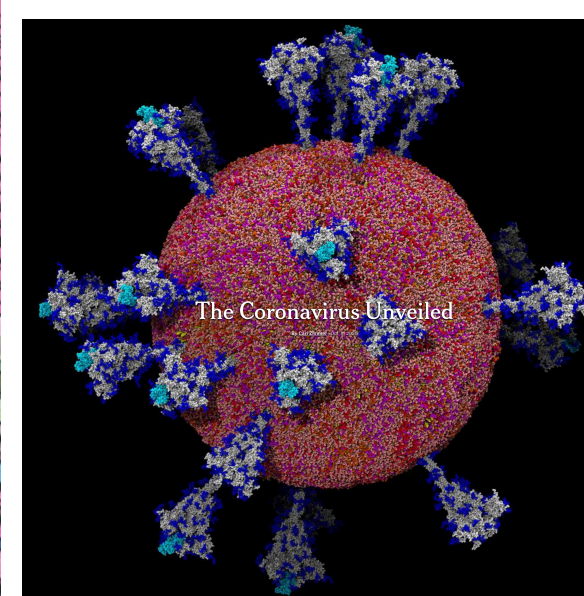
We have simulations!



example: PRACE fast-track call at EU level, >80 projects received, >500 million CPU hours assigned

Visualization

Molecular Landscapes
by David S. Goodsell
Coronavirus
Life Cycle, 2020



Visualization

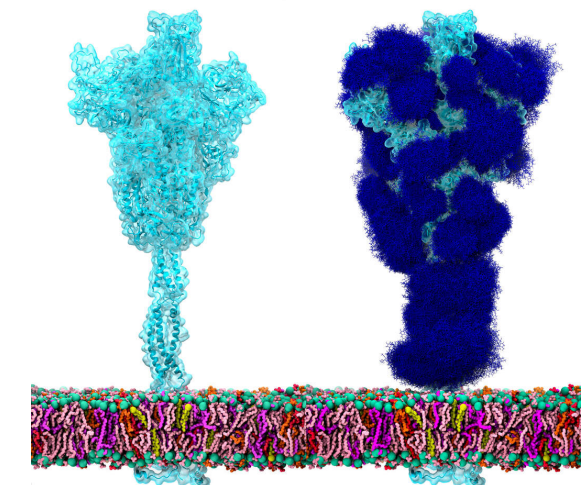
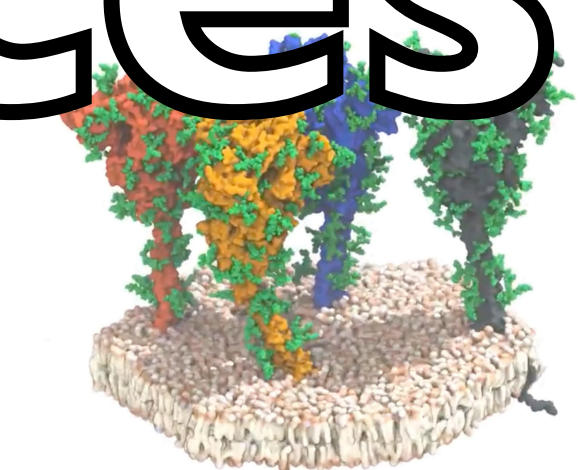
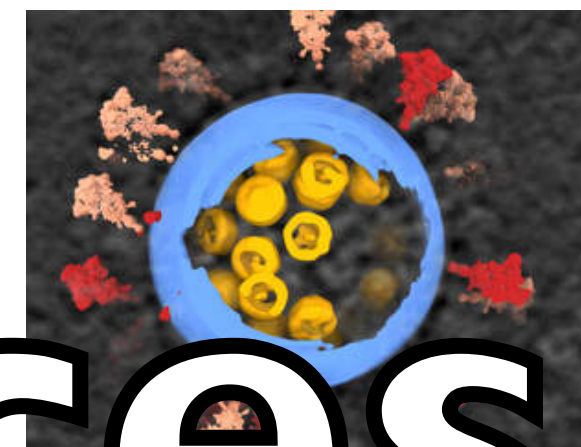
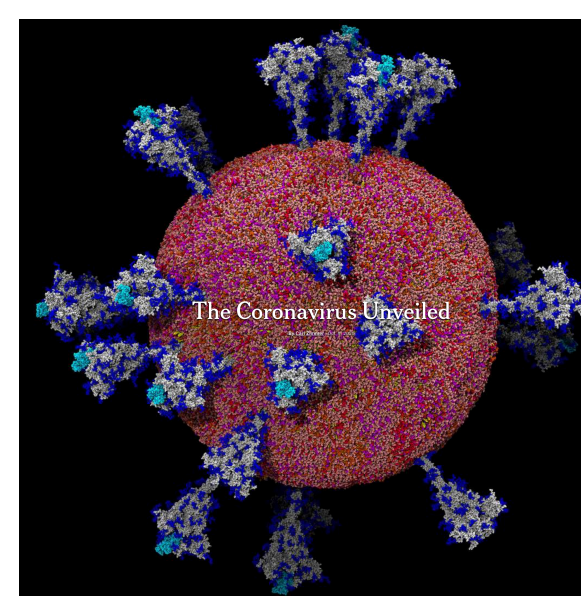
Experiences

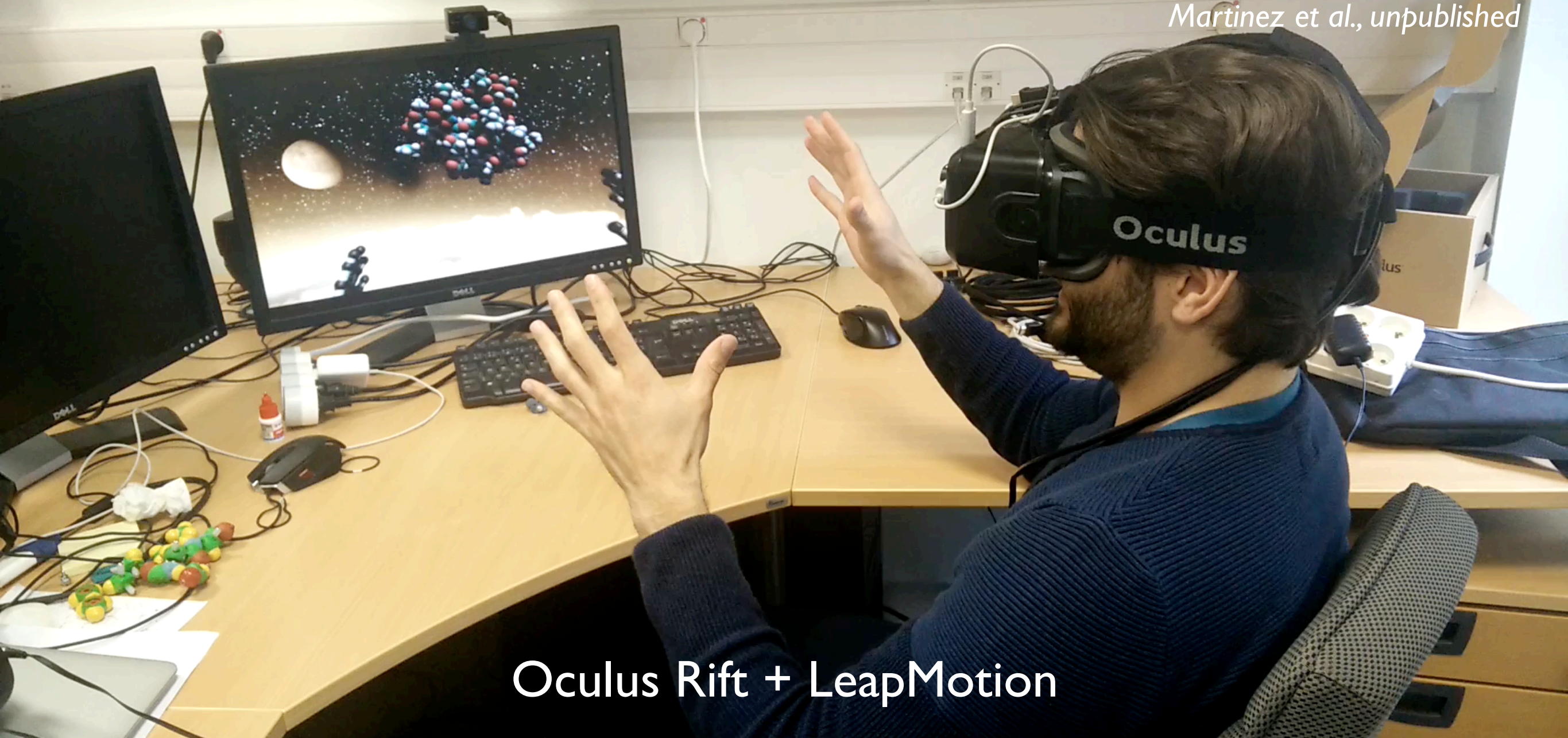
Molecular Landscapes

by David S. Goodsell

Coronavirus

Life Cycle, 2020





Oculus Rift + LeapMotion

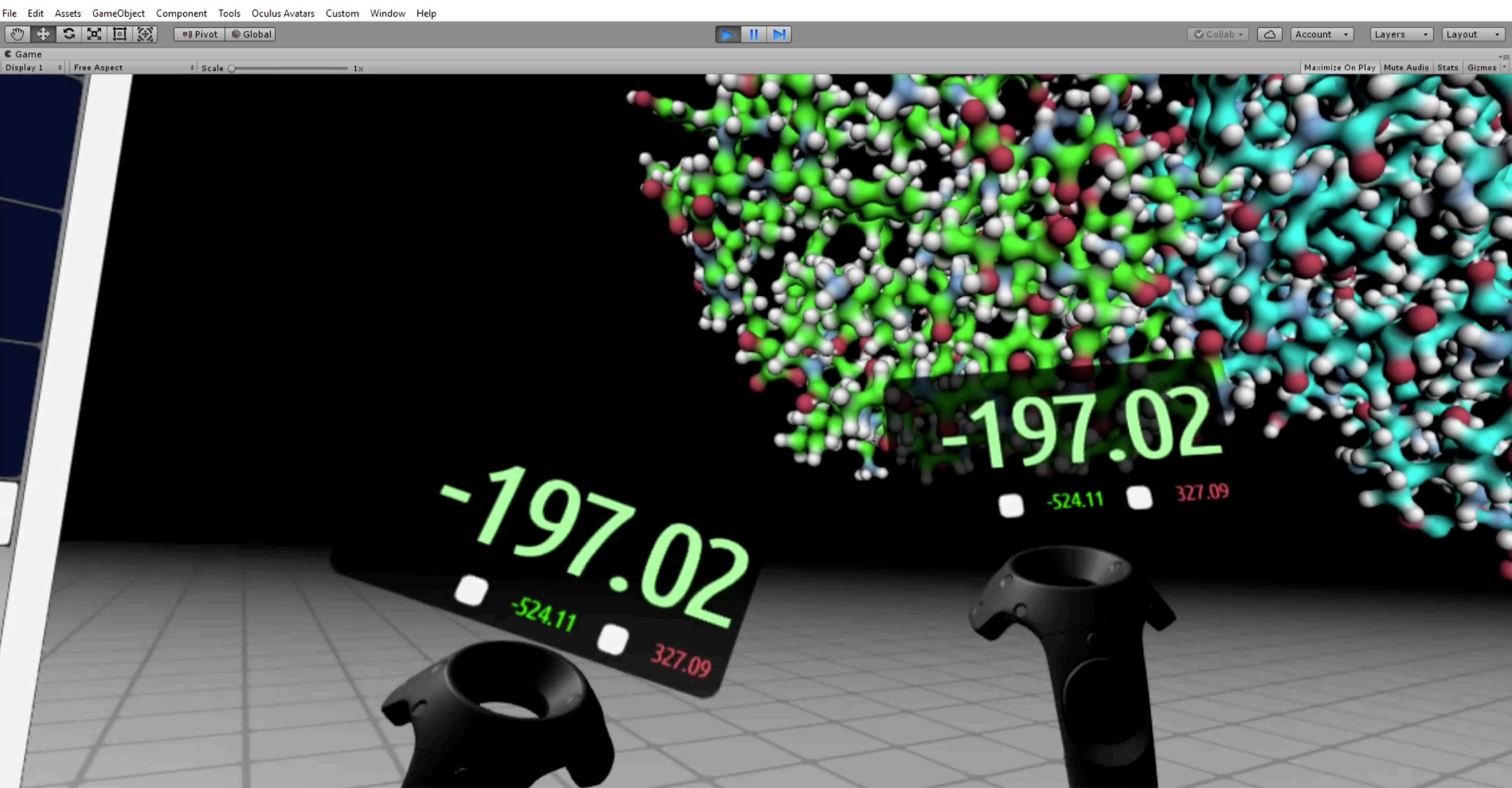


HTC Vive



HoloLens

Protein-Protein docking in UnityMolVR



designed in collaboration with UCB Biopharma

Our VR builds are freely available upon request! And we can give you a demo!

Martinez et al., Unpublished

Protein-Protein docking in UnityMolVR

File Edit Assets GameObject Component Tools Oculus Avatars Custom Window Help

Pivot Global

Game

▶ || ▶

Collab

Account

Layers

Layout

Maximize On Play Mute Audio Stats Gizmos



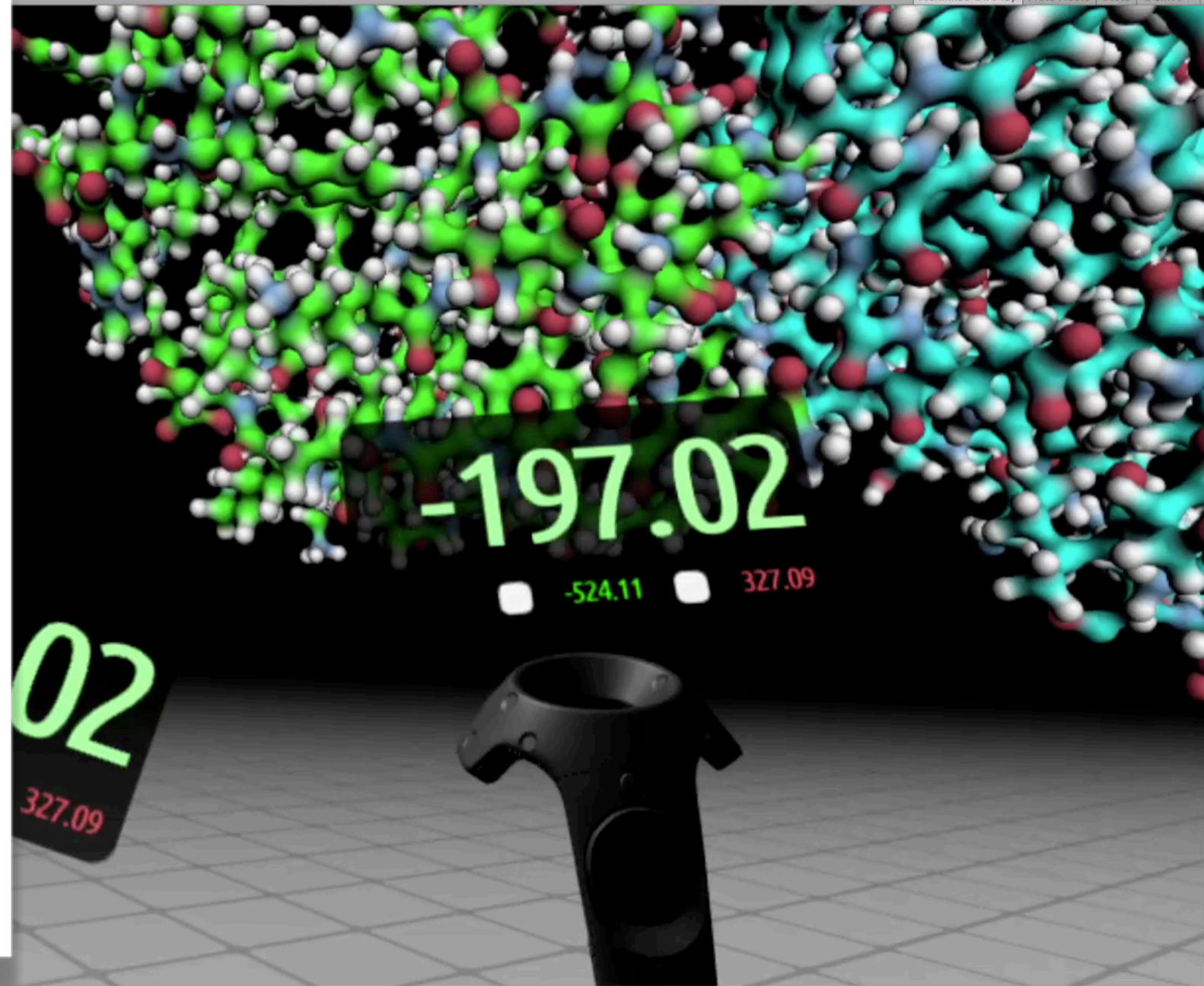
EMBL-EBI Training
@EBItraining



#EventSnapshot: Participants at this week's course 'Structural Bioinformatics' are currently enjoying a demo on the @PDBEurope Virtual Reality game, VR Ventolin during their lunch break.



05:09 - 17 sept. 2019



designed in collaboration with UCB Biopharma

Our VR builds are freely available upon request! And we can give you a demo!

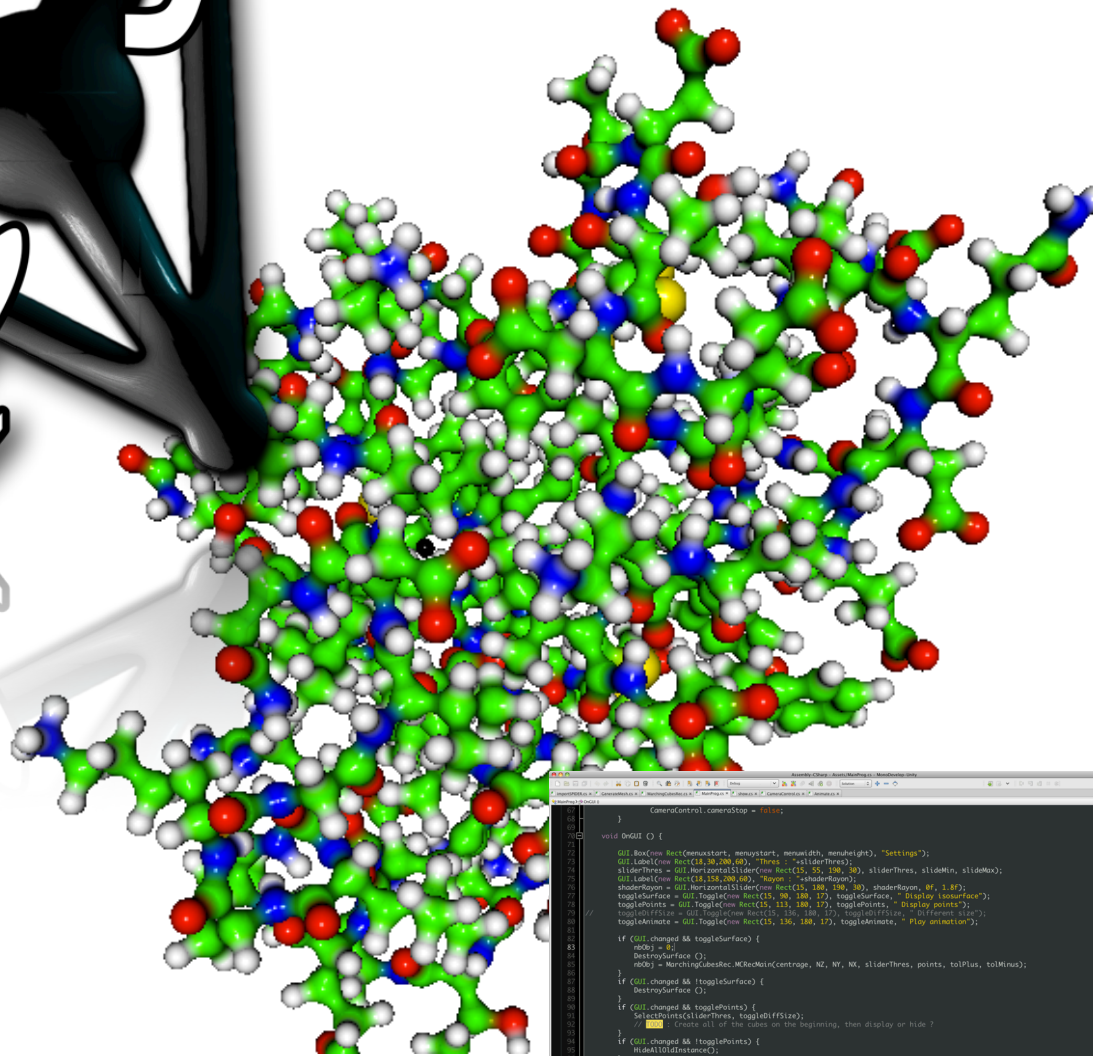
Martinez et al., Unpublished

unity

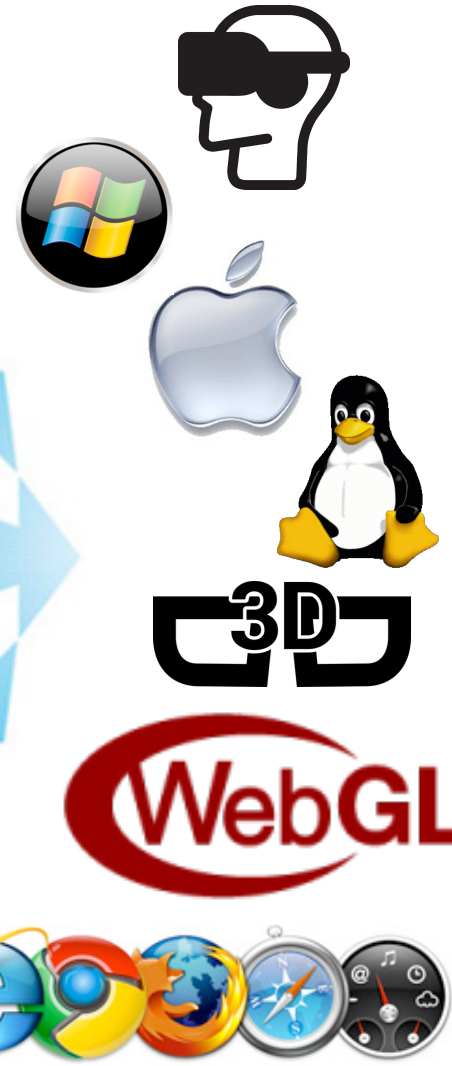
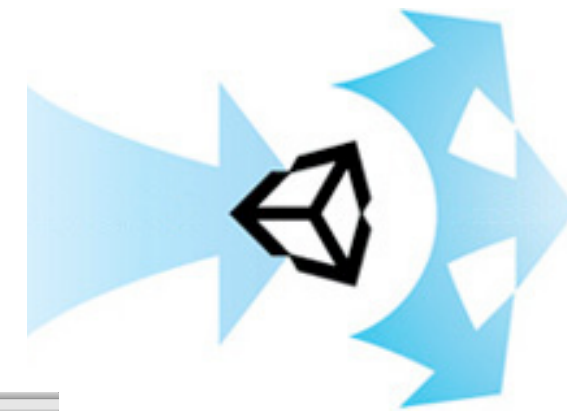
10 years
12 000 downloads



mol



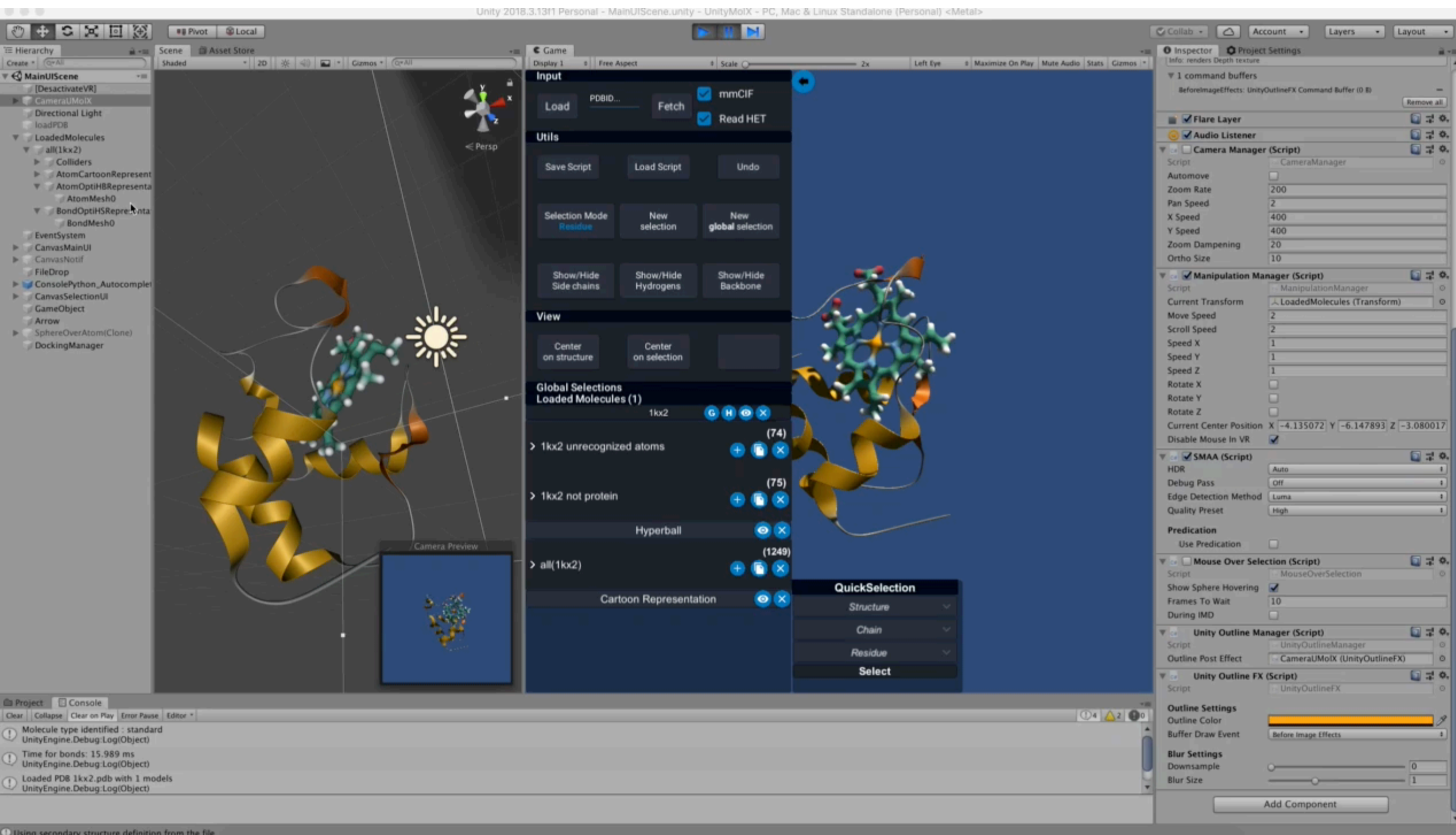
```
void OnGUI () {  
    GUI.Button (GUIRect (10, 200, 40, 220), "Settings");  
    GUI.Label (GUIRect (10, 220, 40, 240), "Times : " + sliderThree);  
    sliderThree = GUI.HorizontalSlider (GUIRect (40, 240, 100, 260), sliderThree, sliderMax, sliderMin);  
    GUI.Label (GUIRect (10, 260, 40, 280), "Rayon : " + shaderRayon);  
    shaderRayon = GUI.HorizontalSlider (GUIRect (40, 280, 100, 300), shaderRayon, 0.1, 0.2);  
    toggleSurface = GUI.Toggle (GUIRect (10, 300, 100, 320), toggleSurface, "Display Isosurface");  
    togglePoints = GUI.Toggle (GUIRect (10, 320, 100, 340), togglePoints, "Display points");  
    toggleFFSize = GUI.Toggle (GUIRect (10, 340, 100, 360), toggleFFSize, "Difference size");  
    toggleAnimate = GUI.Toggle (GUIRect (10, 360, 100, 380), toggleAnimate, "Play animation");  
  
    if (GUI.changed && toggleSurface) {  
        mObj = null;  
        DestroySurface ();  
        mObj = new GameObject ("MCRCenter (Center, NZ, NY, NX, sliderThree, points, tolPlus, tolMinus);");  
        DestroySurface ();  
    }  
    if (GUI.changed && togglePoints) {  
        SelectPoints (sliderThree, toggleFFSize);  
        // Create all of the points on the beginning, then display or hide ?  
        HideAllInstances ();  
    }  
    if (GUI.changed && toggleAnimate) {  
        mObj = AnimateAnim ();  
    }  
    GUI.Label (GUIRect (10, 70, 200, 40), "The points : " + numObj);  
}
```



- Full 3D development platform
- **Advanced graphics engine**
- **Portable, intuitive to use**
- 3 languages : **C#, Boo, Javascript**

- Export to **multiple platforms** :
OSX, Windows, Linux, Android, iOS, ..
WebGL ..

Unity editor: example #1



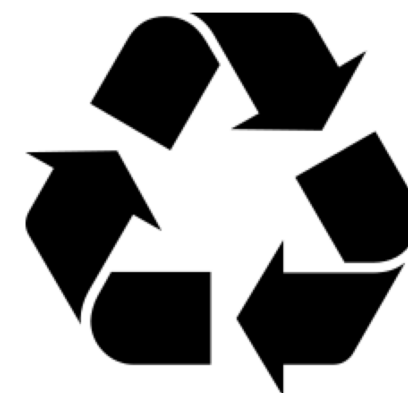
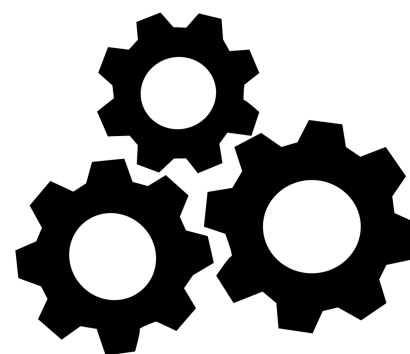
On the fly modification of parameters and object properties



1

Sharing molecular visualizations

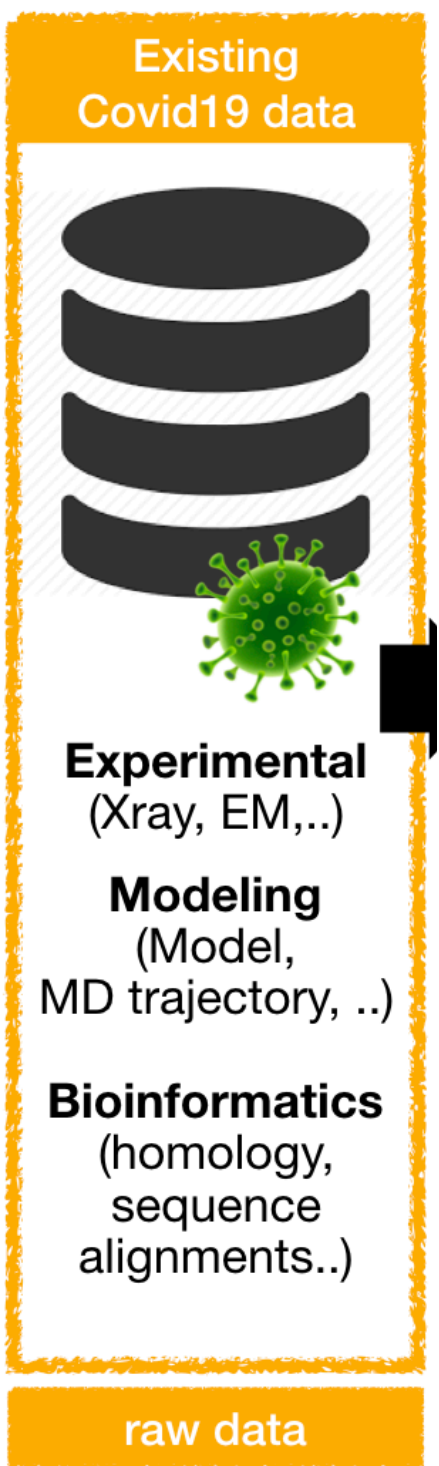
F_{indable} A_{ccessible} I_{nteroperable} R_{eusable}



1

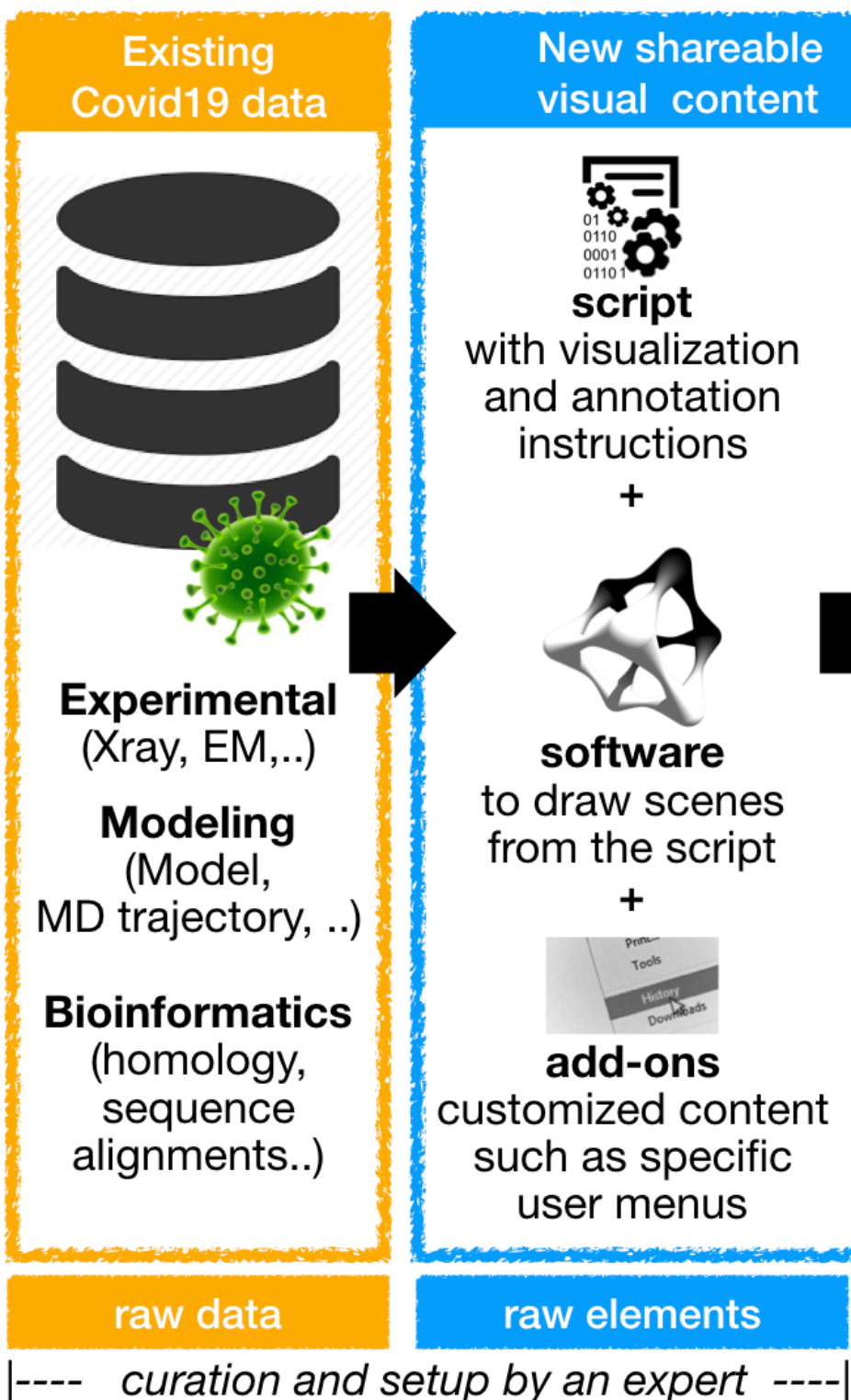
Sharing molecular visualizations

Sharing insights on Covid19 data

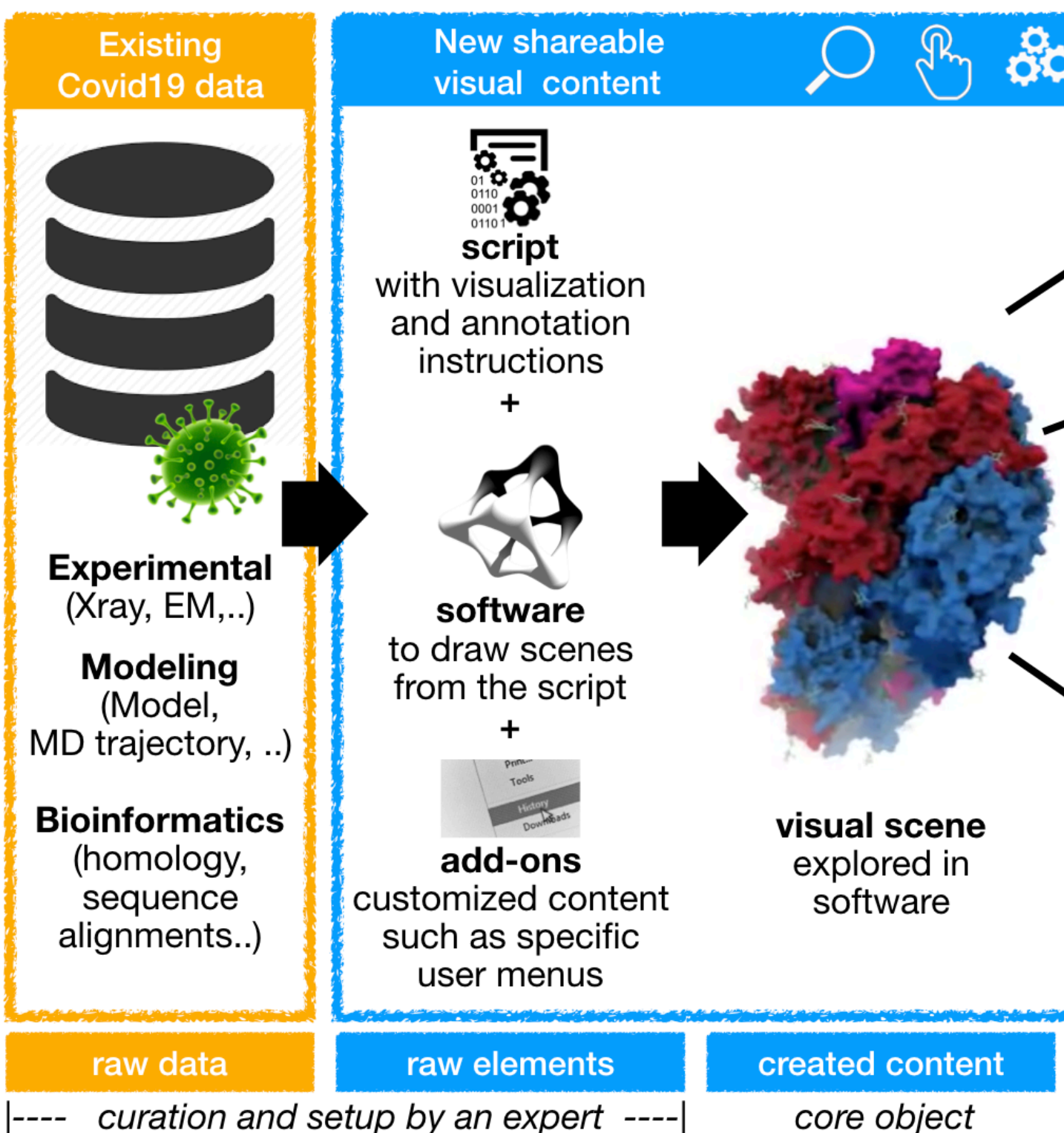


|---- curation and s

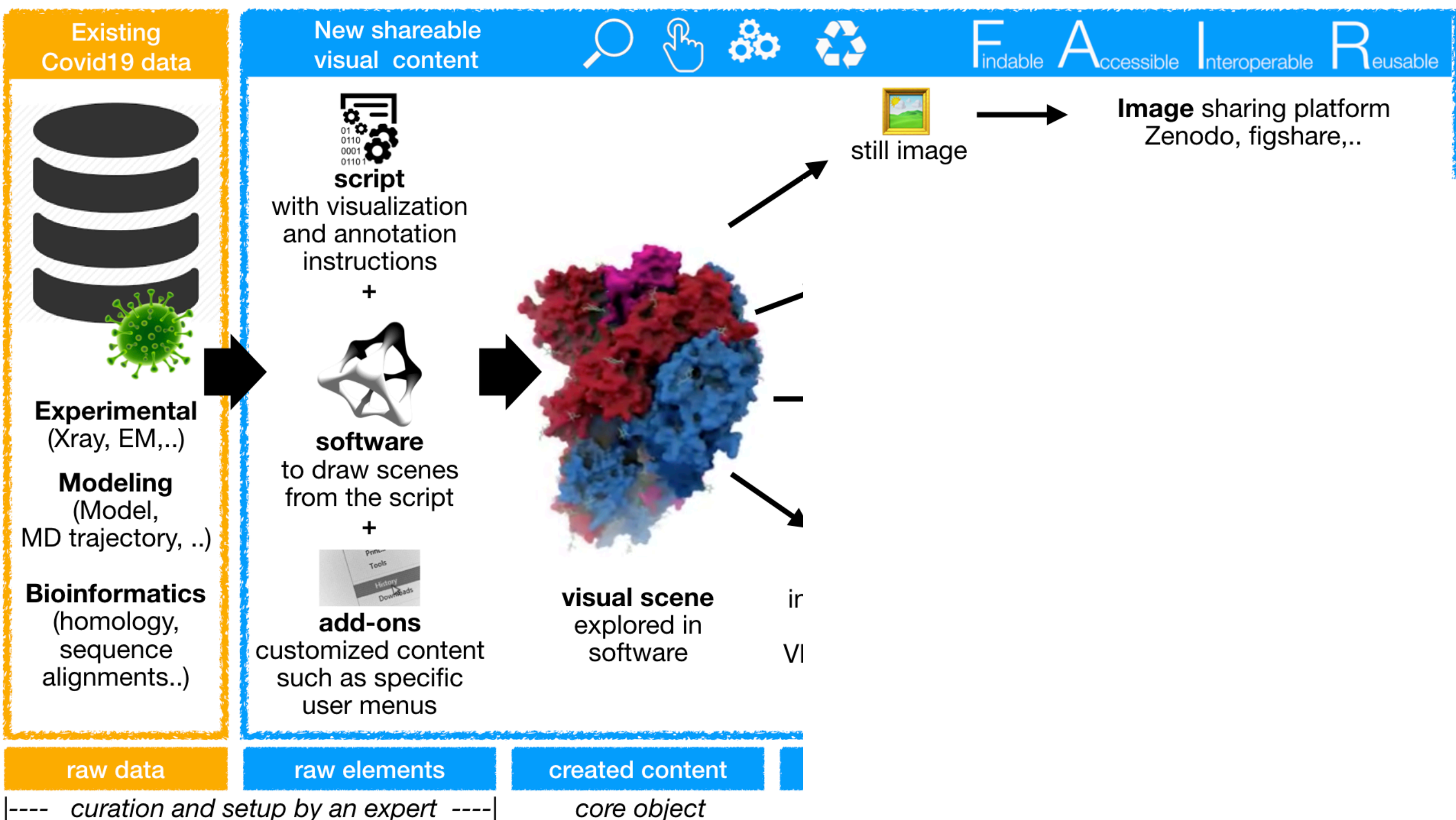
Sharing insights on Covid19 data



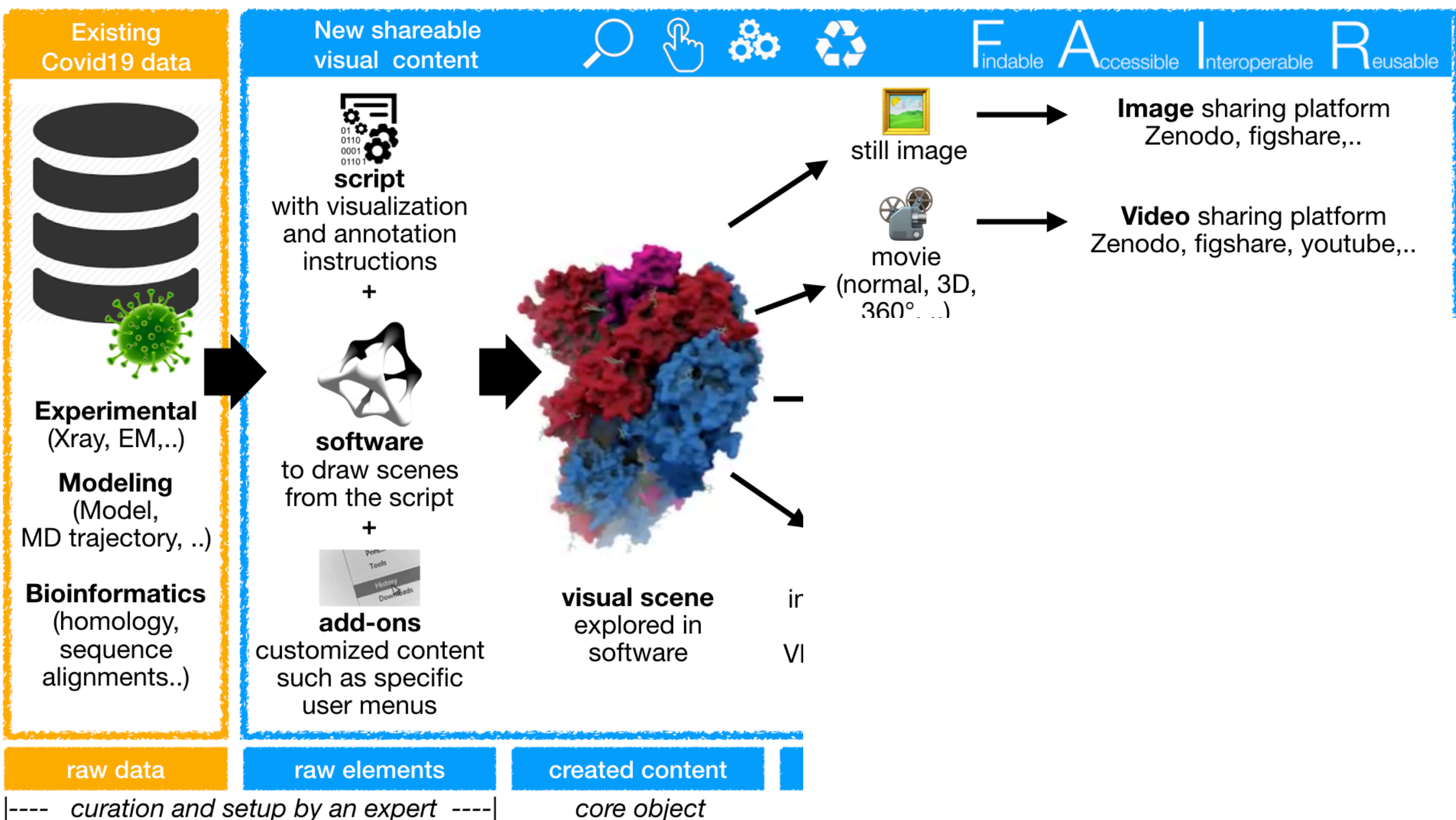
Sharing insights on Covid19 data



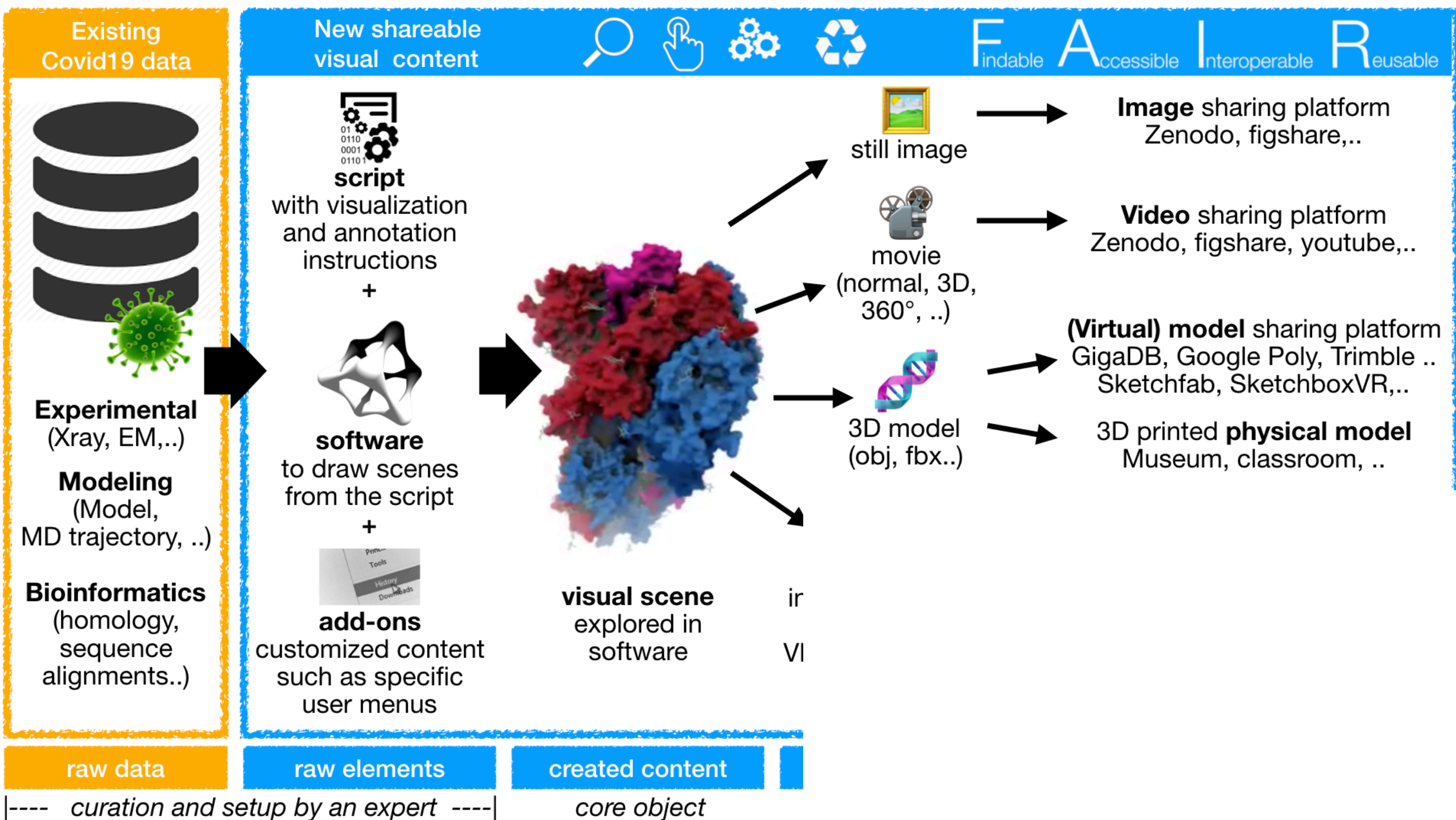
Sharing insights on Covid19 data



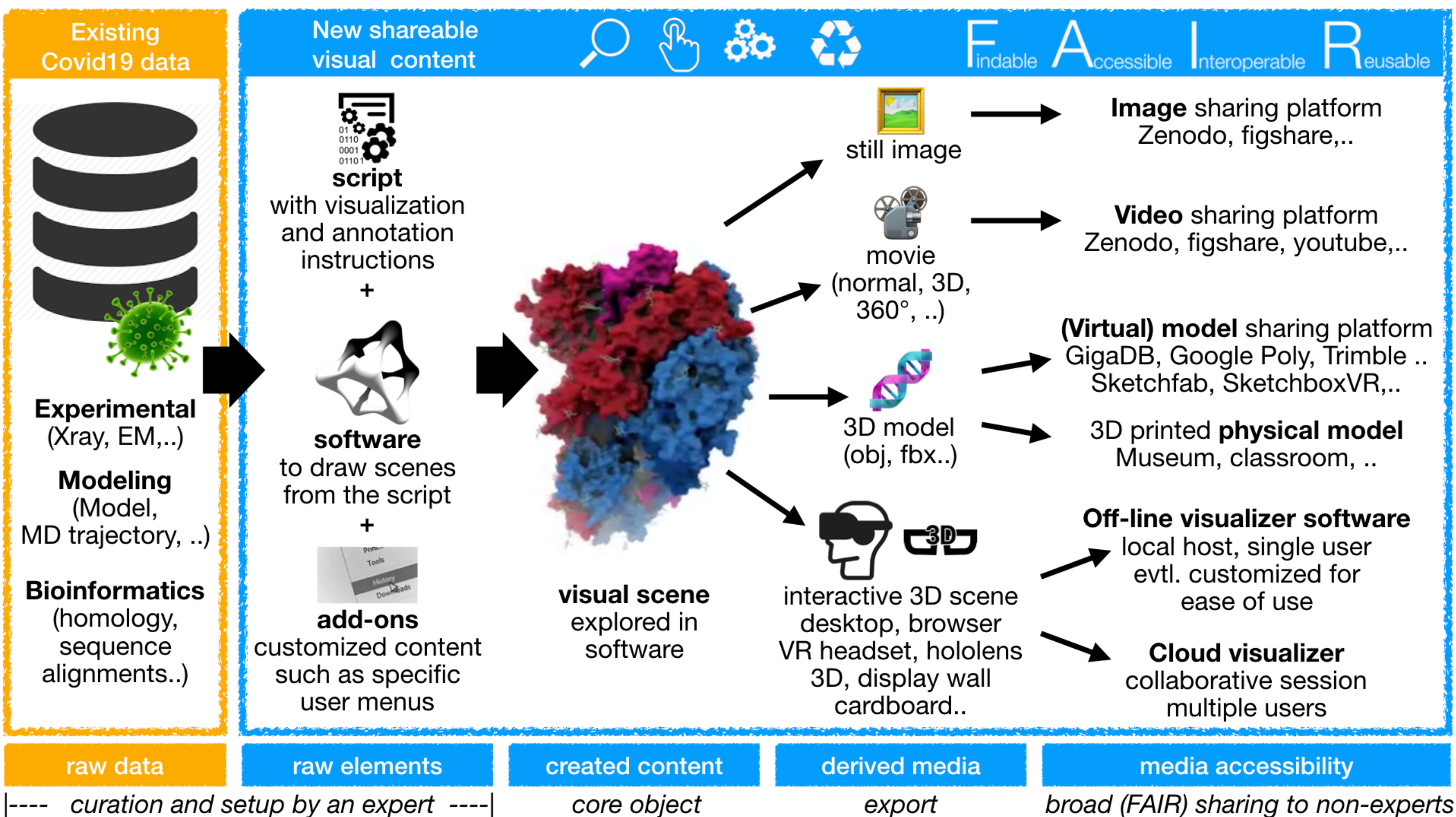
Sharing insights on Covid19 data



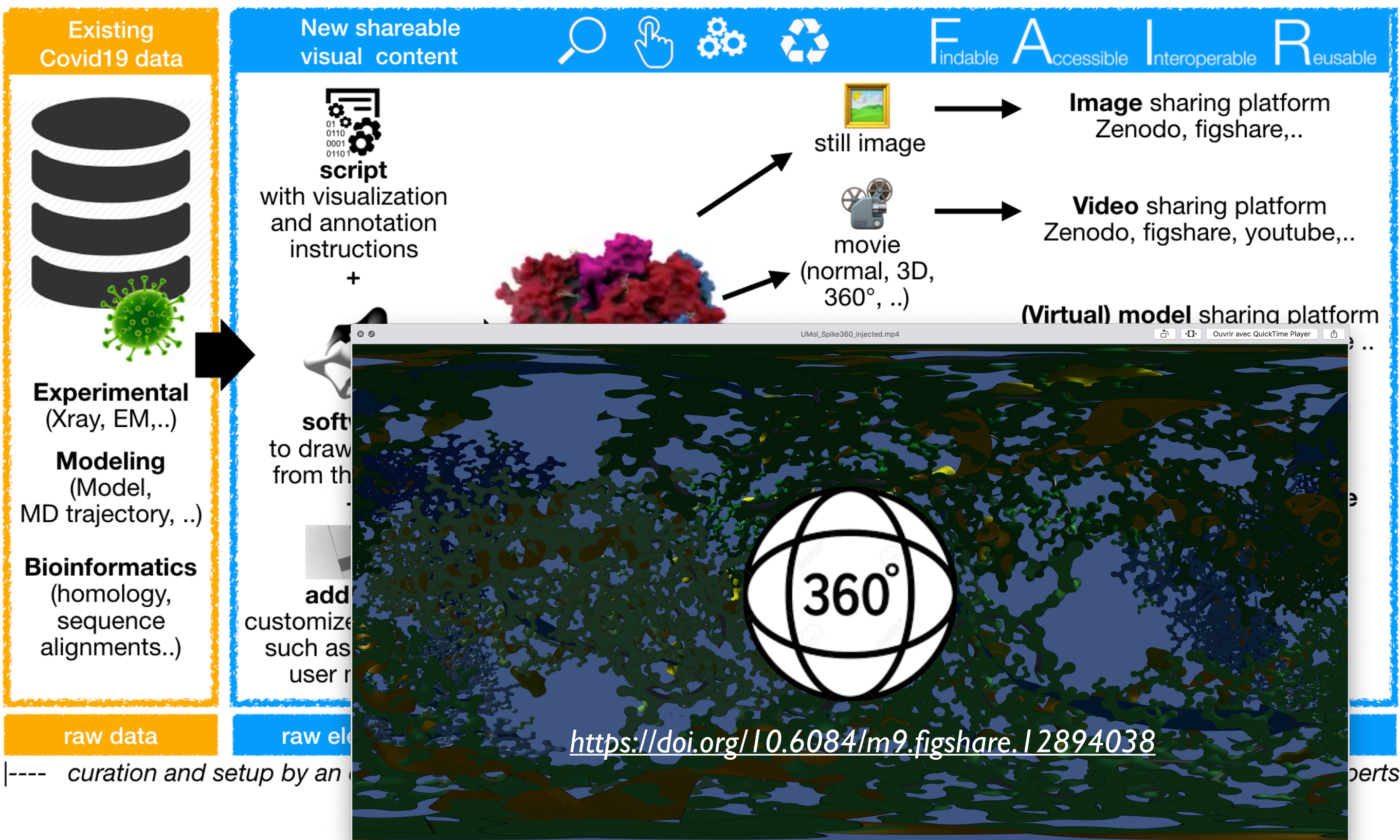
Sharing insights on Covid19 data

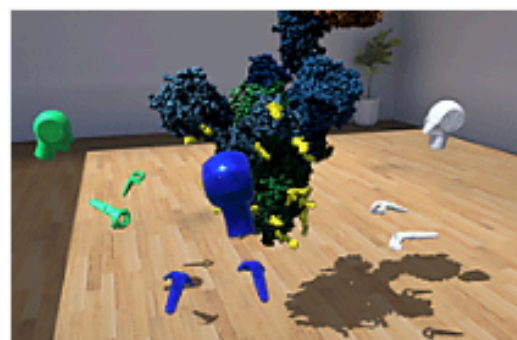


Sharing insights on Covid19 data

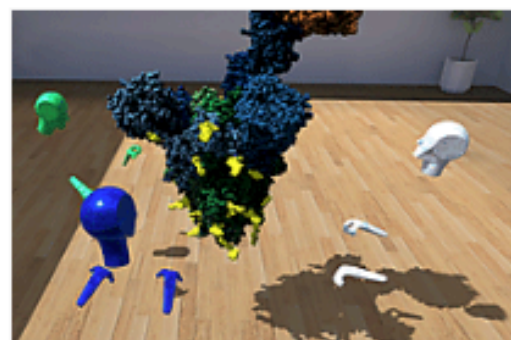


Sharing insights on Covid19 data

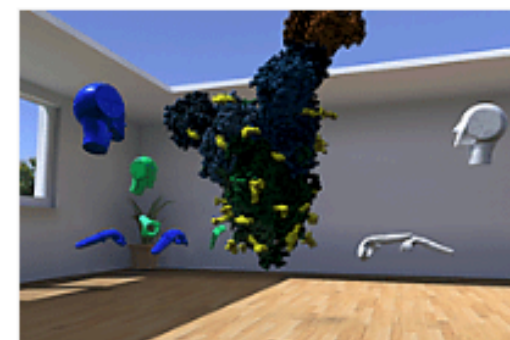




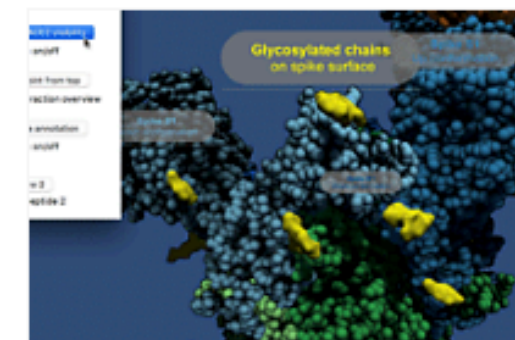
multi3.jpg (514.99 kB)



multi2.jpg (518.91 kB)



multi1.jpg (444.56 kB)



menu.png (875.17 kB)



umol-menu.png (1.08 MB)

[Cite](#)
[Download all \(3.37 MB\)](#)
[Share](#)
[Embed](#)
[+ Collect](#)


5 files



Simple structural views of the SARS spike glycoprotein complex with human angiotensin-converting enzyme 2 (ACE2)

Figure posted on 25.08.2020, 12:18 by [Marc Baaden](#), [Xavier Martinez](#)

A set of 5 screenshots of UnityMol running the first example system. Three screenshots are from a multi-user virtual reality session with 3 participants, two screenshots illustrate

0
views

0
downloads

0
citations

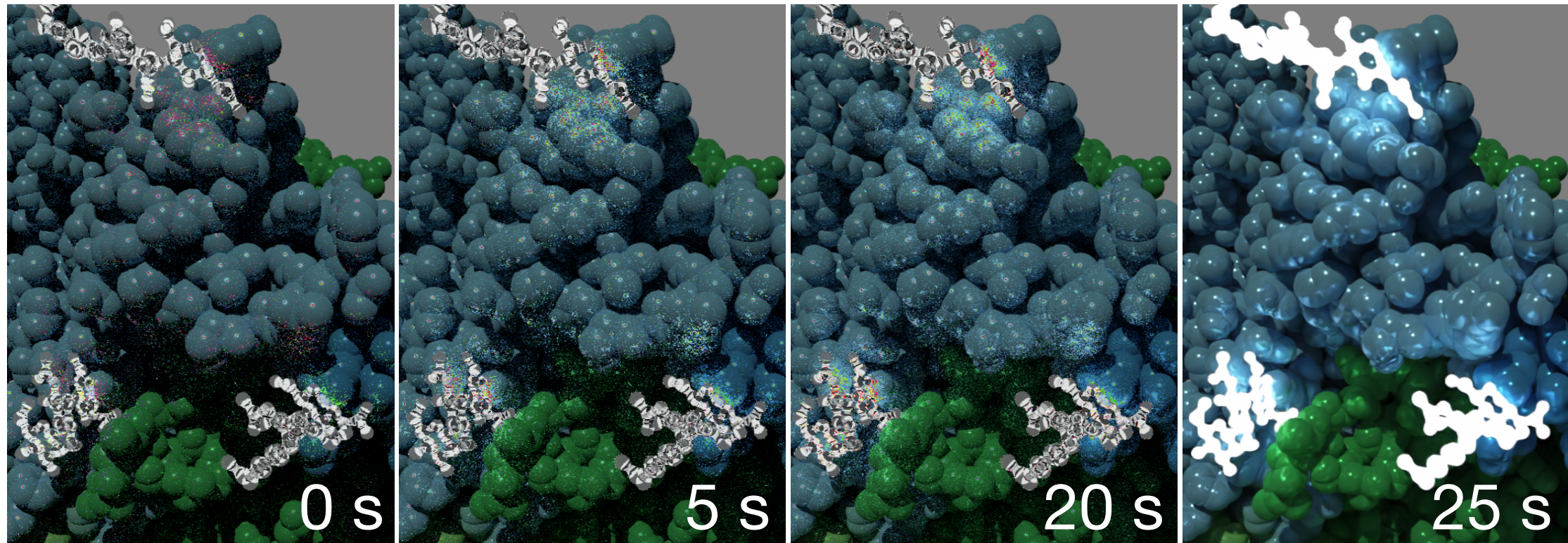
CATEGORIES

- [Structural Biology \(incl. Macromolecular Modelling\)](#)

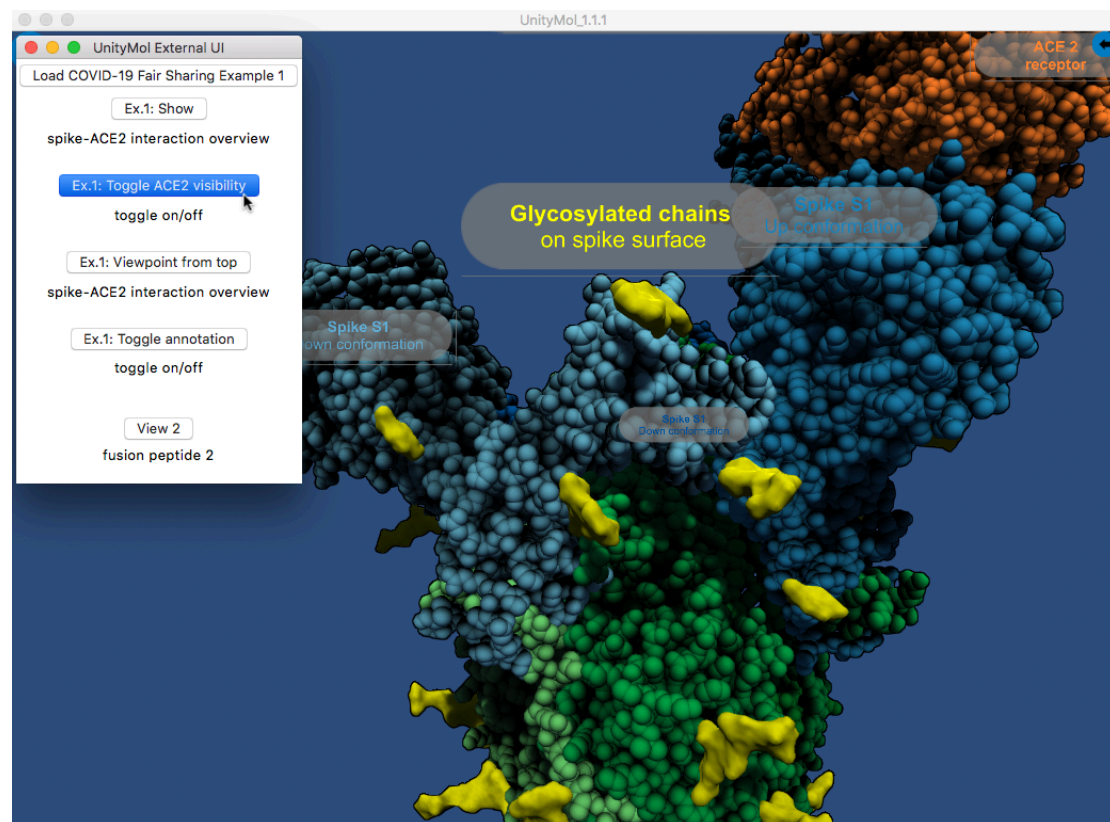
Martinez et al., submitted to Acta Cryst D

Sharing images

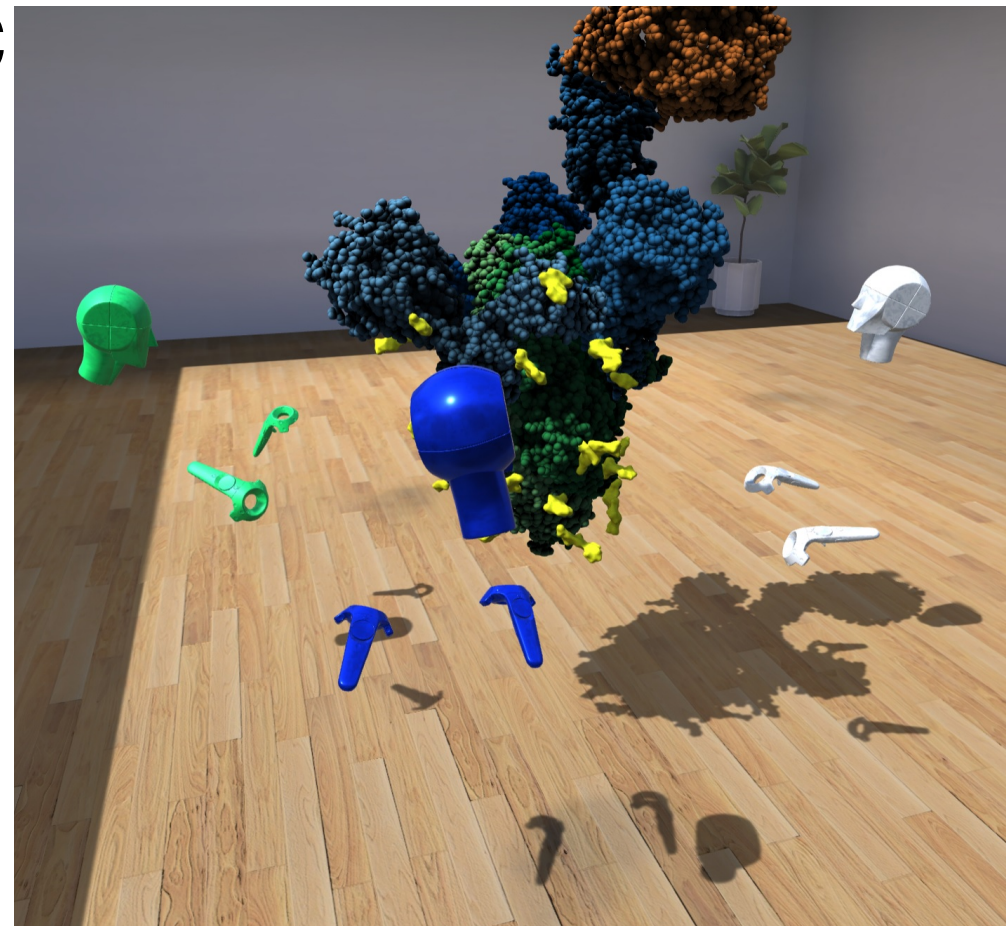
A



B



C



UnityMol External UI

Load COVID-19 Fair Sharing Example 1

Ex.1: Show

spike-ACE2 interaction overview

Ex.1: Toggle ACE2 visibility

toggle on/off

Ex.1: Viewpoint from top

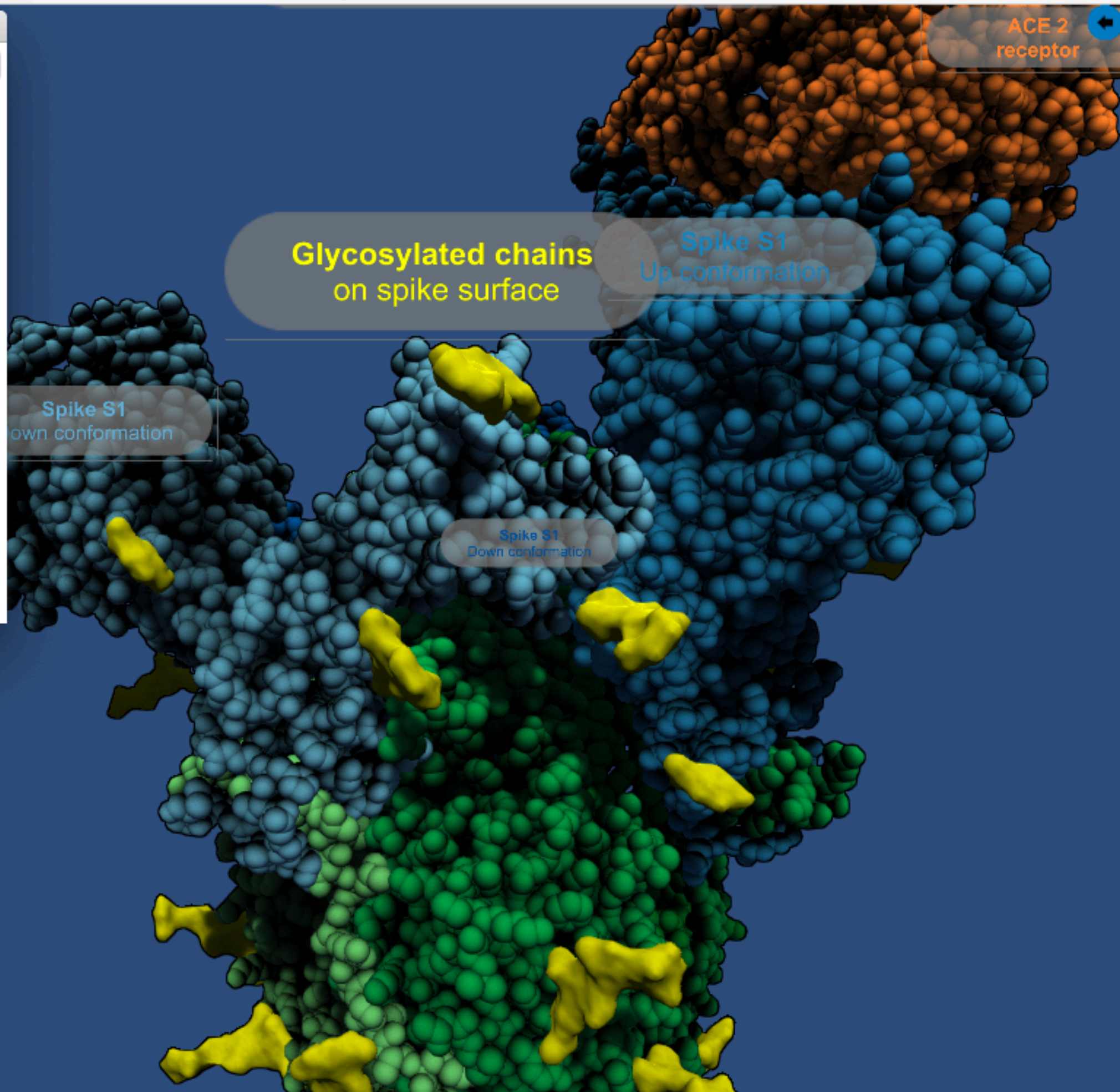
spike-ACE2 interaction overview

Ex.1: Toggle annotation

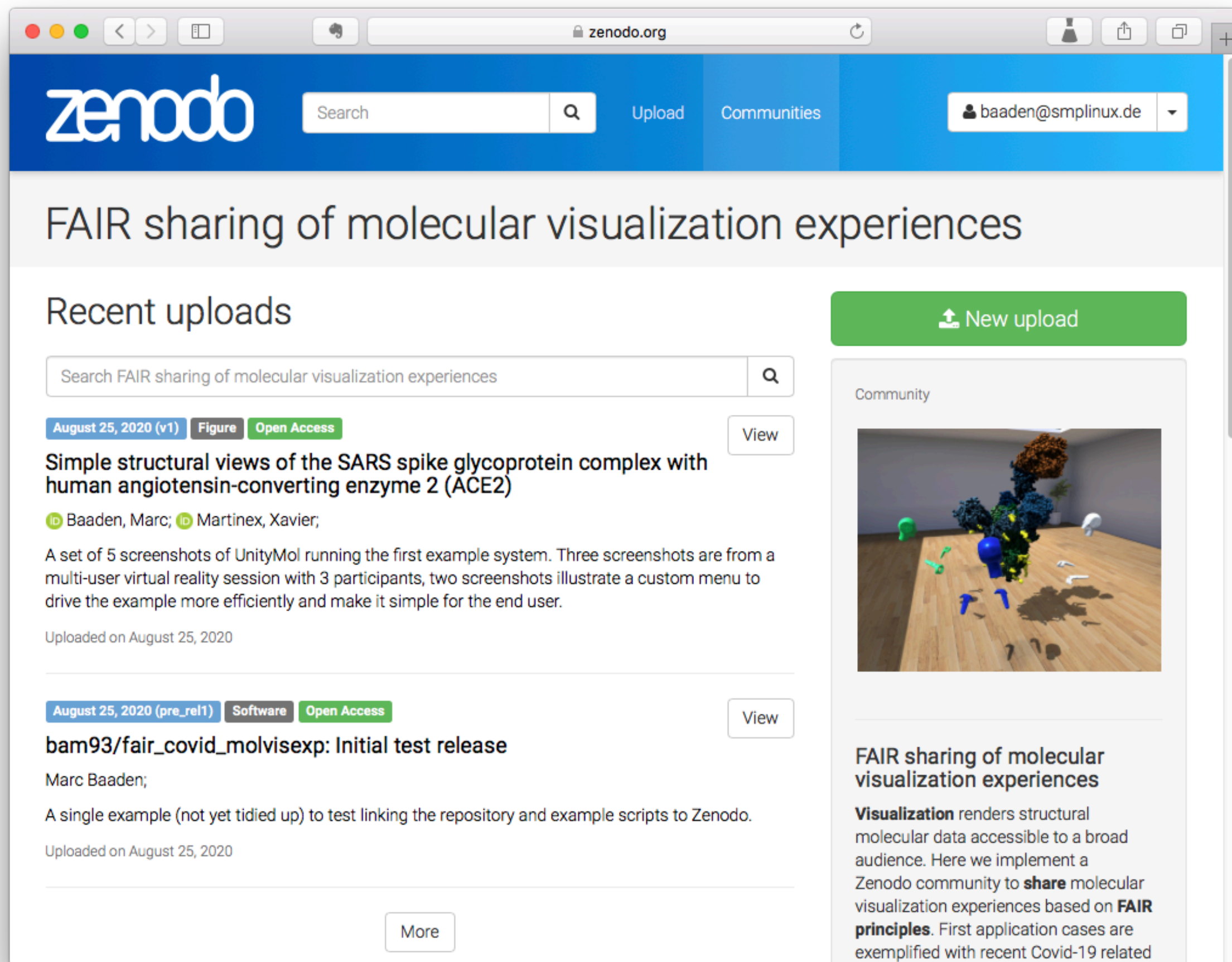
toggle on/off

View 2

fusion peptide 2

Glycosylated chains
on spike surfaceSpike S1
Up conformationSpike S1
Down conformationSpike S1
Down conformation

Zenodo community to centralize



The screenshot shows the Zenodo website interface. At the top, there's a blue header with the Zenodo logo, a search bar, and navigation links for 'Upload' and 'Communities'. A user profile 'baaden@smplinux.de' is logged in. Below the header, a large banner reads 'FAIR sharing of molecular visualization experiences'. The main content area is divided into two columns. The left column, titled 'Recent uploads', contains a search bar and two upload entries. The first entry is titled 'Simple structural views of the SARS spike glycoprotein complex with human angiotensin-converting enzyme 2 (ACE2)' by Baaden, Marc and Martinex, Xavier, dated August 25, 2020 (v1), categorized as 'Figure' and 'Open Access'. The second entry is titled 'bam93/fair_covid_molvisexp: Initial test release' by Marc Baaden, dated August 25, 2020 (pre_rel1), categorized as 'Software' and 'Open Access'. The right column features a green 'New upload' button and a community card for 'Community'. The community card includes a 3D molecular visualization image and a description: 'FAIR sharing of molecular visualization experiences. Visualization renders structural molecular data accessible to a broad audience. Here we implement a Zenodo community to share molecular visualization experiences based on FAIR principles. First application cases are exemplified with recent Covid-19 related'.

zenodo

Search

Upload

Communities

baaden@smplinux.de

FAIR sharing of molecular visualization experiences

Recent uploads

Search FAIR sharing of molecular visualization experiences

August 25, 2020 (v1) Figure Open Access View

Simple structural views of the SARS spike glycoprotein complex with human angiotensin-converting enzyme 2 (ACE2)

Baaden, Marc; Martinex, Xavier;

A set of 5 screenshots of UnityMol running the first example system. Three screenshots are from a multi-user virtual reality session with 3 participants, two screenshots illustrate a custom menu to drive the example more efficiently and make it simple for the end user.

Uploaded on August 25, 2020

August 25, 2020 (pre_rel1) Software Open Access View

bam93/fair_covid_molvisexp: Initial test release

Marc Baaden;

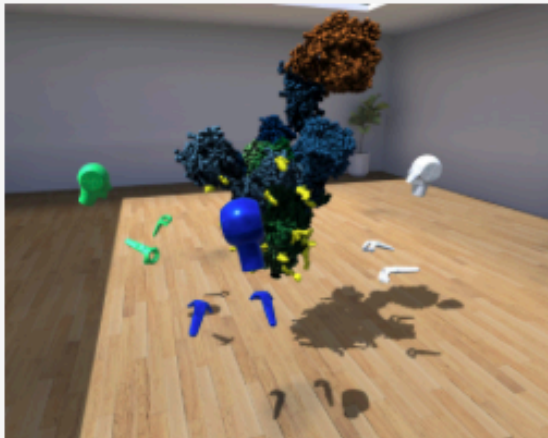
A single example (not yet tidied up) to test linking the repository and example scripts to Zenodo.

Uploaded on August 25, 2020

More

New upload

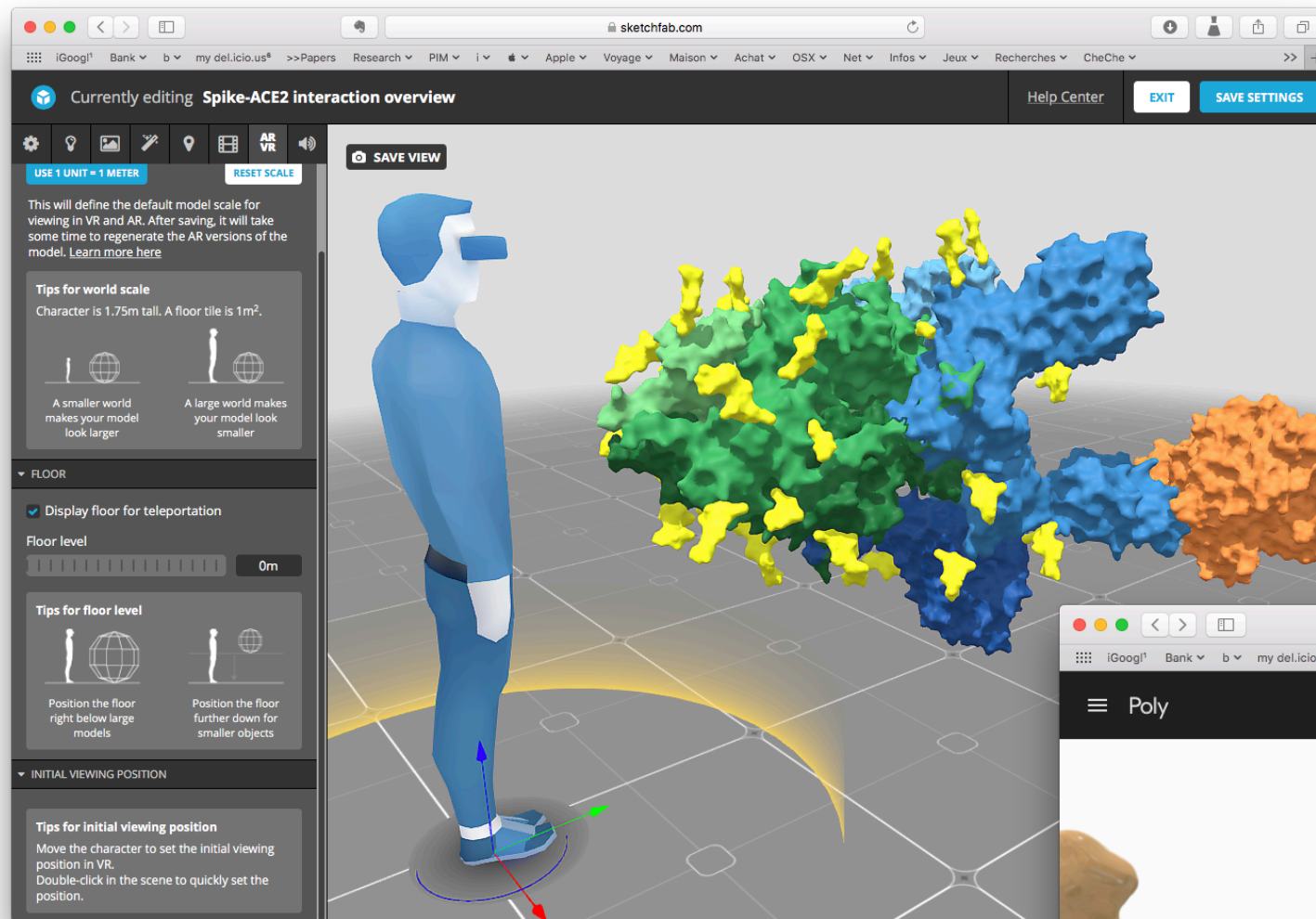
Community



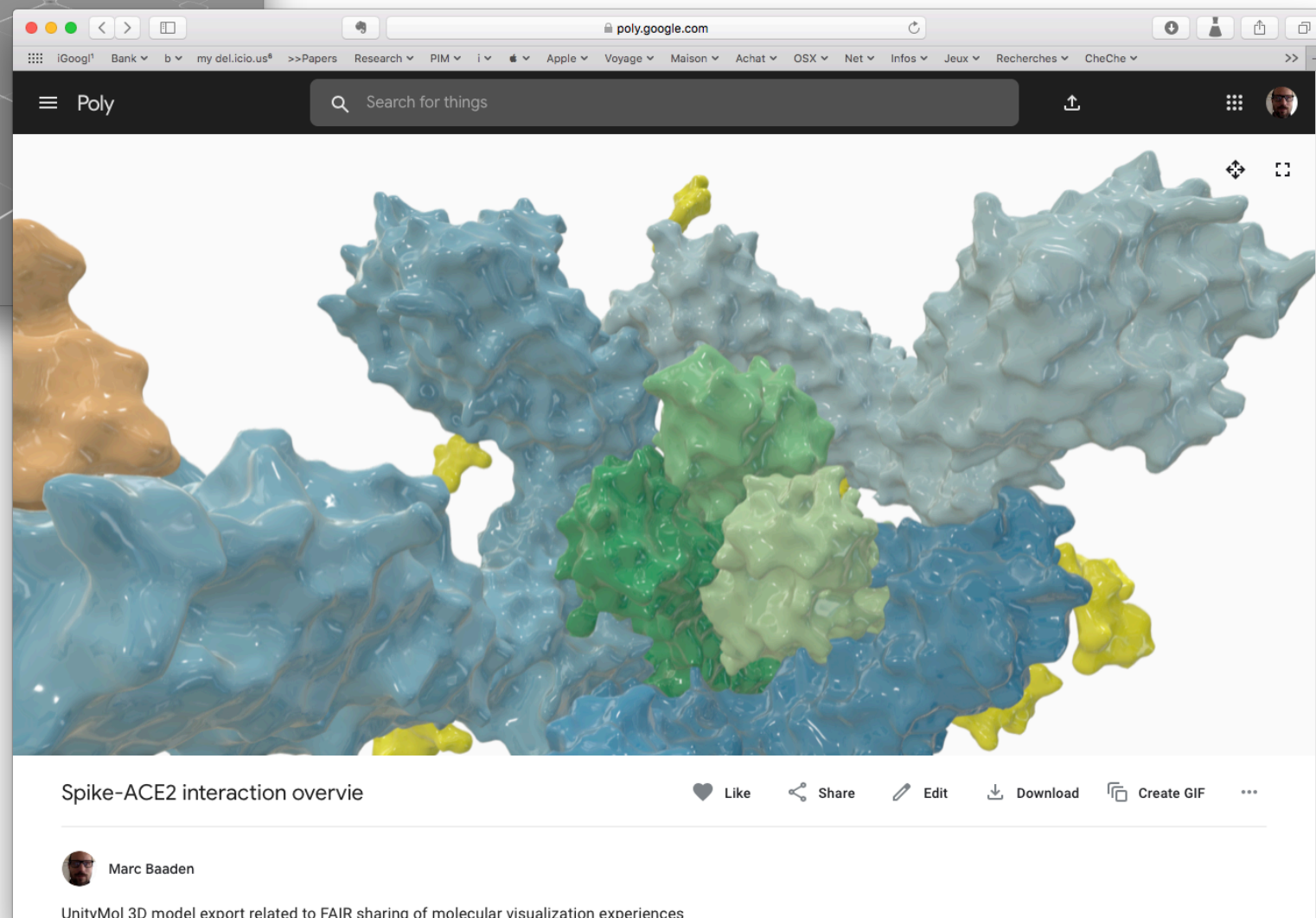
FAIR sharing of molecular visualization experiences

Visualization renders structural molecular data accessible to a broad audience. Here we implement a Zenodo community to **share** molecular visualization experiences based on **FAIR principles**. First application cases are exemplified with recent Covid-19 related

Sharing 3D models



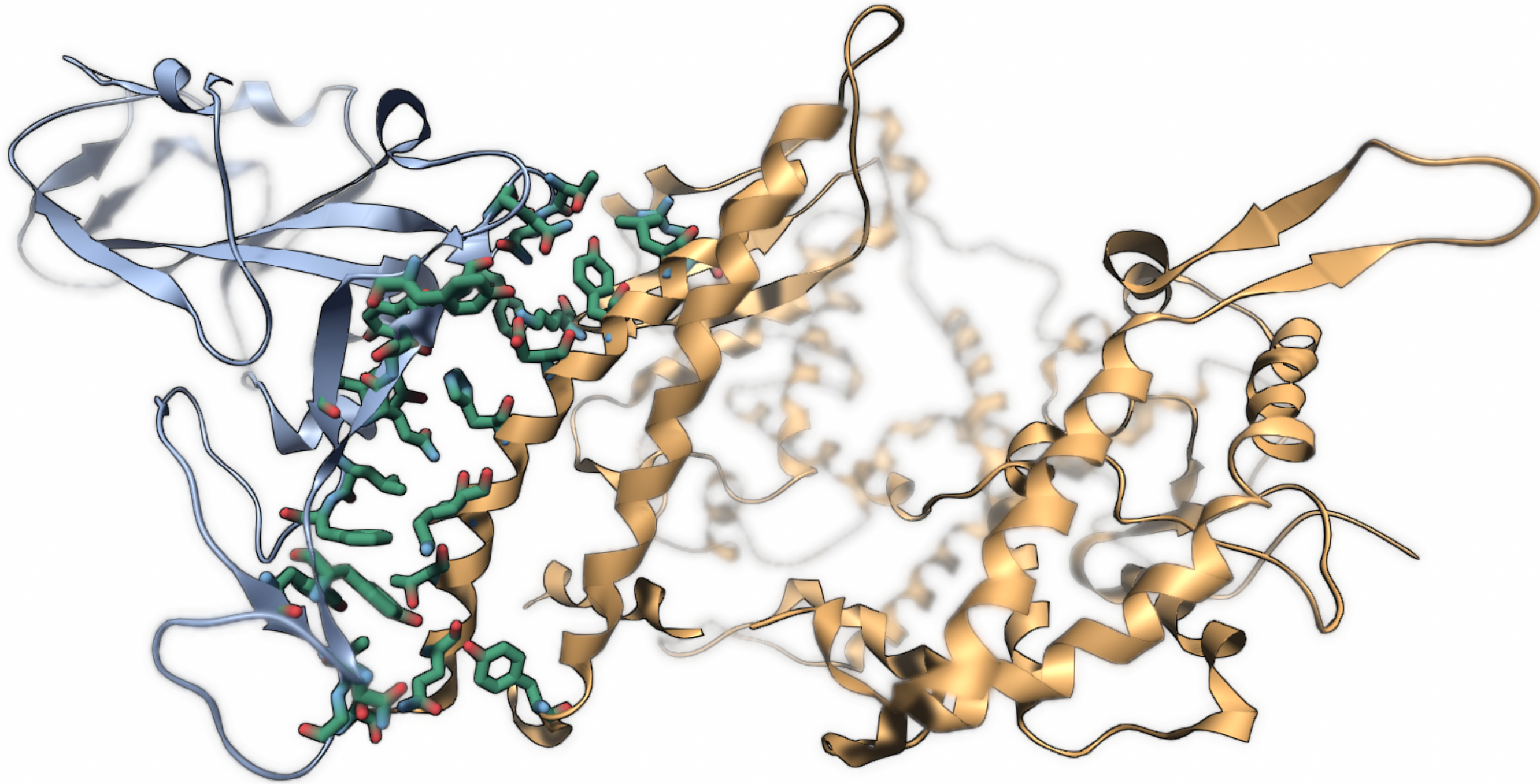
Sketchfab



Google Poly

Martinez et al., submitted to Acta Cryst D

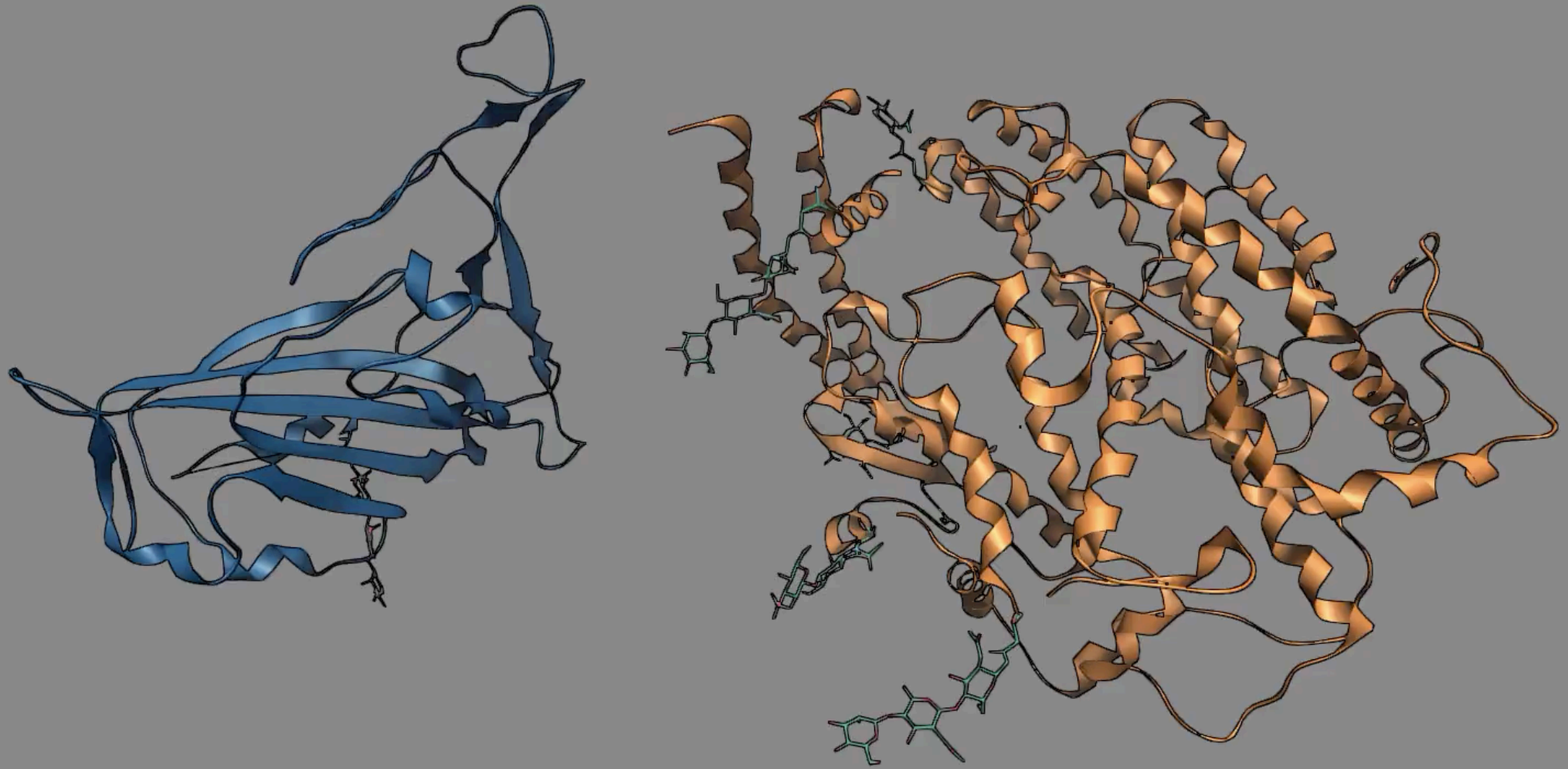
Animations



D. E. Shaw Research (2020) Molecular Dynamics Simulations Related to SARS-CoV-2

Martinez et al., submitted to Acta Cryst D

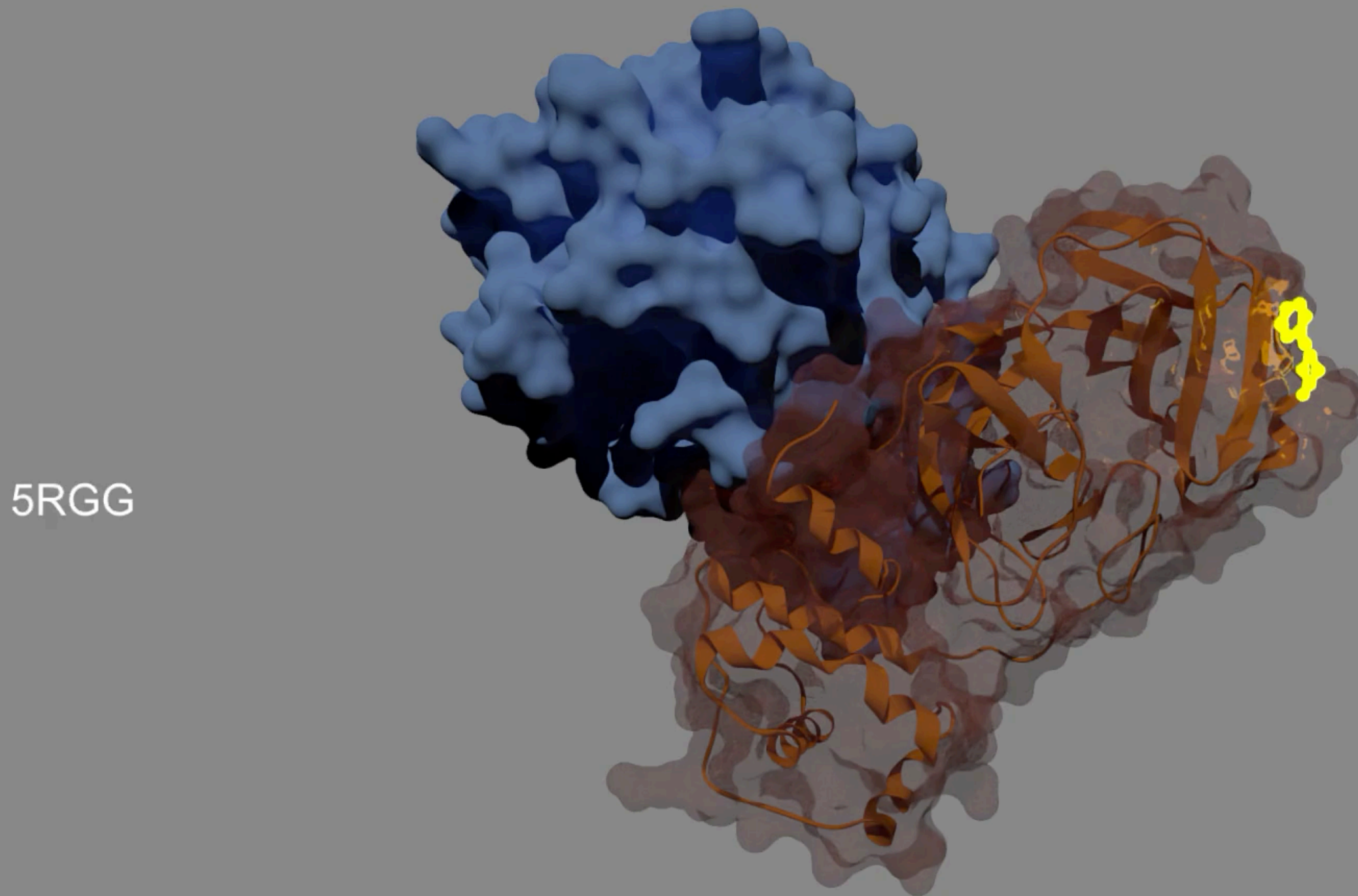
Animations



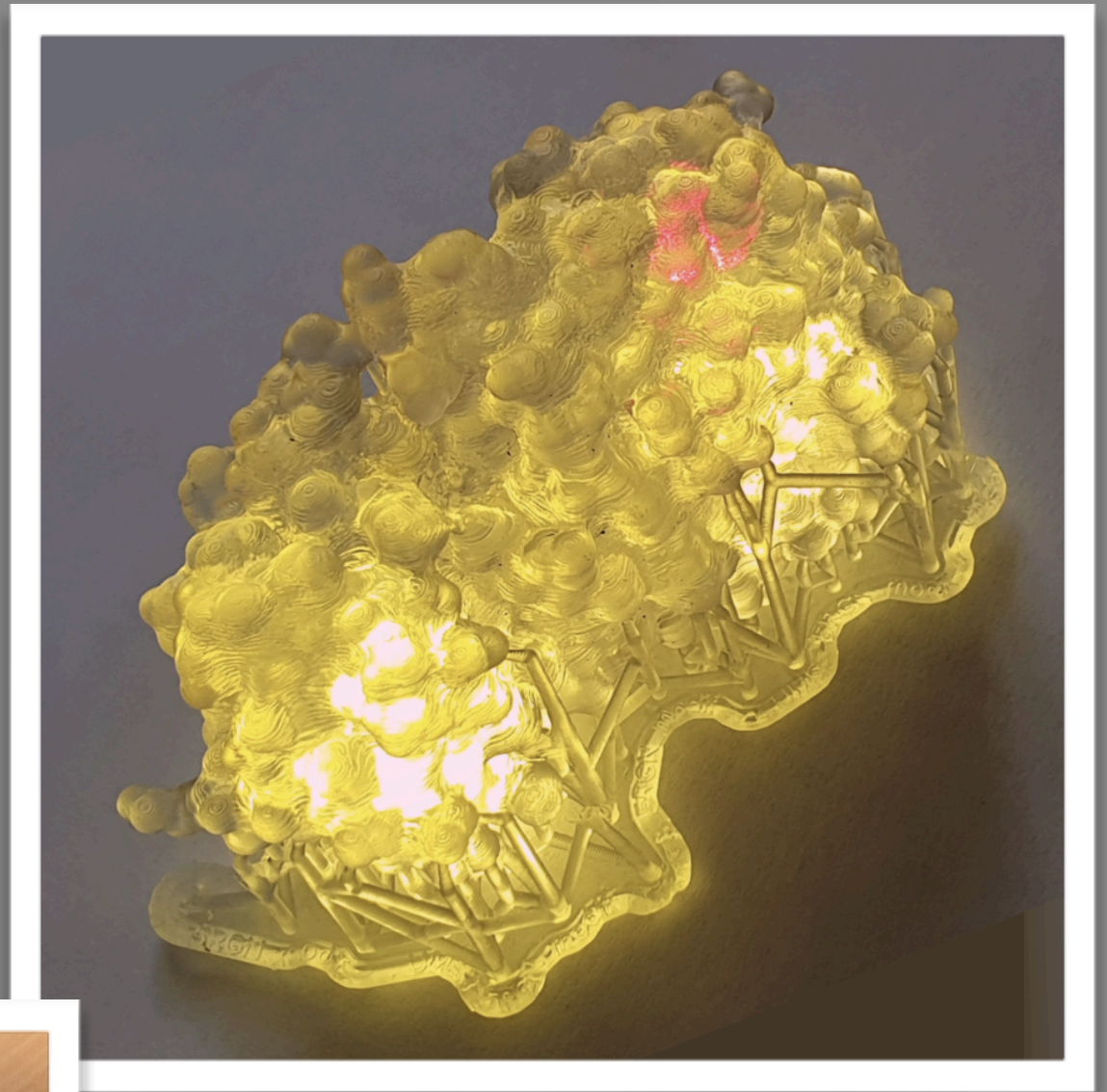
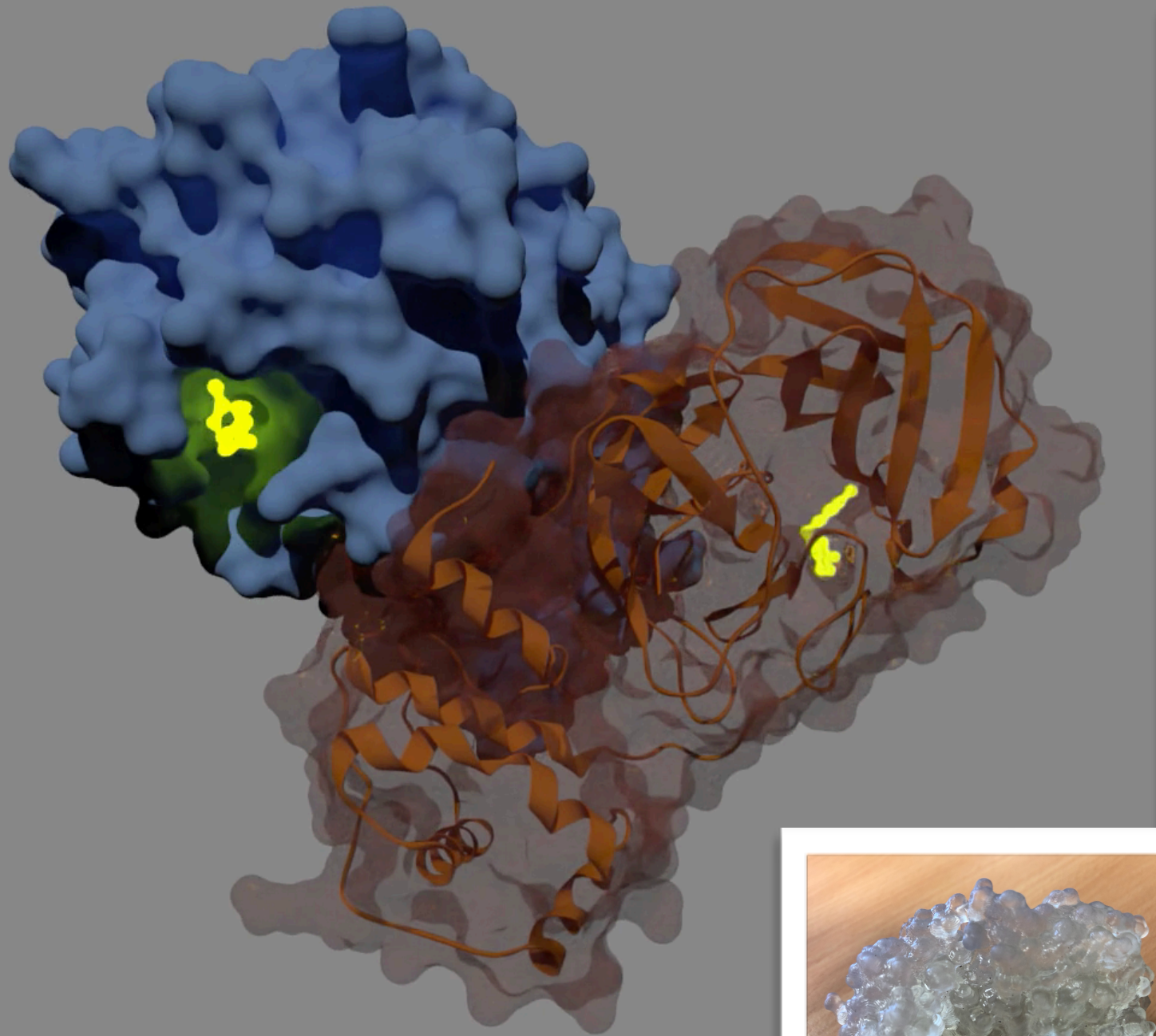
D. E. Shaw Research (2020) Molecular Dynamics Simulations Related to SARS-CoV-2

Martinez et al., submitted to Acta Cryst D

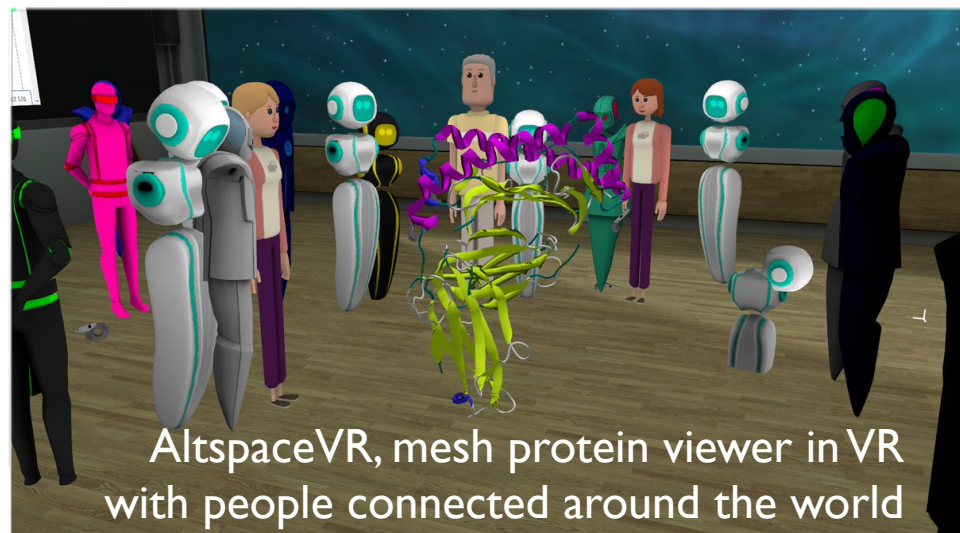
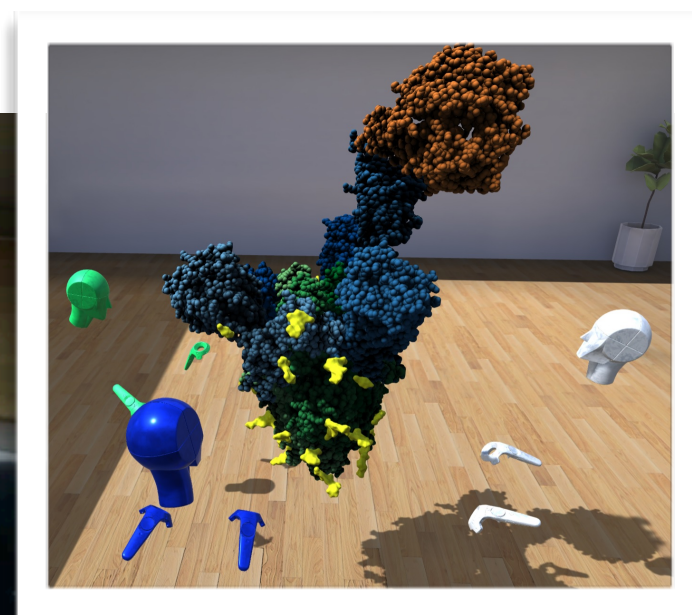
From virtual to real



From 3D models to printed objects



Collaborative multi-user sessions



Soon to come in *UnityMol!* For now:

AltPDB.info by T. Skillman

More details in our preprint



[HOME](#) | [ABOUT](#)

bioRxiv is receiving many new papers on coronavirus SARS-CoV-2. A reminder: these are preliminary reports that have not been peer-reviewed, should not guide clinical practice/health-related behavior, or be reported in news media as established information.

New Results

[Comment on this paper](#)

FAIR sharing of molecular visualization experiences: from pictures in the cloud to collaborative virtual reality exploration in immersive 3D environments

Xavier Martinez, Marc Baaden

doi: <https://doi.org/10.1101/2020.08.27.270140>

This article is a preprint and has not been certified by peer review [what does this mean?].

Abstract

[Full Text](#)

[Info/History](#)

[Metrics](#)

[Preview PDF](#)

Abstract

Motivated by the current Covid-19 pandemic that has spurred a substantial flow of structural data we describe how molecular visualization experiences can be used to make these datasets accessible to a broad audience. Using a variety of technology vectors related to the

<https://doi.org/10.1101/2020.08.27.270140>



FAIR sharing of molecular visualization experiences - overview

This page is an inventory of all media, data, code examples and instructions related to our preprint on [biorxiv](#) which lay the foundation for a Zenodo community and a figshare collection on FAIR sharing of molecular visualization experiences.

Collections and communities

Item	Link
Zenodo community incorporating all media, models, codes, executables etc.	Zenodo
figshare collection incorporating all elements deposited via figshare	Figshare

Media

Type	Description	Link(s)
Image	Five simple structural views (still images) of the SARS spike glycoprotein complex with human angiotensin-converting enzyme 2 (ACE2)	DOI 10.5281/zenodo.3999339 figshare
Image	Screen captures illustrating molecular 3D model sharing through Sketchfab, Google Poly and NIH Print Exchange	DOI 10.6084/m9.figshare.12881606
Image	Screen captures illustrating example 4 (bioinformatics data mapping on a 3D structure)	DOI 10.6084/m9.figshare.12894077
Movie	Animation of drug molecules binding to Covid-19 main protease	DOI 10.6084/m9.figshare.12860069
360 Movie	UnityMol 360 degree video with a camera path through the COVID19 spike protein-ACE2 complex	DOI 10.6084/m9.figshare.12894038 youtube
3D movie	to come	to come

Models

Item	Description	Link(s)
3D Model (fbx)	A 3D model of the spike-ACE2 interaction exported from UnityMol. The raw fbx file can be downloaded, or the 3D model can be directly viewed on Google Poly or on Sketchfab. This also allows viewing in AR/VR with various devices	DOI 10.6084/m9.figshare.12866981.v2 Google_Poly Sketchfab
Printable Model (stl)	A 3D model and related files for 3D printing of the SARS-CoV-2 main protease monomer	DOI 10.6084/m9.figshare.12867314 NIH_Print_Exchange

Code and executables

Item	Link
UnityMol scripts and required files to reproduce the examples described in our paper	DOI 10.5281/zenodo.4007911
UnityMol 1.1.1 executable build for MacOSX to run the above scripts	DOI 10.6084/m9.figshare.12866804
UnityMol 1.1.1 executable build for Windows 64 to run the above scripts	DOI 10.6084/m9.figshare.13050770
UnityMol 1.1.3beta executable build for Windows 64 Virtual Reality to run the above scripts	DOI 10.6084/m9.figshare.13238081
More executable builds to run the above scripts	(to come)
UnityMol source code release of related versions	(to come)

Documents

Item	Link
Preprint of the paper underlying this repository available from biorxiv	DOI 10.1101/2020.08.27.270140
Documentation on how to create the various media and models above with UnityMol	(to come once the code is stabilized)

License

Martinez et al., submitted to Acta Cryst D



X Martinez (post-doc) * **A Lanrezac** (PhD student)
* **H Santuz** (engineer)



Collaborations

CryoEM / SAXS

AE Molza, E Giudice
O. Delalande

MinOmics

S Lemaire, A Maes
C Marchand, B Laurent

VR contributors & users

S Doutreligne, N Férey
M Trellet, J Rodriguez
AMJJ Bonvin, M Levitt

UCB Biopharma

Z Sands, S Grootjans

Amgen Corp

D Kostin, PK Ghatti

Visualization. IMD etc.

S Pasquali, A Taly,
P Derreumaux
C Gageat, J Jonquet
P Bourdot
B Raffin, S Limet
S Robert, M Dreher
M Chavent

Thank you !