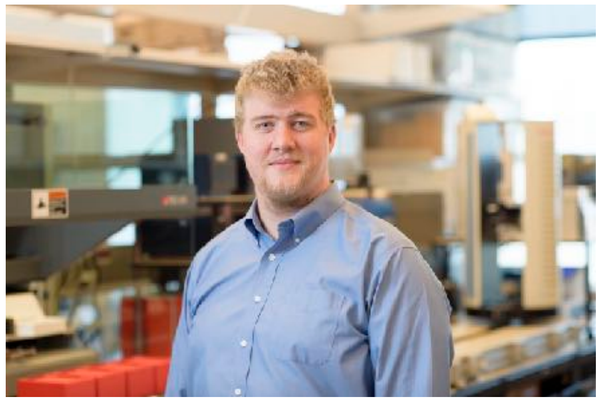
BioExcel Webinar Series #47

COVID-19 Molecular Structure and Therapeutics Hub

Presenter: Levi Naden (Molecular Sciences Software Institute (MolSSI))

Host: Rossen Apostolov (KTH Royal Institute of Technology)

Today's Presenter



Levi Naden

Software Scientist at MolSSI
lnaden@vt.edu

Levi Naden is a Software Scientist at MolSSI and lead for COVID-19 Molecular Structure and Therapeutics Hub project. Levi has a background in computational free energy algorithms, scientific software development and deployment, and software interoperability. He has a Bachelors in Chemical Engineering from Kansas State University and a PhD in Chemical Engineering from University of Virginia.

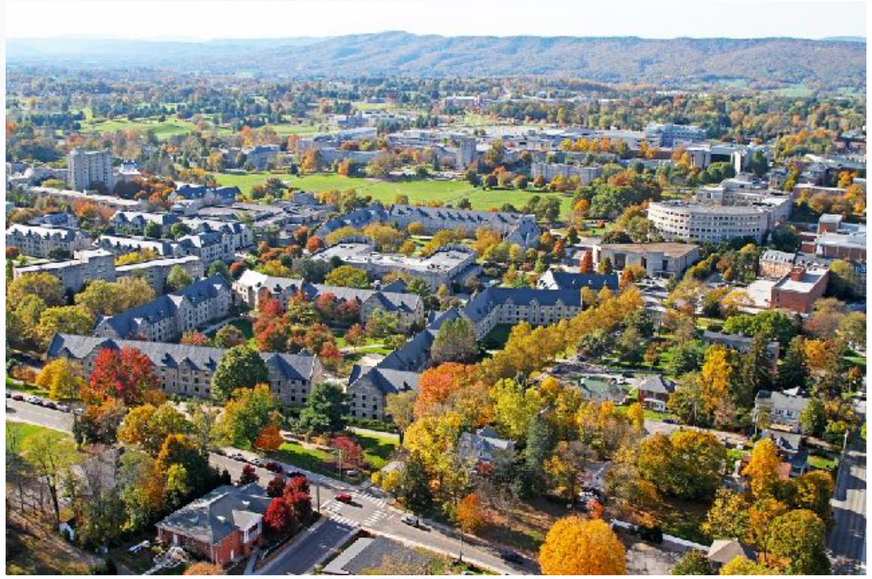
The Molecular Sciences Software Institute: https://www.molssi.org/

What is MolSSI?

Designed to serve and enhance the software development efforts of the broad field of computational molecular science (CMS) – a domain that includes quantum chemistry, computational materials science, and biomolecular simulation.

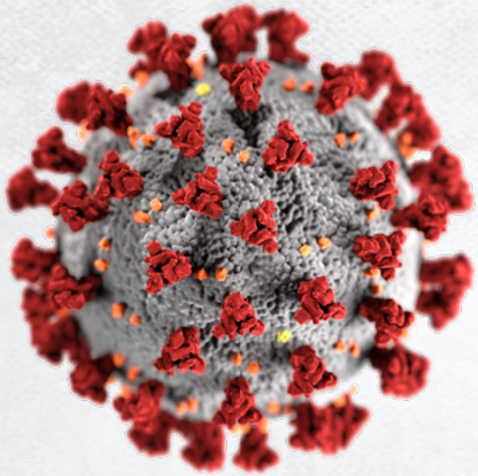
Goals:

1. Provide software expertise and infrastructure
2. Provide education and training
3. Provide community engagement and leadership



There are ups and downs to the current state of research

The Enemy



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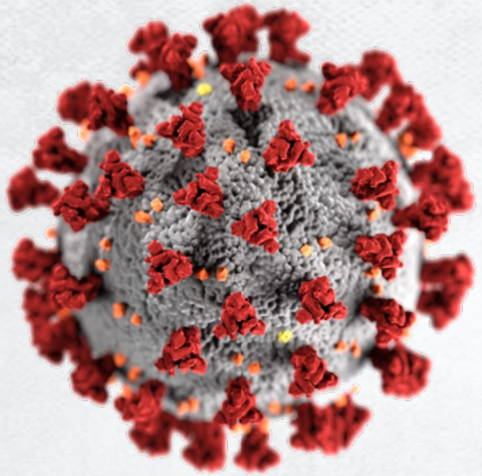

The Good

Covid-19 Changed How the World Does Science, Together

Never before, scientists say, have so many of the world's researchers focused so urgently on a single topic. Nearly all other research has ground to a halt.

Source: New York Times

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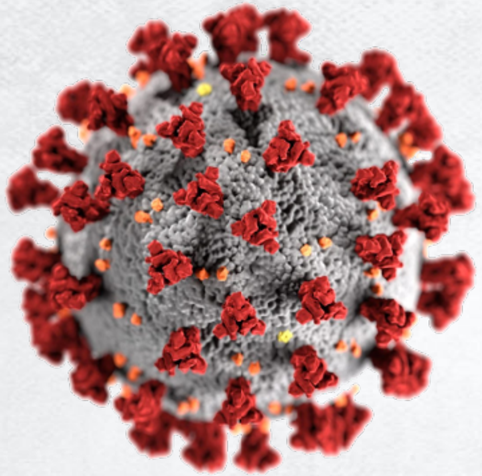

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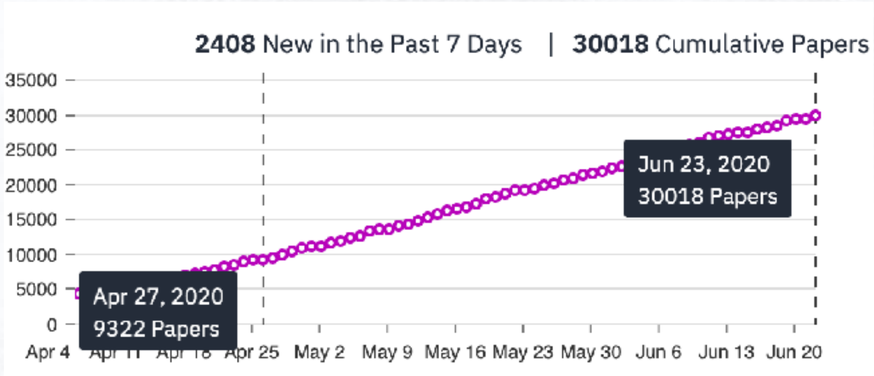

Total Volume of COVID-19 Research Papers
Source: covid19primer by Primer.ai.

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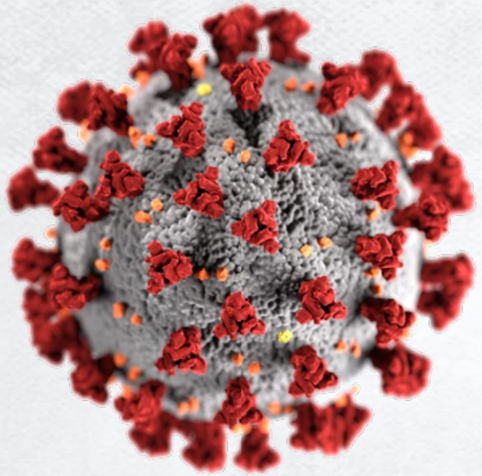

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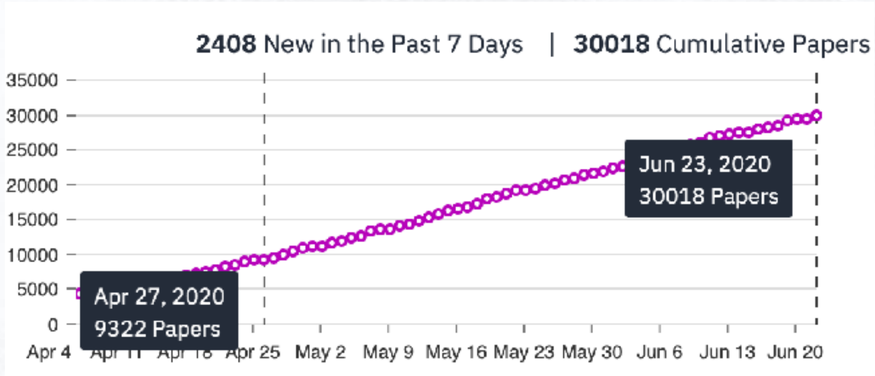

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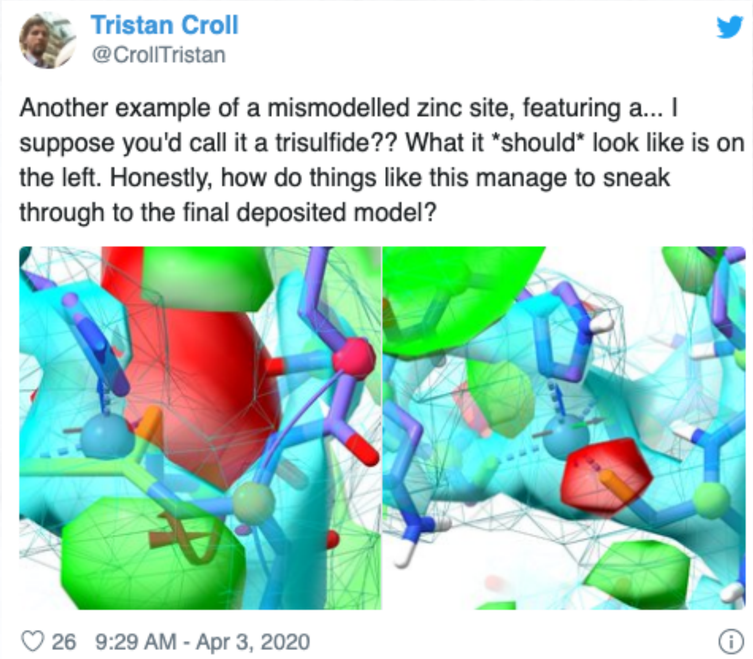
Lots of scientists stuck at home right now looking to help

Source: First google search for "antsy person"

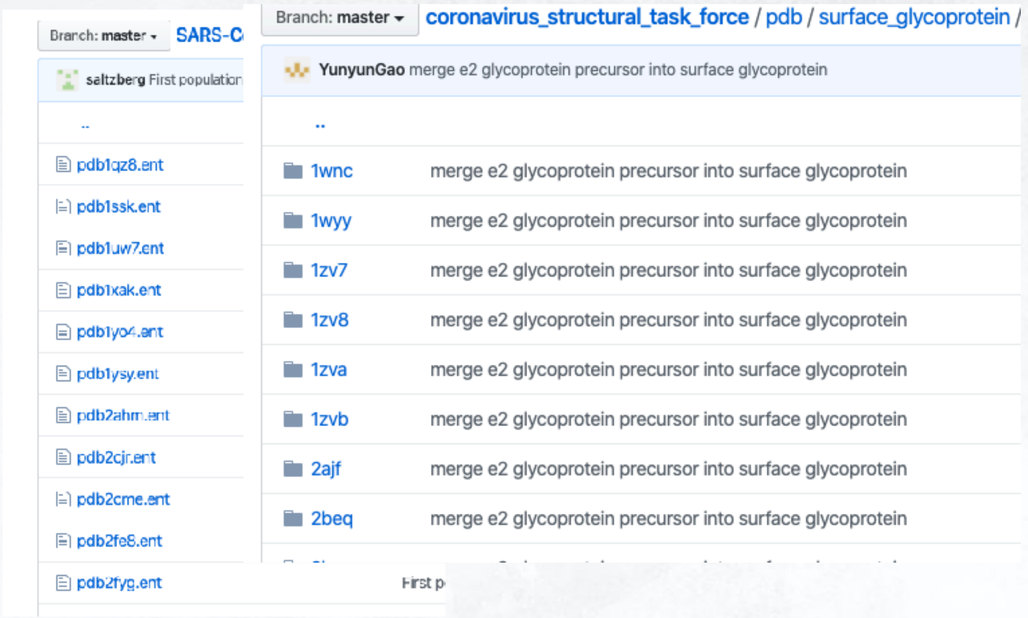
Every institute and lab under the sun is doing something with SARS-CoV-2

- Overall a good thing, but has downsides
  - Editors: “We are being overwhelmed with papers”
  - Quality: Mixed bag
  - Collaborators: We have data, people want data, how do I get them data?



Even good data are nebulous

- Everyone does their own work
  - And is great in their own rights!



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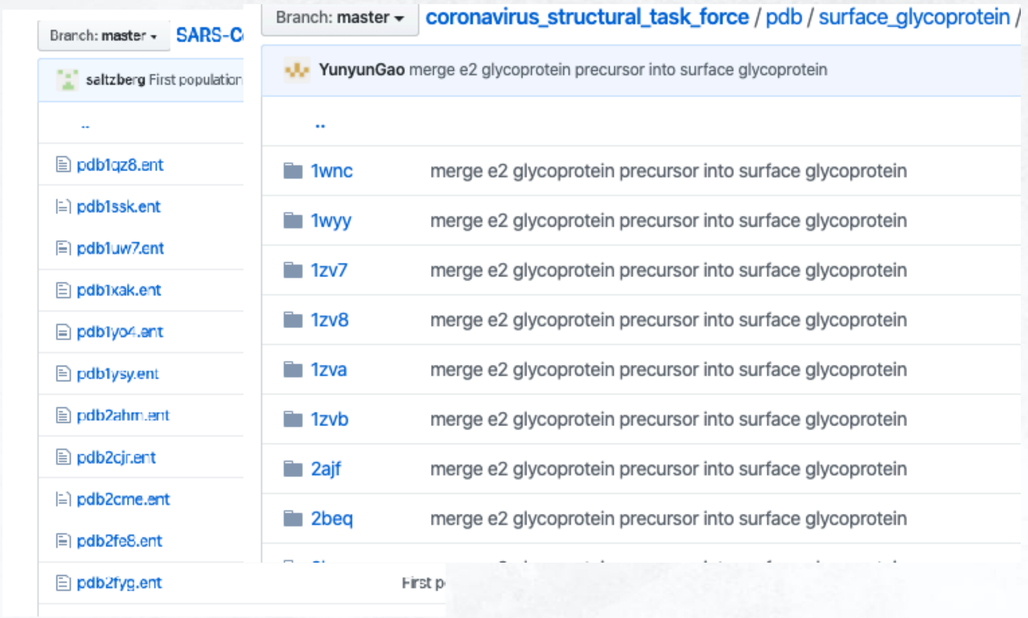

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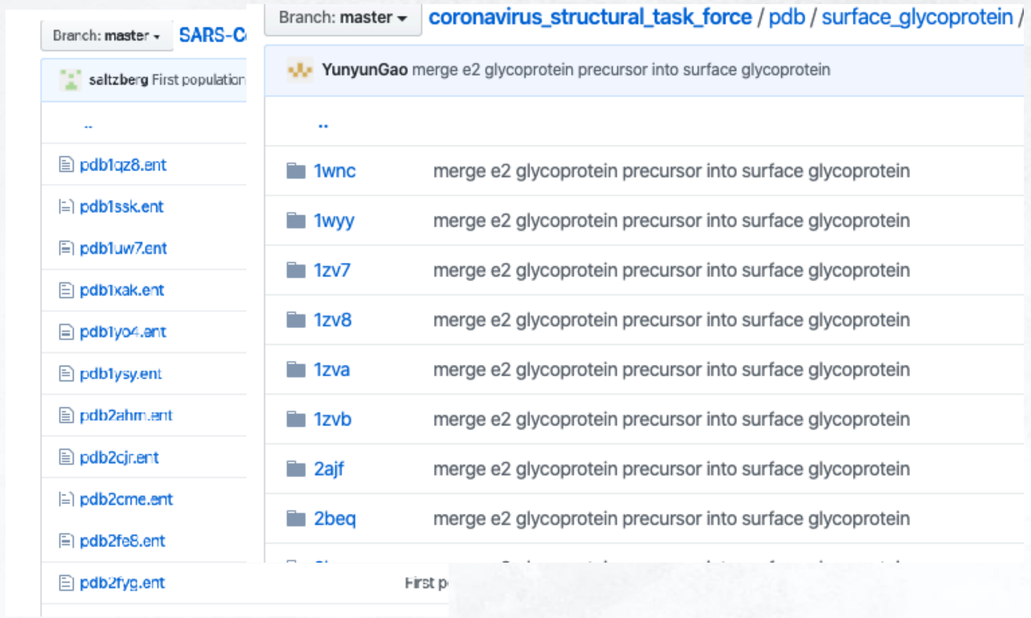

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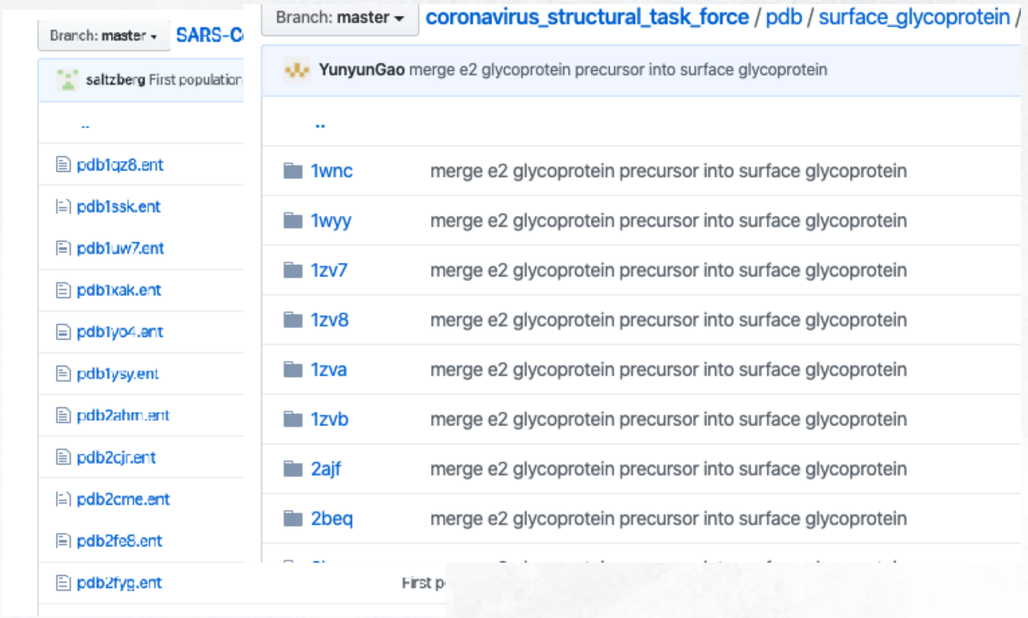

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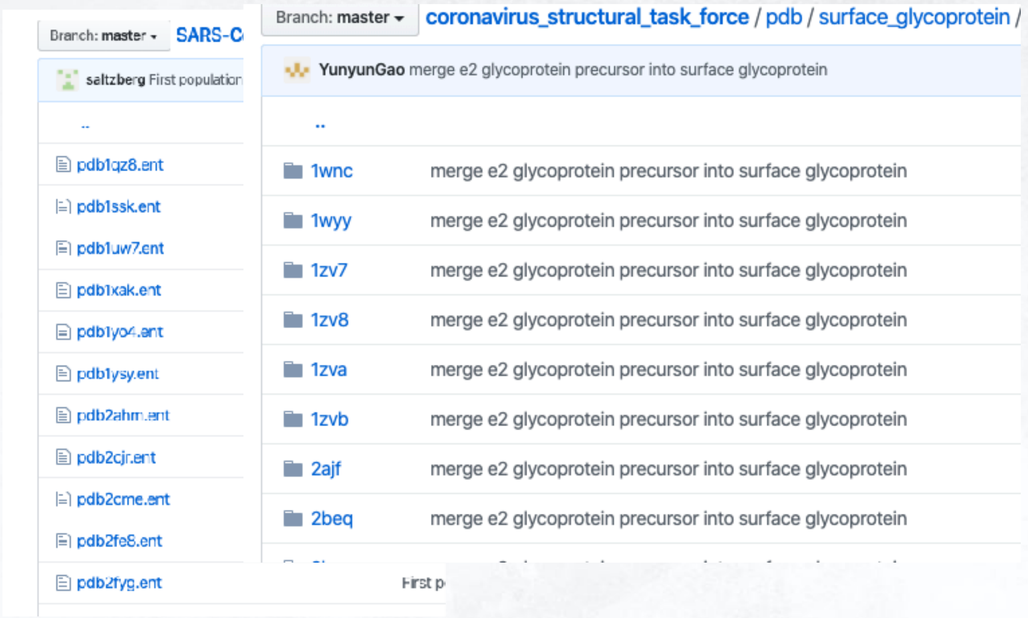

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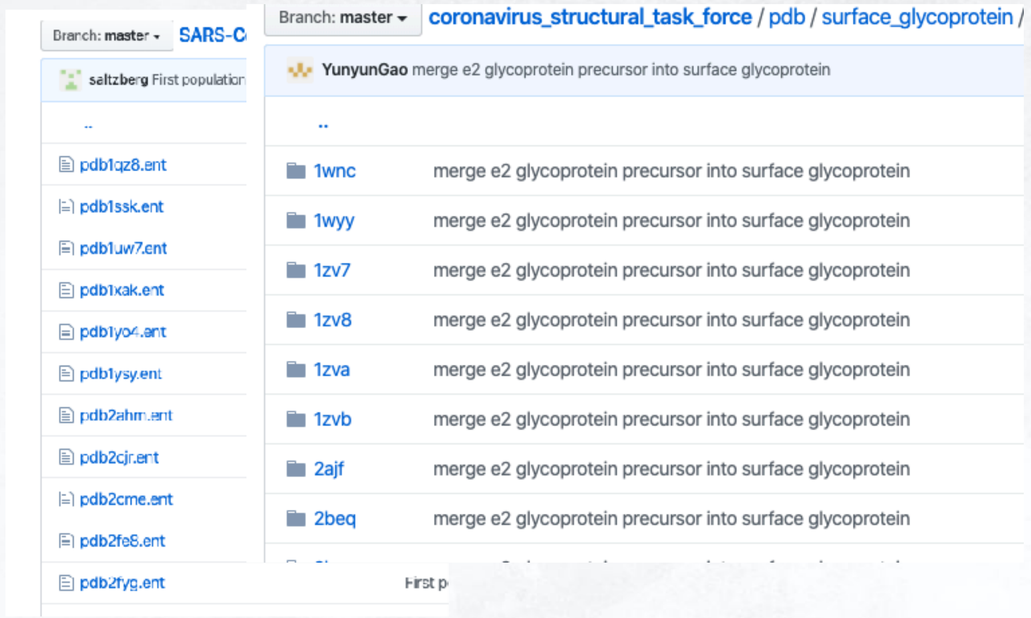

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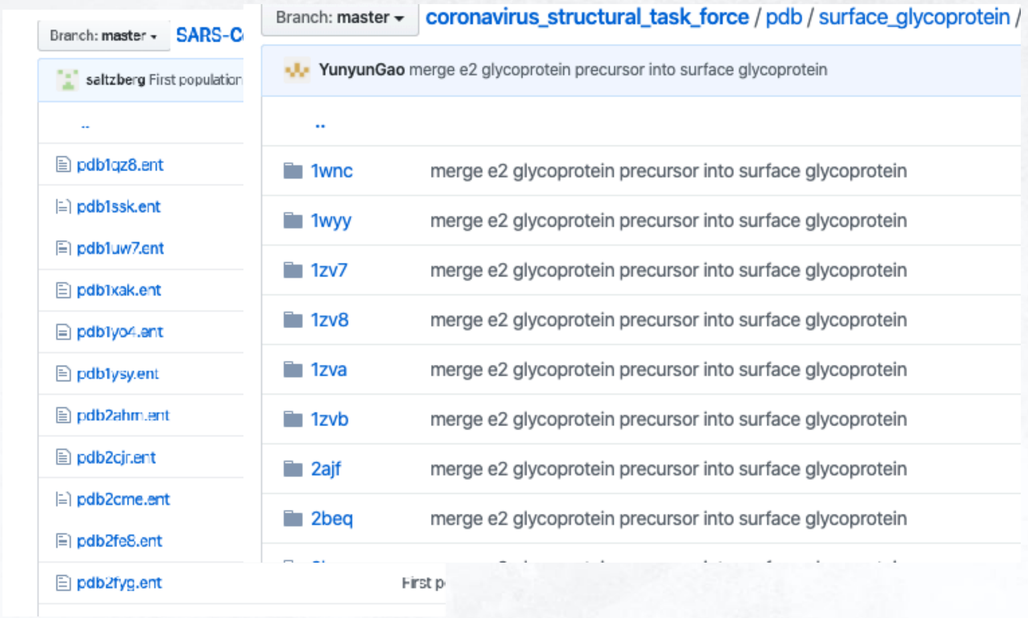

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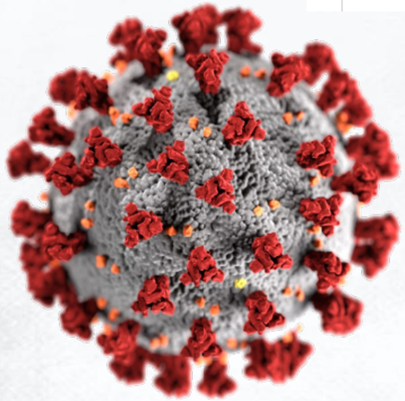

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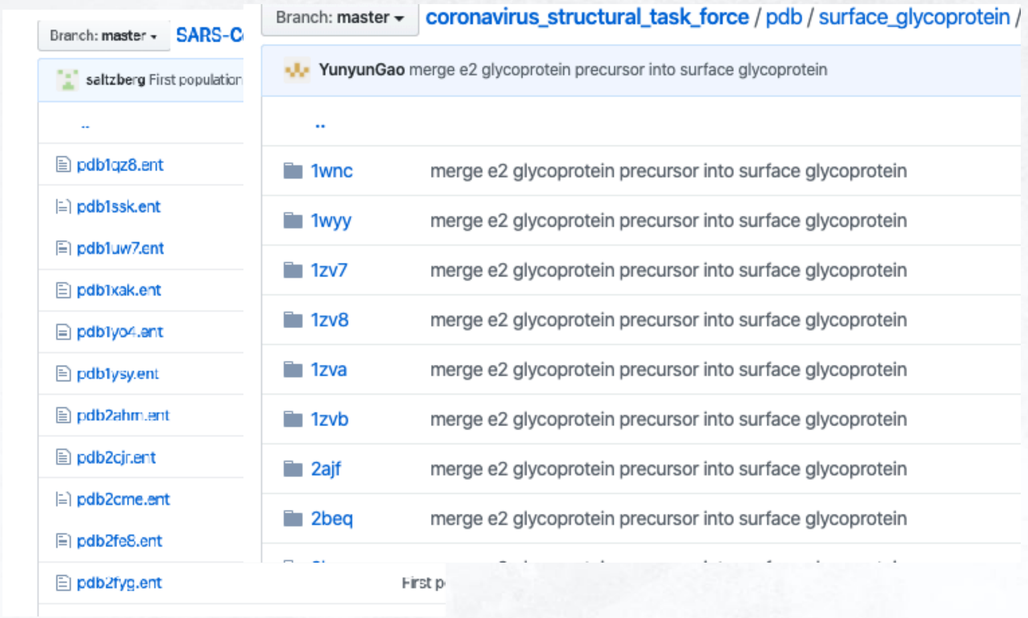

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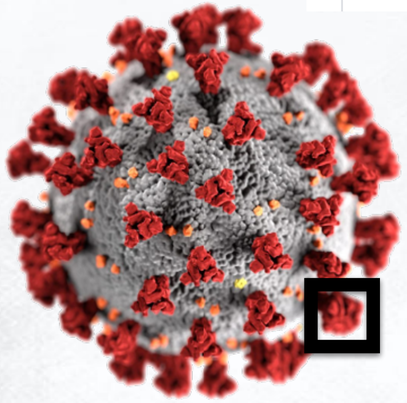

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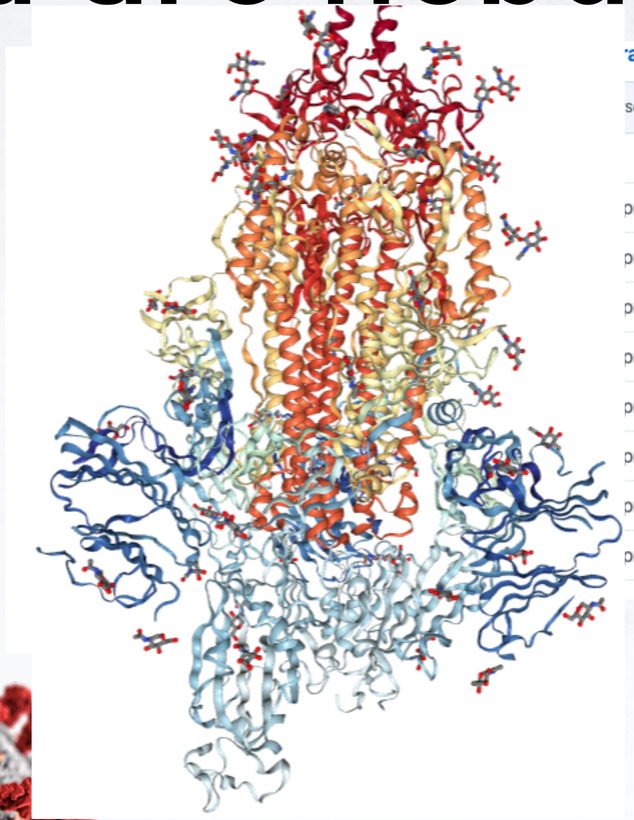

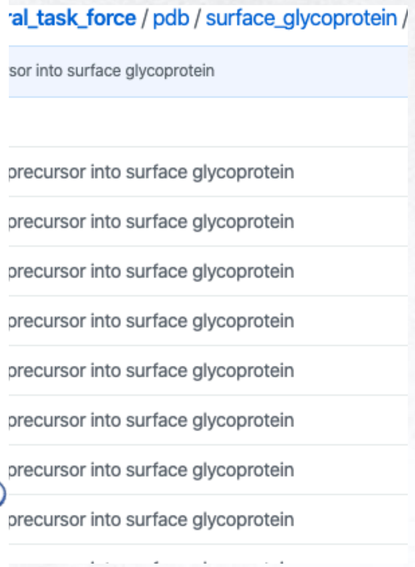

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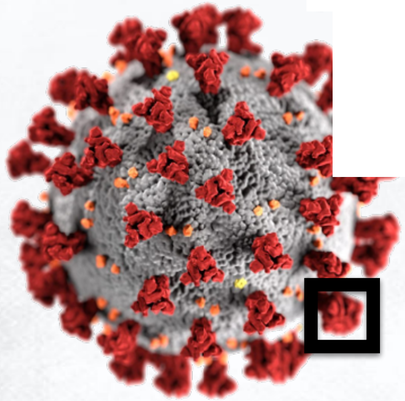

Spike

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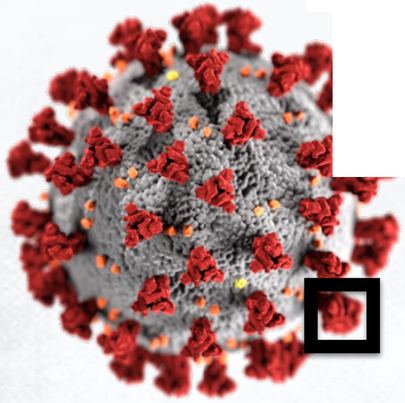
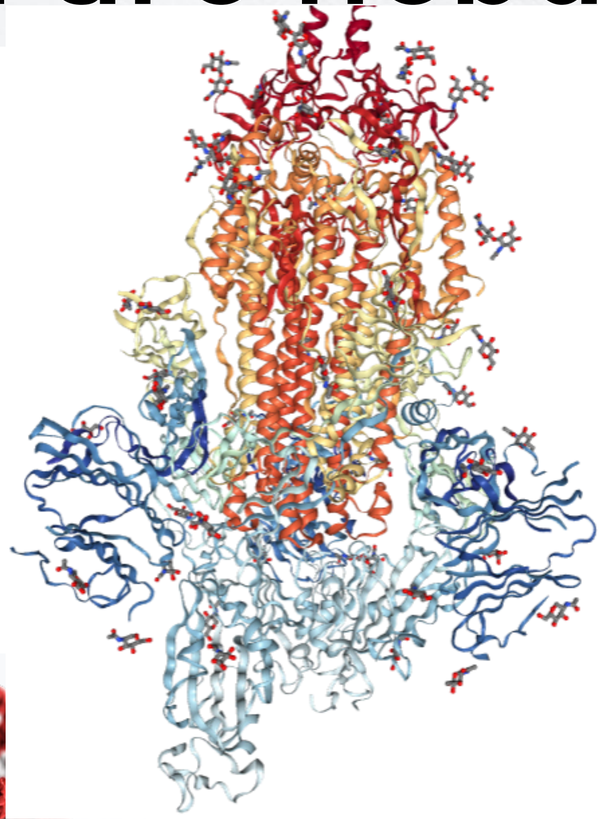
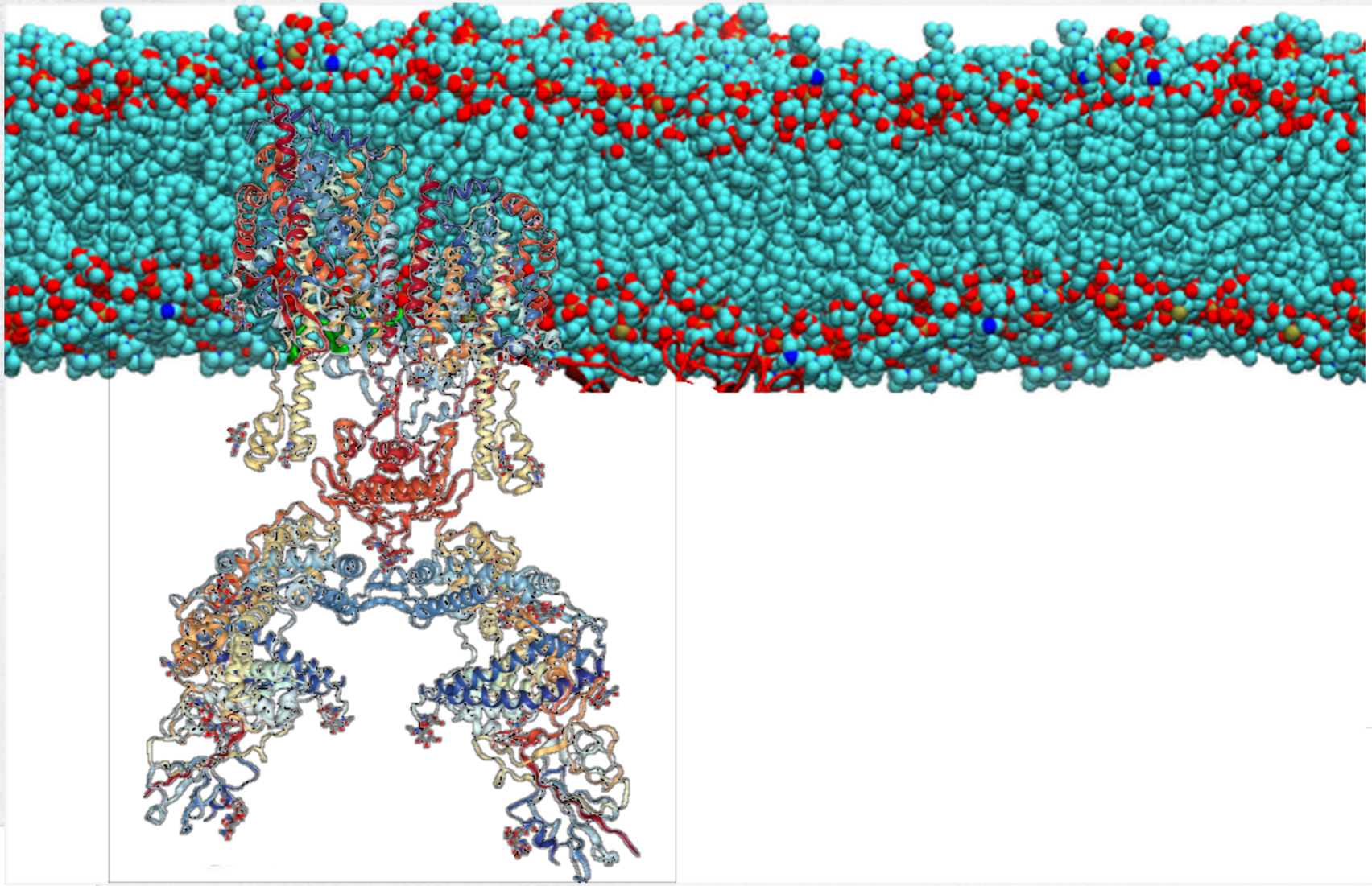
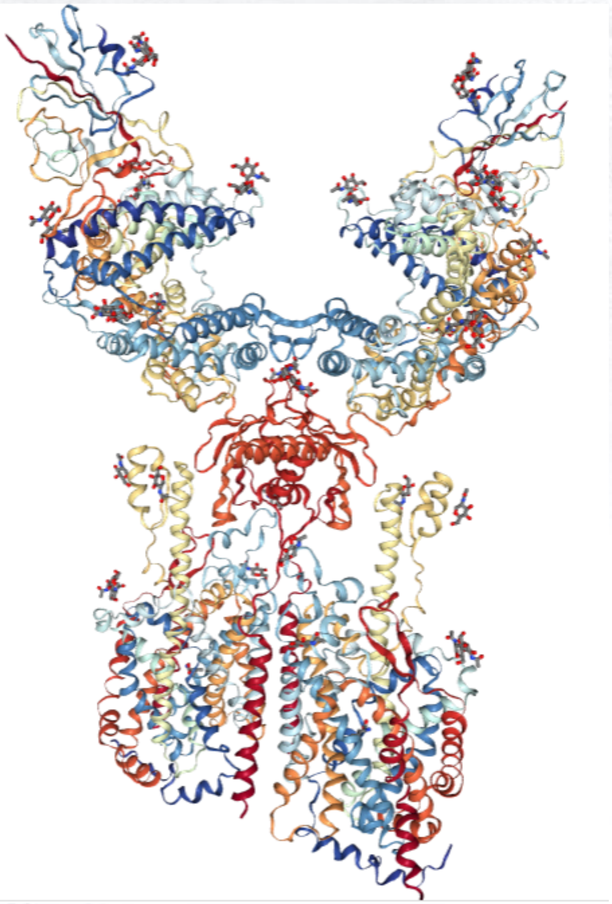




Spike

ACE2





ACE2

Modified from: Human Brain Project

We needed a hub for easily conveyed science

Simple descriptors
Community peer reviewed
Centralized or pointers to data
Accessible to experts in all domains

Two PI's sparked what is now a global network of cooperation

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Rommie Amaro

Adrian Mulholland

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Prototype (3 months ago)

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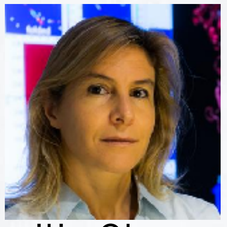

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JCIM JOURNAL OF CHEMICAL INFORMATION AND MODELING

D E Shaw Research

RIKEN BDR

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MOLSSI

bioexcel

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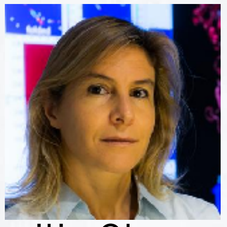

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One month a whole bunch of this later...

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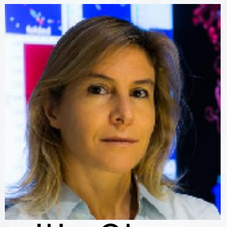

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Dozens of individual contributors

Community in US, EU, Switzerland, Korea, Japan

Upwards of a dozen Orgs./Institutes aiding or in talks

covid.molssi.org

MOLSSI

bioexcel

covid.molssi.org

Let's take a look at what is there!

github.com/MolSSI/covid

The Hub is bringing in companies to better aid researchers

- DataCite for issuing DOIs on demand
  - Make data citable in papers!

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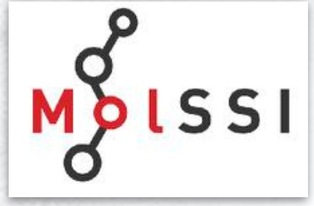
- AWS Open Data Program for storage
  - 100+ TB of storage
  - Explore options of storing the data we generate correctly



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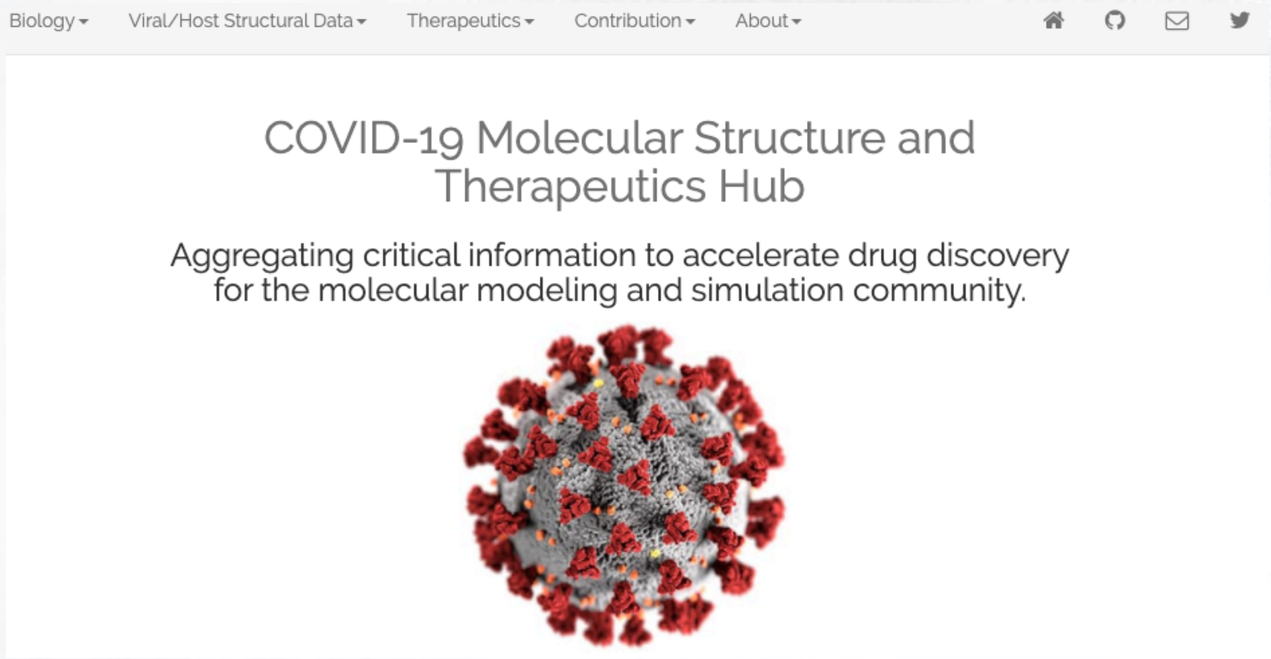
- Potential Improvements:
  - Knowledge Graphs for data
  - Data licensing schemes

The Hub showed unexpected social insights

- Simple descriptors:
  - Positive response, effective.
  - Iteration and Expansion



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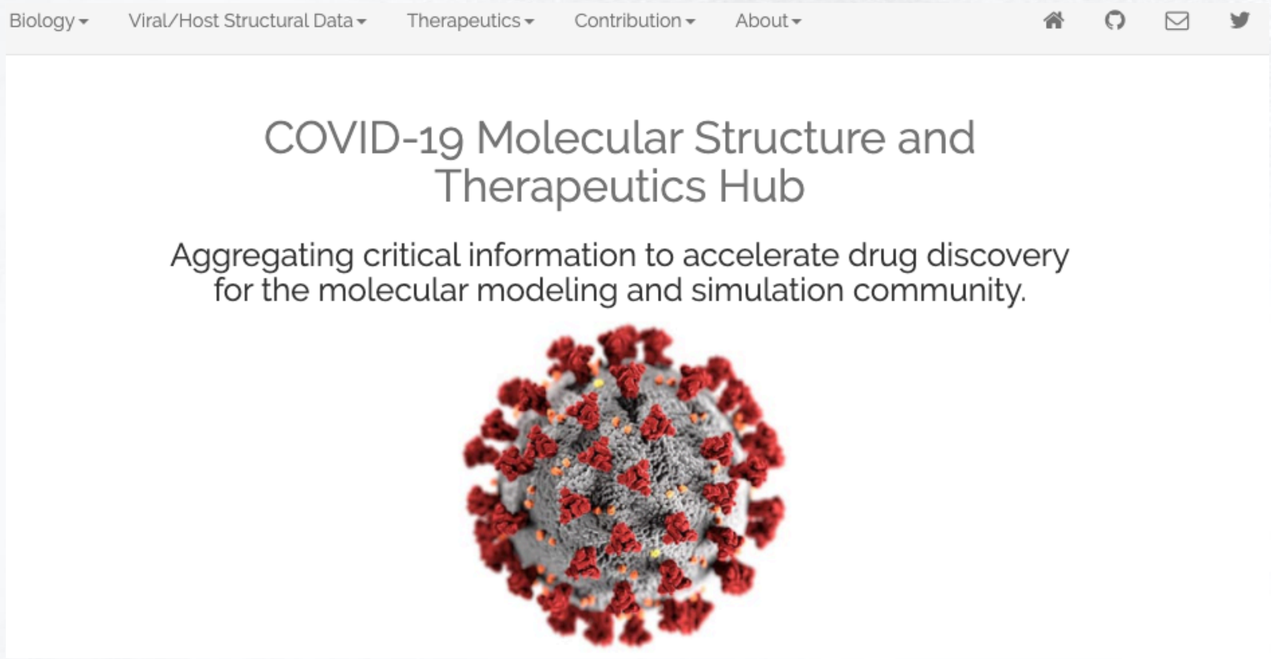
  - Original: Data ASAP - Review after
  - Actual: Reluctant* data additions



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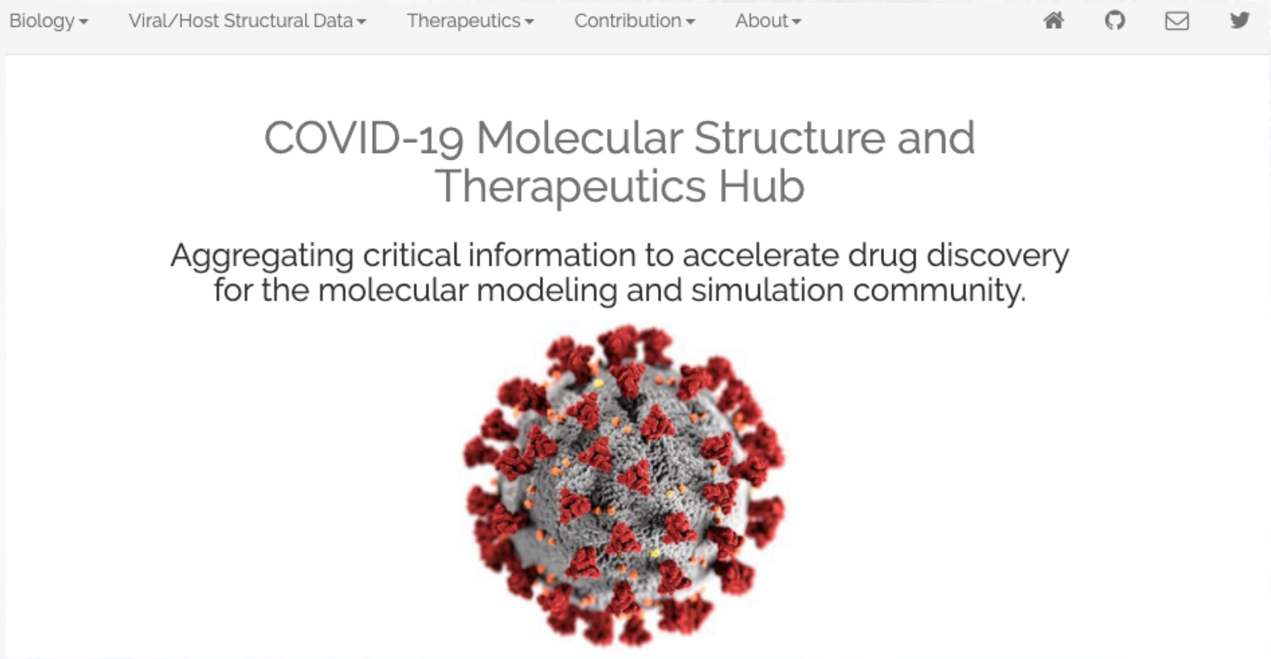
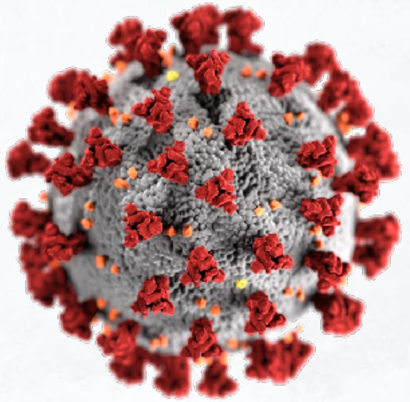
  - Actual: Reluctant* data additions
- Centralized or pointers to data
  - Can we link to it? We'll share it.
  - Can we quantify access? Even better.



What can we learn for the next research cohesion?



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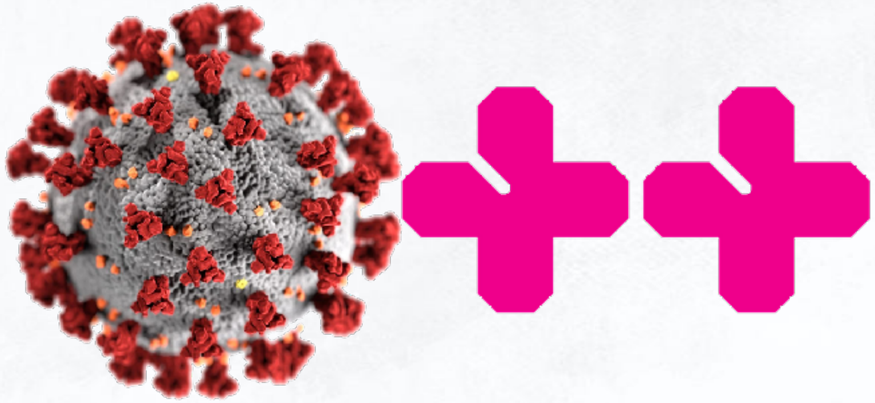

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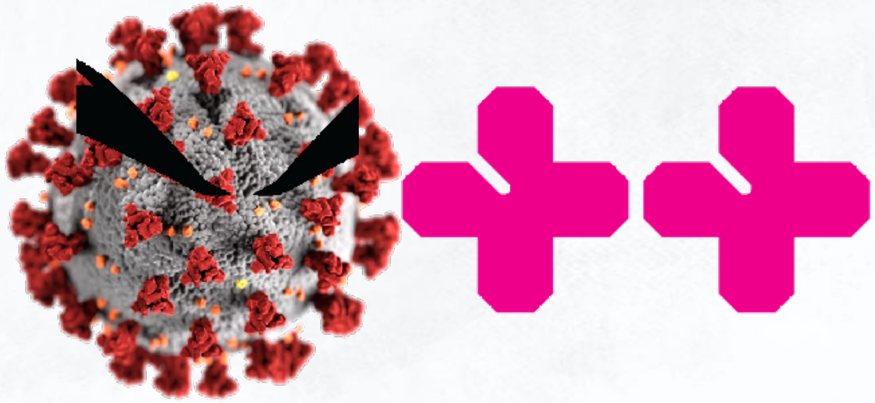

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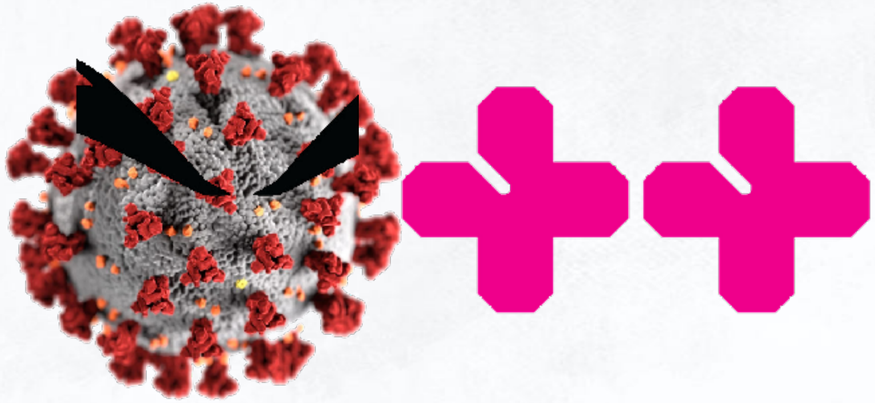

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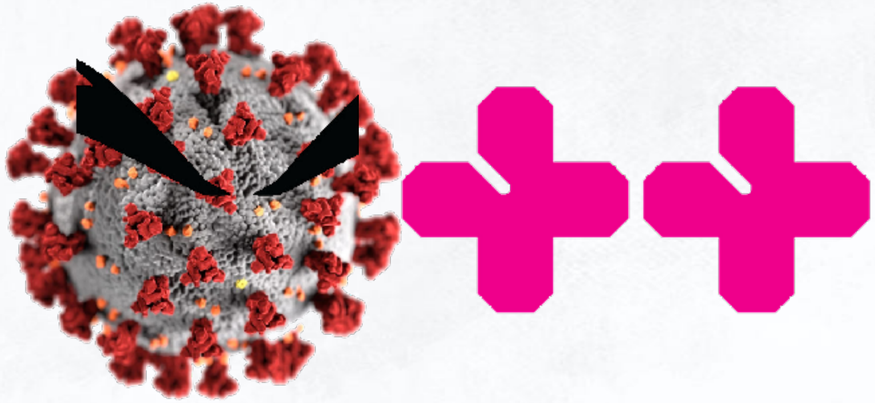

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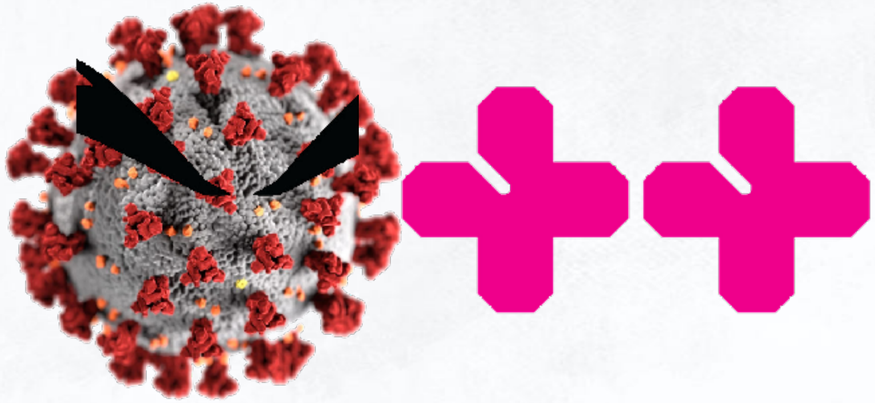

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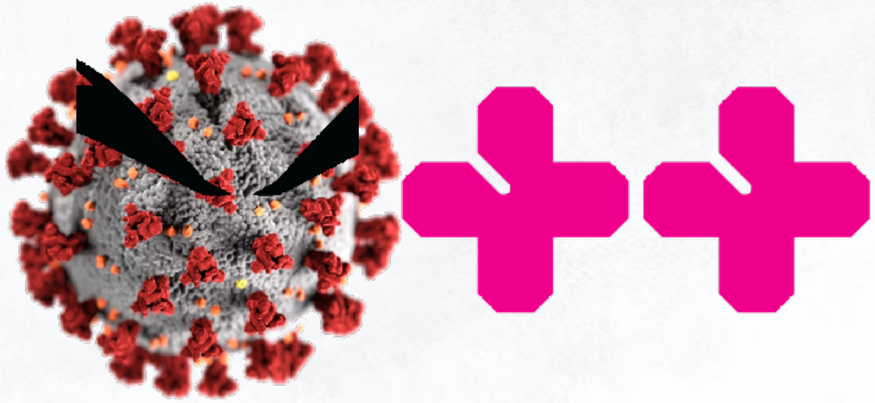
- Network data then connect people



What can we learn for the next research cohesion?

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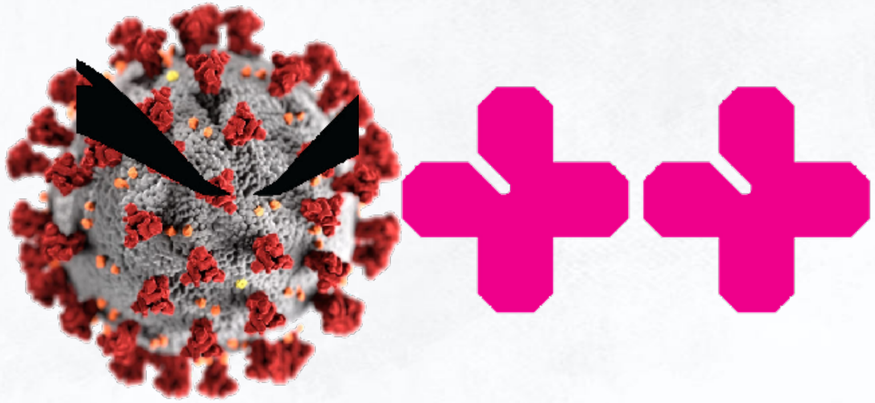

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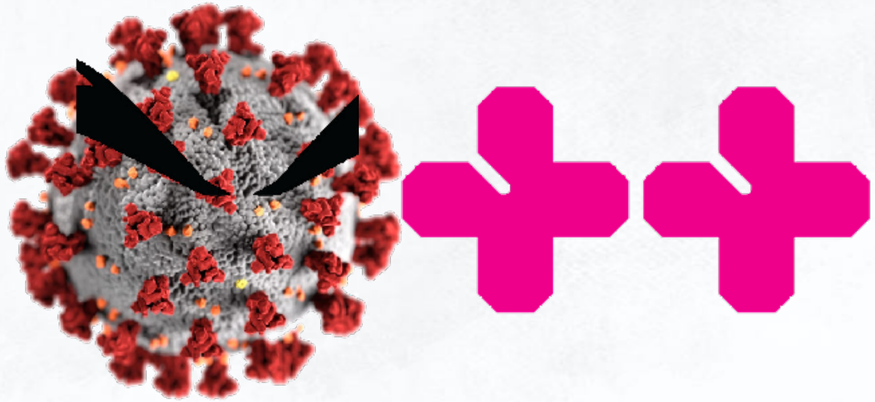

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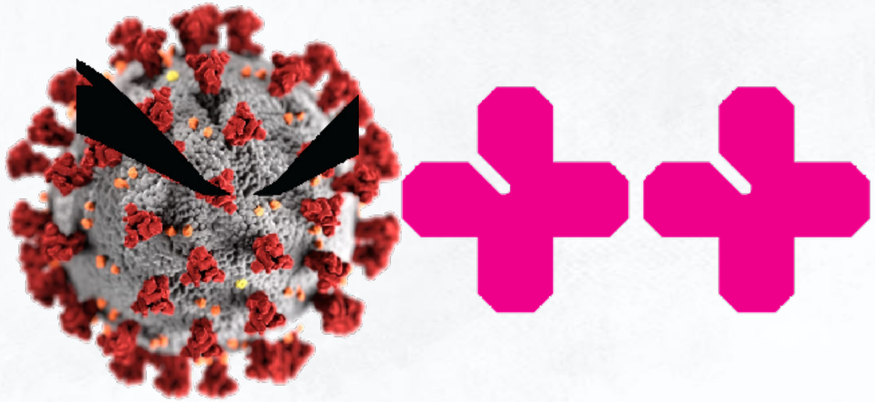

Sam Ellis

Andrew Abi-Mansour

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Thank you for listening!

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