

Coronavirus Antibodies & Emerging Vaccines

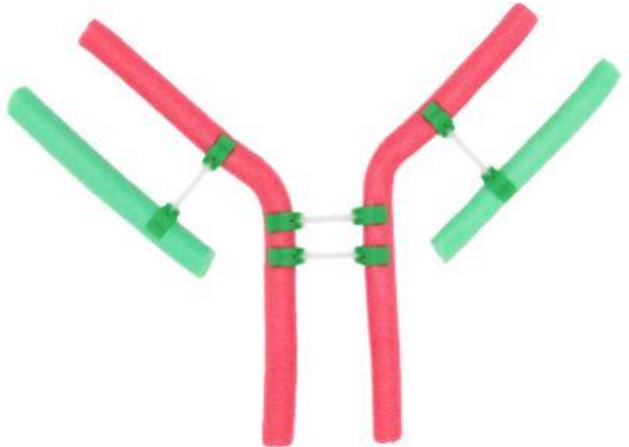




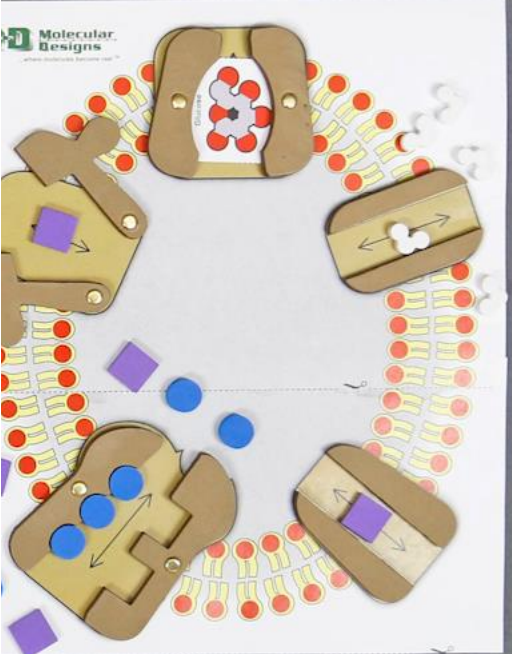
Field Test

 **Student Modeling Packs**
Home and School!

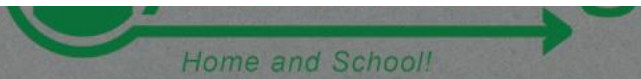
Antibody Student Modeling Pack[®]



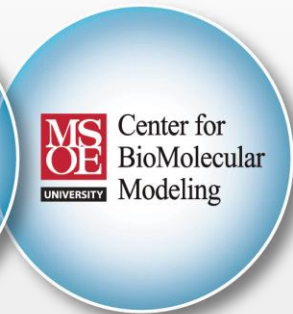
The image shows a Y-shaped antibody molecule model. It consists of two red arms and two green arms, connected by green cross-links. The model is set against a white background.



cks



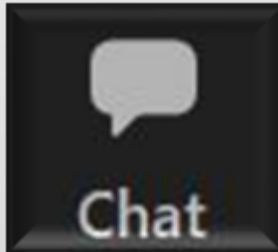




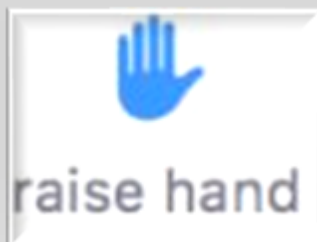
Webinar Norms



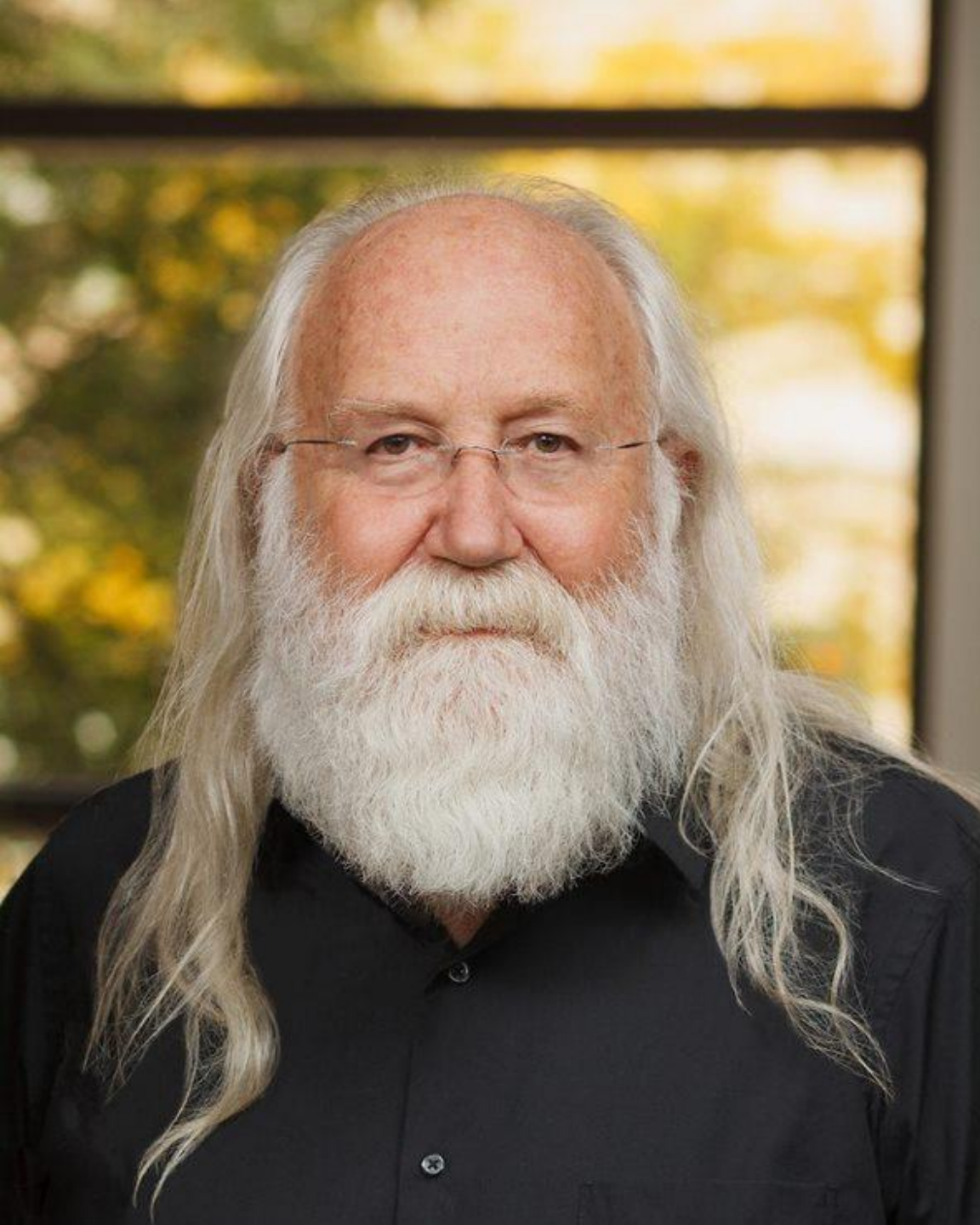
Questions for the Speaker should be entered into the Q&A Box



Comments and Questions for 3D Molecular Designs Staff should be entered into the Chat box.



Use the Raise Hand button to participate in discussion when applicable.

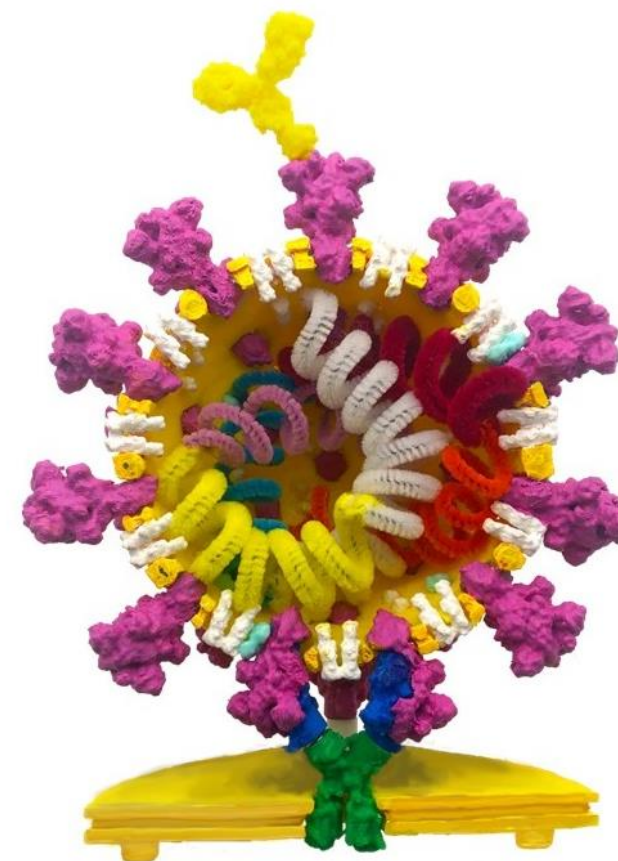


Timothy Herman, PhD

- Director of the Center for BioMolecular Modeling at MSOE
- Founding Partner of 3D Molecular Designs
- B.S. in Chemistry from the University of Nebraska
- Ph.D. in Biochemistry from Oregon State University.
- Post-doctoral studies in Molecular Biology at Harvard Medical School.

The science of **CORONAVIRUS**

...from the perspective of a
reductionist biochemist.



My job? ... to keep up with recent developments in the molecular biosciences,... and to interpret/communicate these developments for educators and their students.

*We do this through **modeling!***

MAPS Teams
Modeling **A P**rotein **S**tory

CORONAVIRUS

The AeroNab Story

And now,....

Antibodies,...and the AeroNab Story!



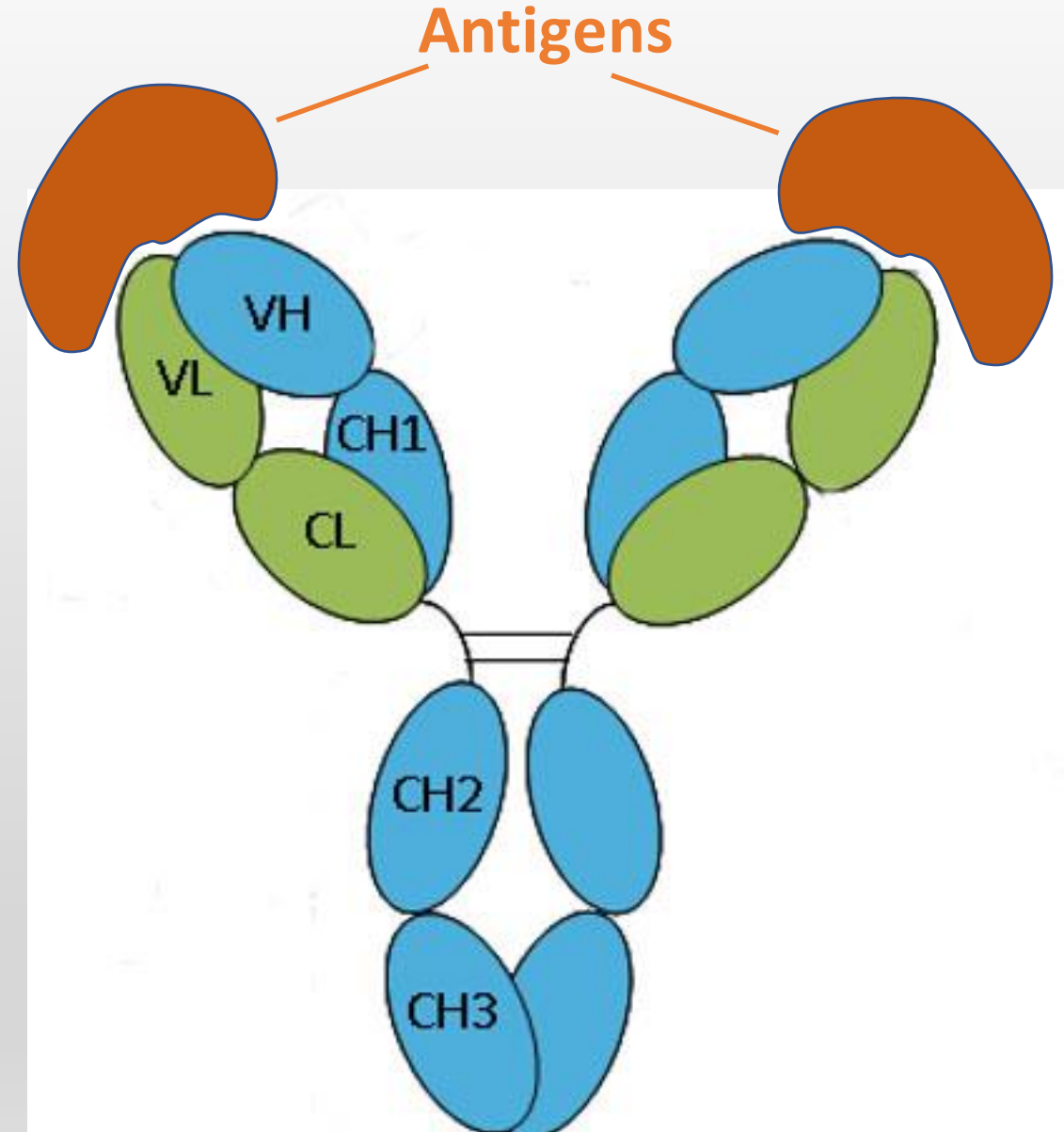
Antibodies have a modular design

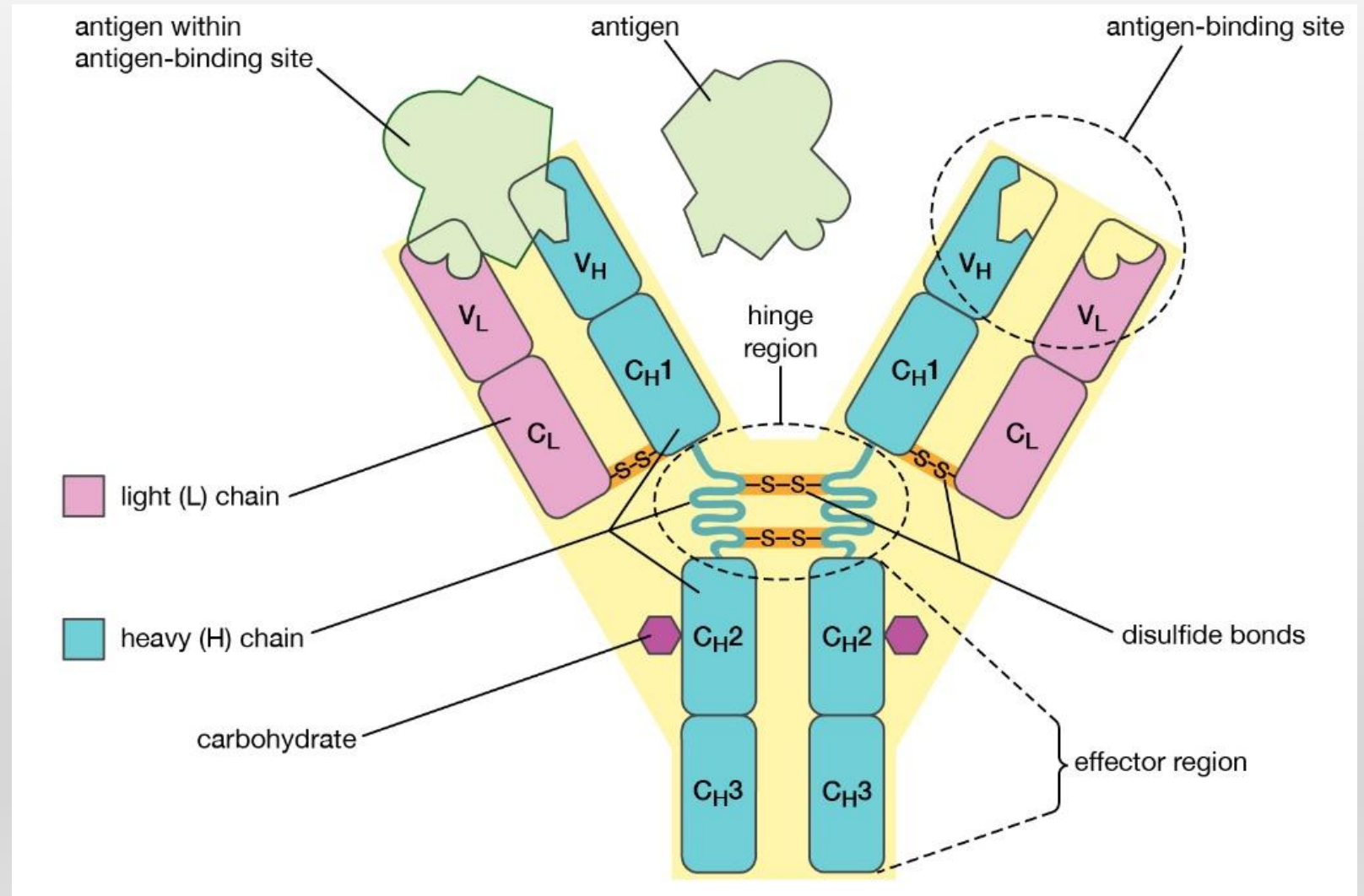
They are composed of 12 immunoglobulin folds

Each IgG fold is made up of ~120 amino acids

Each IgG fold consists of 2 beta-sheets....connected by a disulfide bond.

An antibody is composed of 2 Light Chains,
and 2 Heavy Chains





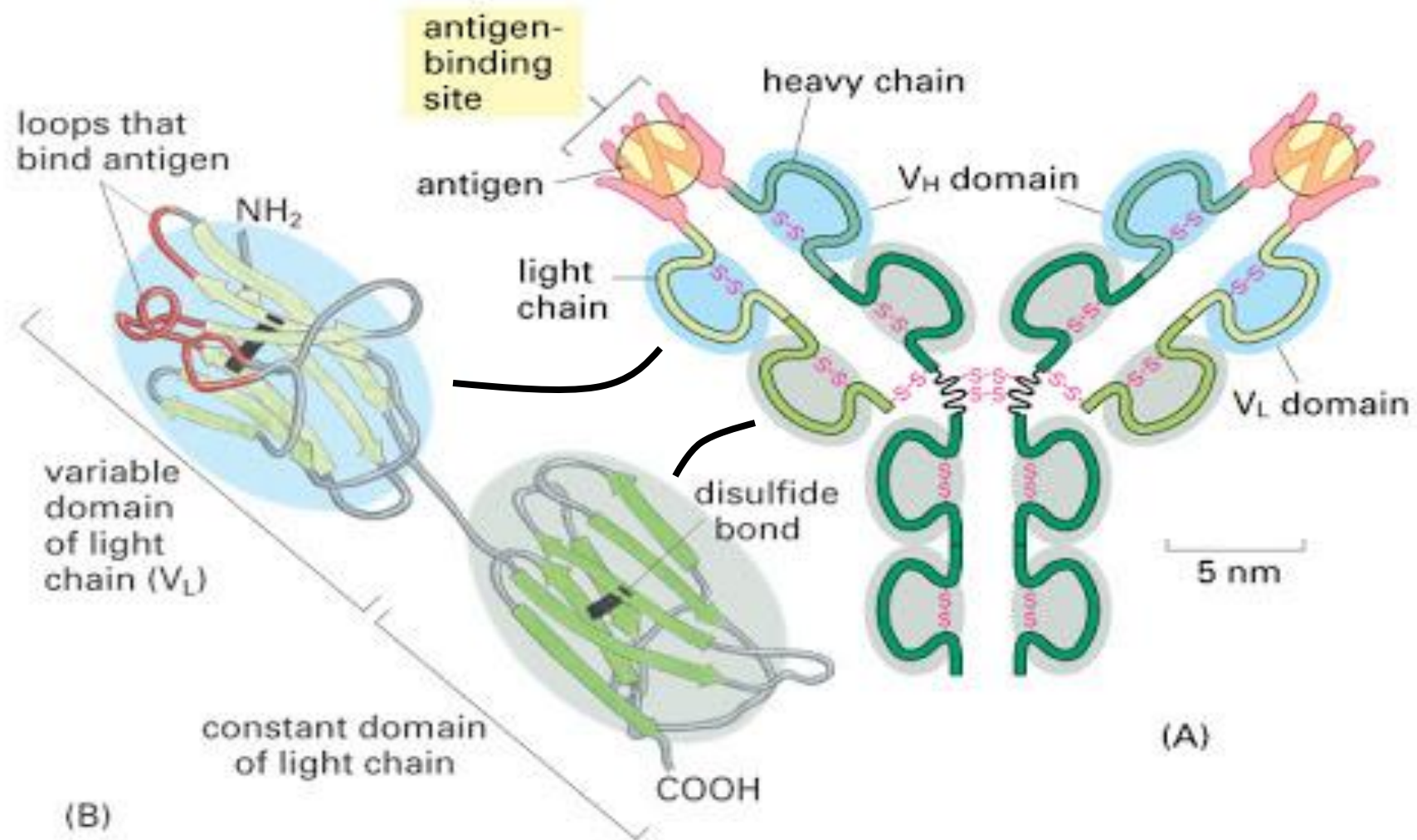
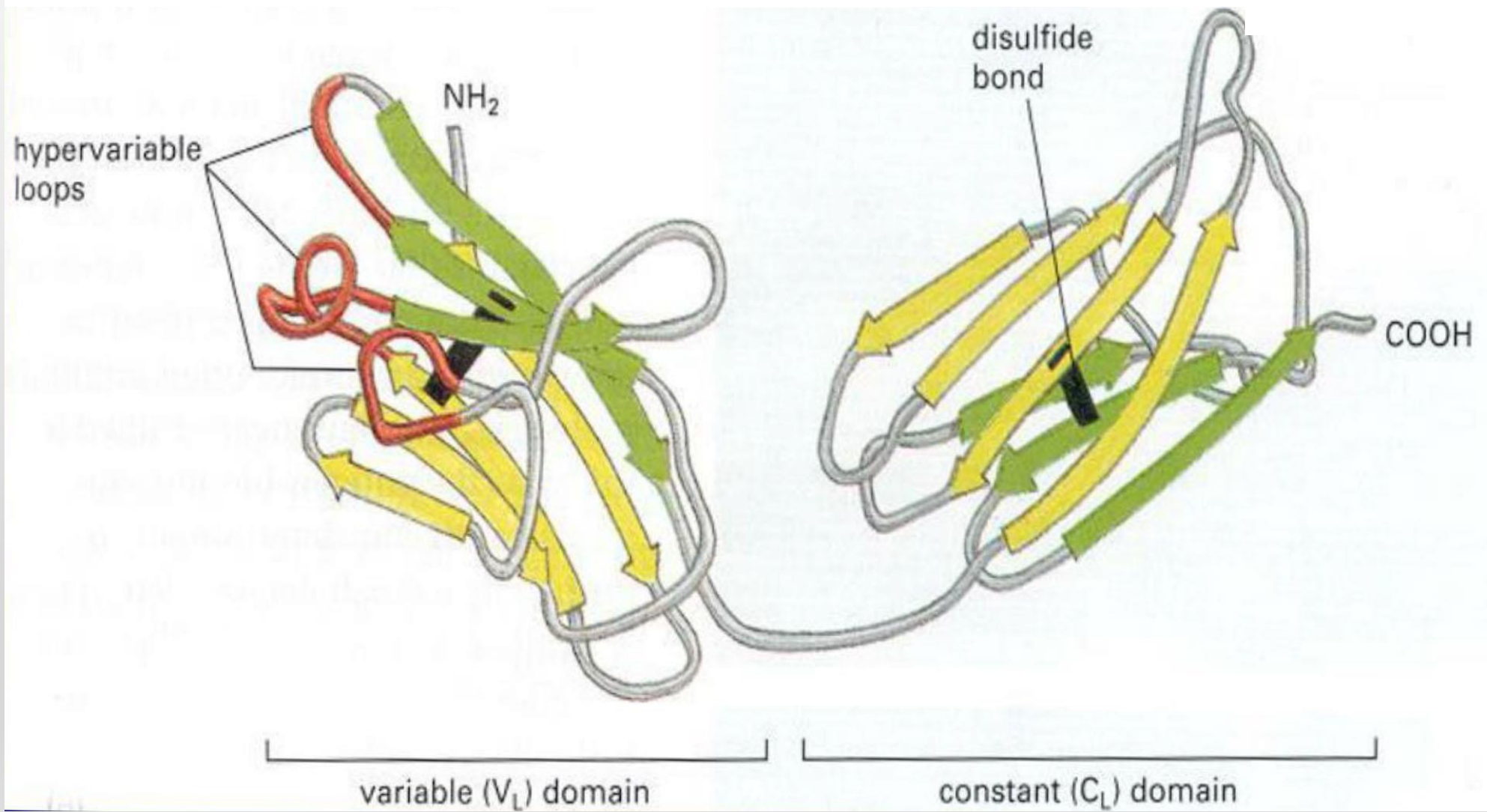
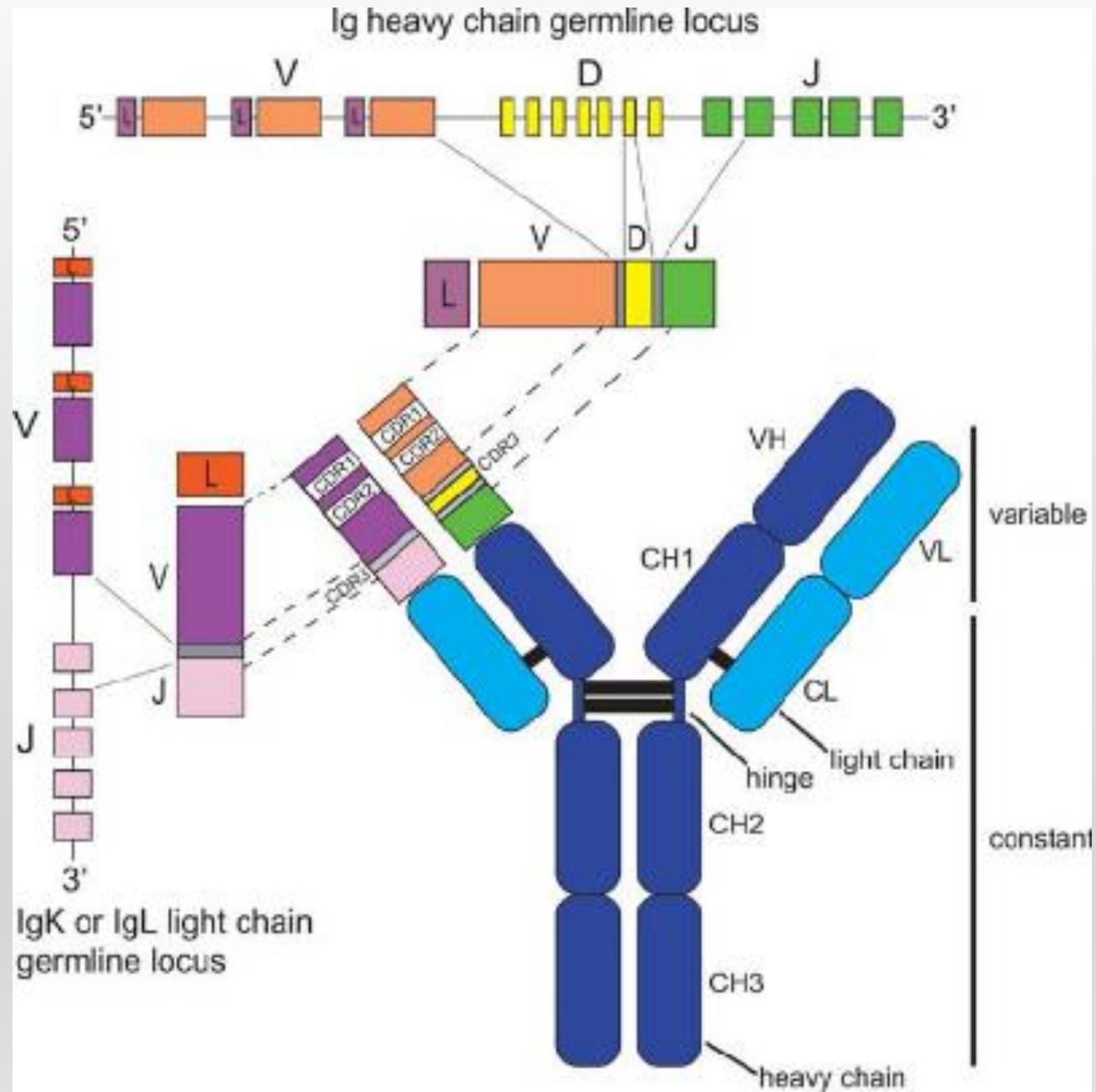


Figure 4-32 Essential Cell Biology, 2/e. (© 2004 Garland Science)





First Antibody Structure...Saul et.al,...1973

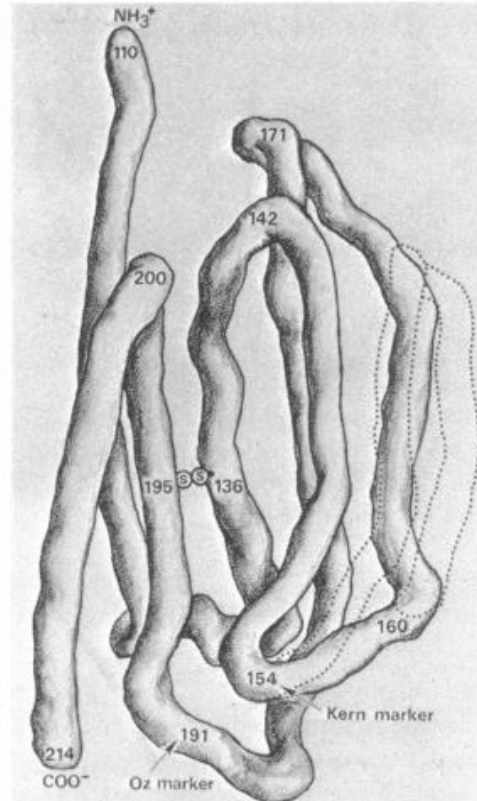


FIG. 4. Diagram of the basic "immunoglobulin fold". *Solid trace* shows the folding of the polypeptide chain in the constant subunits (C_L and C_{H1}). *Numbers* designate L (λ)-chain residues, beginning at " NH_3^+ " which corresponds to residue 110 for the L chain. *Broken lines* indicate the additional loop of polypeptide chain characteristic of the V_L and V_H subunits.

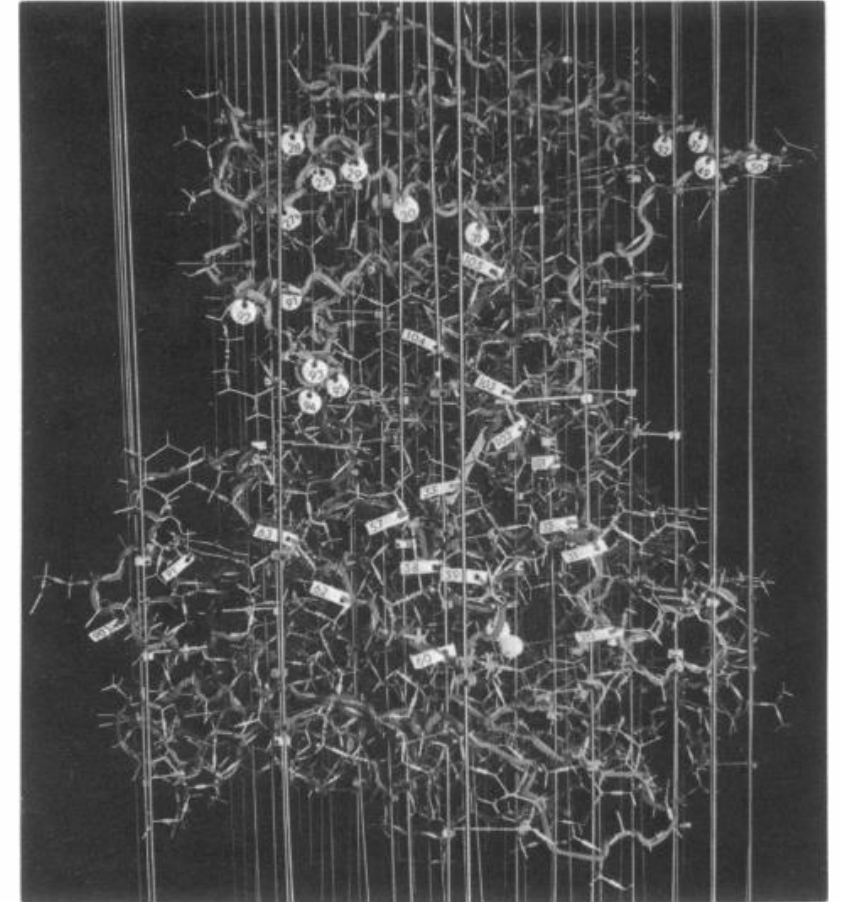
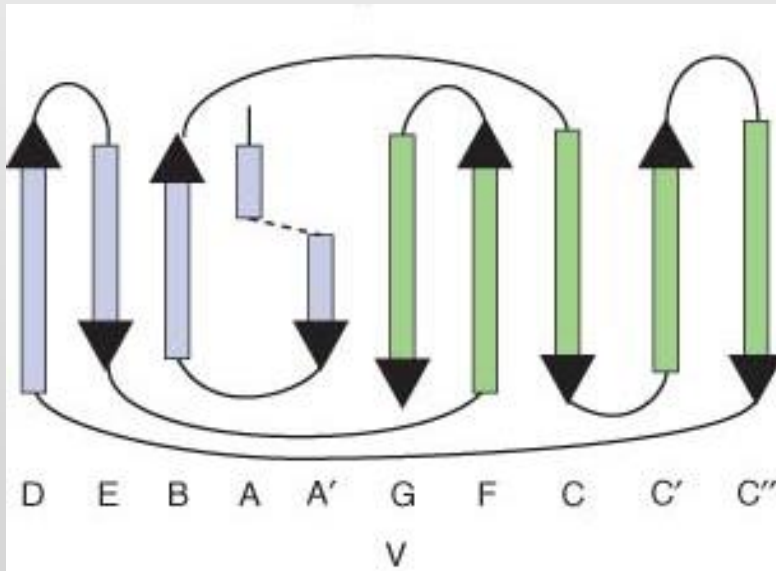


FIG. 5. View of the Fab' model showing the spatial relationship of the hypervariable positions. Numbers in *round* and *rectangular* tags correspond to L-chain and H-chain hypervariable positions, respectively. The longer axis of the V_H subunit (bot-

The IgG Fold....

2 beta-sheets, connected by a disulfide bond



An ultra-high affinity synthetic nanobody blocks SARS-CoV-2 infection by locking Spike into an inactive conformation

a bioRxiv preprint: <https://doi.org/10.1101/2020.08.08.238469>

Michael Schoof^{1,2#*}, Bryan Faust^{1,2,3,4#}, Reuben A. Saunders^{1,5#}, Smriti Sangwan^{1,2#}, Veronica Rezelj^{6#}, Nick Hoppe^{3,4}, Morgane Boone^{1,2}, Christian Bache Billesbølle^{3,4}, Marcell Zimanyi^{1,2,3}, Ishan Deshpande^{3,4}, Jiahao Liang³, Aditya A. Anand^{1,2}, Niv Dobzinski^{1,2}, Beth Shoshana Zha⁷, Benjamin Barsi-Rhyne³, Vladislav Belyy^{1,2}, Andrew W. Barile-Hill⁸, Sayan Gupta⁹, Camille R. Simoneau^{10,11,12}, Kristoffer Leon^{10,11,12}, Kris M. White^{13,14}, Silke Nock^{1,2}, Yuwei Liu^{1,2}, Nevan J. Krogan^{4,5,10,11}, Corie Y. Ralston⁹, Danielle L. Swaney^{4,5,10,11}, Adolfo García-Sastre^{13,14}, Melanie Ott^{10,11,12}, Marco Vignuzzi⁶, QCRG Structural Biology Consortium⁴, Peter Walter^{1,2*}, Aashish Manglik^{3,4,10,15*}

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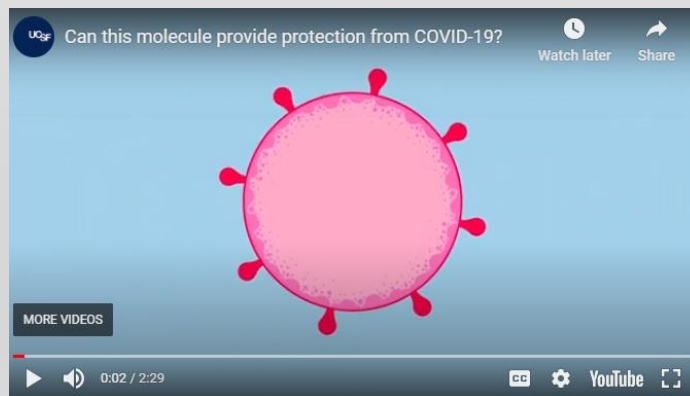
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An ultra-high affinity synthetic nanobody blocks SARS-CoV-2 infection by locking Spike 2 into an inactive conformation

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<https://www.universityofcalifornia.edu/news/aeronabs-promise-powerful-inhalable-protection-against-covid-19>



← **AeroNab** – a single domain nanobody that binds the coronavirus Spike protein....and protects us from infection??

https://www.youtube.com/watch?v=WjhbexLtYts&feature=emb_logo



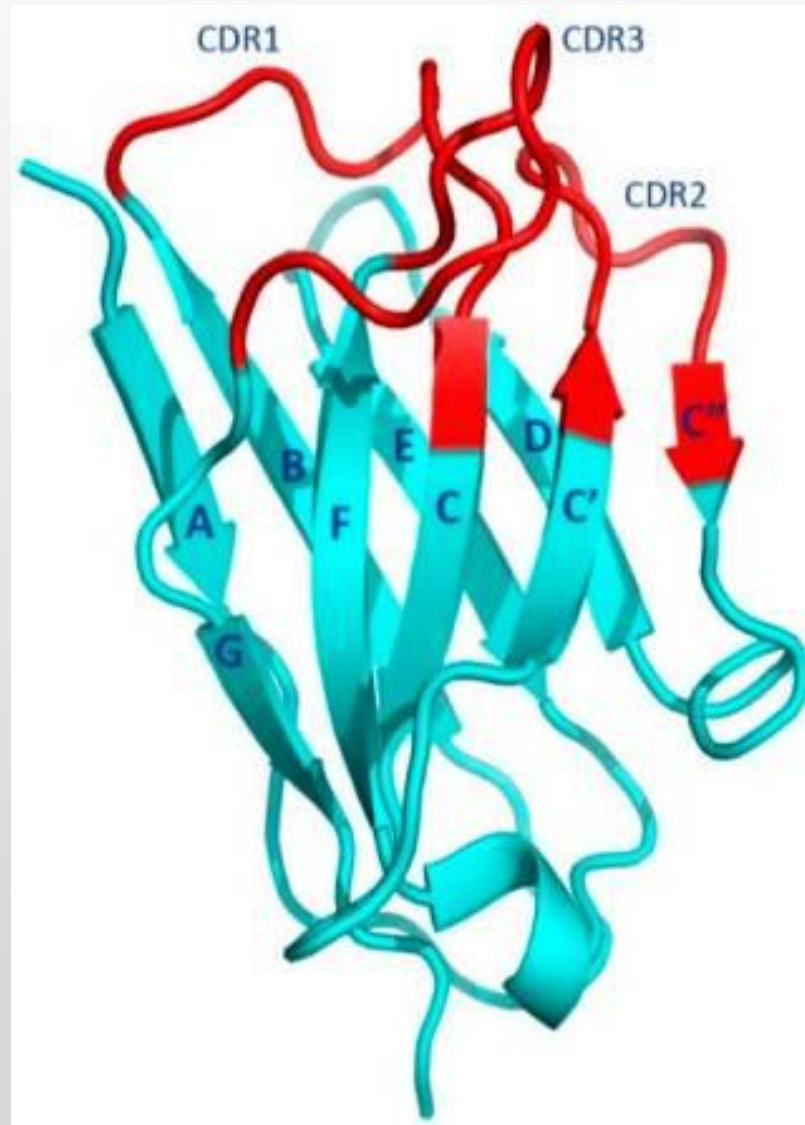
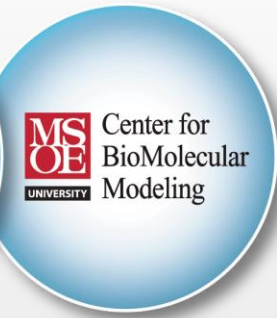
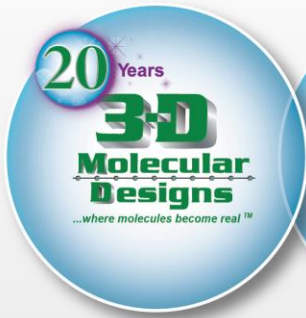
AND NOW,...an update....

On Nov. 23, we learned that the work described in the bioRxiv pre-preprint has been peer-reviewed and accepted for publication in Science.

And more importantly, this means that the pdb files describing the structure of the Nb6 nanobody bound to the coronavirus spike protein is available to everyone,... from the Protein Data Bank. The relevant pdb file is 7KKK.pdb.

A pdf of the Science paper that will soon be published is available here:

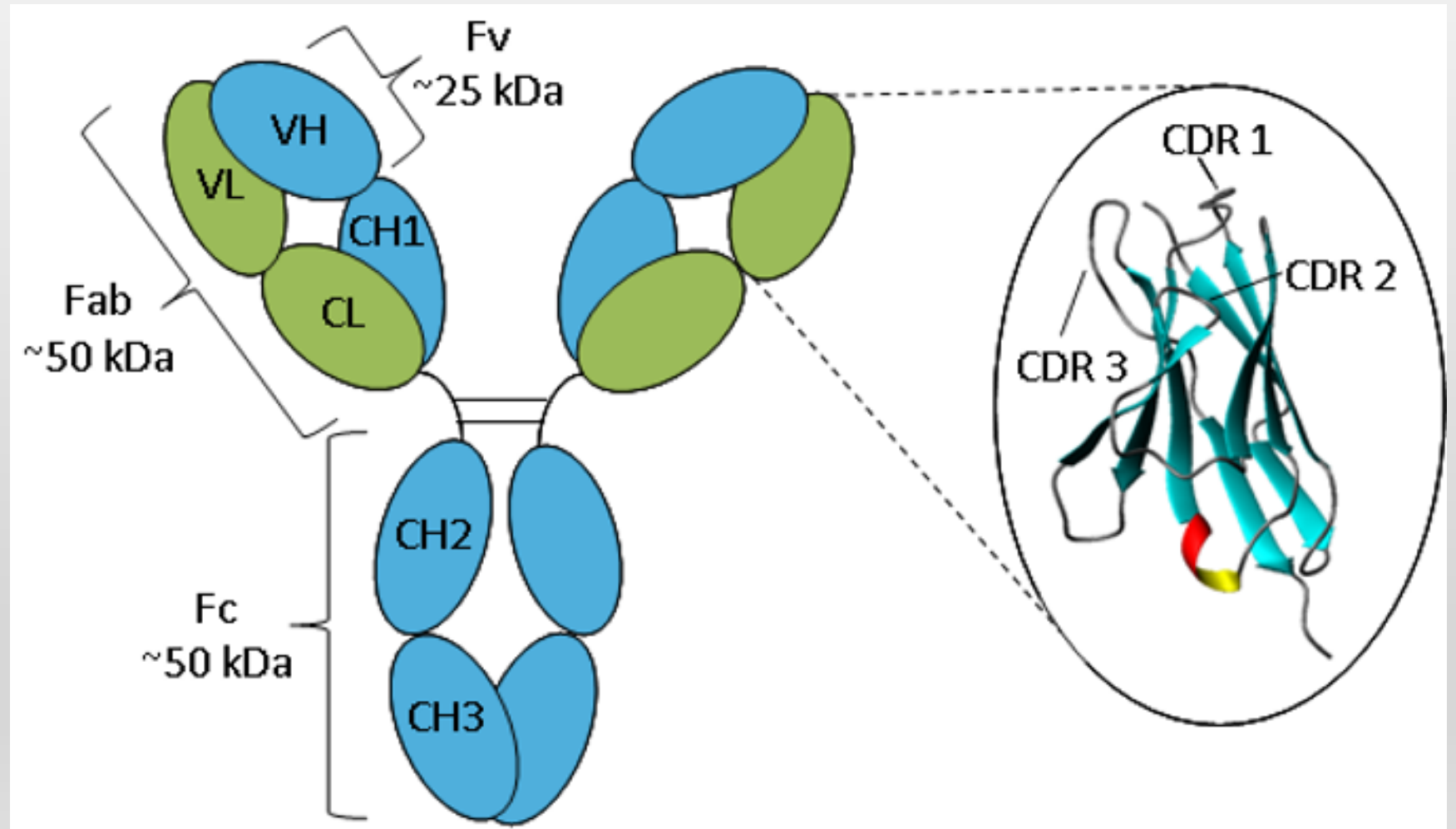
Happy Modeling.....



Variable domain



Constant domain



What are we **NOT** going to talk abouttonight?

Virology.... *But check out TWIV: a podcast about viruses - "the kind that make you sick".*

Immunology..... *Innate vs Adaptive Immunity
Humoral vs. Cellular Immunity*

Public Health Issues.... *Viral diagnostics
PCR vs. Rapid tests*

Vaccines.... *mRNA vaccines*

Summer Professional Development Courses
From the MSOE Center for BioMolecular Modeling

The CBM hosts a collection of professional development courses that provide teachers with the experience and community necessary to confidently use models in their classroom



★★ NOTE: Do to Covid-19, we plan to offer this workshop June 22-26, 2020 as a virtual workshop. ★★



Mark Hoelzer

- Director of Digital Media at the Center of BioMolecular Modeling
- Partner of 3D Molecular Designs and Lead Model Designer
- Masters of Fine Art (2014) in New Media from the Academy of Art University

Thank you for attending!

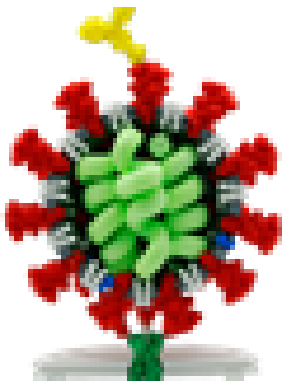
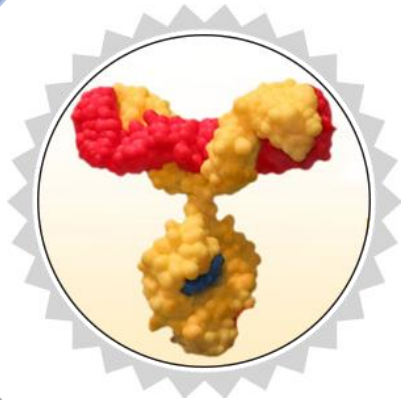
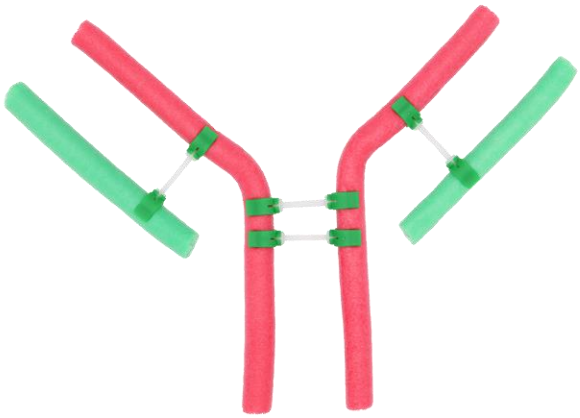
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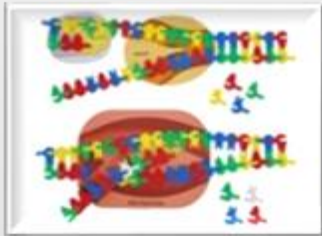
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A Tale of Two Sisters, Modeling Transcription & Protein Synthesis

Wednesday, January 27, 2021 at 6:00 PM Central



Neurotransmitters, Synapses & Acetylcholinesterase

Modeling How Cells Talk – Making Sense of Synapses and Signals

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Proteins & the Protein Folding Problem

Proteins – Now that Everything has Changed

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