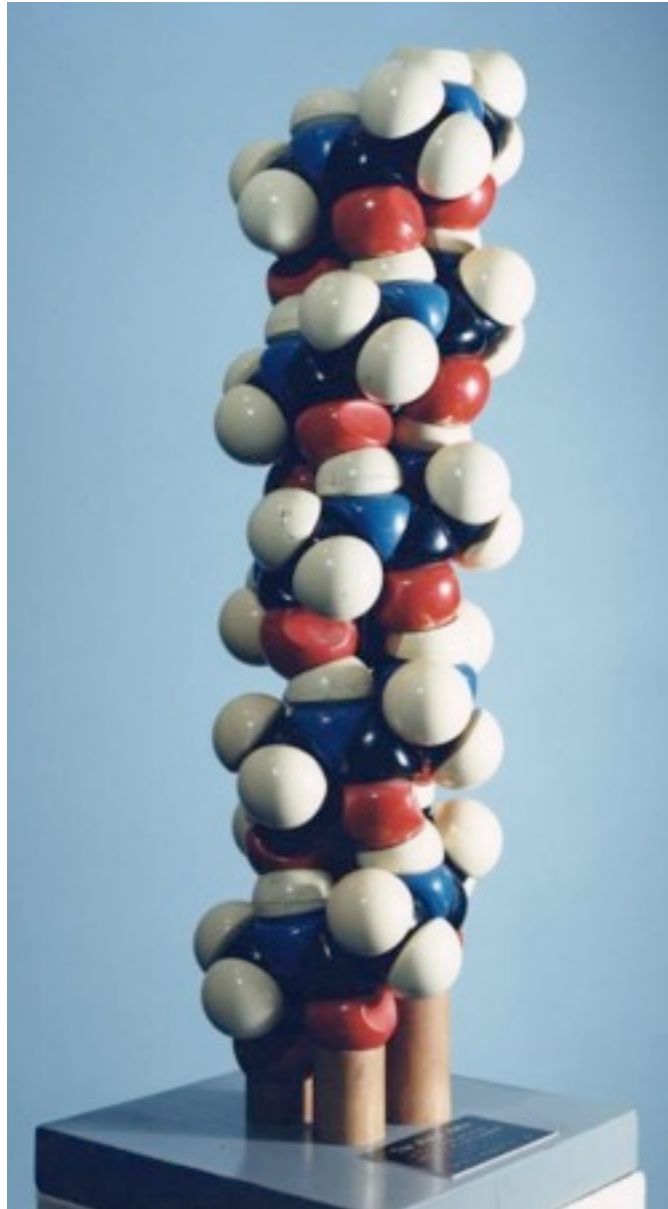


La chimie fait son cinéma en visualisation moléculaire

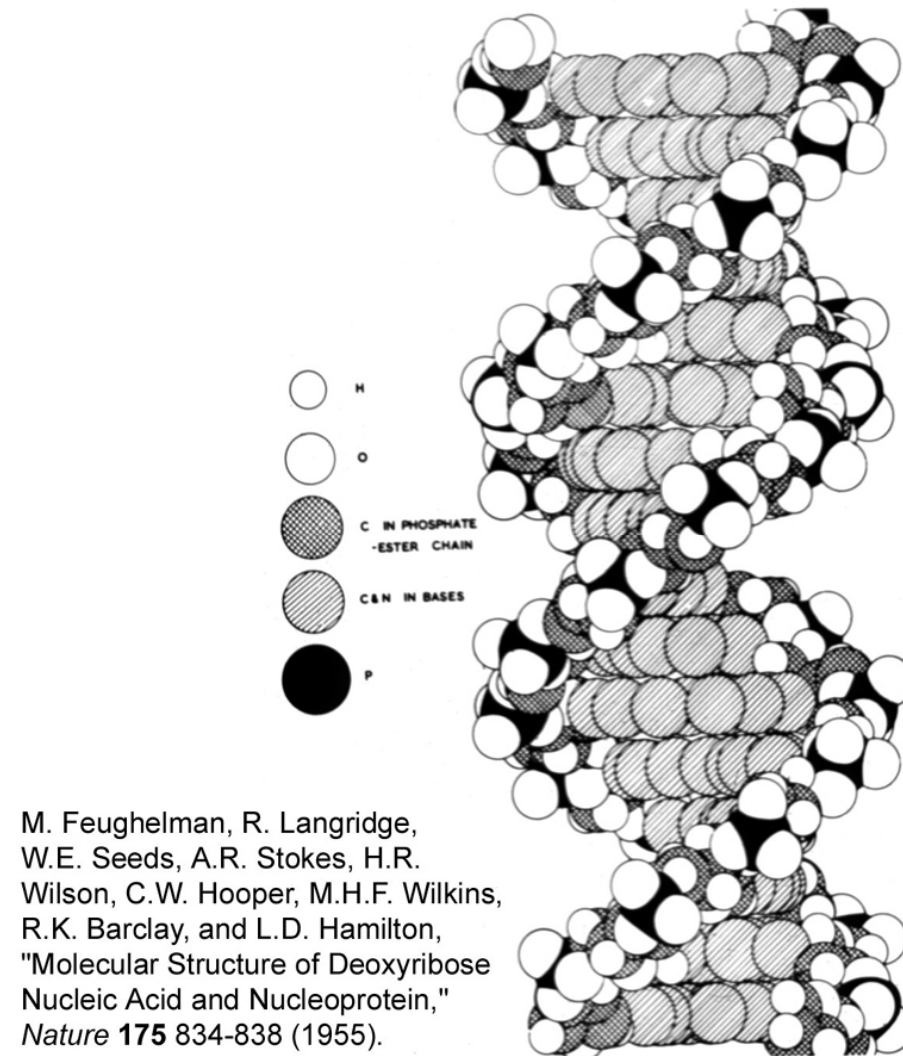
Marc Baaden, CNRS

CNRS UPR 9080, IBPC, Paris - <http://www.baaden.ibpc.fr>

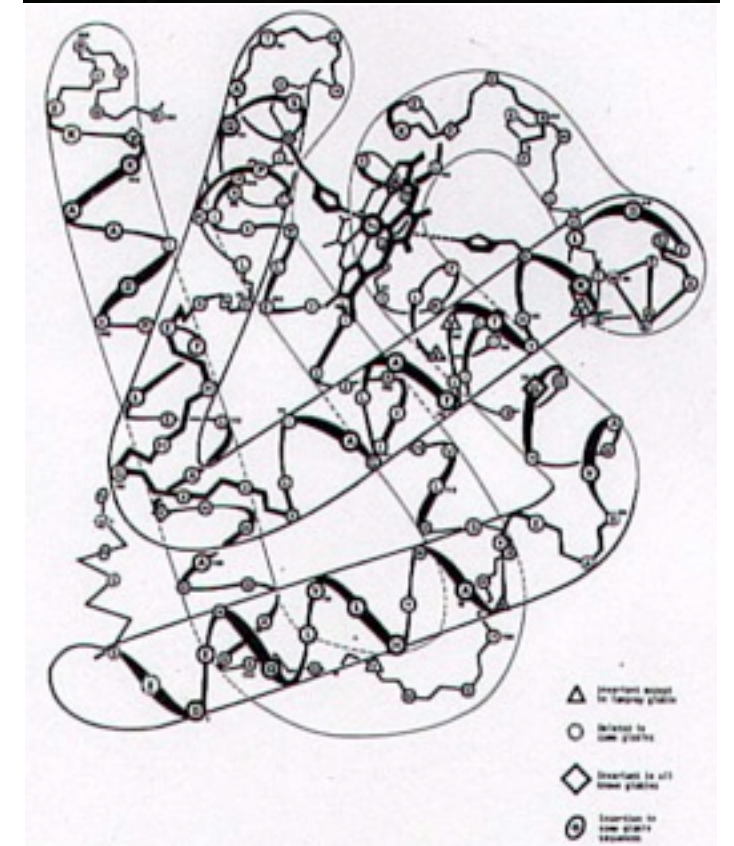
De Pauling à Kendrew: les années 1950-60



Modèle CPK - **1953**
(Corey-Pauling-Koltun)



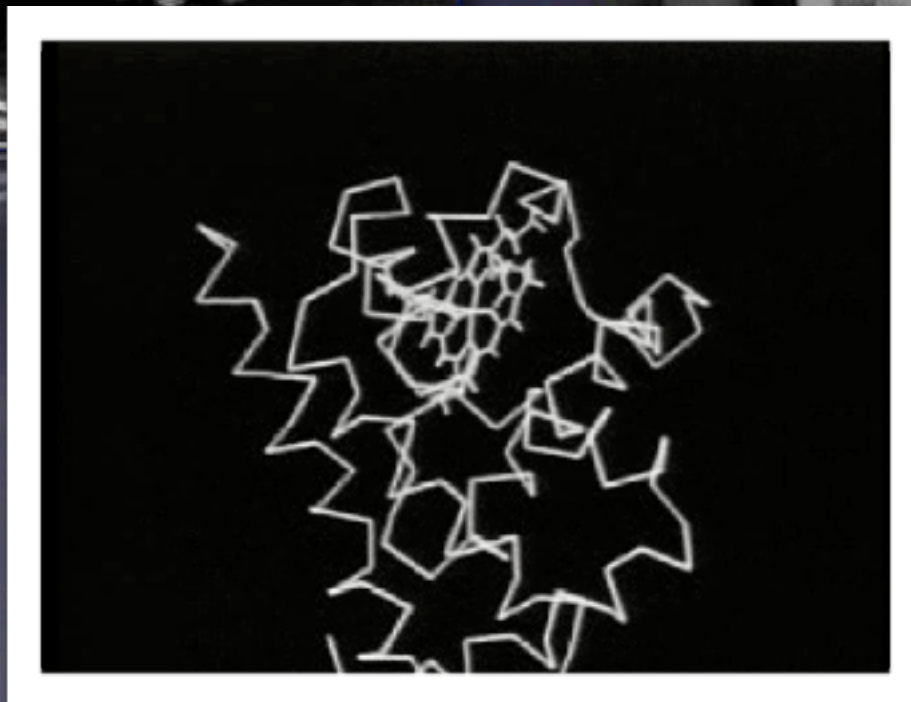
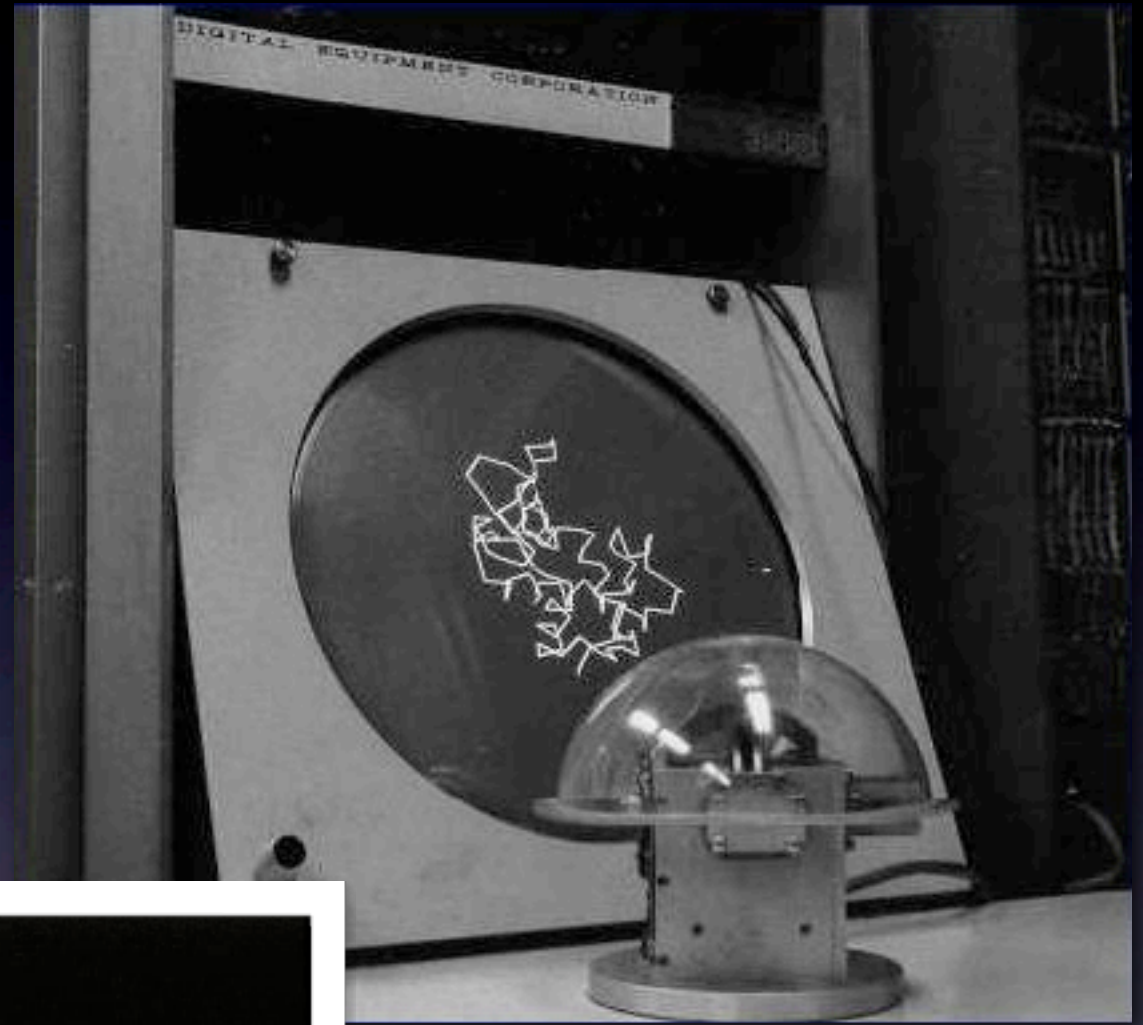
Molecular Structure
of DNA - **1955**



Modèle de Myoglobine
(Kendrew) - **1957**

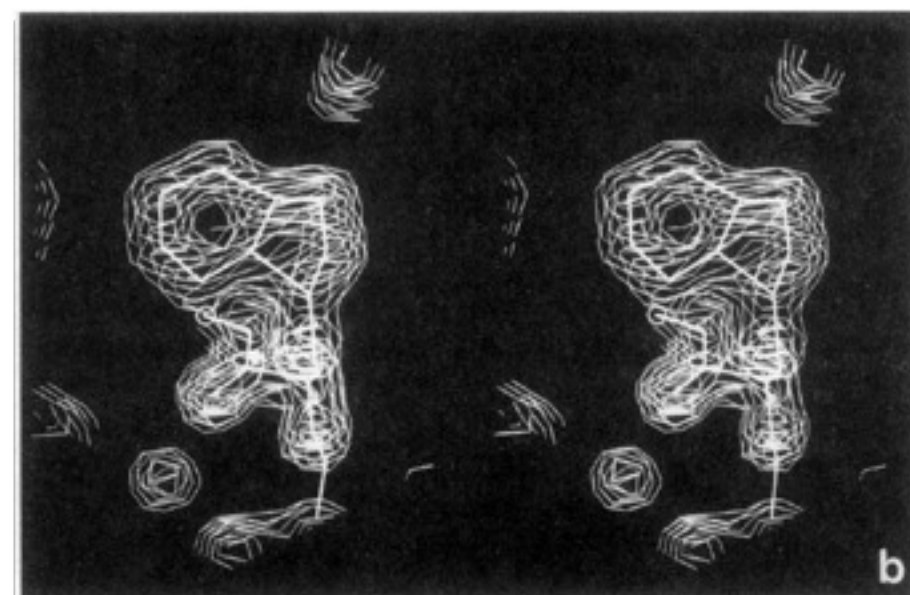
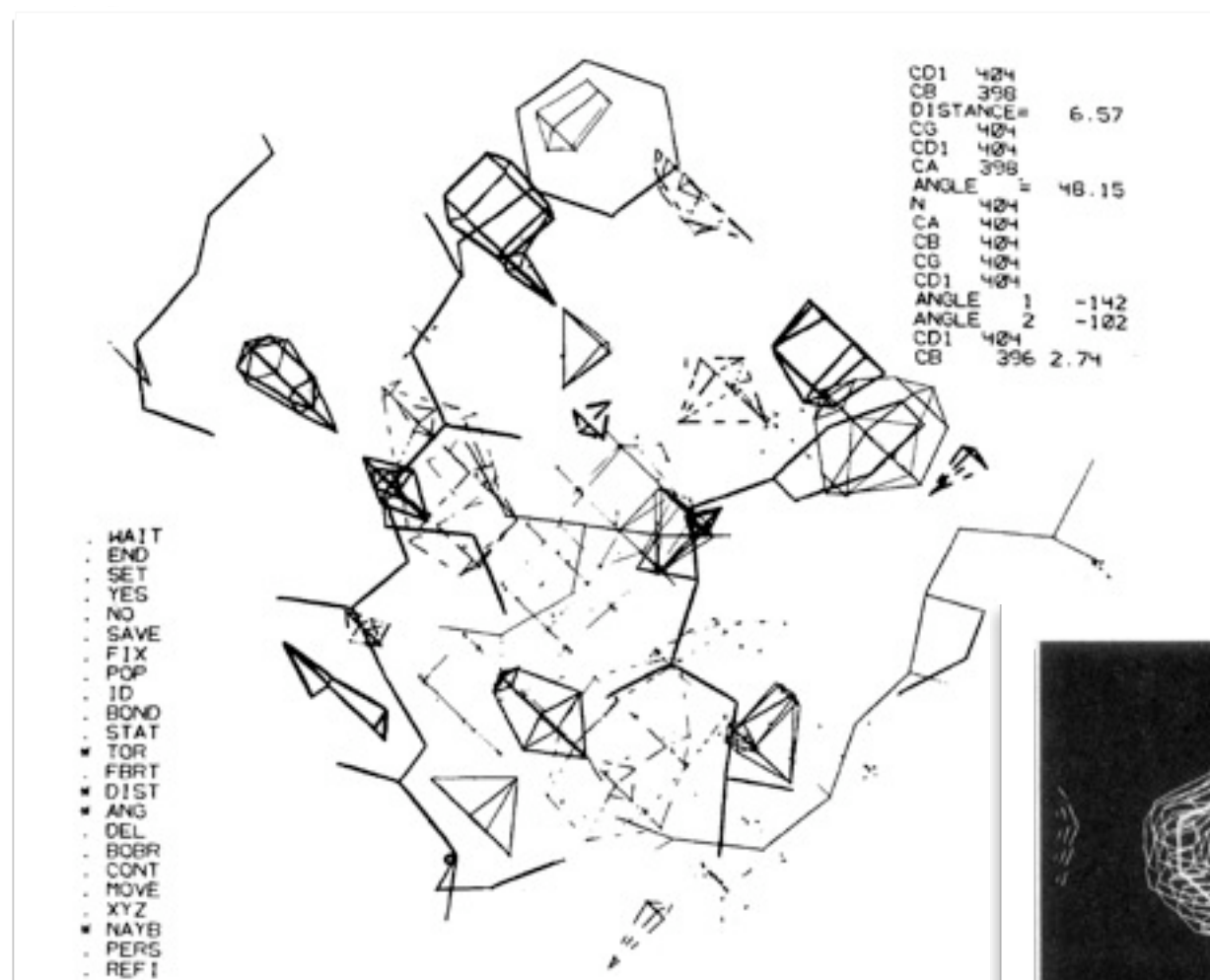
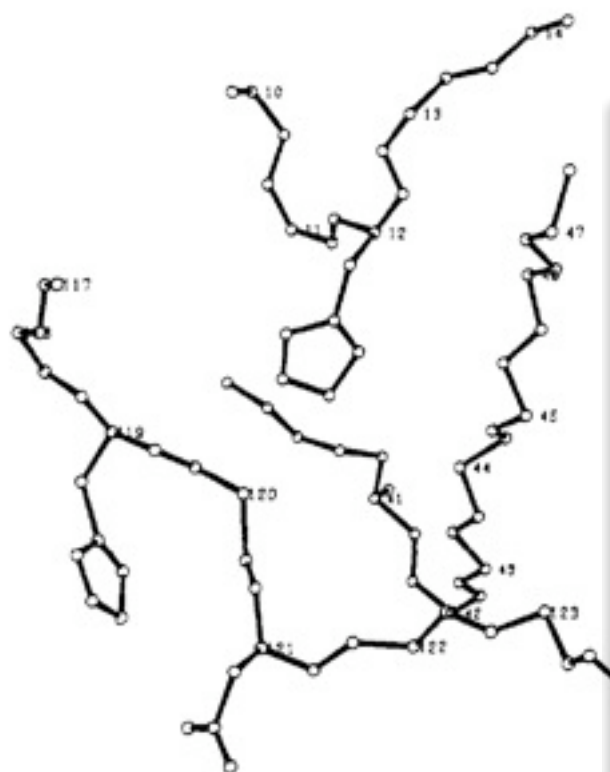
The sixties.. Levinthal's "Kluge"

by Marc Baaden, 2011



oscilloscope line drawing
1960s, MIT

Dessins de traits: les années 1970

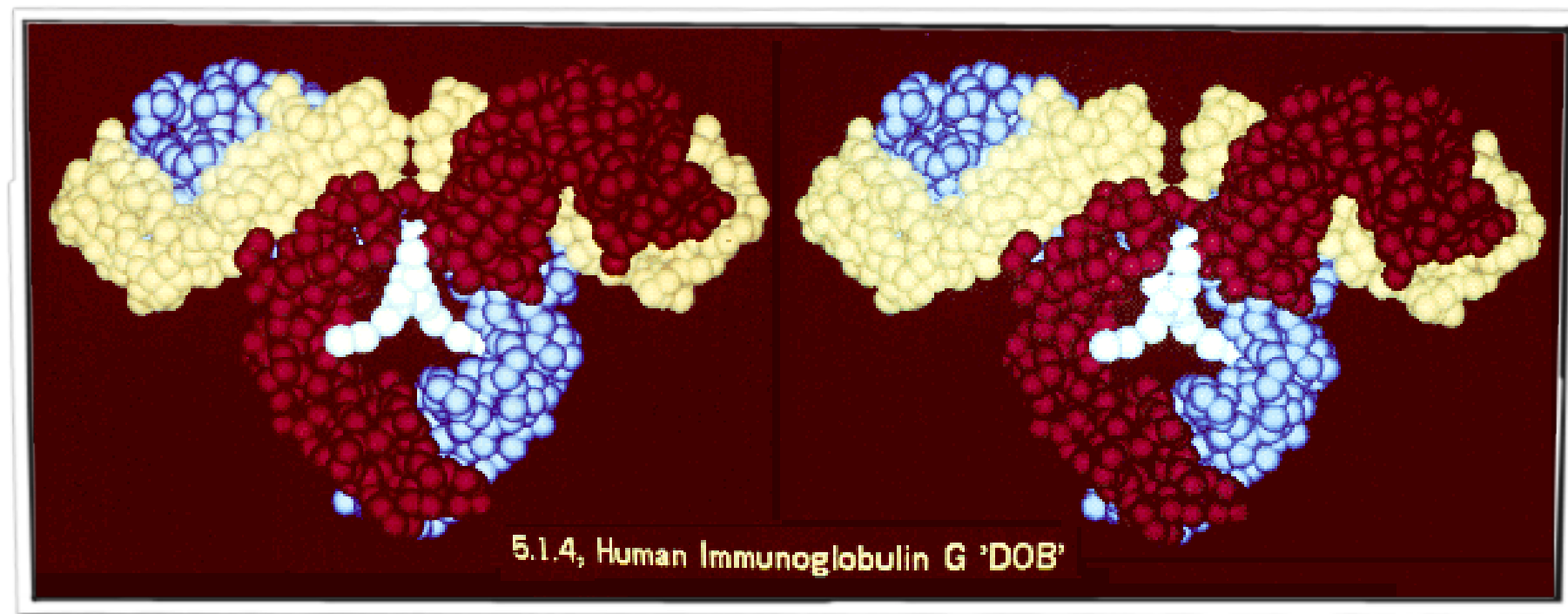


ORTEP (Johnson)
1970

FRODO (Jones)
1978

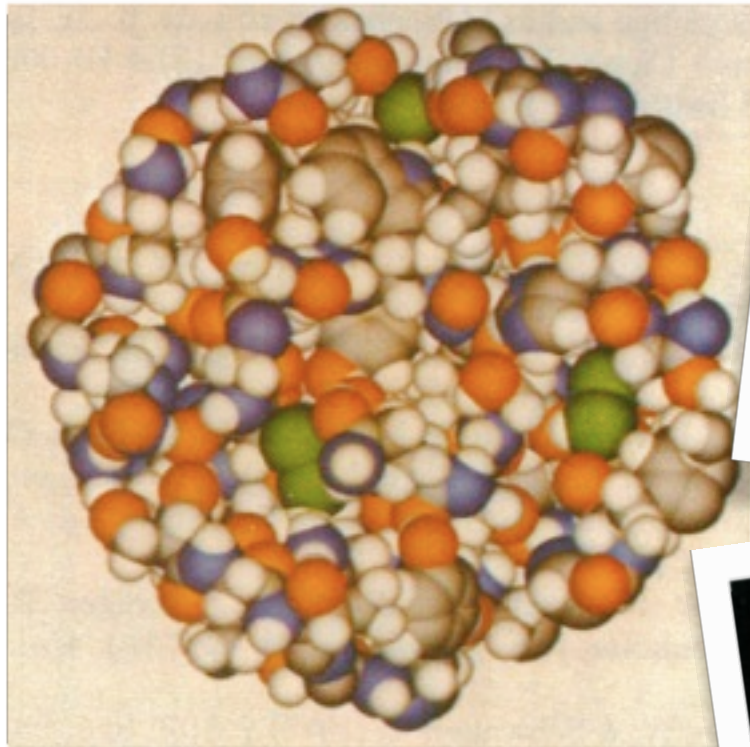
Structure + carte de
densité (Collins) **1975**

Longtemps avant la télévision 3D...

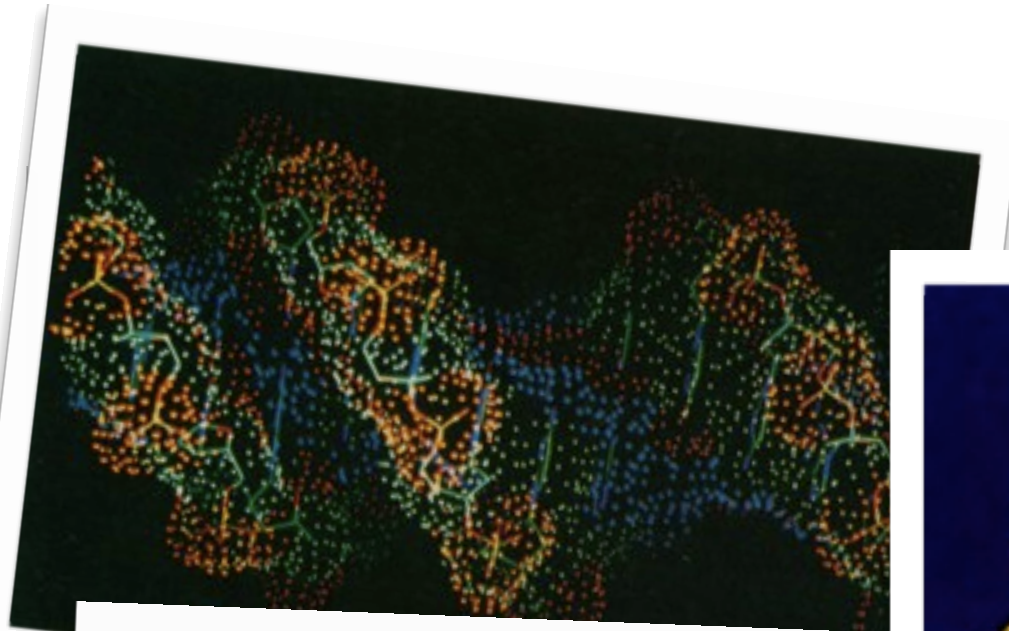


Teaching Aids for Macromolecular Structure, 1980

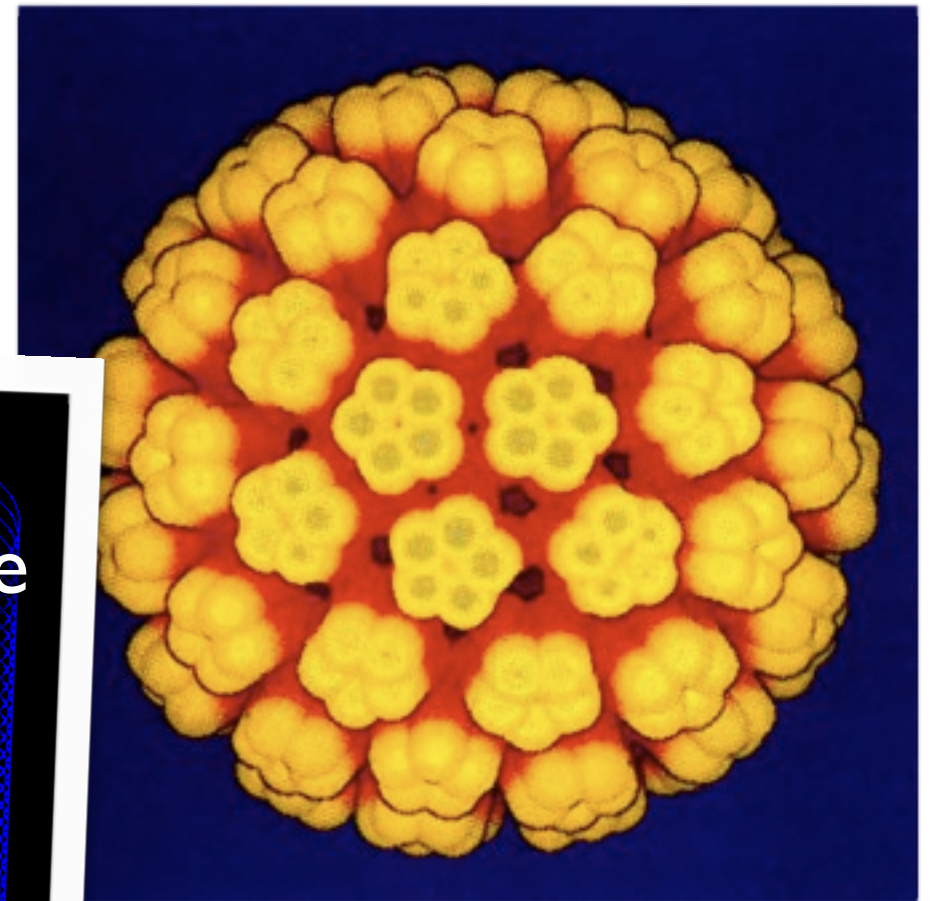
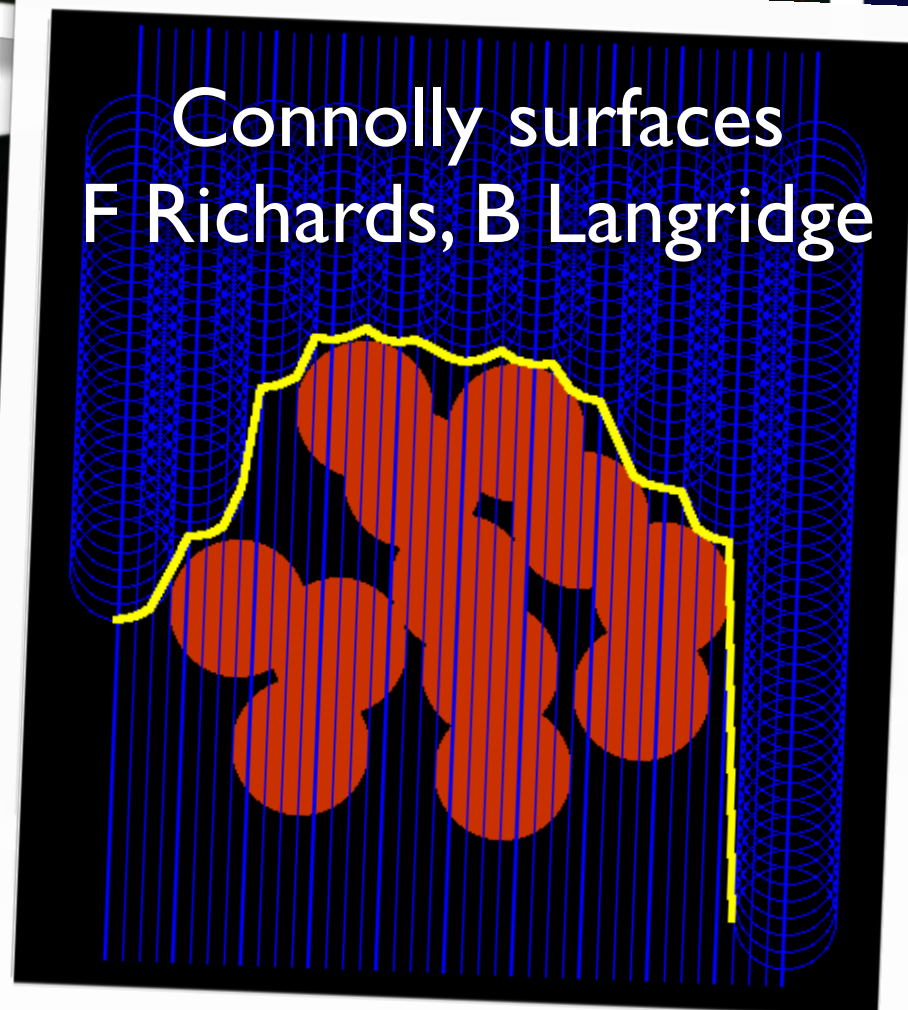
Et la couleur fut... les années 1980-90



(Feldmann) **1978**



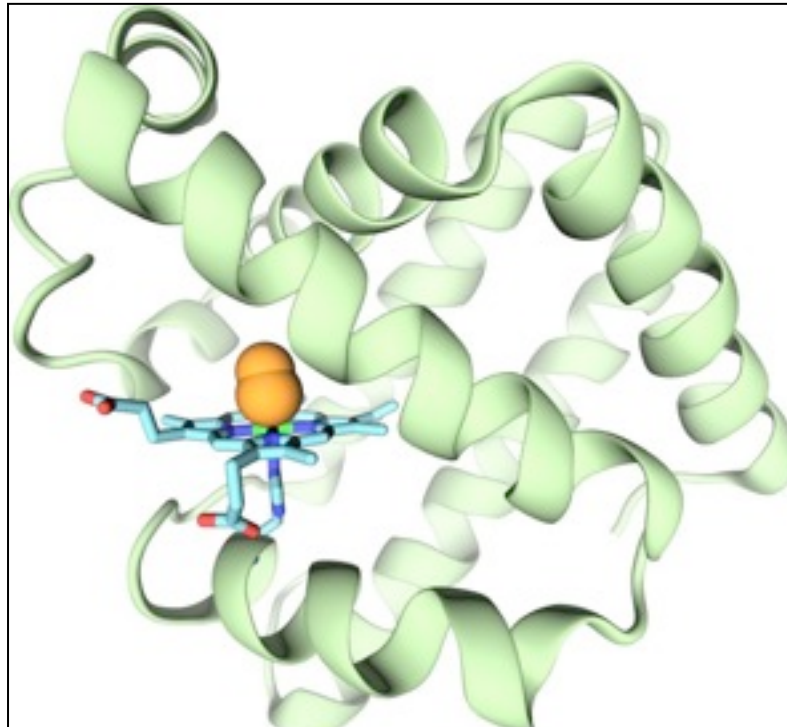
Connolly surfaces
F Richards, B Langridge



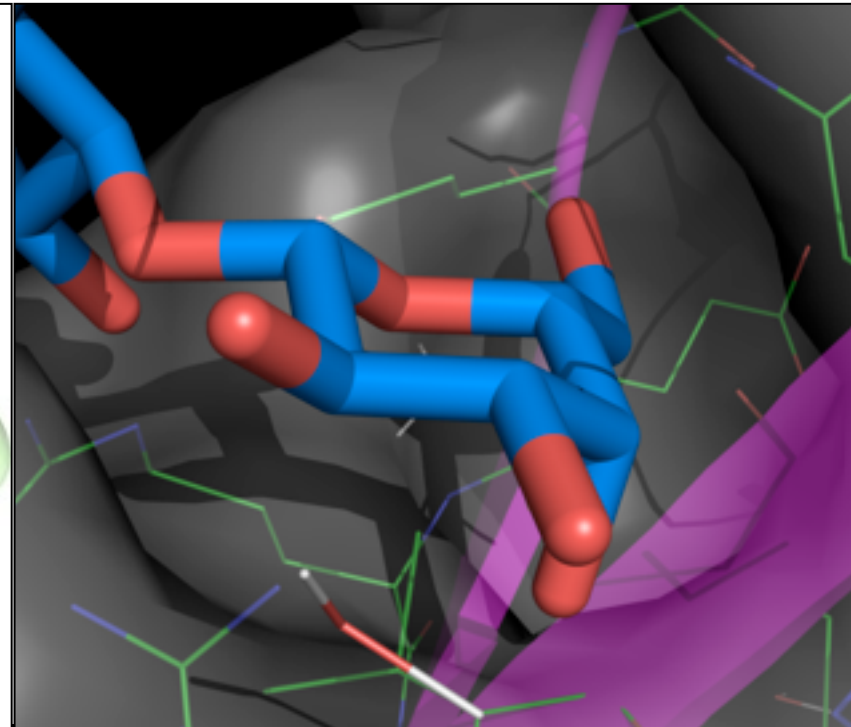
Capside de Virus
(Namba) **1988**

Plus beau, plus grand, plus vite, gratuit 90's à nos jours

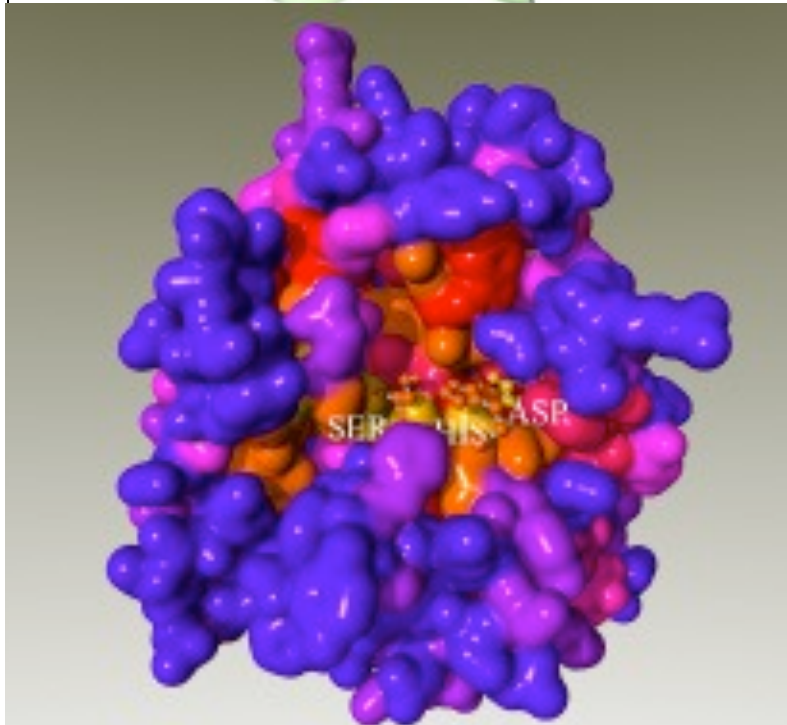
VMD
(J. Stone)
1996



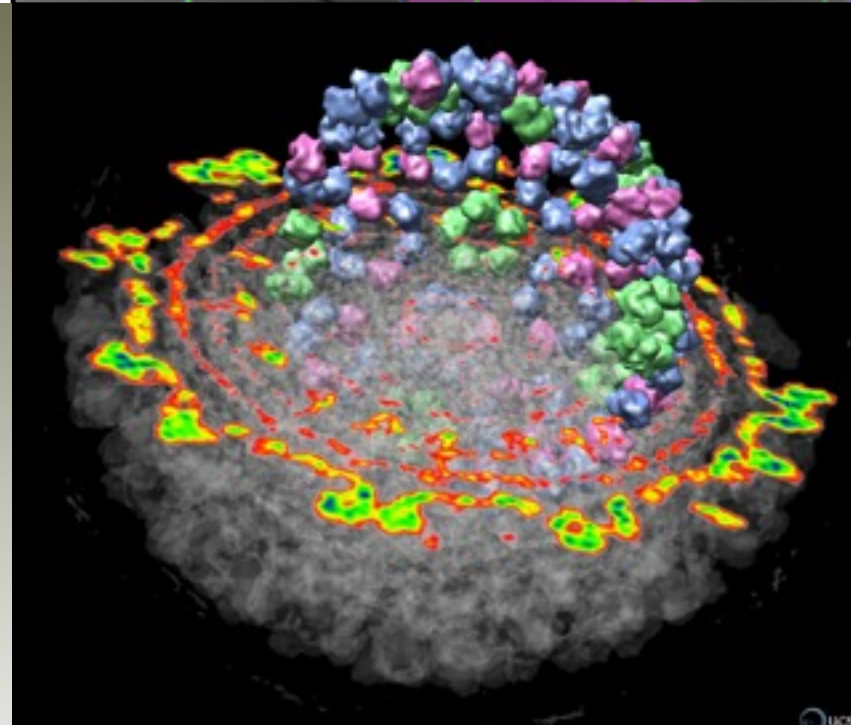
PyMol
(W. L. Delano)
2000



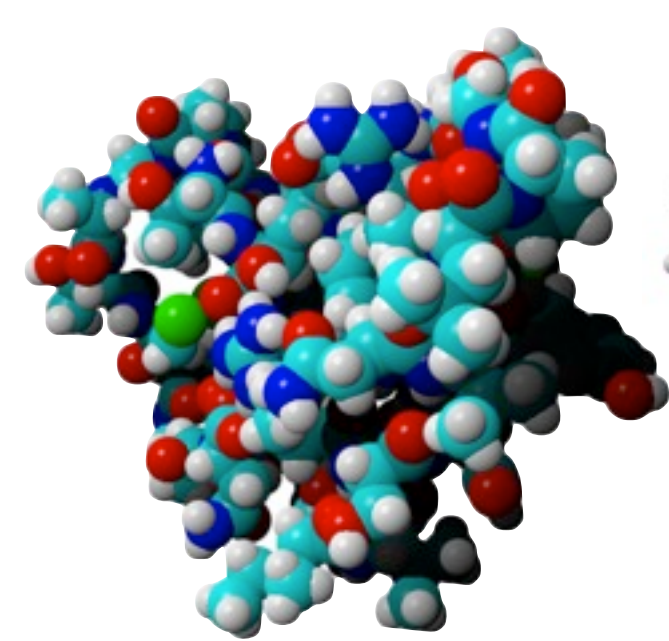
Yasara
(E. Krieger)
2002



Chimera
(T. Ferrin)
2007

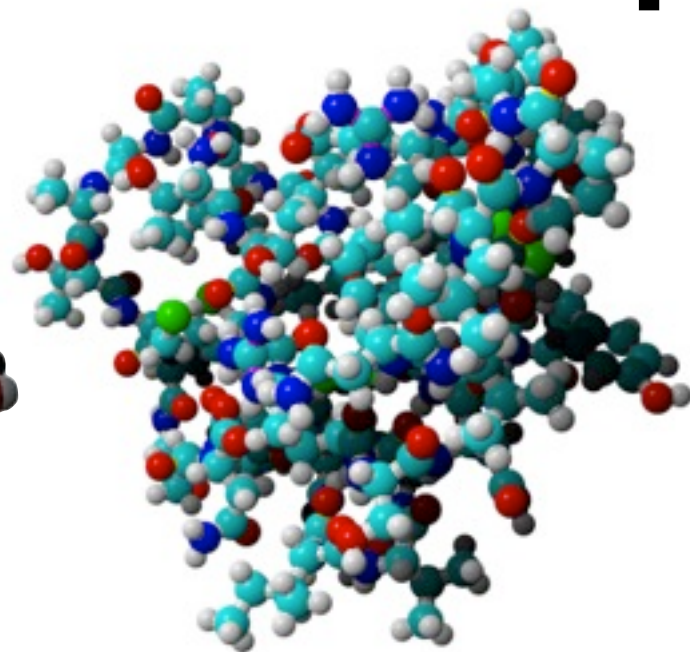


Standard representations



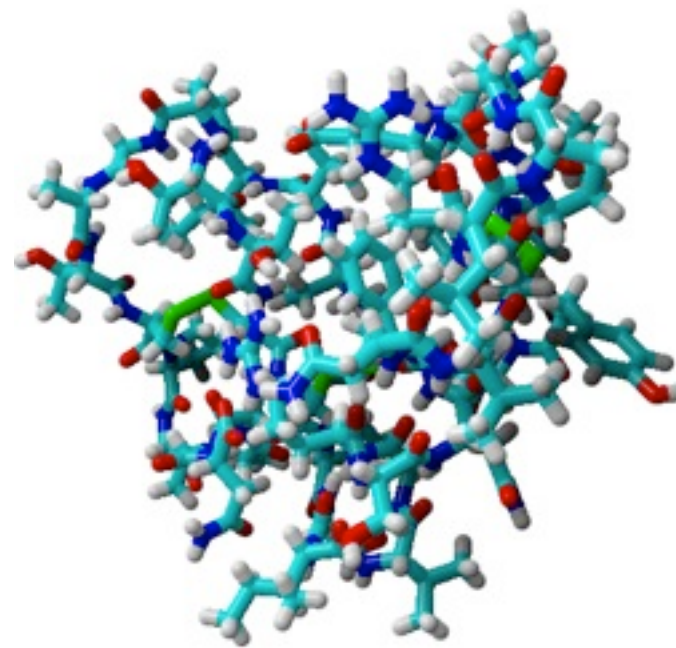
CPK spheres

31k / 10k
vertices / faces



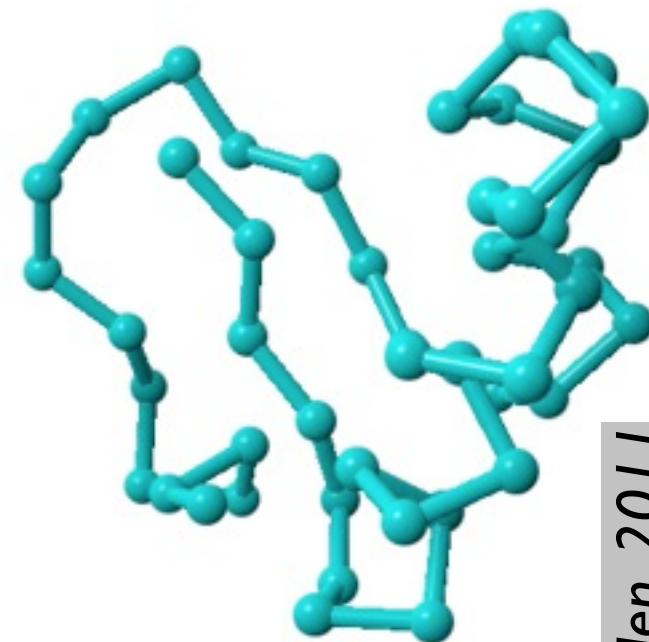
ball & stick

112k / 37k



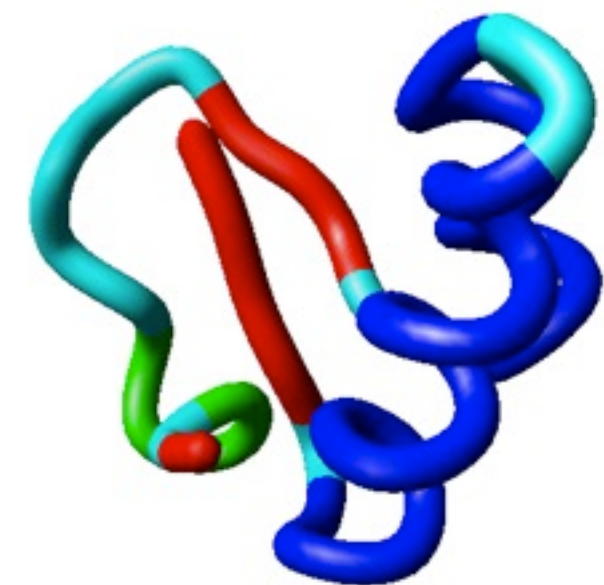
licorice

112k / 37k



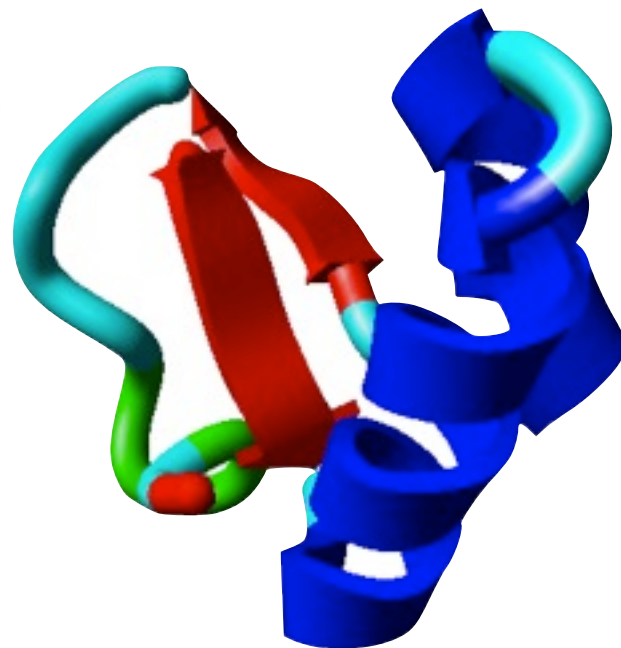
trace

11k / 4k



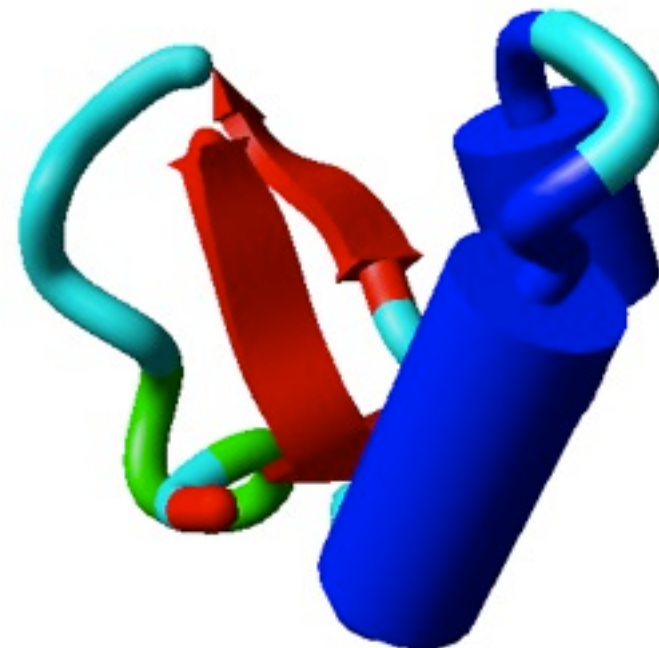
tube

33k / 11k



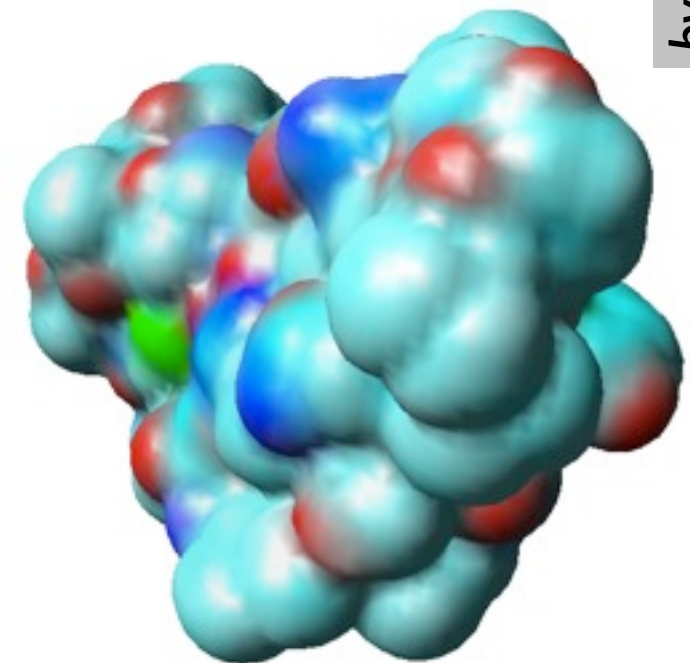
ribbon

68k / 23k



cartoon

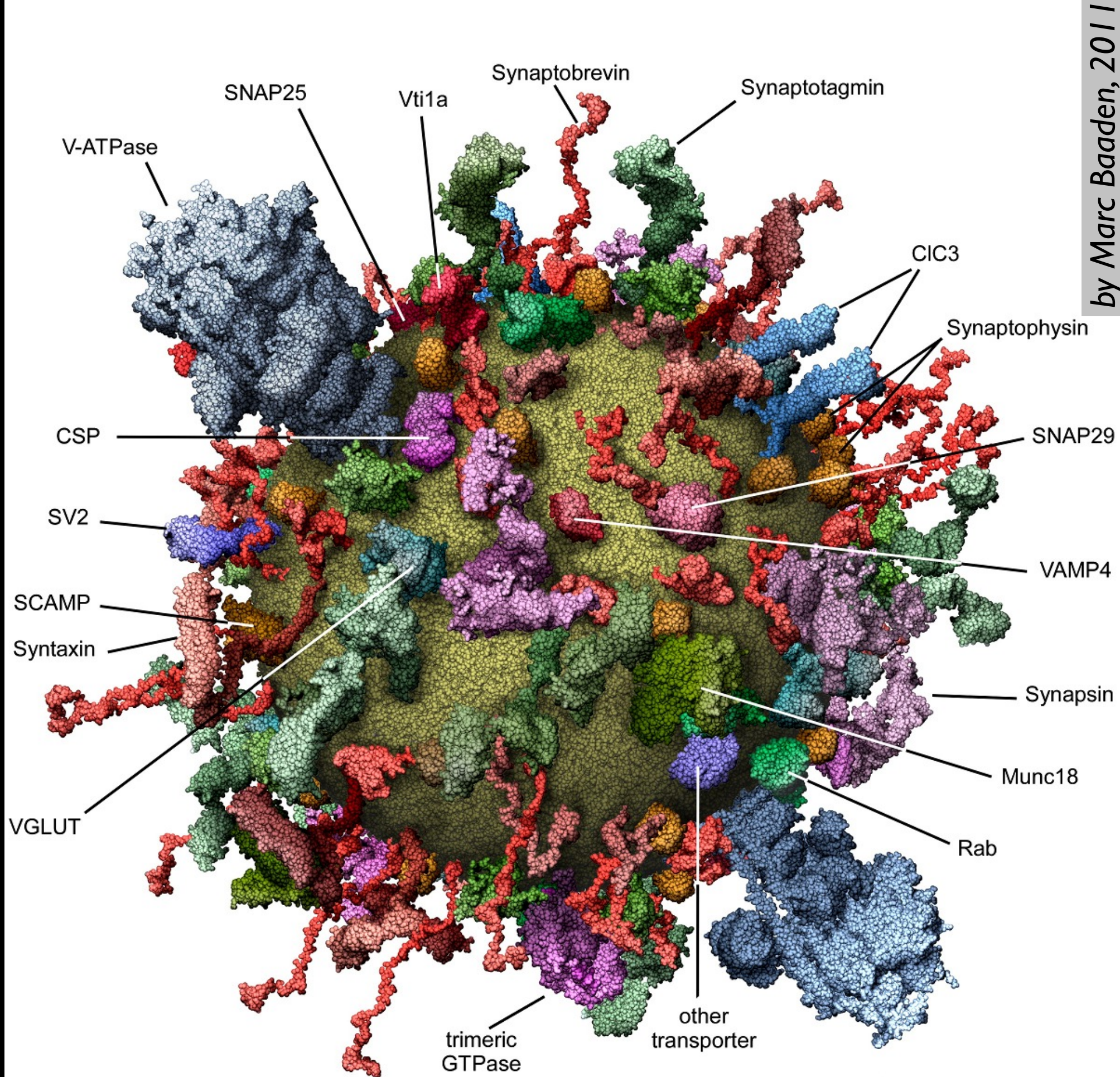
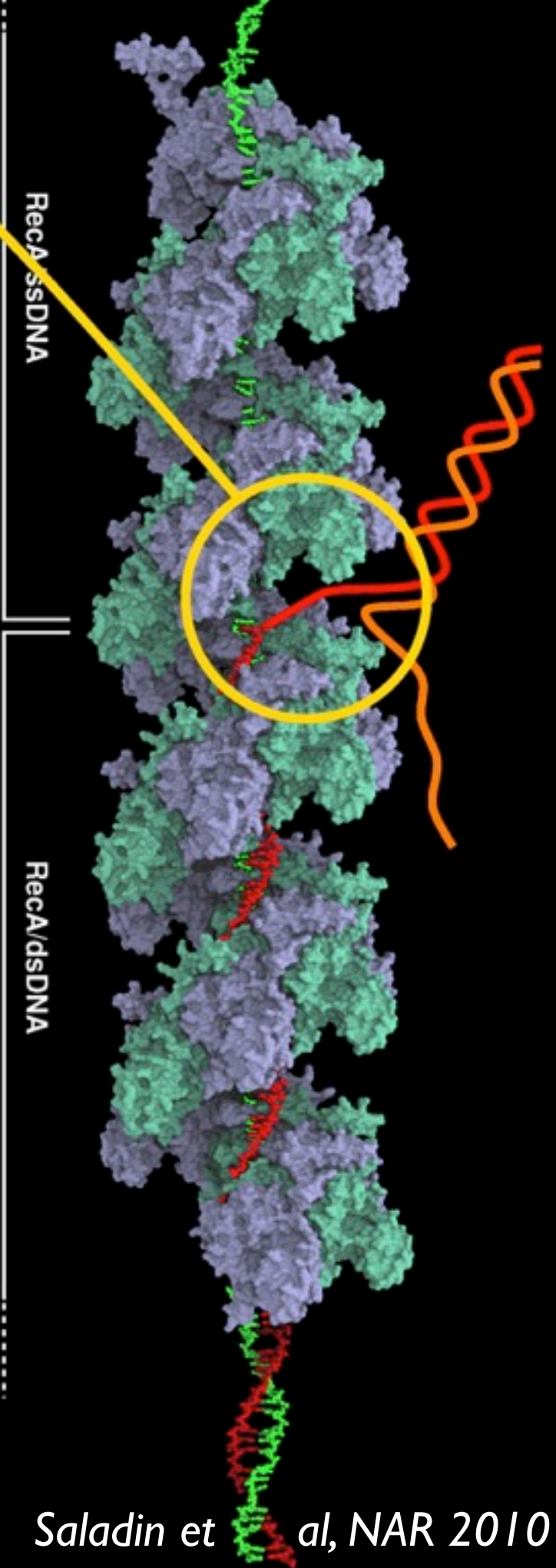
23k / 8k



surface

50k / 17k

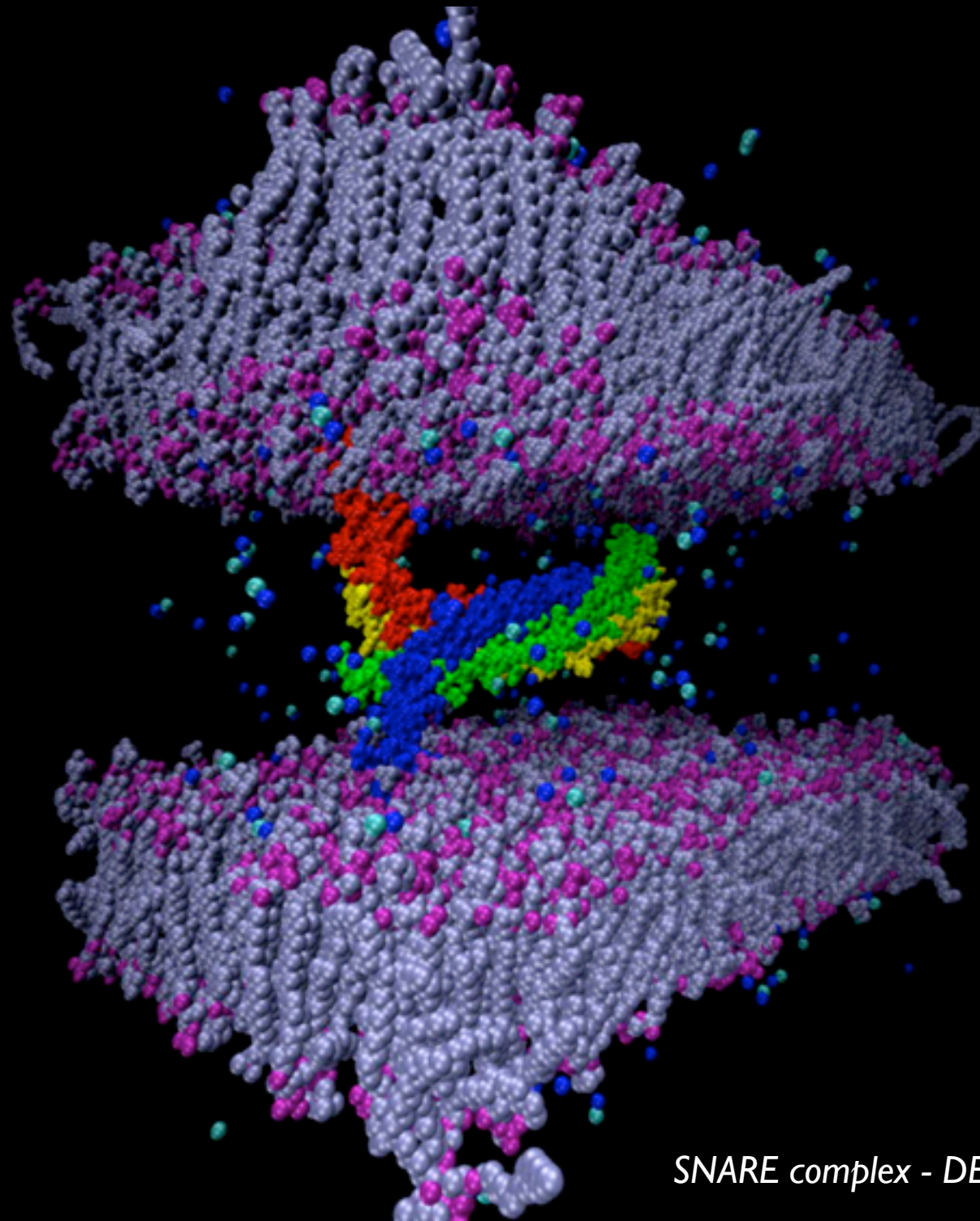
by Marc Baaden, 2011



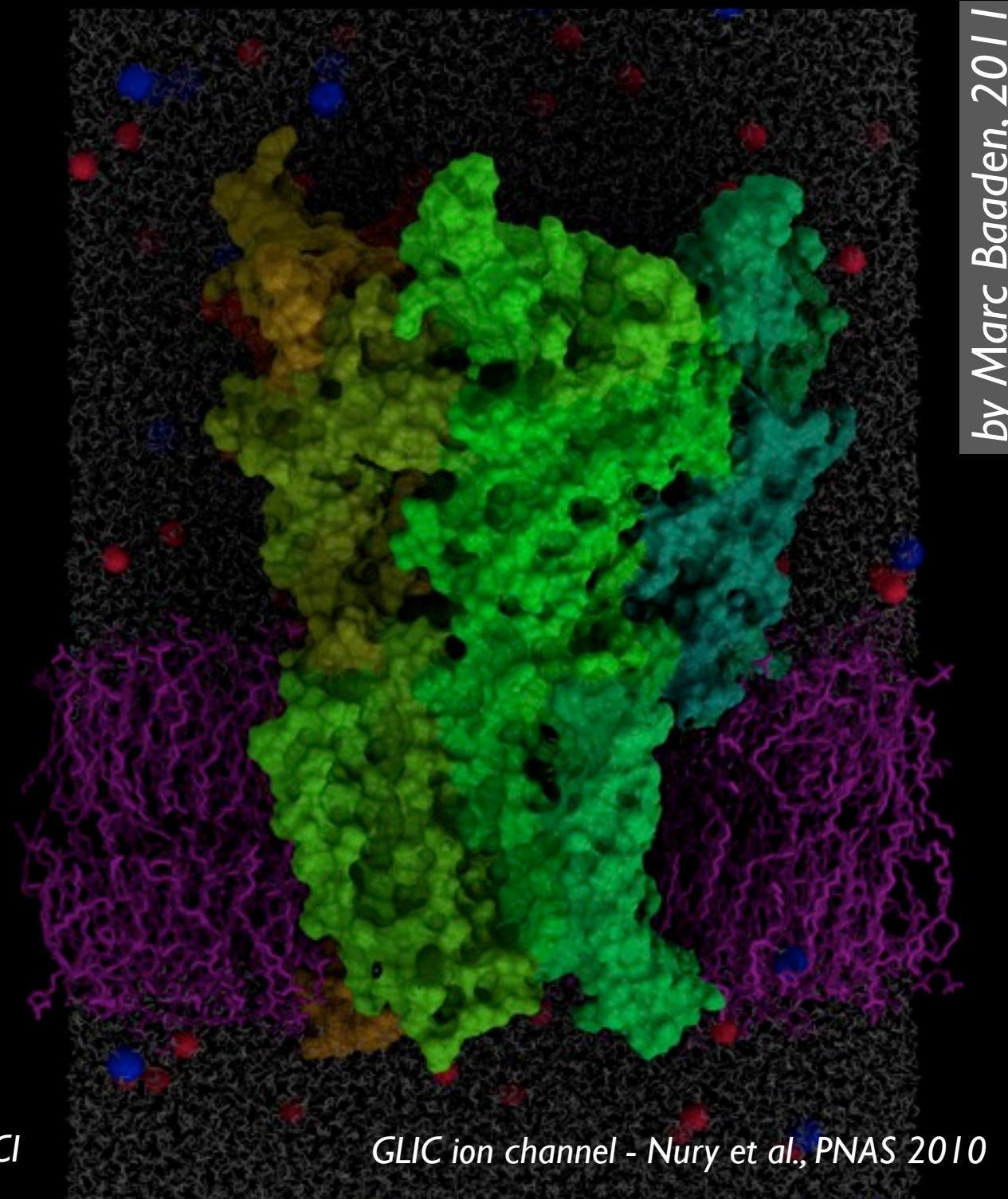
by Marc Baaden, 2011

Takamori, Cell 2006

Large Dynamic datasets



- 339 792 atoms
- 75 Gb of data (compressed)
- > 40 000 frames

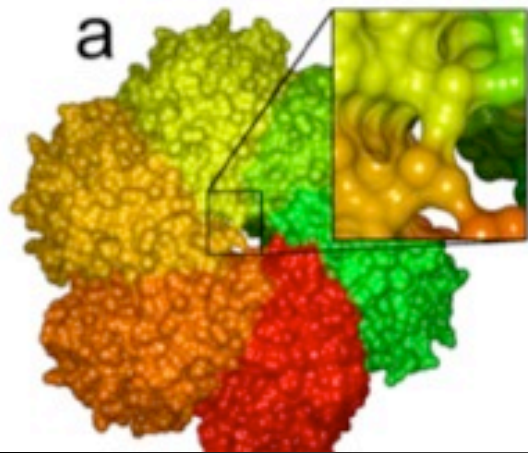


- 198 567 atoms
- 169 Gb of data (compressed)
- > 20 000 frames

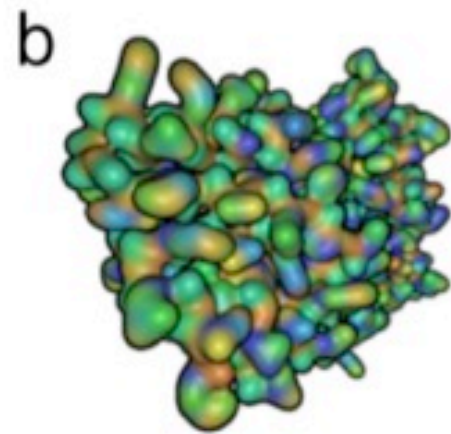
New developments on GPUs

by Marc Baaden, 2011

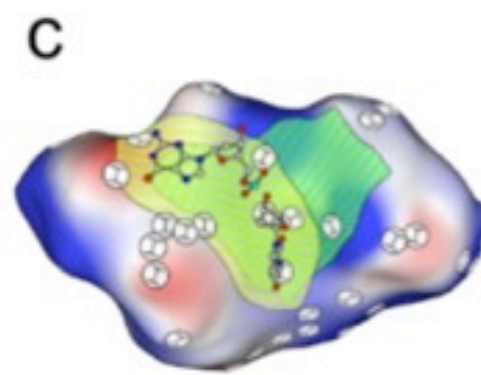
SURFACES



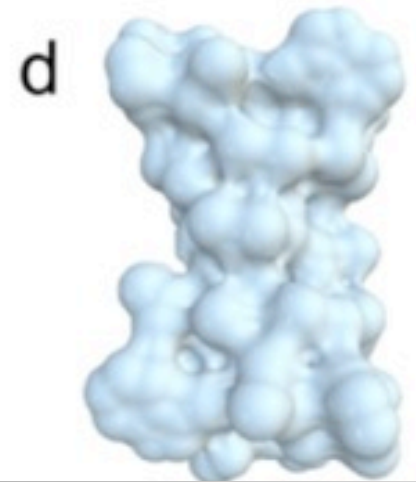
Connolly / ray-casting



metaballs / ray-casting

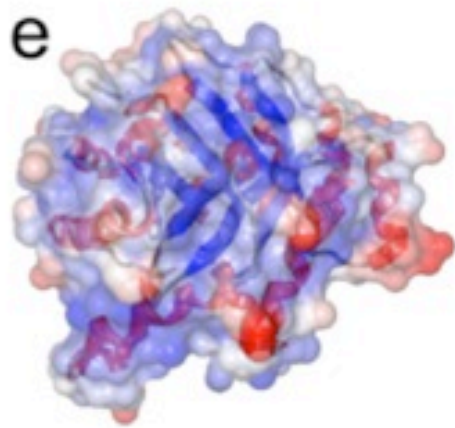


abstracted

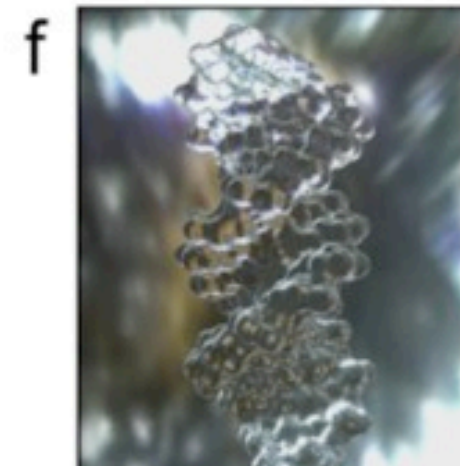


skin / ray-casting

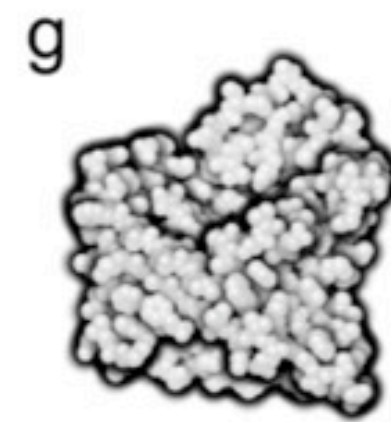
LIGHTING



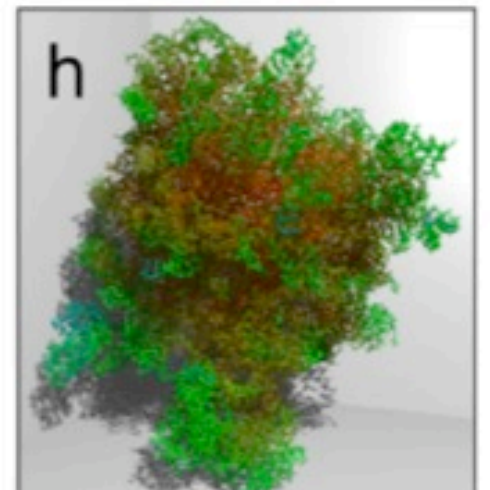
transparency



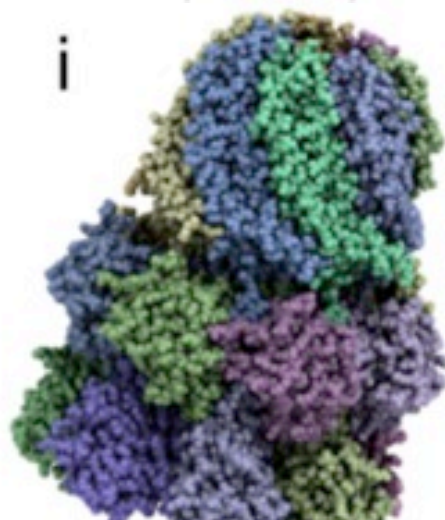
high dynamic range



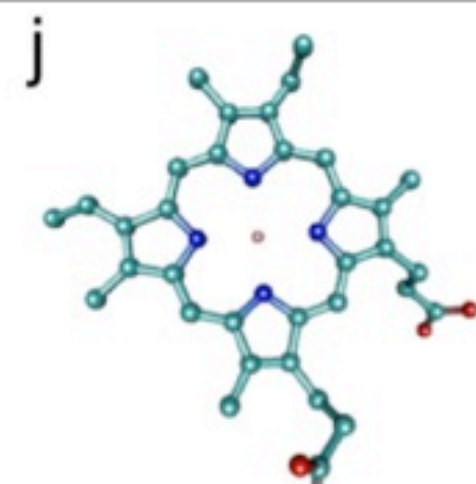
halo effect



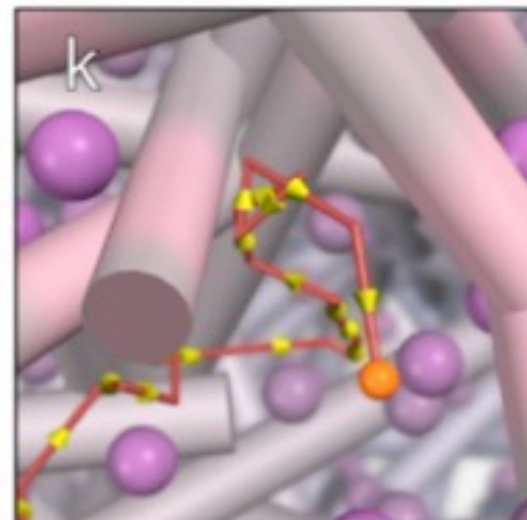
global shadowing



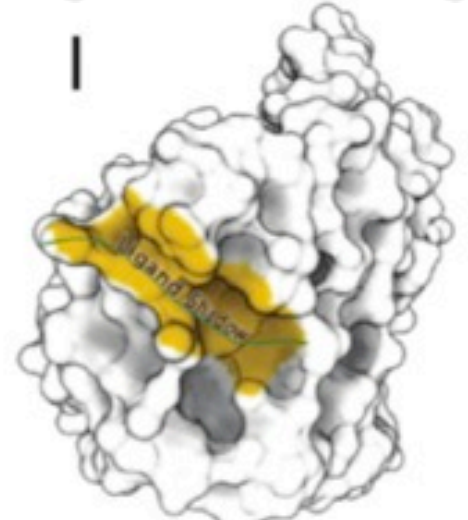
ambient occlusion



ray-casted CPK
& HyperBalls

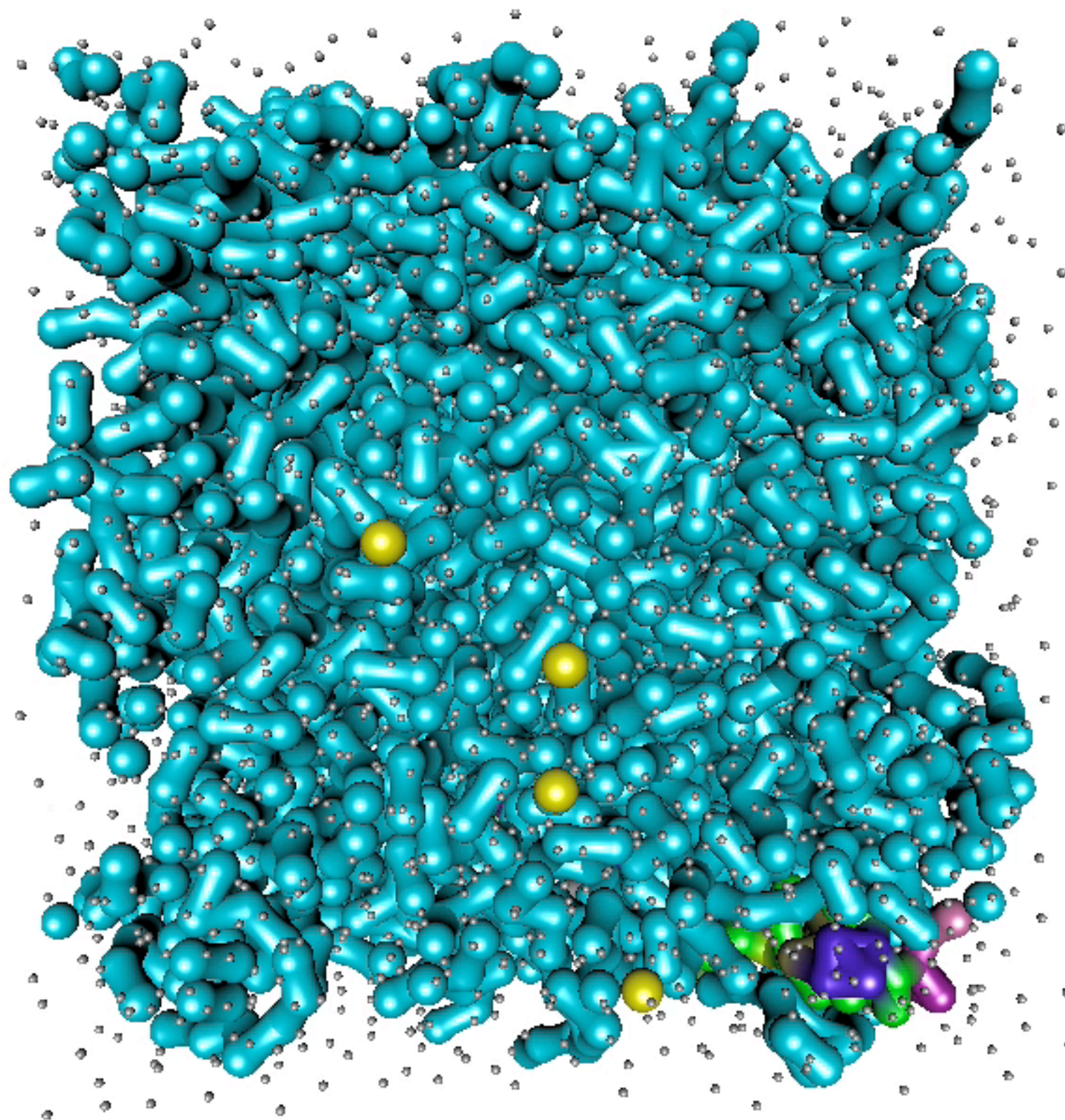


dof / desaturation

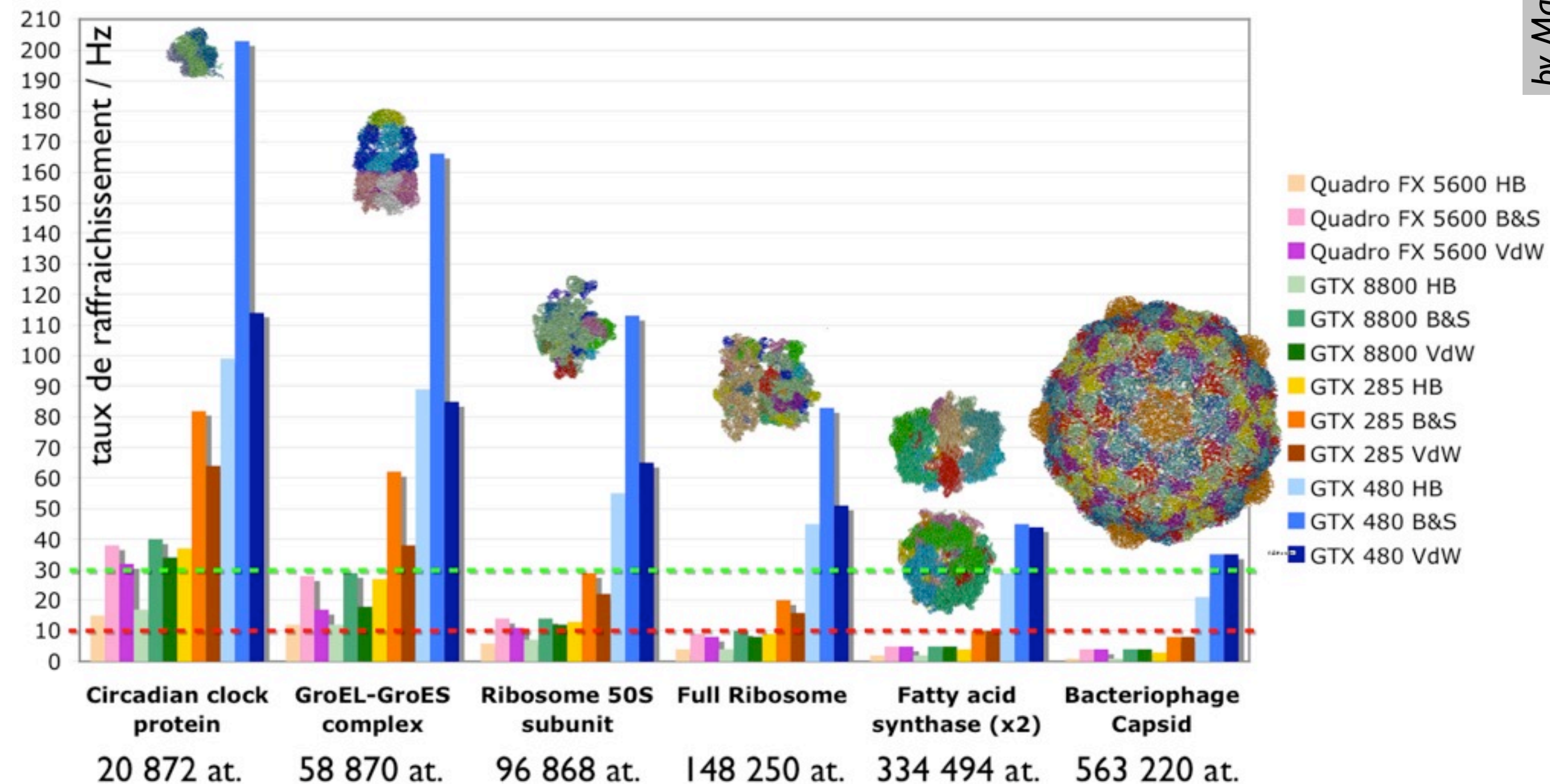


3D annotation

Chavent et al, Brief BioInf 2011

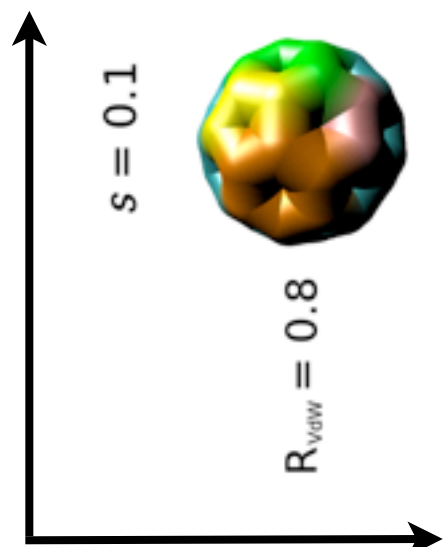


Performance

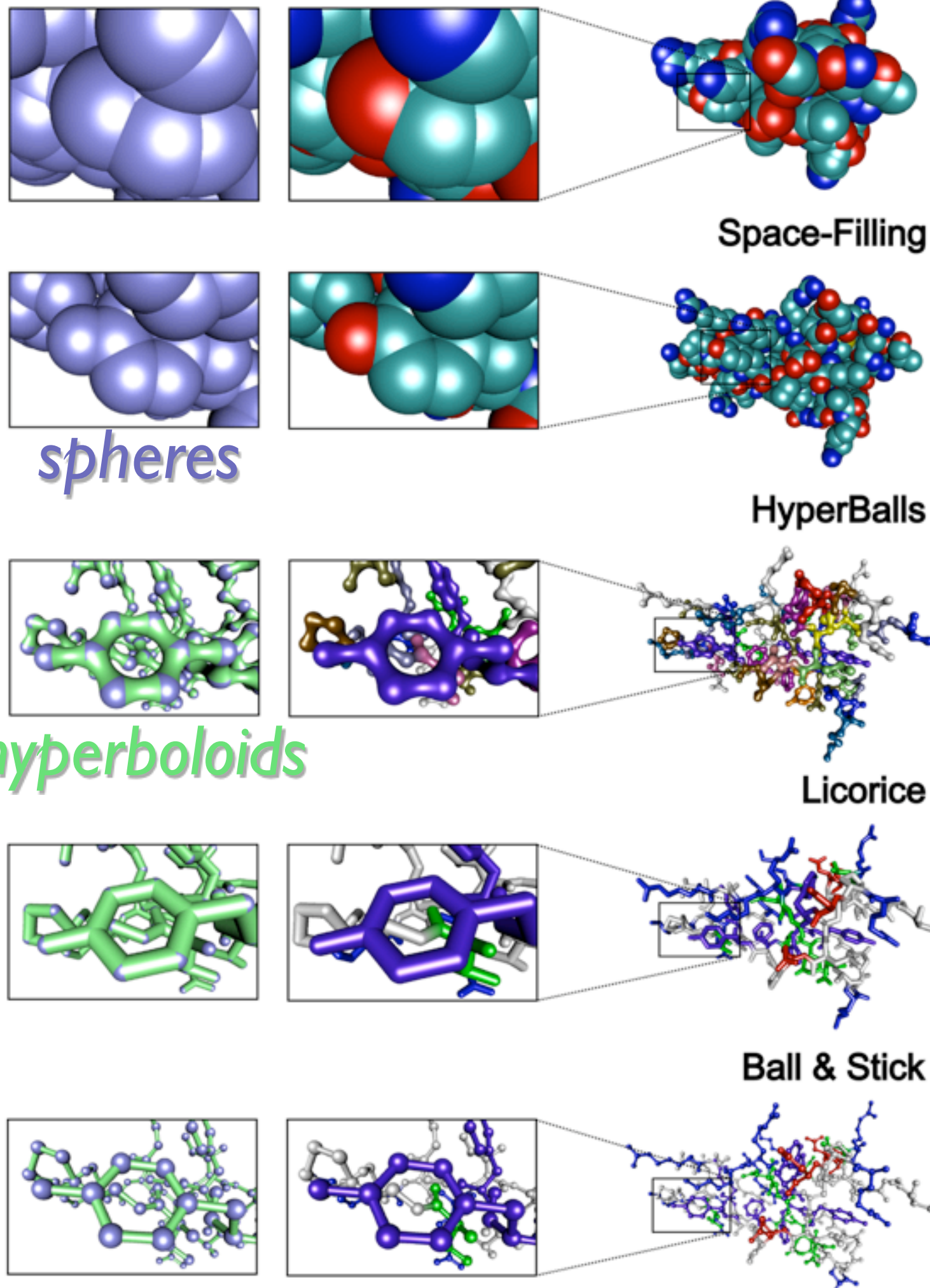
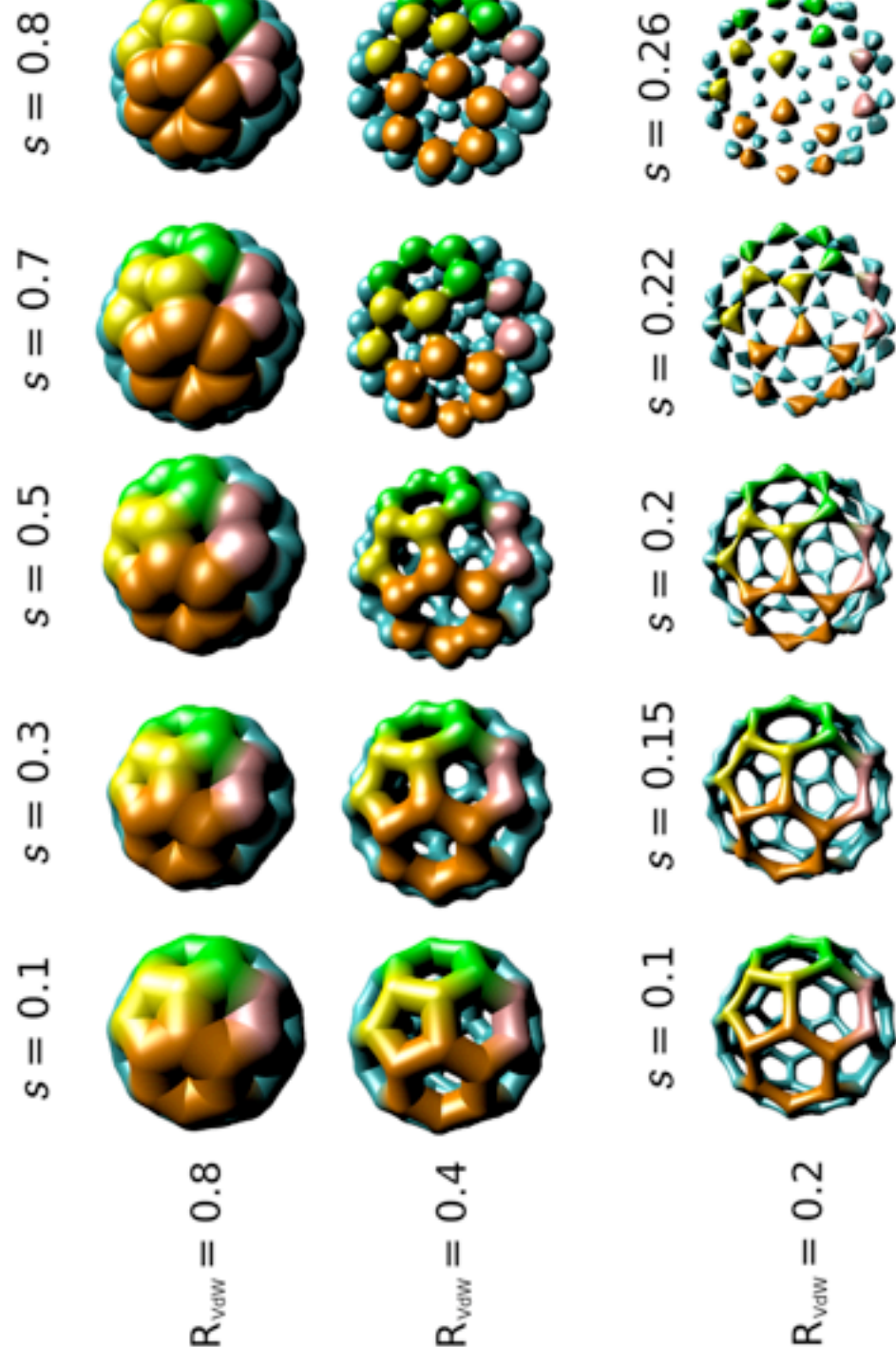


A unified representation

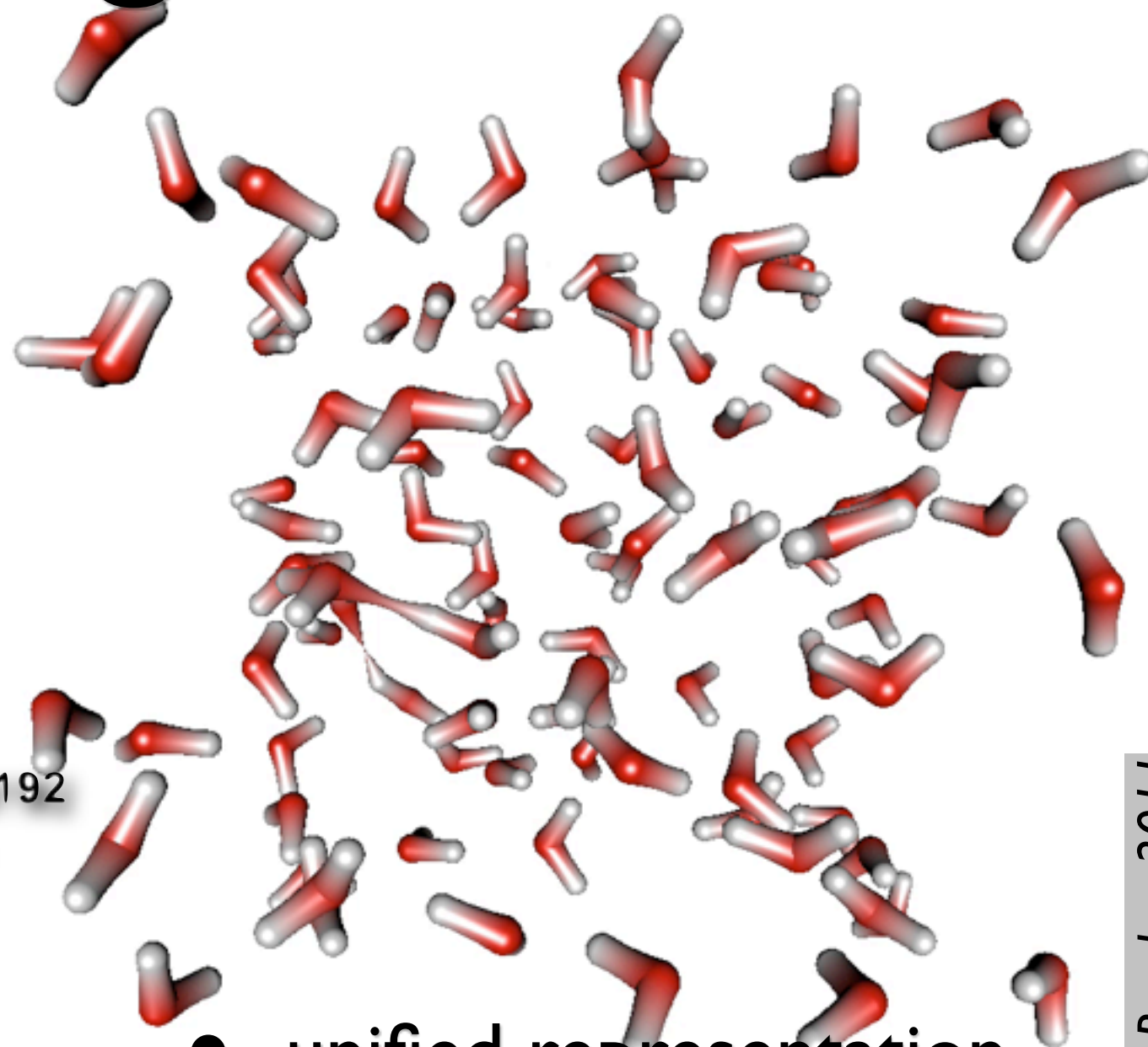
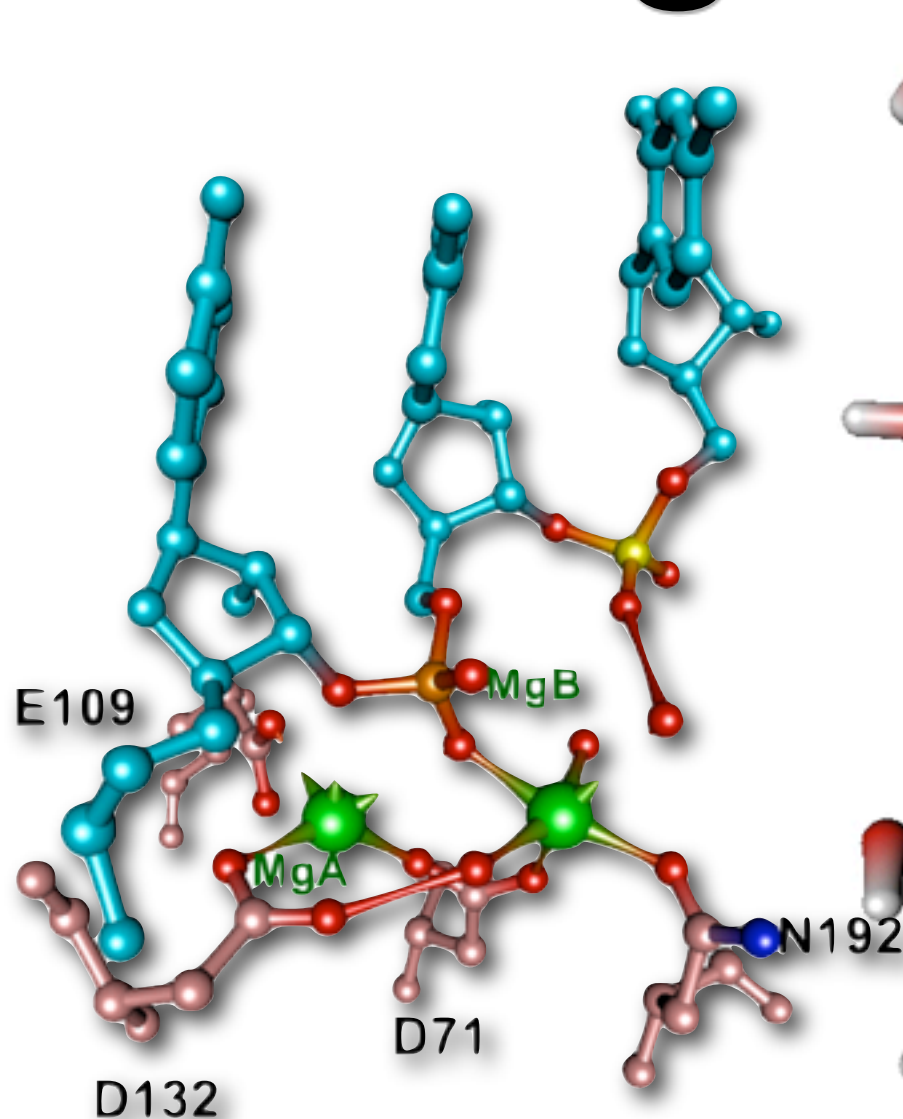
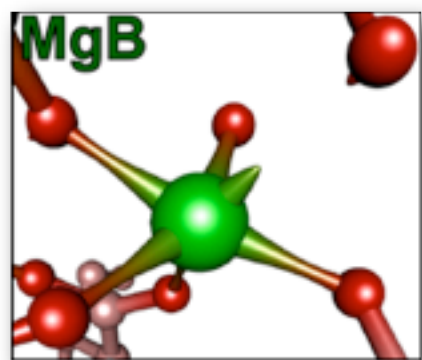
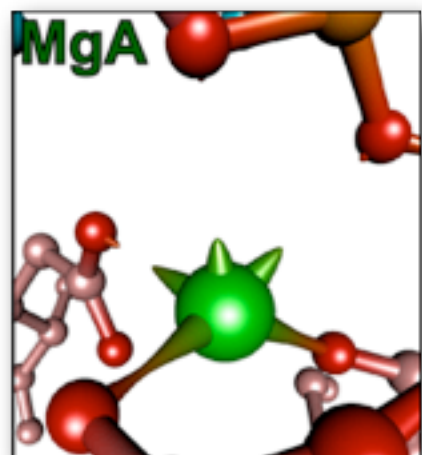
"shrink factor"



radii



Highlights



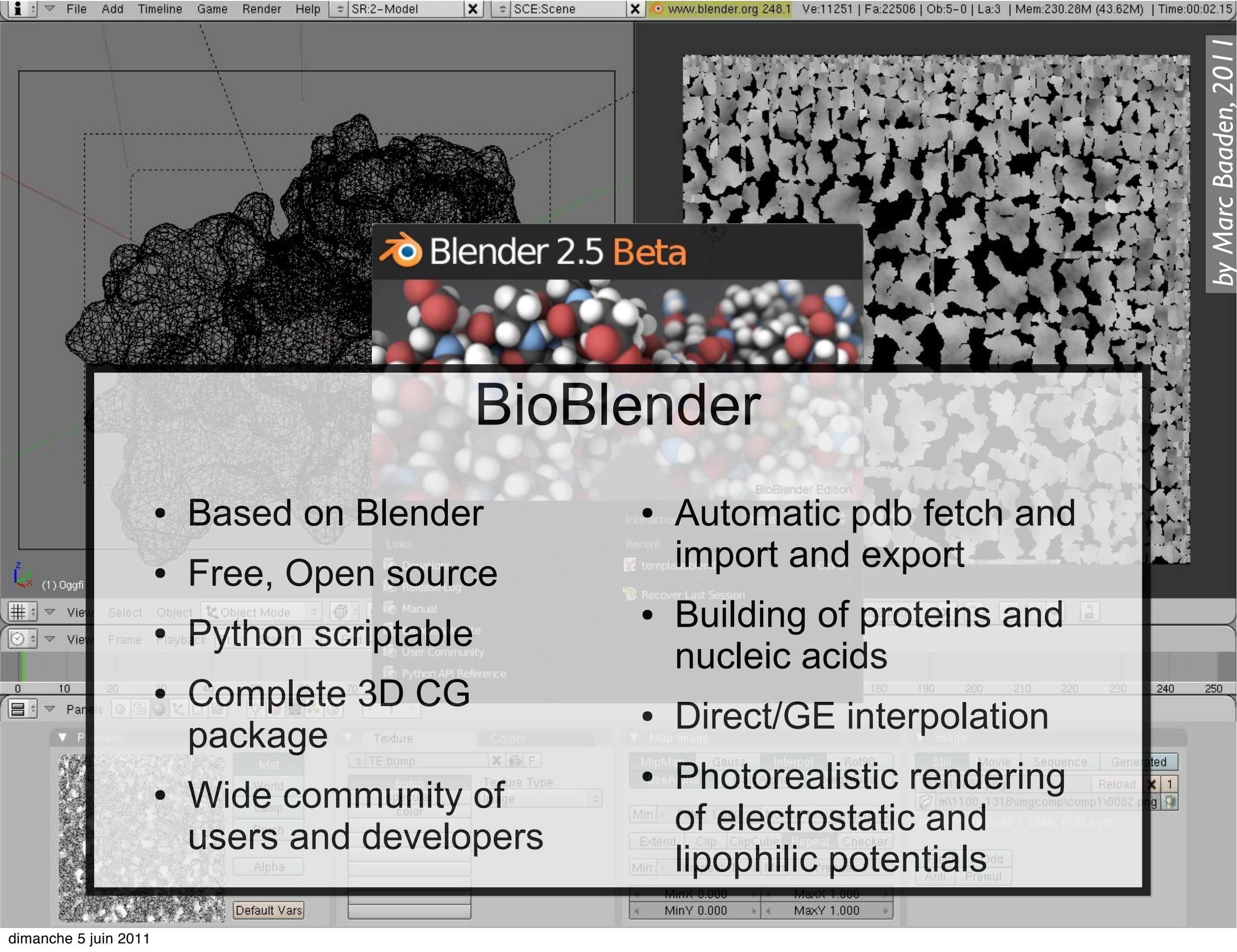
- coordination bonds
- asymmetry
- symbolize strength

- unified representation

- HyperBalls

- dynamic representation

Chavent et al, J Comput Chem, accepted



Blender 2.5 Beta

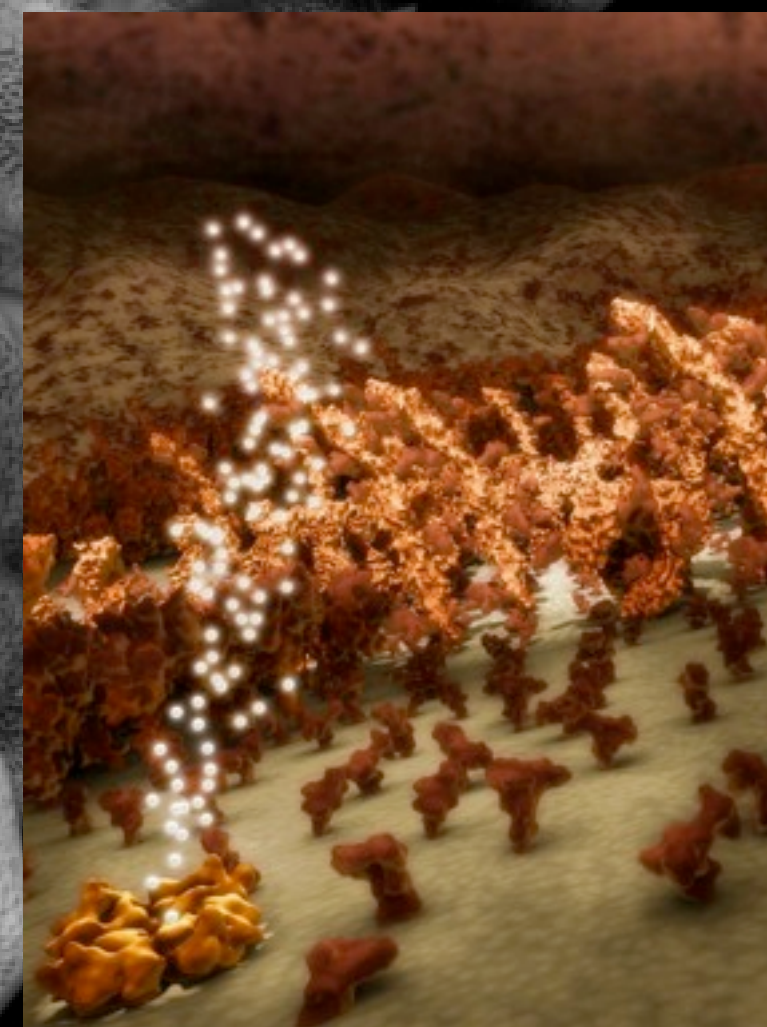
BioBlender

- Based on Blender
- Free, Open source
- Python scriptable
- Complete 3D CG package
- Wide community of users and developers

- Automatic pdb fetch and import and export
- Building of proteins and nucleic acids
- Direct/GE interpolation
- Photorealistic rendering of electrostatic and lipophilic potentials

www.BioBlender.org

by Marc Baaden, 2011



www.scivis.ifc.cnr.it
Pisa, Italy

“démon”

SpiderGL : BLT2 GPCR receptor (Baaden et Catoire)

http://www.baaden.ibpc.fr/pub/blt2/jbn11.html

bioblender

Carnet d'adresses Bonjour i Apple PIM Maison Voyage Research Bank Achat OSX Net Jeux Infos Recherches iGoogl¹ 2CiteULike²

SpiderGL : BLT2 GPCR receptor (B...

HOME **baaden@ibpc**

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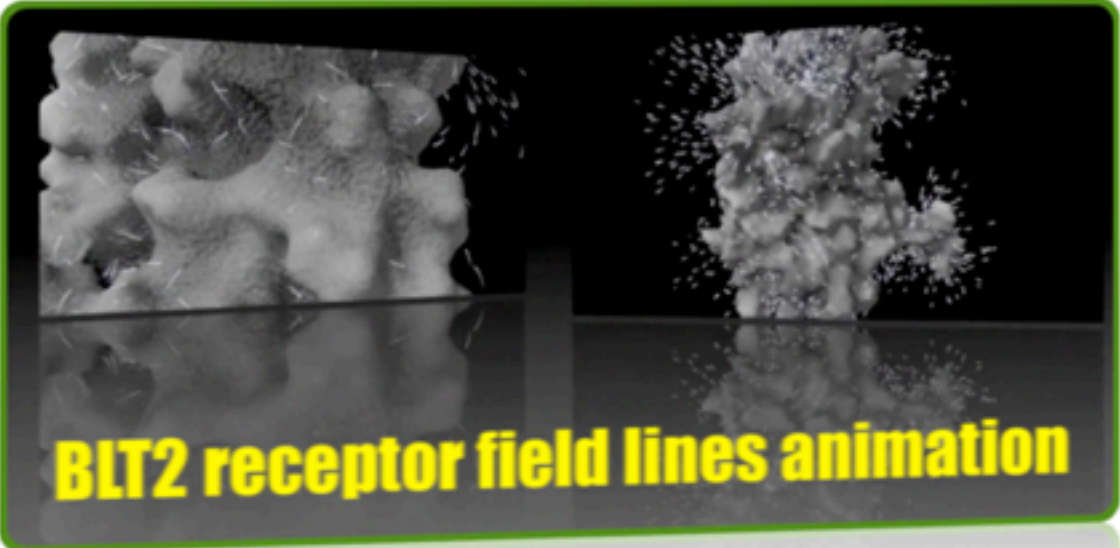
Xing

RSS feed

SpiderGL : BLT2 GPCR receptor electrostatic potential

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Supplementary material to Catoire et al., JBN 2011



BLT2 receptor field lines animation

< Visualization courtesy of Monica Zoppè and colleagues >

Visualization of field lines of the membrane-inserted BLT2 GPCR, with a particularly strong attraction to its extracellular binding site, implemented in a modern WebGL-capable web-browser. This animation is supplementary material to the article *Electrostatically-driven fast association and perdeuteration allow transferred cross-relaxation detection for G protein-coupled receptor ligands with equilibrium dissociation constants in the high-to-low nanomolar range* by Catoire et al. *Journal of Biomolecular NMR* 2011

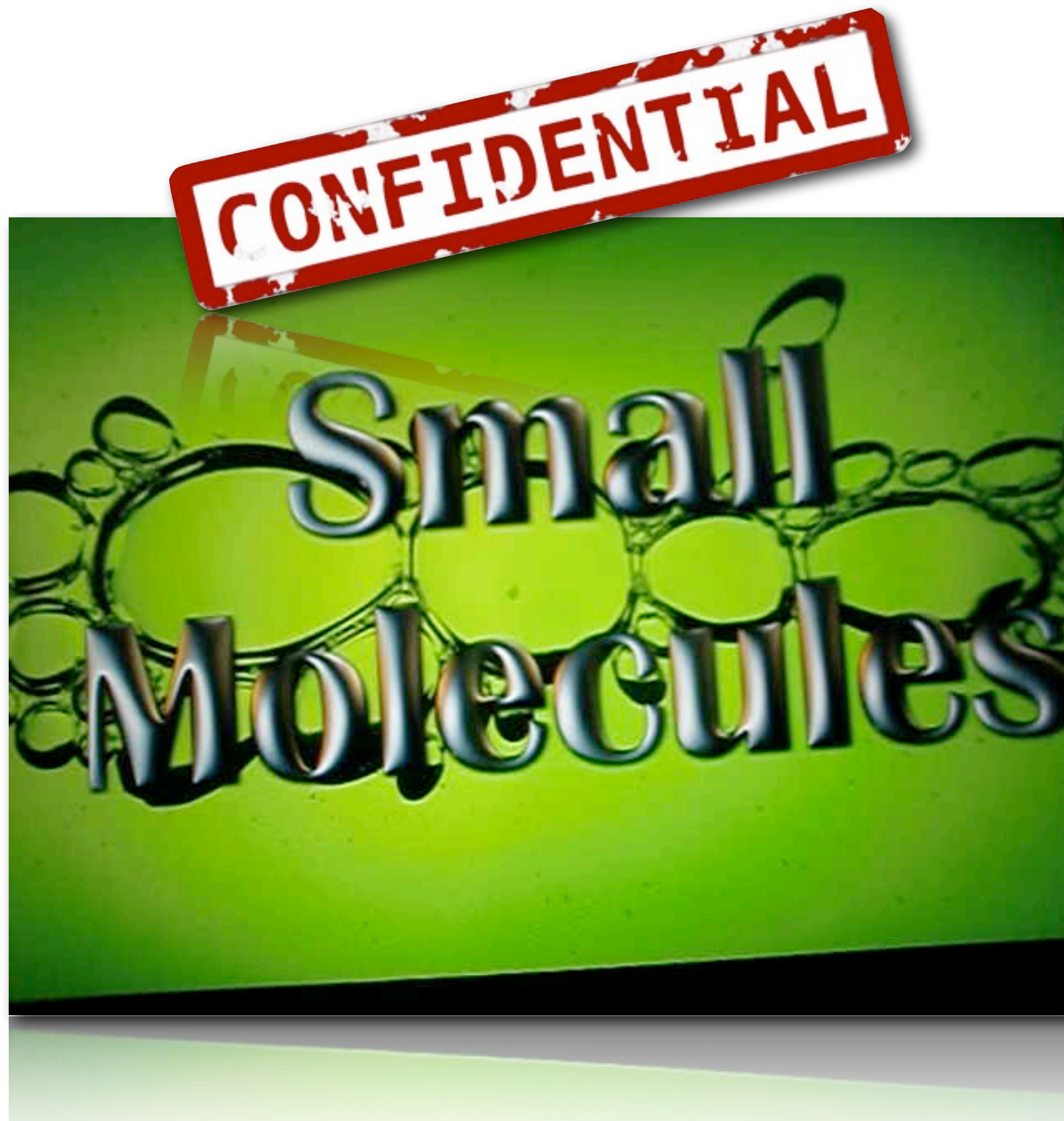
<http://www.baaden.ibpc.fr/pub/blt2/jbn11.html>

Appareils mobiles

- Visualisation encore très limitée
- Trouver des astuces techniques
 - *Triangulation ok si pas trop de triangles*
 - *Lancer de rayon: pour l'instant impossible*

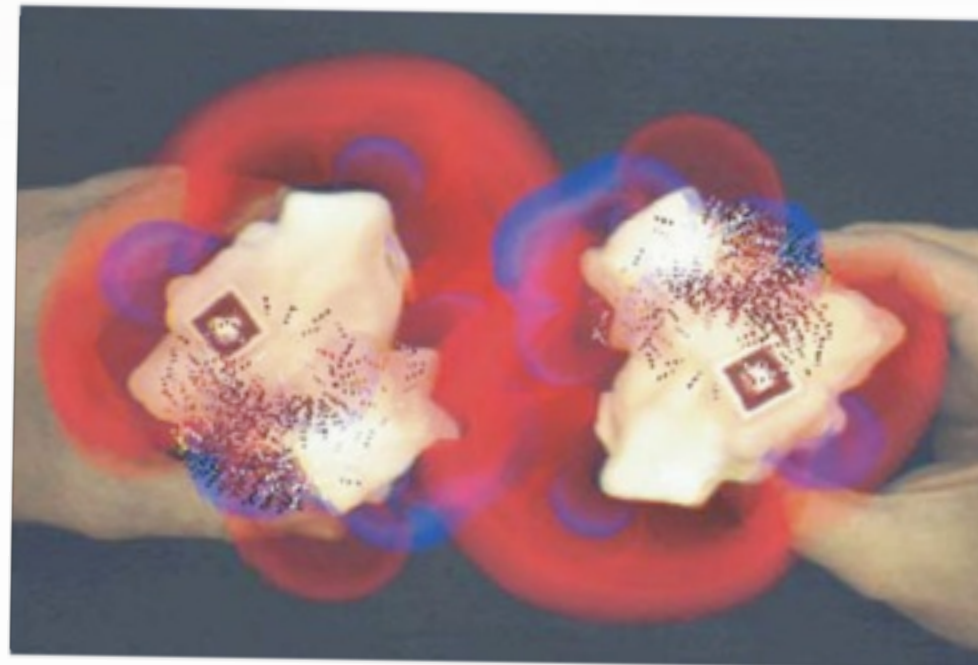
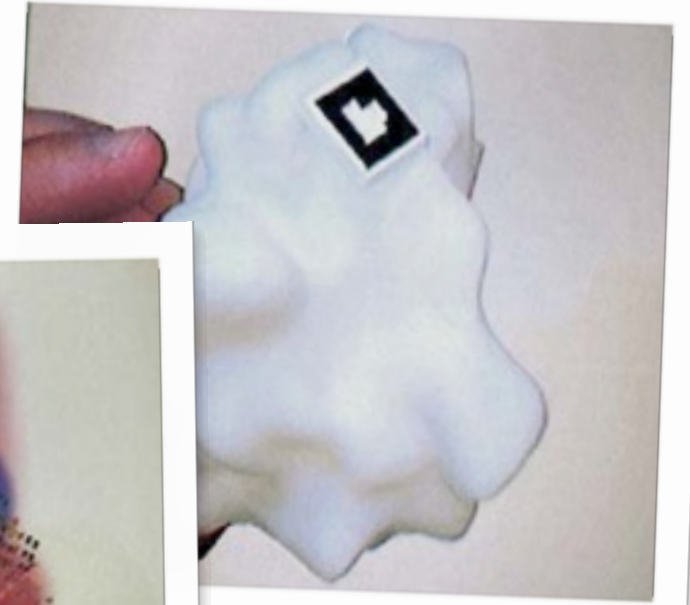
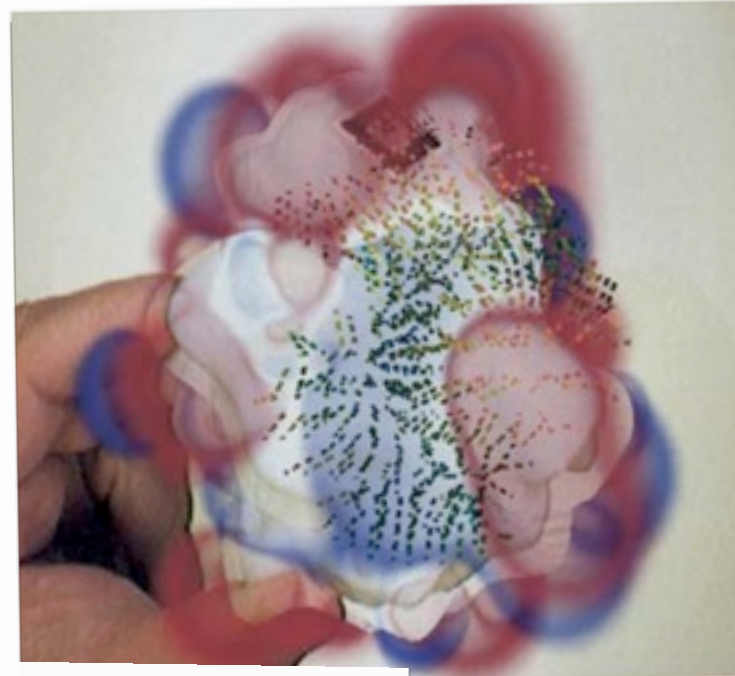


La 3ème dimension entre vos mains

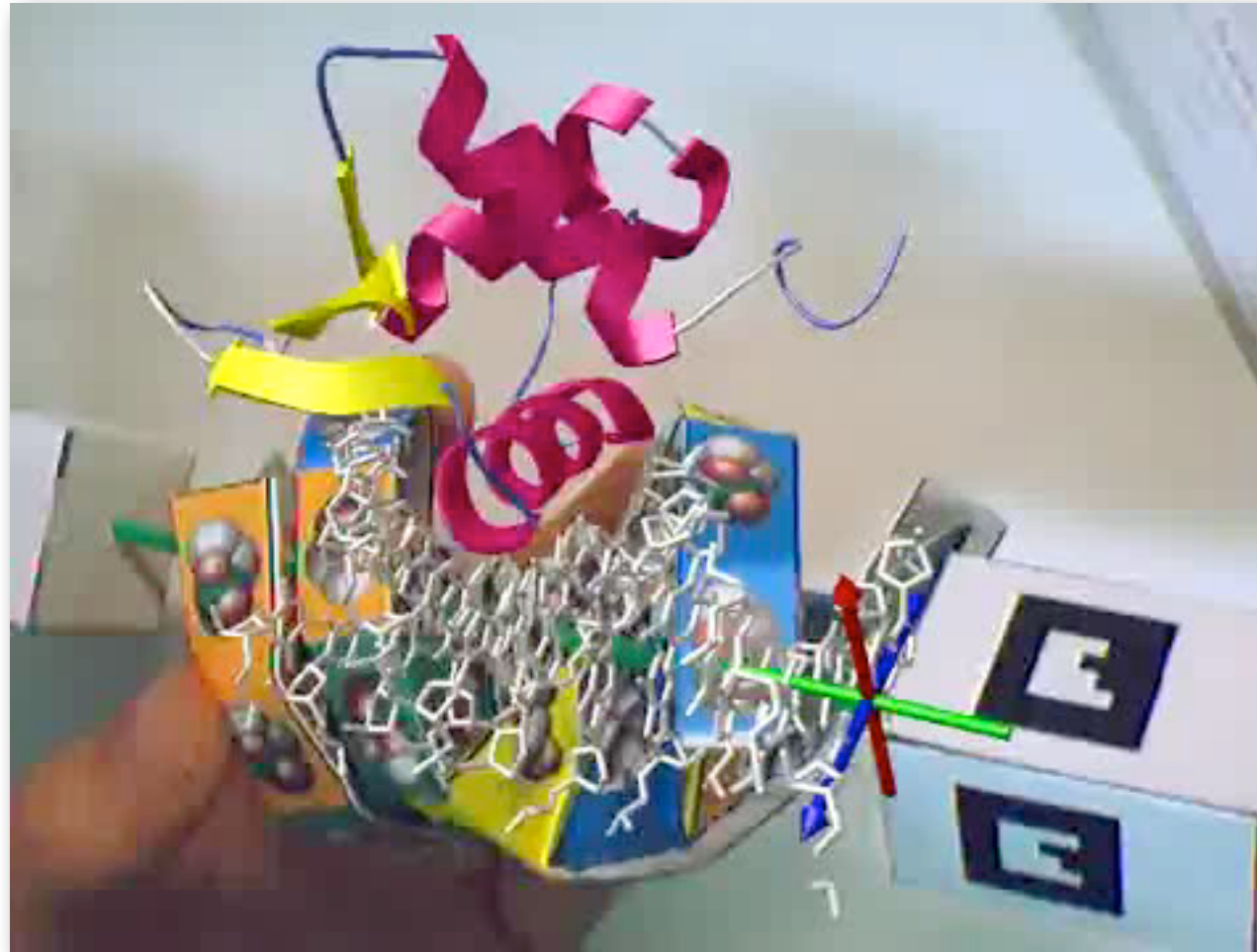


Vers une réalité augmentée

Exemple de modèles 3D (Gillet 2005)



Augmented reality

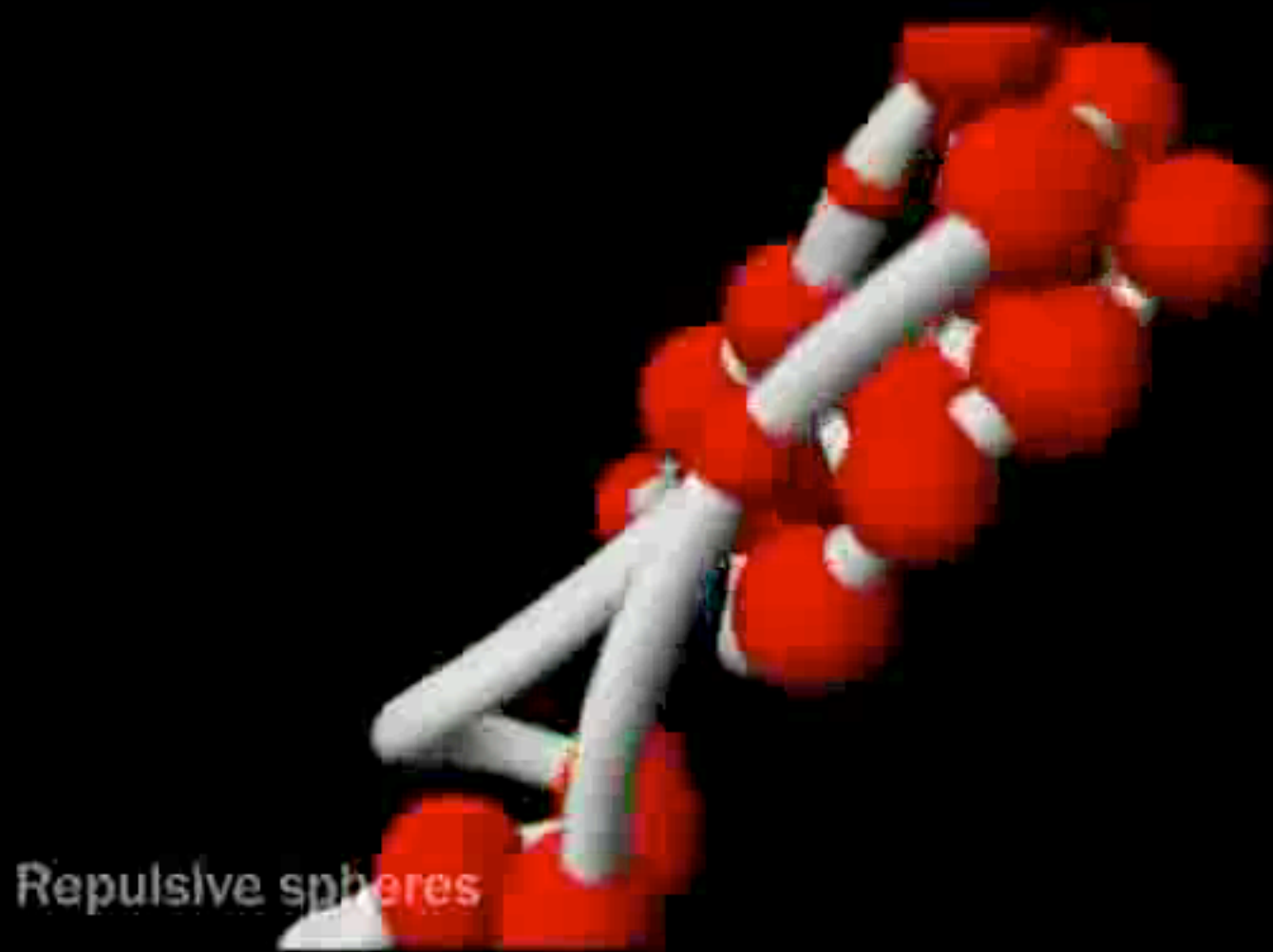


*Molecular Graphics lab, **A Olson & al**, Scripps*

<http://mgl.scripps.edu/>

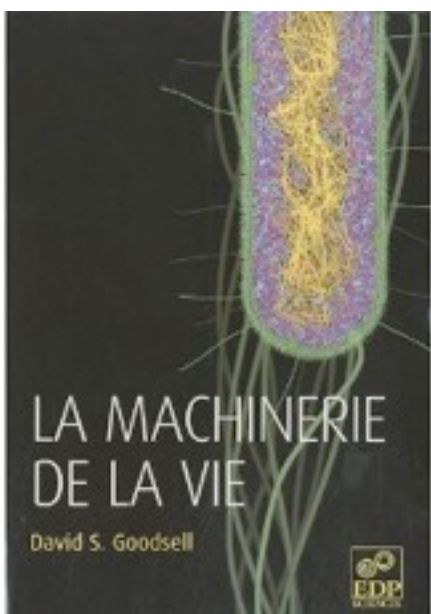
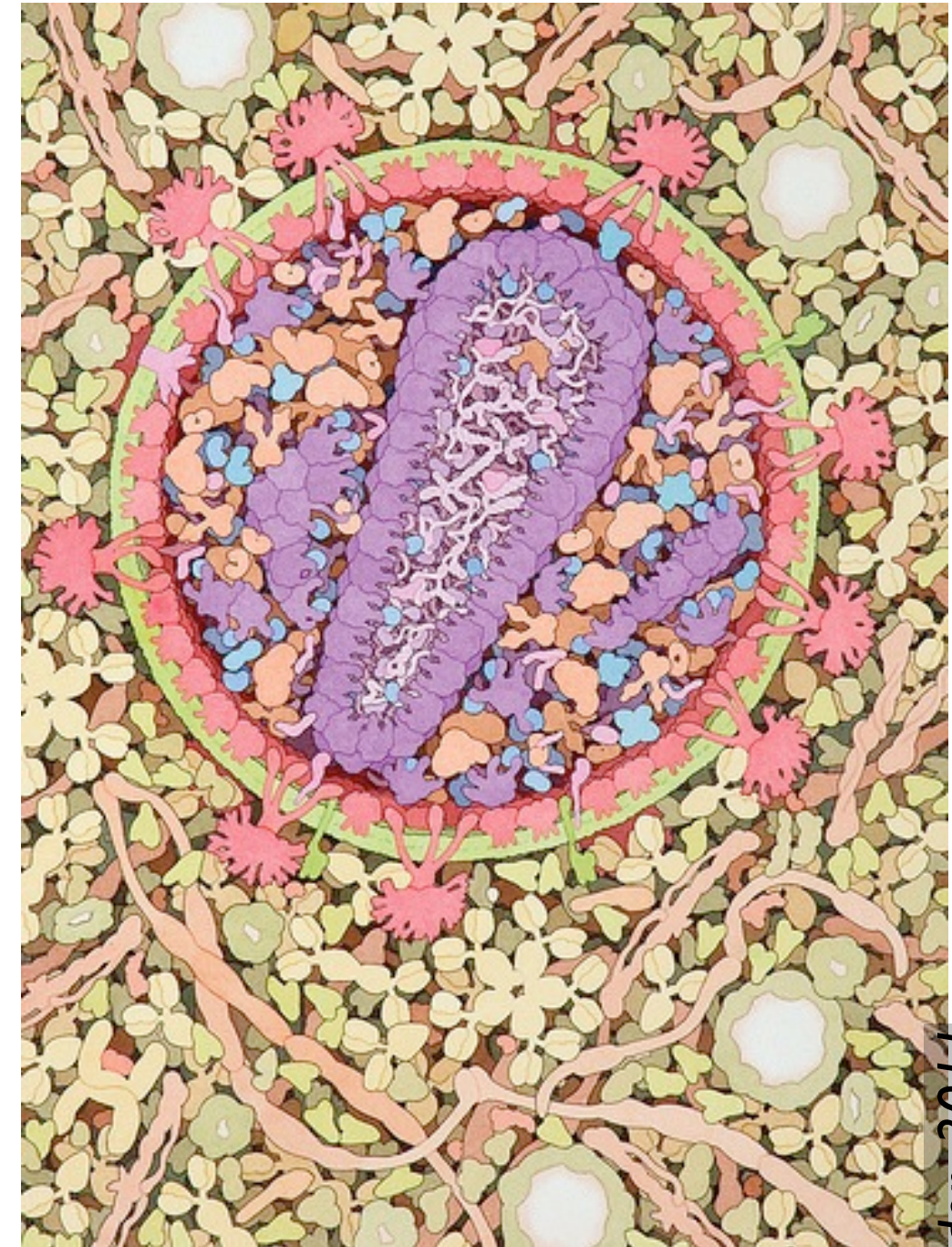
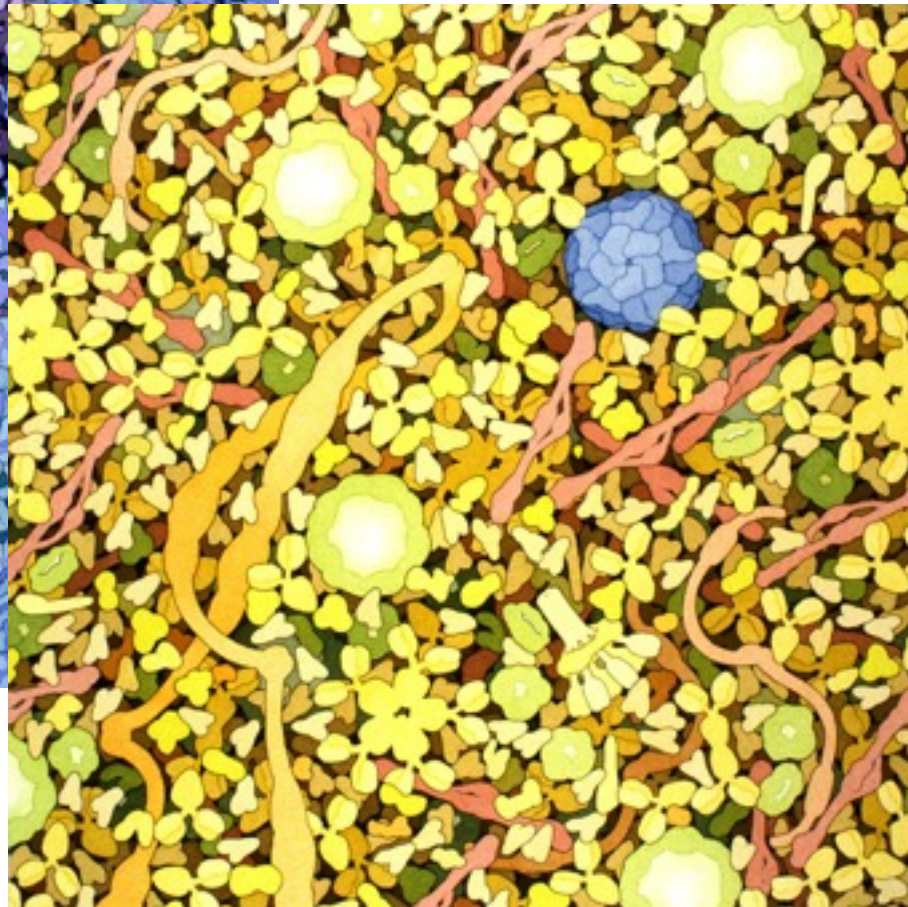
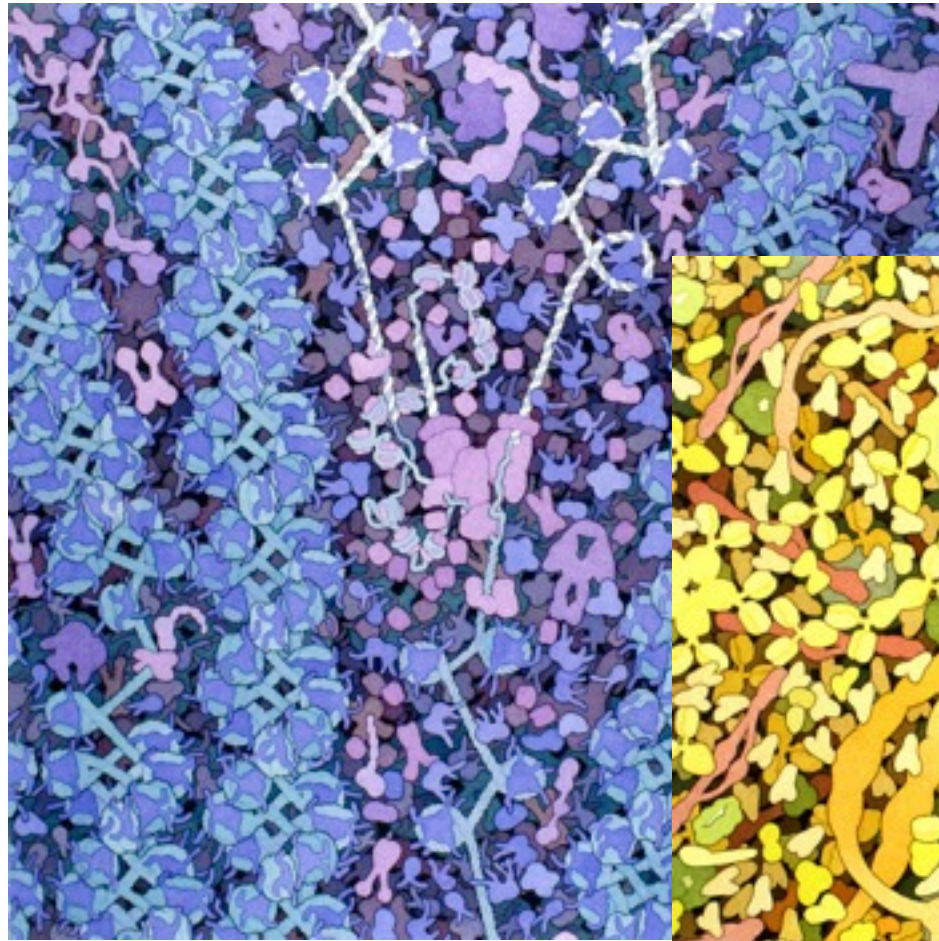
Artistic example: foldgrow

by Marc Baaden, 2011

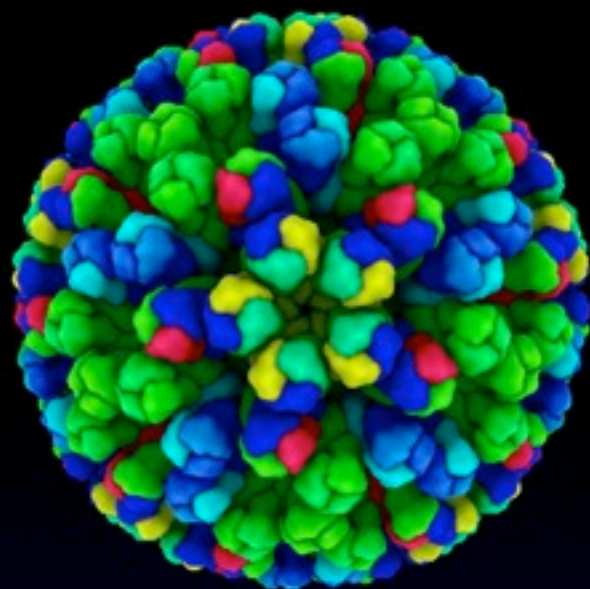


<http://www.youtube.com/watch?v=TU5DVA7fii4>

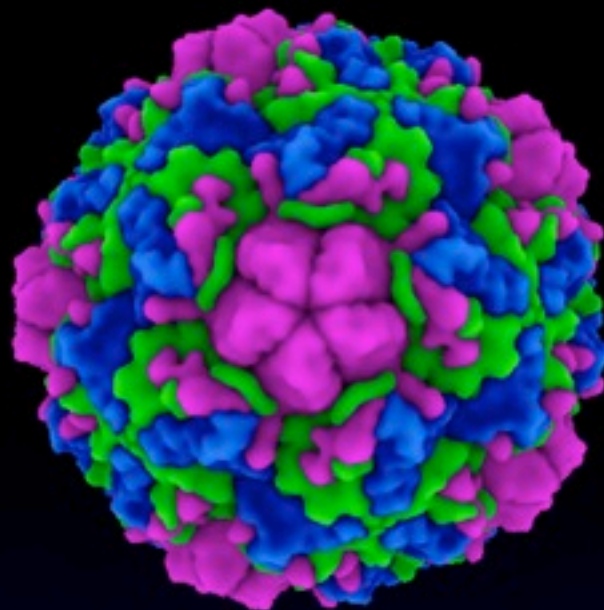
Tableaux de D. Goodsell



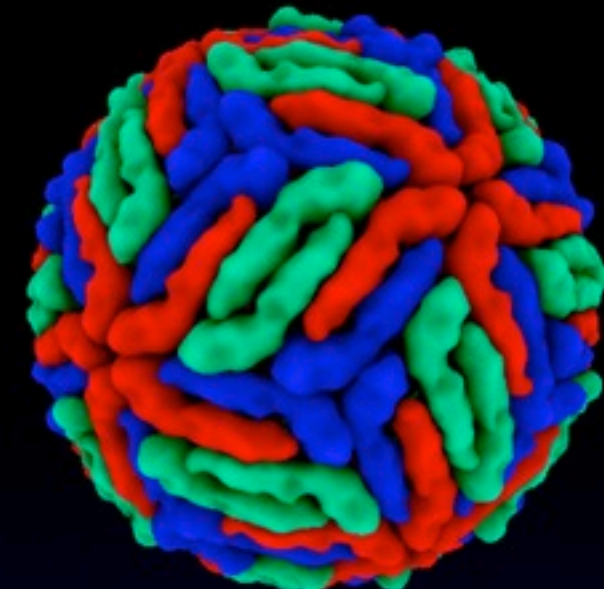
La machinerie de la vie
David S. Goodsell



rotavirus core



rhinovirus

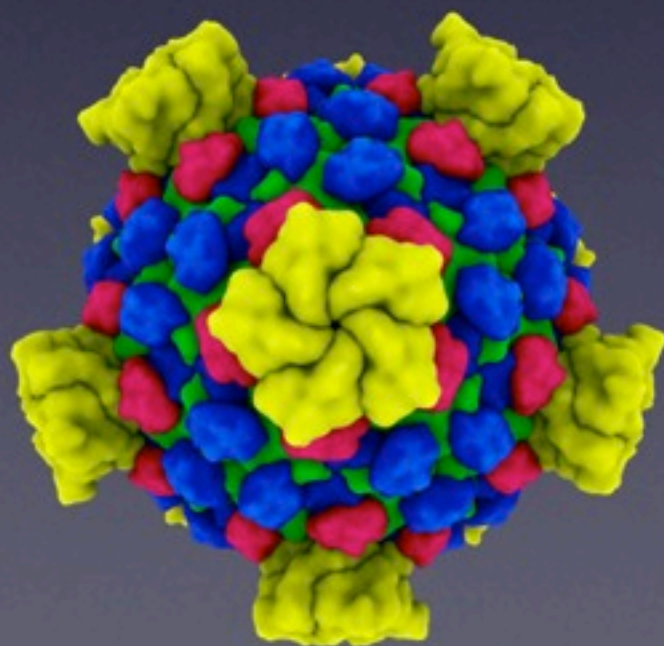


dengue

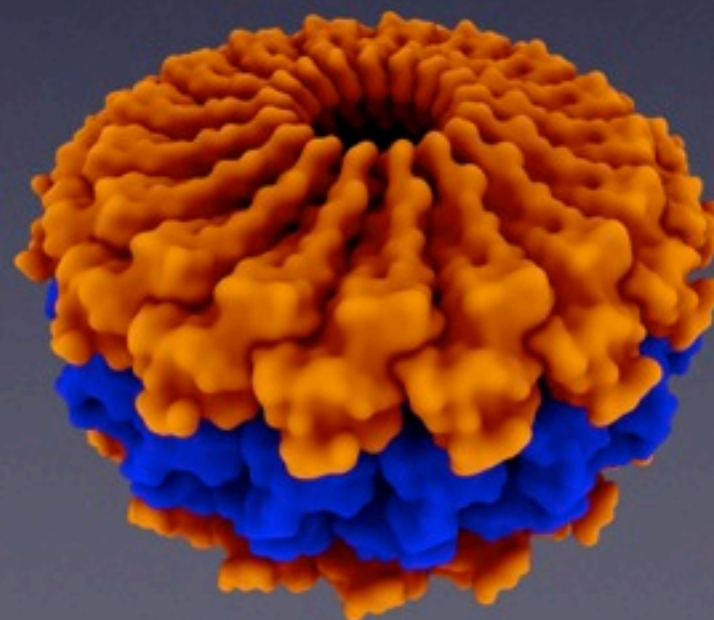
Molecular Maya (mMaya)

A free, open-source software toolkit that extends Maya's capabilities by allowing users to import, model, rig and animate molecular structures

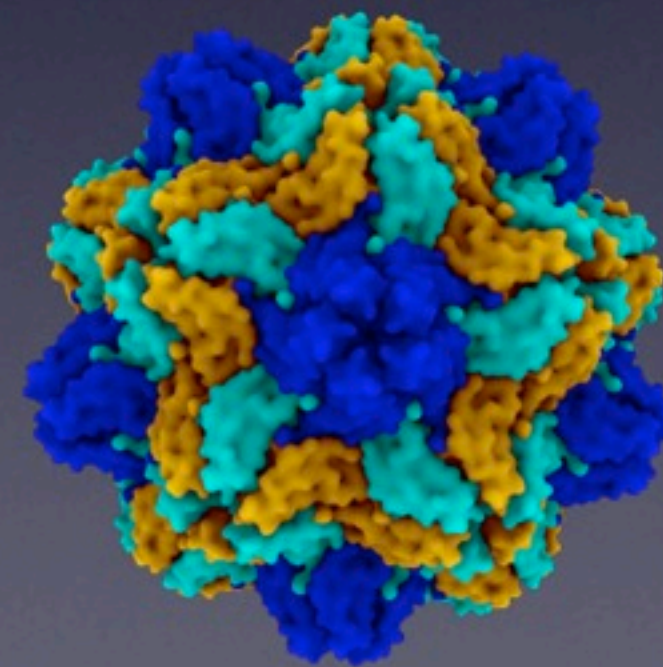
G McGill - <http://www.molecularmovies.com/toolkit/>



reovirus



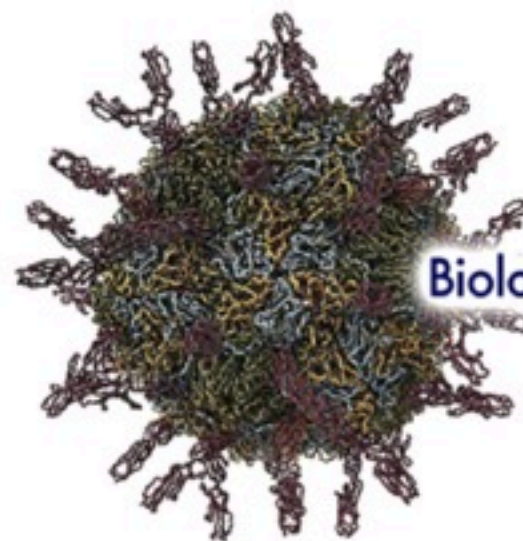
tobacco mosaic virus



tymovirus

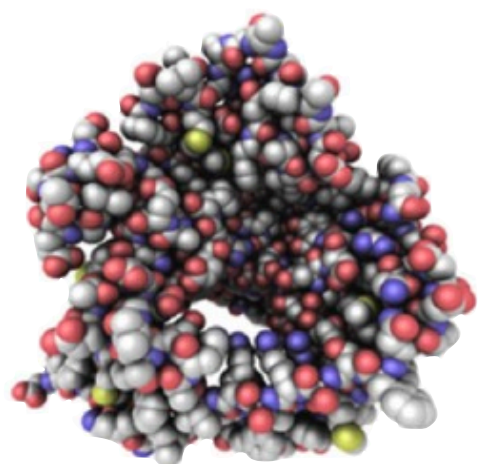
Quelques exemples...

Other Features



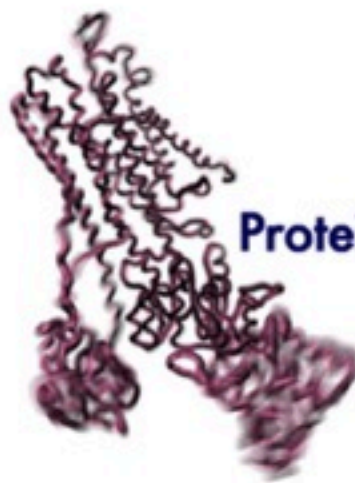
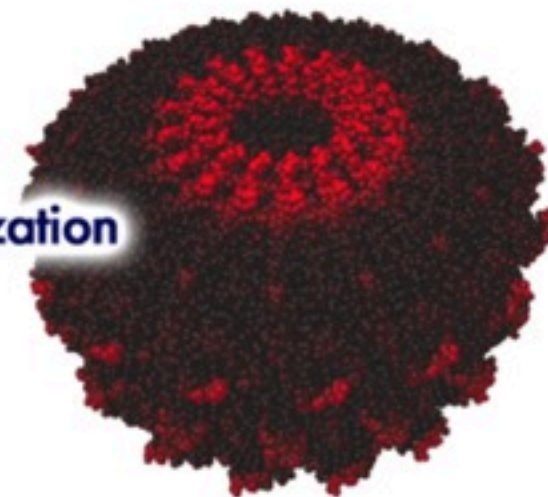
Biological Unit Builder (BioUnit)

Molecular Representations



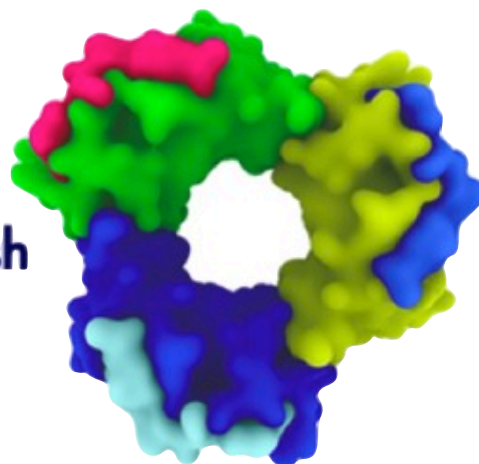
Atoms & Bonds

Temperature/B-factor Visualization

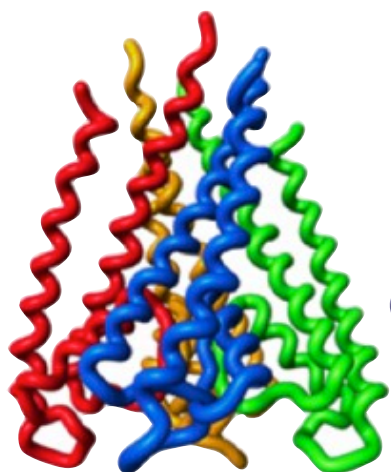


Protein Morphing Module

Surface Mesh

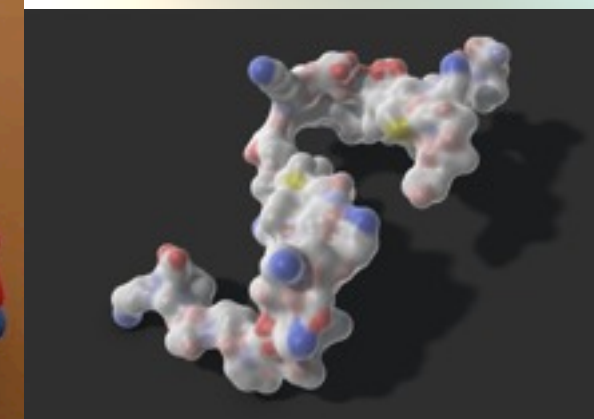


α Carbon Backbone

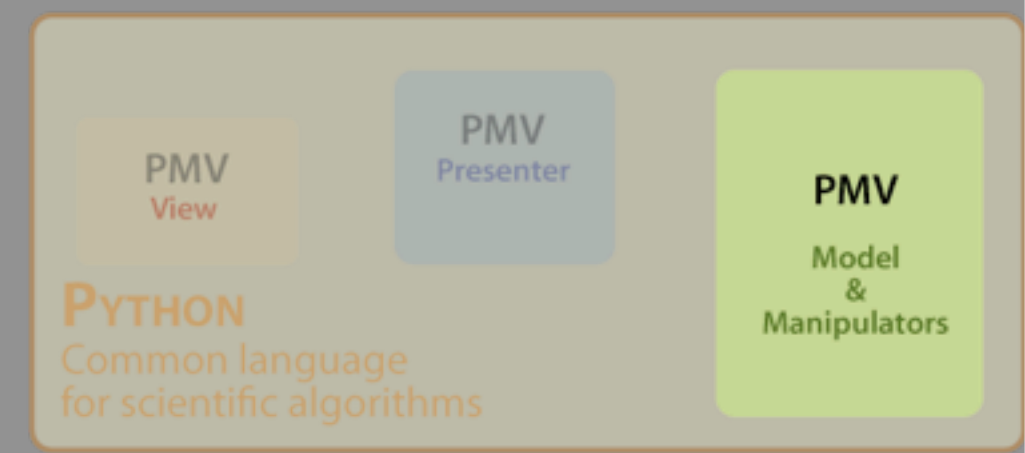
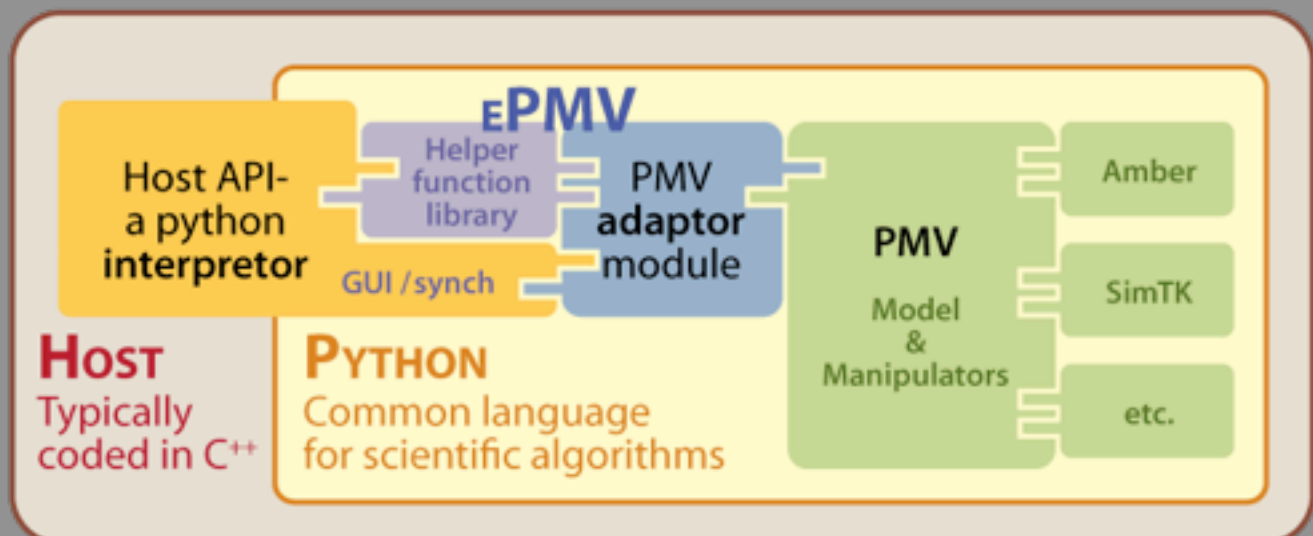


mMaya v1.0
Molecular Maya Toolkit

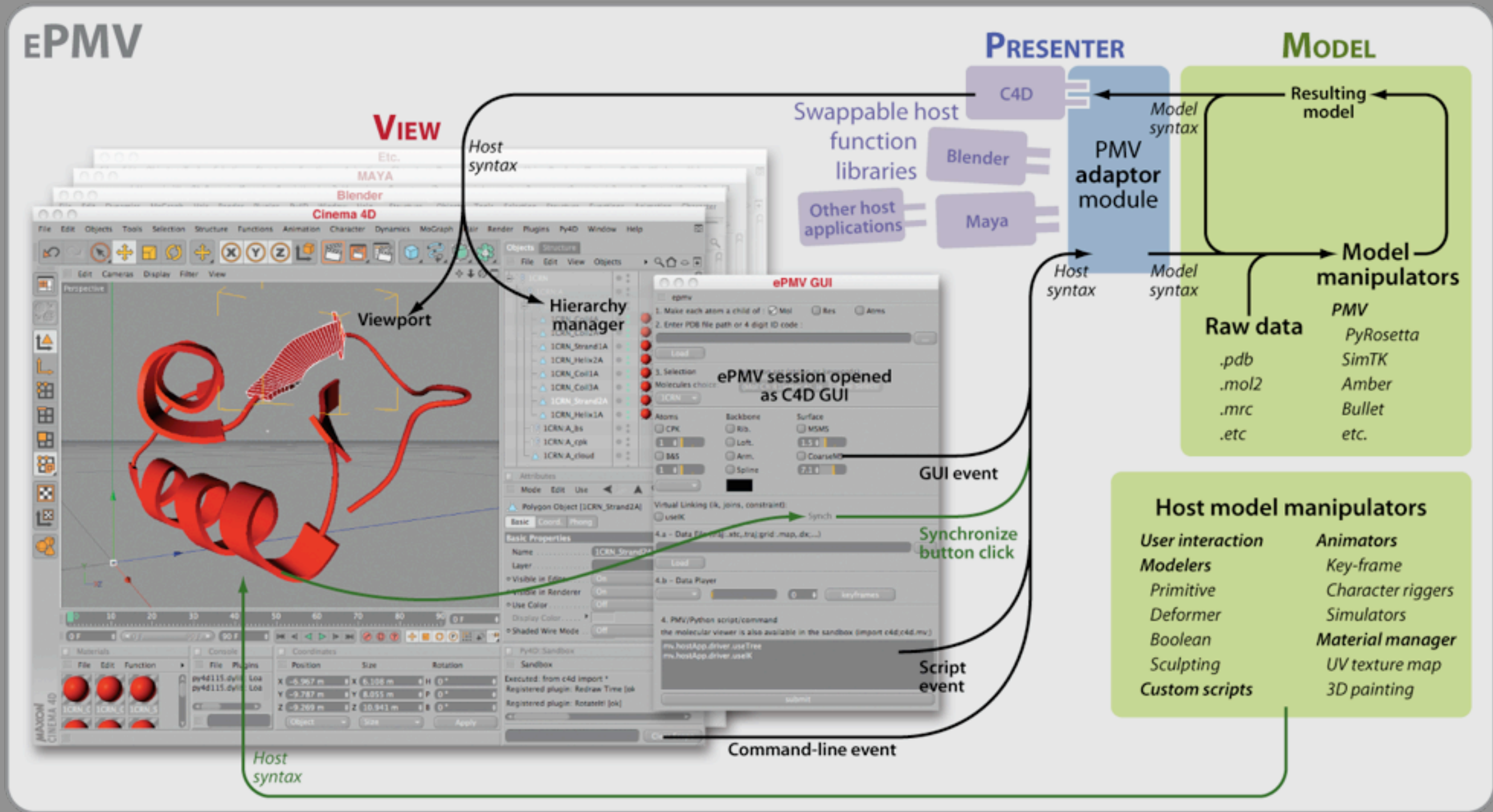
G McGill



by Marc Baaden, 2011



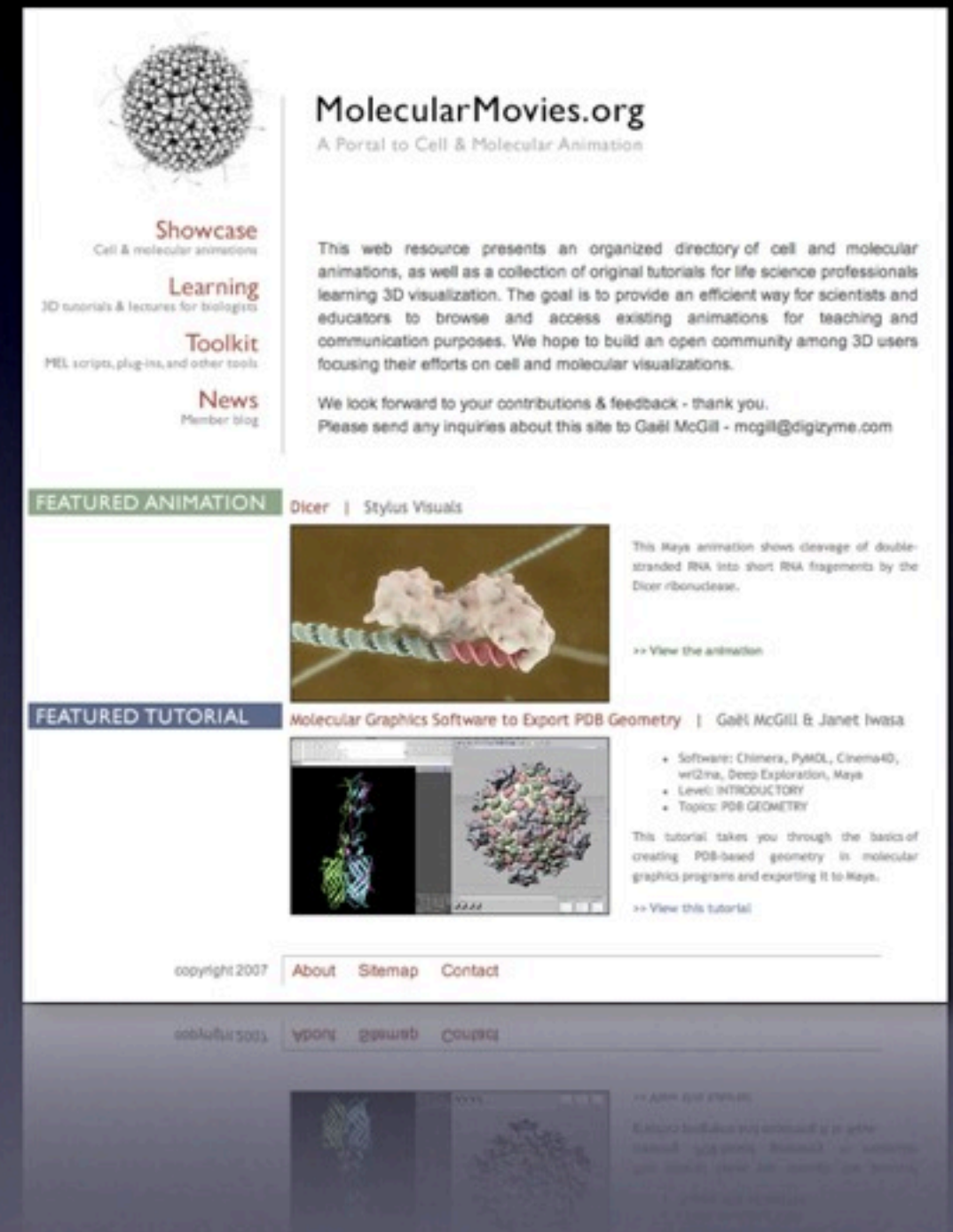
by Marc Baaden, 2011



Audience: Scientists, educators & animators interested in biovisualization.

Purpose:

1. To compile and organize a collection of high quality cellular/molecular visualizations
2. To offer tutorials (text & video) and other learning resources for scientists & animators interested in cell & molecular visualization.
3. To provide free software tools that facilitate the creation of accurate and high quality molecular & cellular visualizations (mMaya)



Showcase section (organized by scientific topic)



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A Portal to Cell & Molecular Animation

Showcase
Cell & molecular animations

Learning
3D tutorials & lectures for biologists

Toolkit
MEL scripts, plug-ins, and other tools

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By Scientific Area | By Animator / Studio

Adhesion / Extracellular Matrix Angiogenesis / Metastasis Apoptosis Chemistry / Organic Synthesis Cytoskeleton / Molecular Motors Developmental Processes Disease / Immune System DNA / Chromatin Drug / Mechanism of Action Evolution / Origins of Life Metabolic / Respiration	Neuronal Signaling Prokaryotes Protein Folding & Stability Replication RNA Stability / RNAi RTKs & Signal Transduction Stem Cells Transcription Translation Viruses / Infectious Disease
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Adhesion / Extracellular Matrix

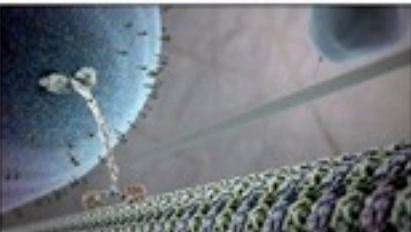
Cell Invasions | Jason Sharpe, Donald Ly, Charles Lumsden et al



This Maya animation provides a visual simulation of fibroblasts moving through extracellular matrix - the 3D matrix and behavior of the cell population through the matrix are based on mathematical models implemented in MEL.

>> View the animation at U. Toronto

The Inner Life of the Cell | XVIVO & Harvard University



This Siggraph award-winning animation depicts the molecular players and signaling processes underlying leukocyte migration, adhesion and extravasation. Structural components of the cytoskeleton and the extracellular matrix, in particular, are highlighted.

>> View the animation at Harvard BioVisions

T-Cell Mobility from Blood to Lymph | Marc Dryer



An interpretative visualization of T-cell mobility from blood to lymph through the thymus-dependent zone of the lymph node using evidence-

Viruses / Infectious Disease

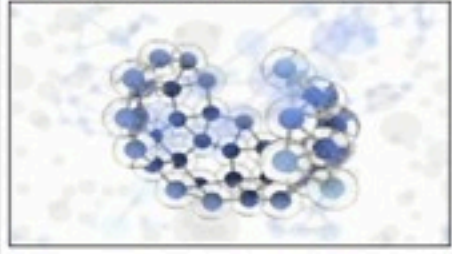
Bacteriophage T4 | Seyet, LLC



An accurate visualization of the Bacteriophage T4 based on Cryo-EM datasets of the virus. The scope of the animation is to show the infection process of T4 into an E. coli cell. All scientific data sets and motion based off of research from Michael Rossmann Laboratory (Purdue University).

>> View the animation

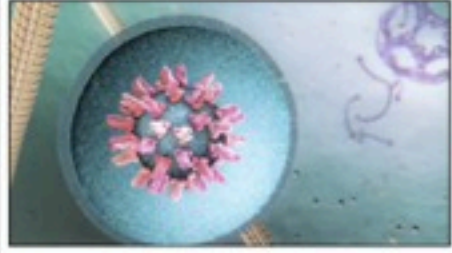
Capsid Molecular Dynamics Simulation | Geordie Martinez / Stylus Visuals



A Maya-rendered visualization of a VMD molecular dynamics simulation. Created for David Chandler's lab at UC Berkeley, this movie depicts the physics of viral capsid formation while summarizing some of the technical steps involved in its creation.

>> View the animation (~41 MB)

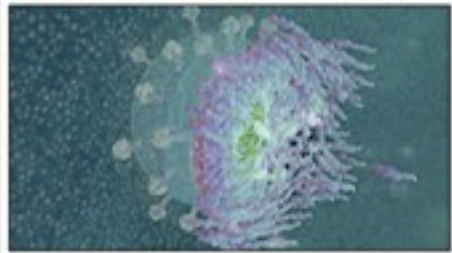
Dengue Virus Entry | Janet Iwasa, Gaël McGill (Digizyme) & Michael Astrachan (XVIVO)



A narrated animation depicting the events that lead to Dengue virus entry into a host cell. In particular, rearrangements and conformational changes in the Dengue glycoprotein E are shown. These lead to membrane fusion and subsequent release of the viral payload into the host cell cytoplasm. Created for WGBH.

>> View the animation (~9 MB)

HIV Assembly, Budding and Maturation | Ken VanderStoep



A visualization of the capsid protein lattice structure that forms during the assembly of immature HIV-1 particles. (Click on the icon in the "Master's Research Project Examples 2002-2005" area of the page).

>> View the animation at U. Toronto

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Merci pour votre attention ! Questions ?

Collaborations & Remerciements

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