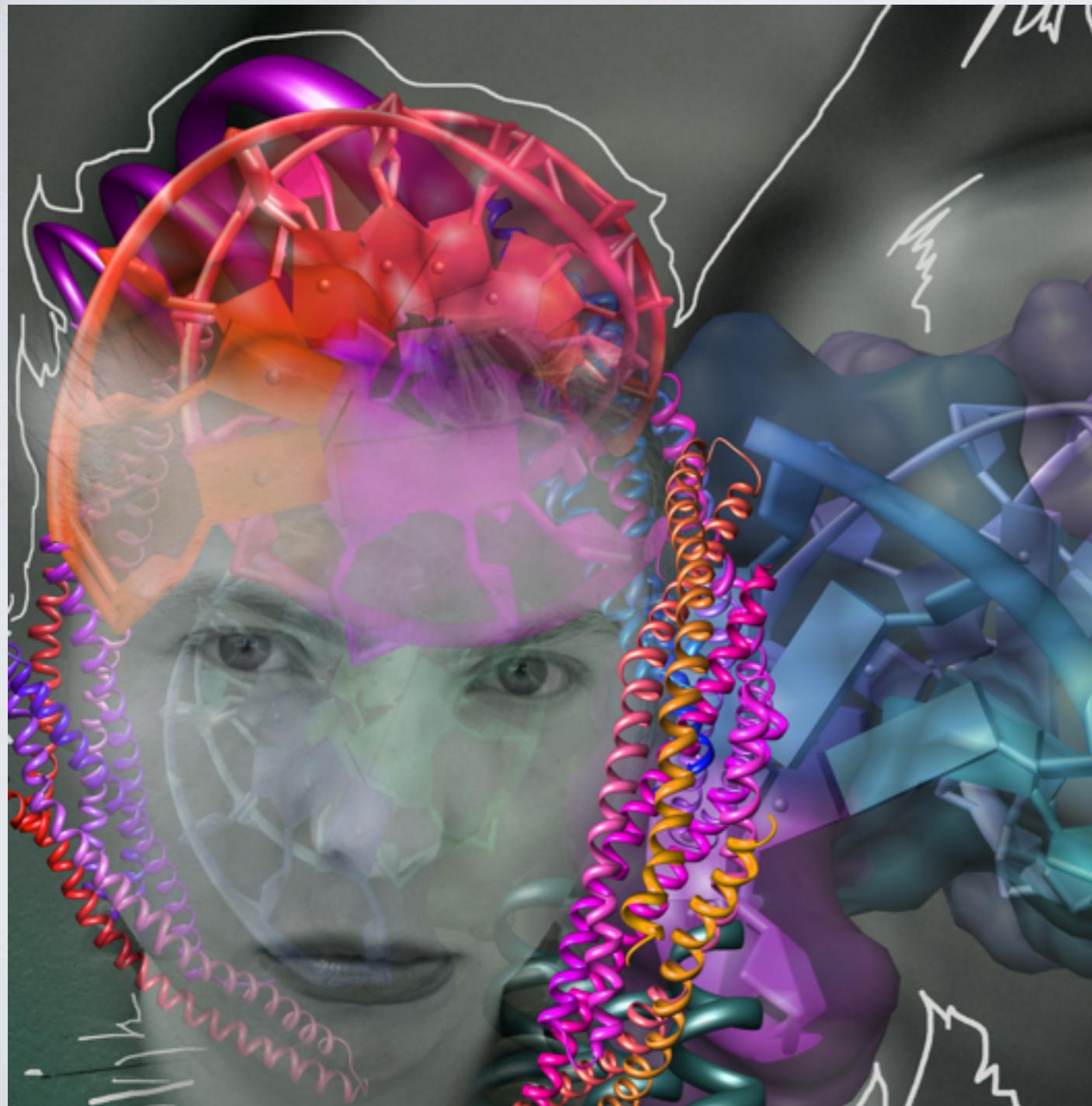


# VISUAL REPRESENTATIONS: FROM ATOMS TO ORGANISMS

Dr. Agnieszka “Bronka” Bronowska

Heidelberg Institute for Theoretical Studies,  
f.r.u. Studio  
Heidelberg, Germany

# INTRODUCTION - WHO I AM



| 12+ years of experience in research: computational chemistry, biophysics, and molecular modelling;

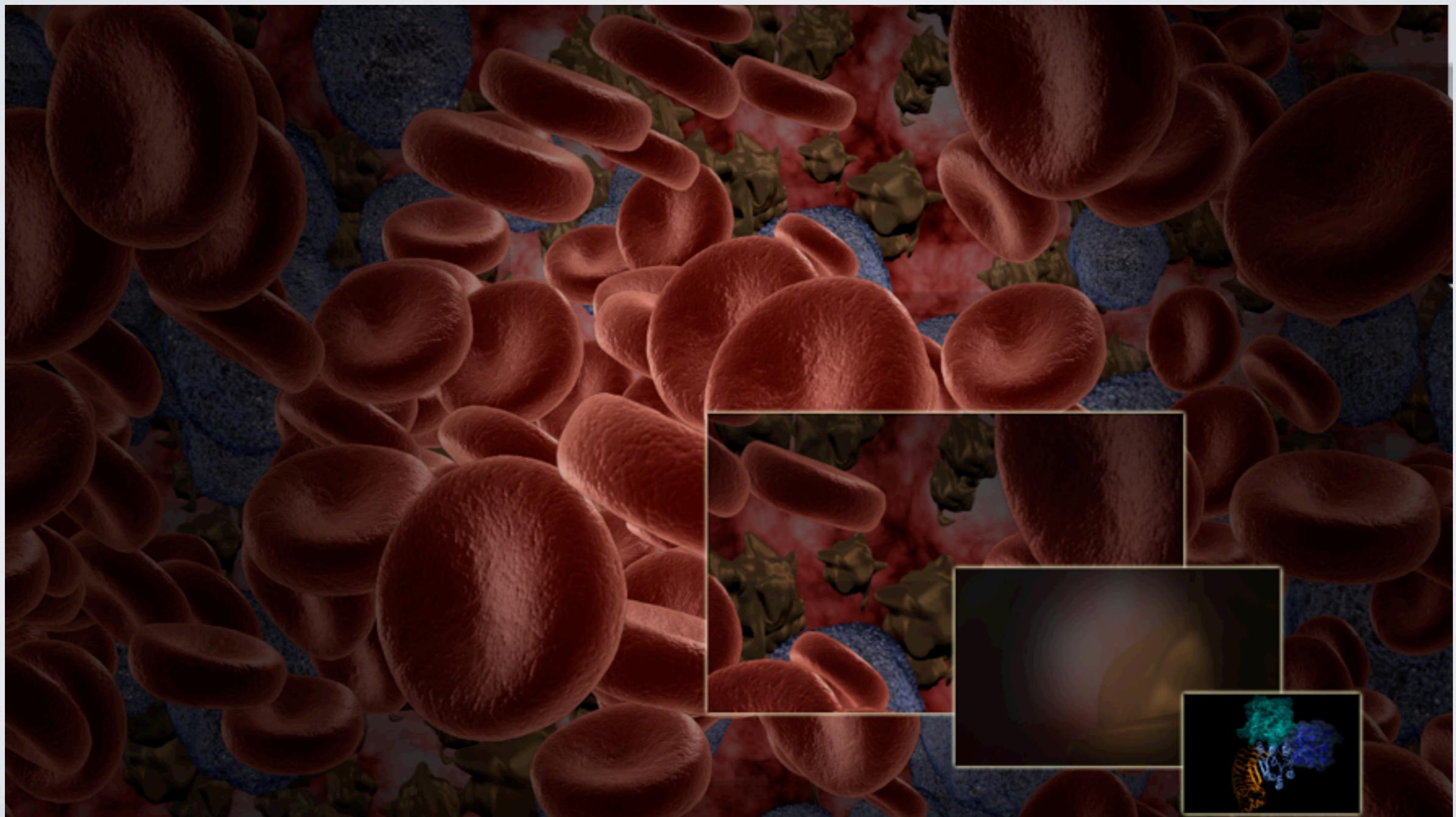
| 15+ years of experience in visual arts: painting, graphical design, motion graphics, animations;

at HITS (formerly EML-Research)  
since 2009;

Artistic Director of f. r. u. Studio  
(since 2011);

# BIOINFOGRAPHICS

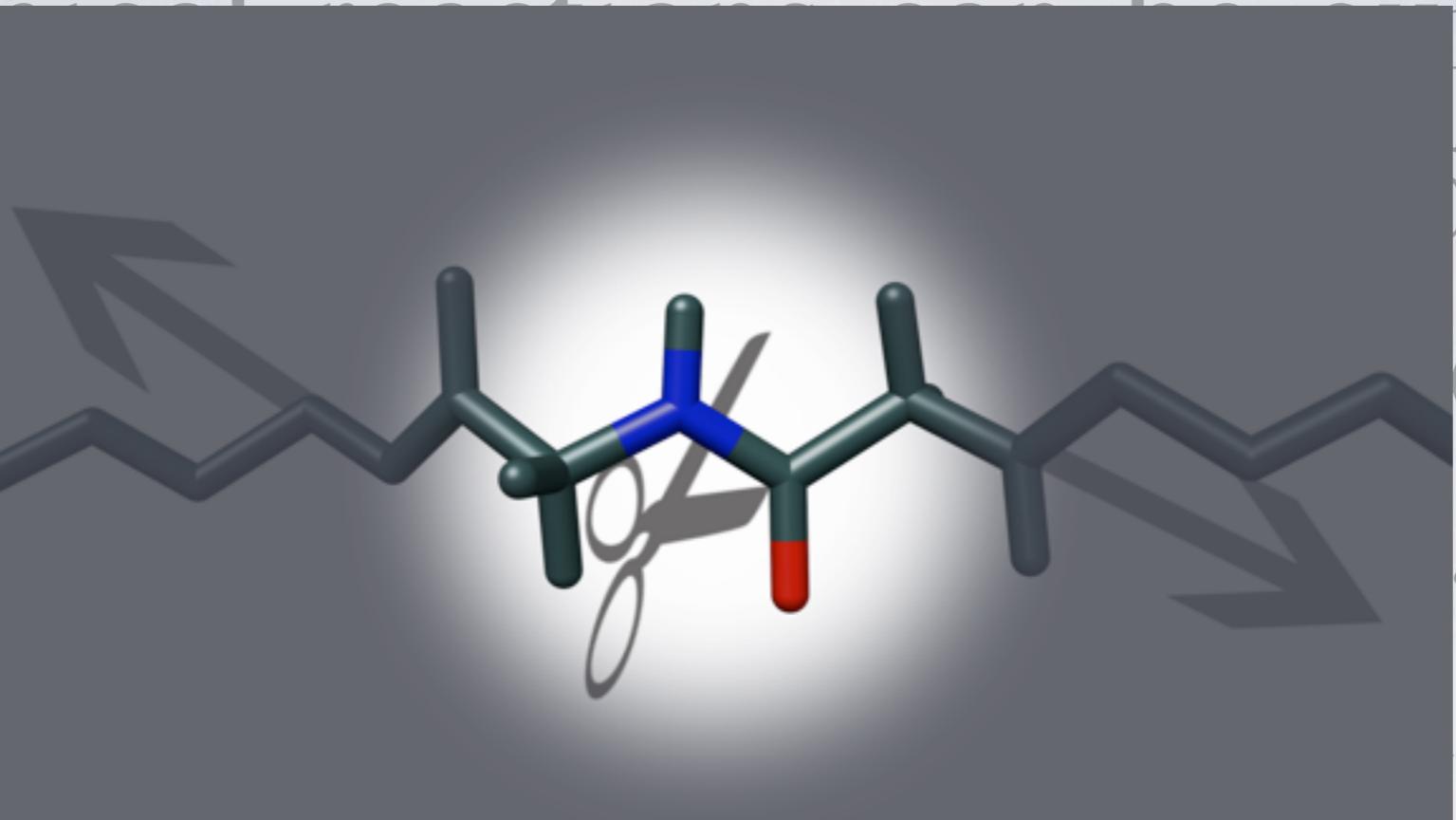
A picture worth a thousands words



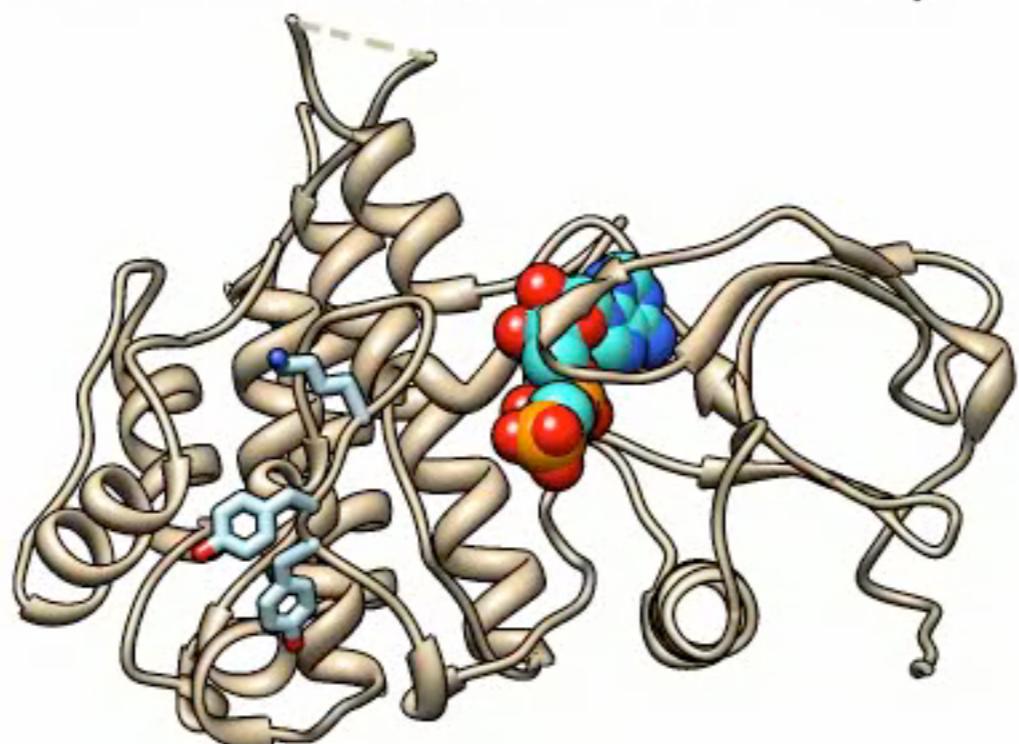
Biochemical reactions can be guided by mechanical forces. It has been shown that the rate of a reaction can be increased in thick protein networks by applying a force. This effect is most prevalent in the combined quenching and stretching experiments. However, the mechanism, is influenced by the mechanical force. Our simulations predict mechanical force-dependent morphing of the FGFR1 kinase domain.

Fei et al., J. Phys. Chem. B, 2011

Morris, Meng & Ferrin, Mol. Cell. Proteomics, 2010



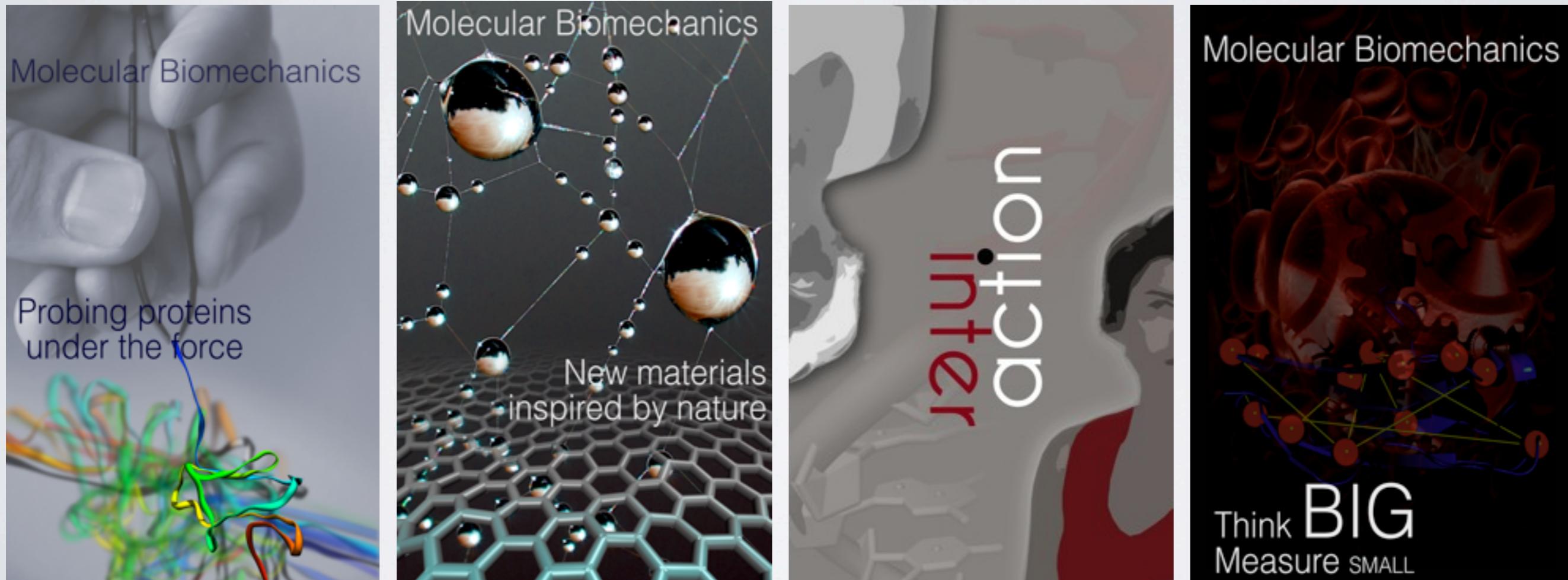
FGFR1 kinase domain morph



# THE ART OF SCIENCE

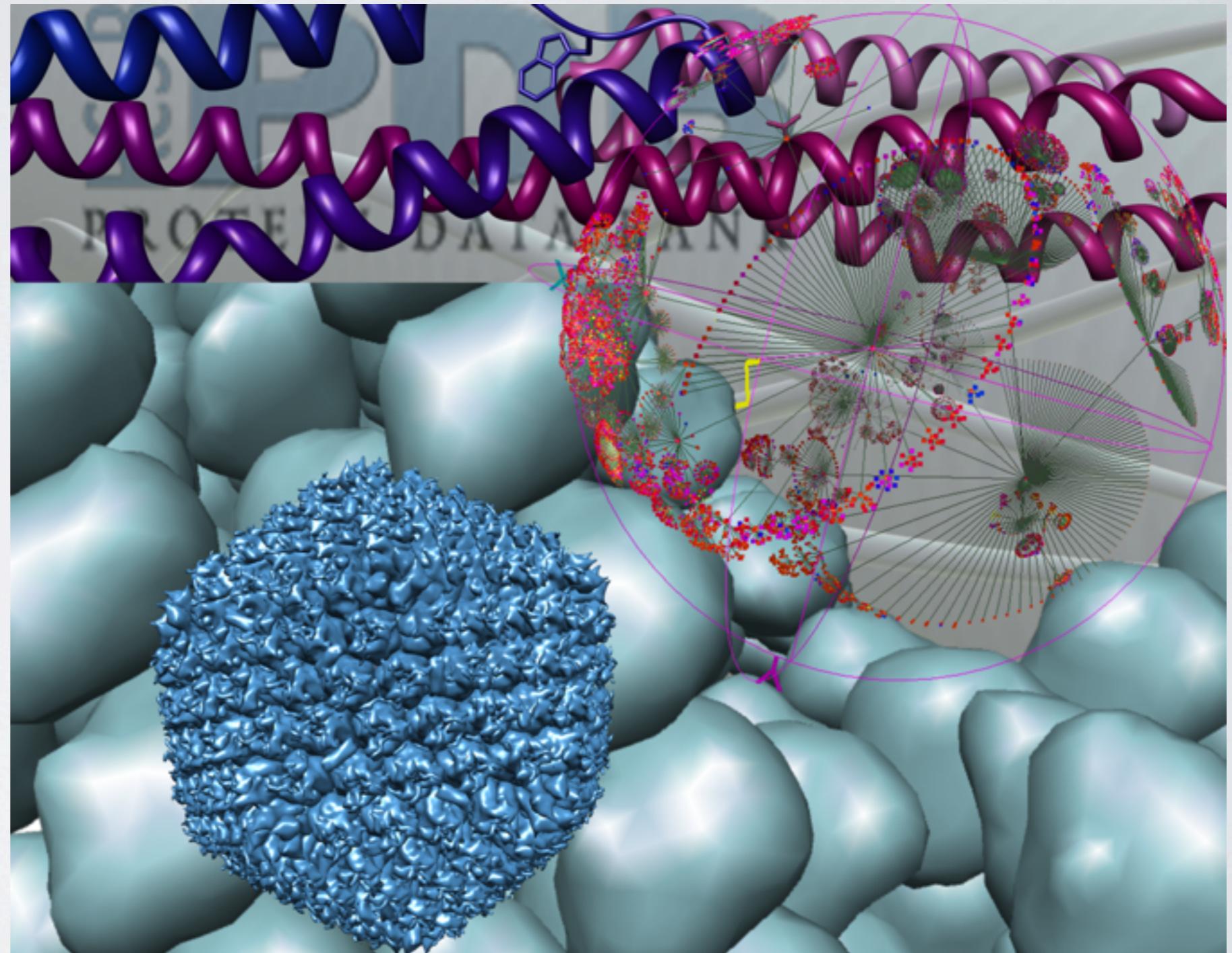
"Science and art are interdependent and inseparable.  
Without some art to it, the best science is reduced to its  
unimaginative mechanics; without science, art becomes  
chaos."

I. J. Singh



# VISUAL REPRESENTATIONS

- Data sources
- Aims
- Available tools
- Representations
- Integration and extending





# DATA SOURCES

Computational chemistry:  
molecular interactions, dynamic behaviour

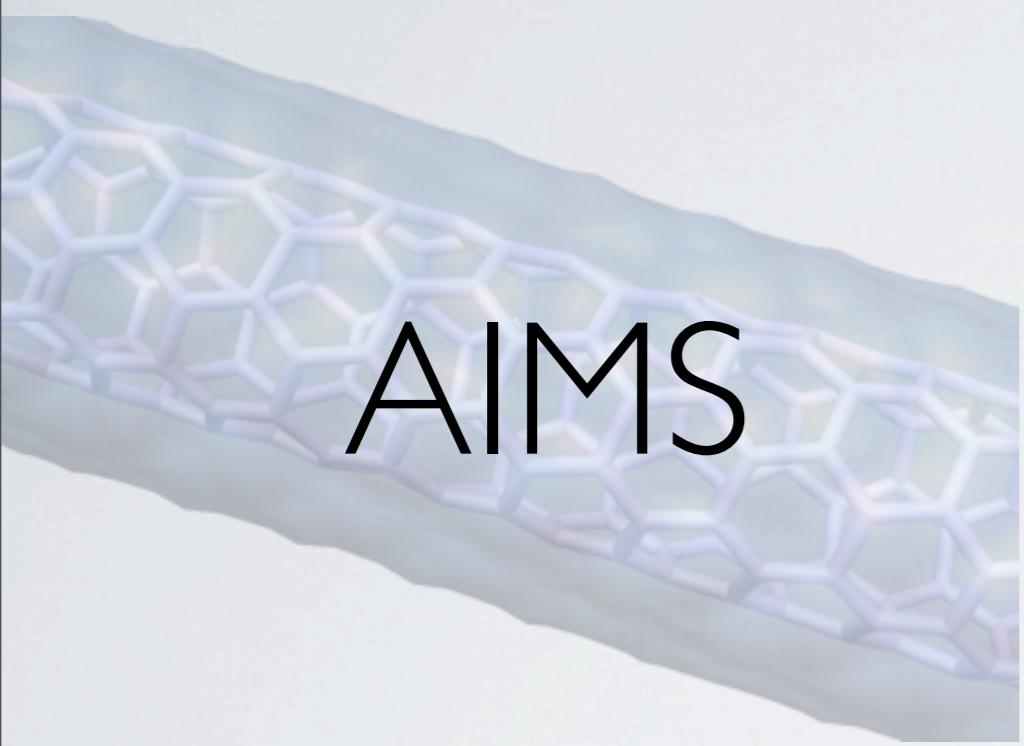
Structural biology:  
crystal structure, NMR

Physical chemistry:  
calorimetric data, SPR, MS

Microscopy:  
volumetric and low-resolution (e.g. EM,  
confocal) data

Systems biology:  
relationships between sequences, structures,  
and functions, a broad view across variety of  
data

High-dimensional techniques (e.g. MRI)



AIMS

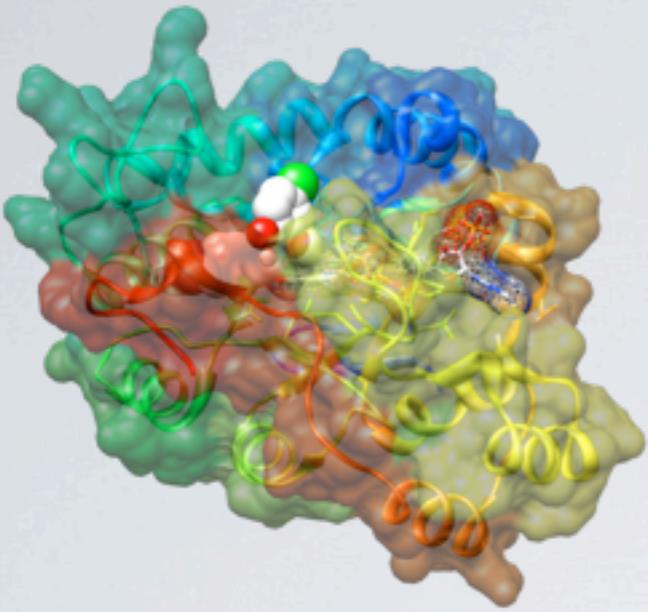
Directing research: fostering new ideas, forming hypotheses;

Publications: clean, informative, high-quality images (static or motion);

Lectures;

Increasing the visibility of results;

Communication within scientific community: collaborative projects, context, perspective;



# TOOLS

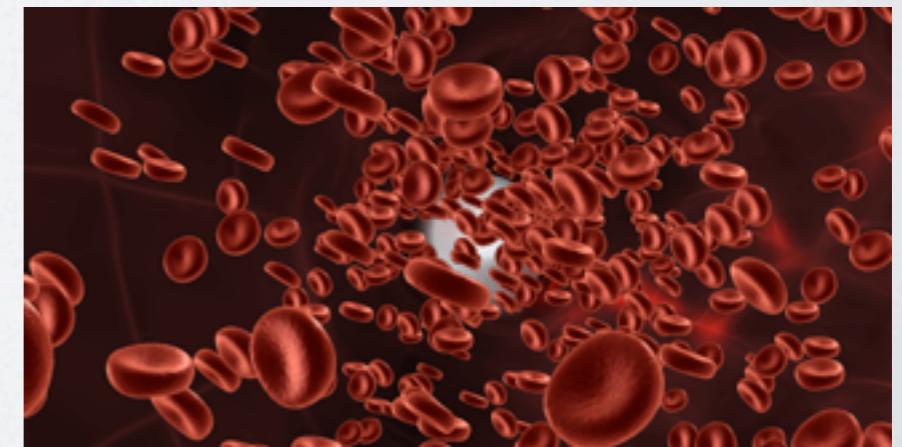
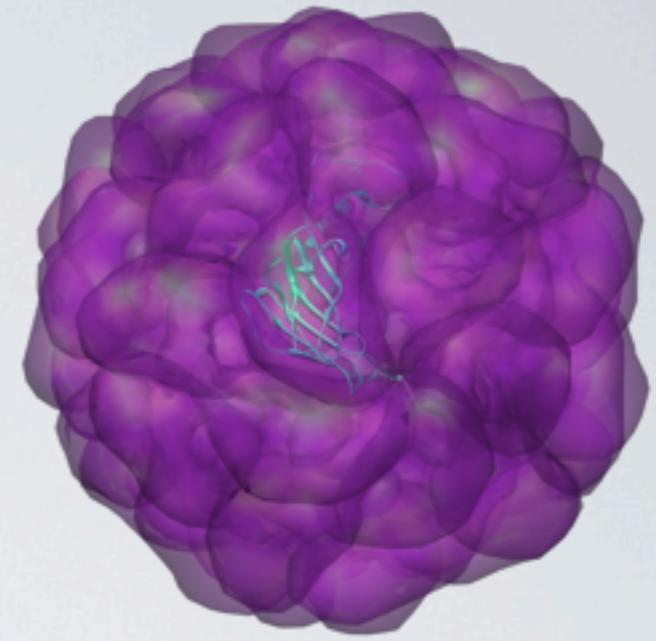
“Full feature” software packages for structural biology:  
UCSF Chimera, VMD, PyMOL

Software packages for systems biology:  
Cytoscape, VisANT, Osprey,  
Skyrails, Walrus

Graphical software:  
Photoshop, Illustrator, GIMP

Motion graphics and video editing:  
After Effects, Premiere, Final Cut, Trapcode

Animations:  
Maya, 3D StudioMax, Zbrush



# BEYOND THE STANDARDS

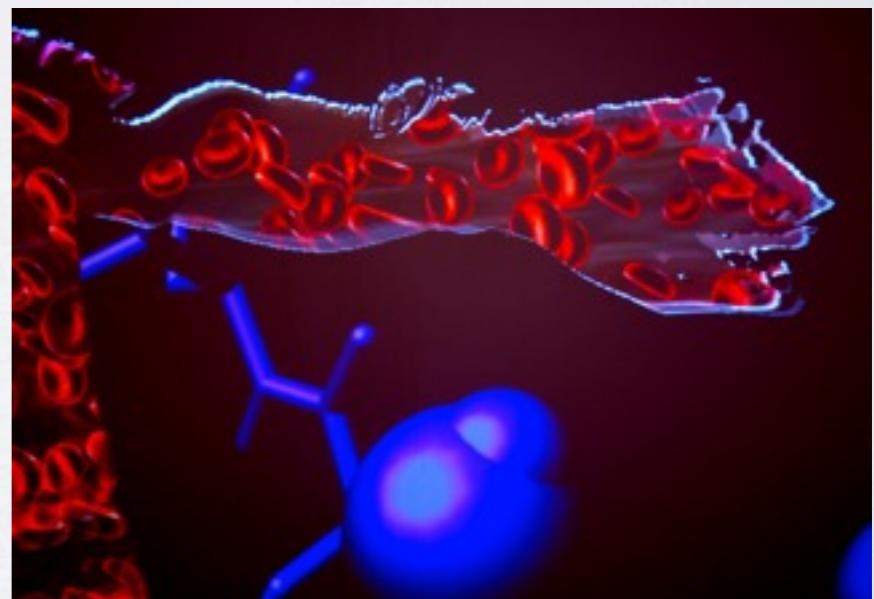
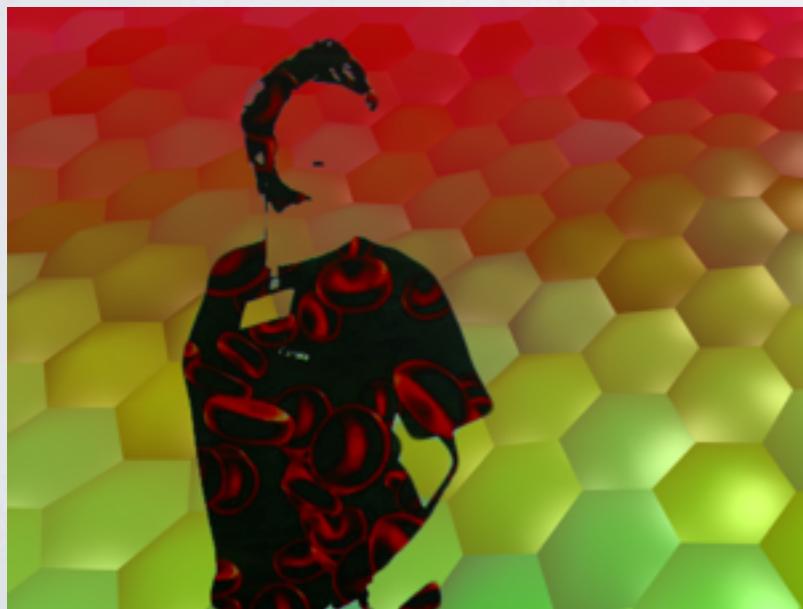


**Video mixers**  
(Modul8, VDMX)

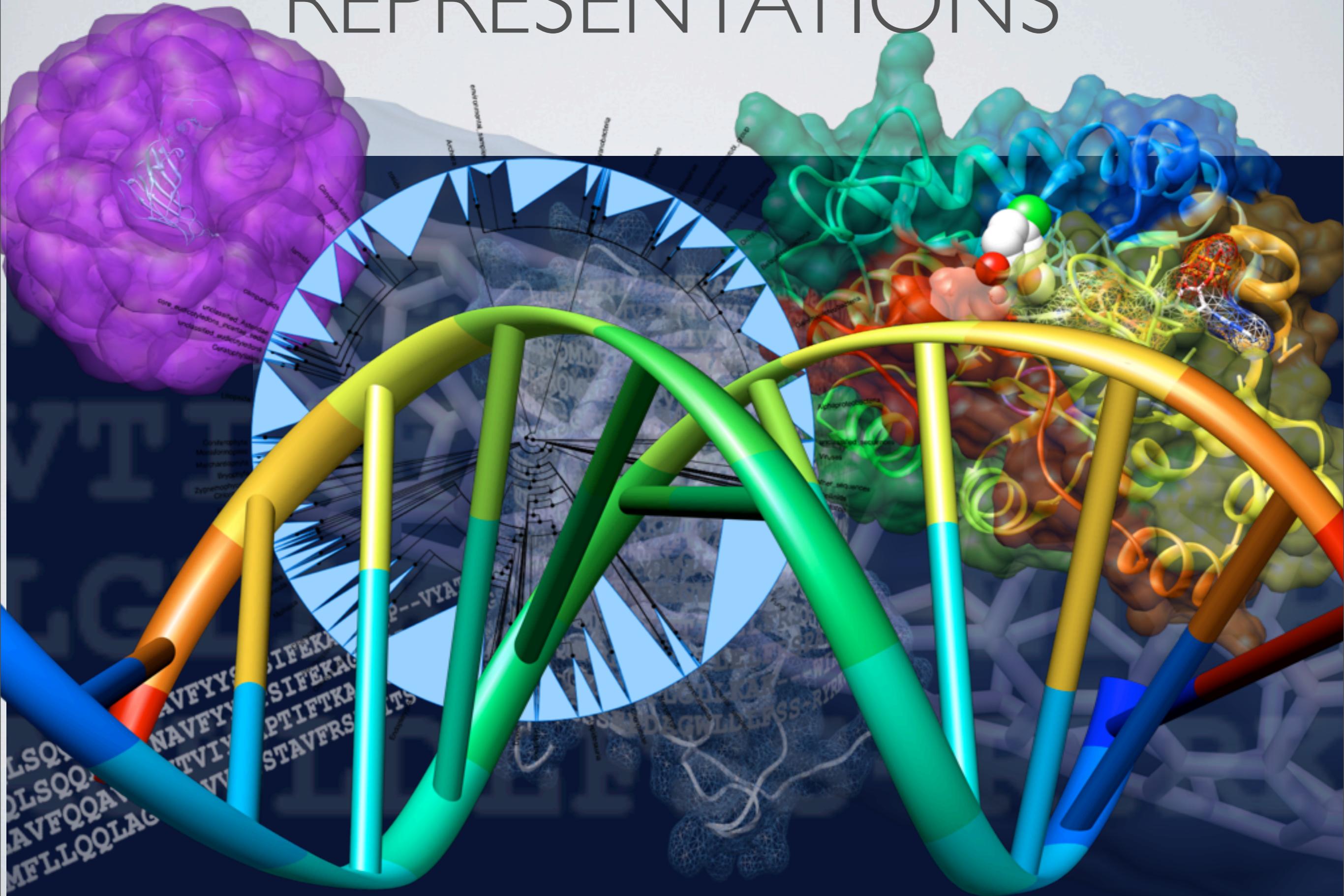
**3D mapping and  
display**

(stereoscopy-capable  
workstations, AE,  
MadMapper, VideoBlocks)

**“New technologies”**  
(Kinect, Arduino-based  
sensors)



# REPRESENTATIONS



# MOTION GRAPHICS

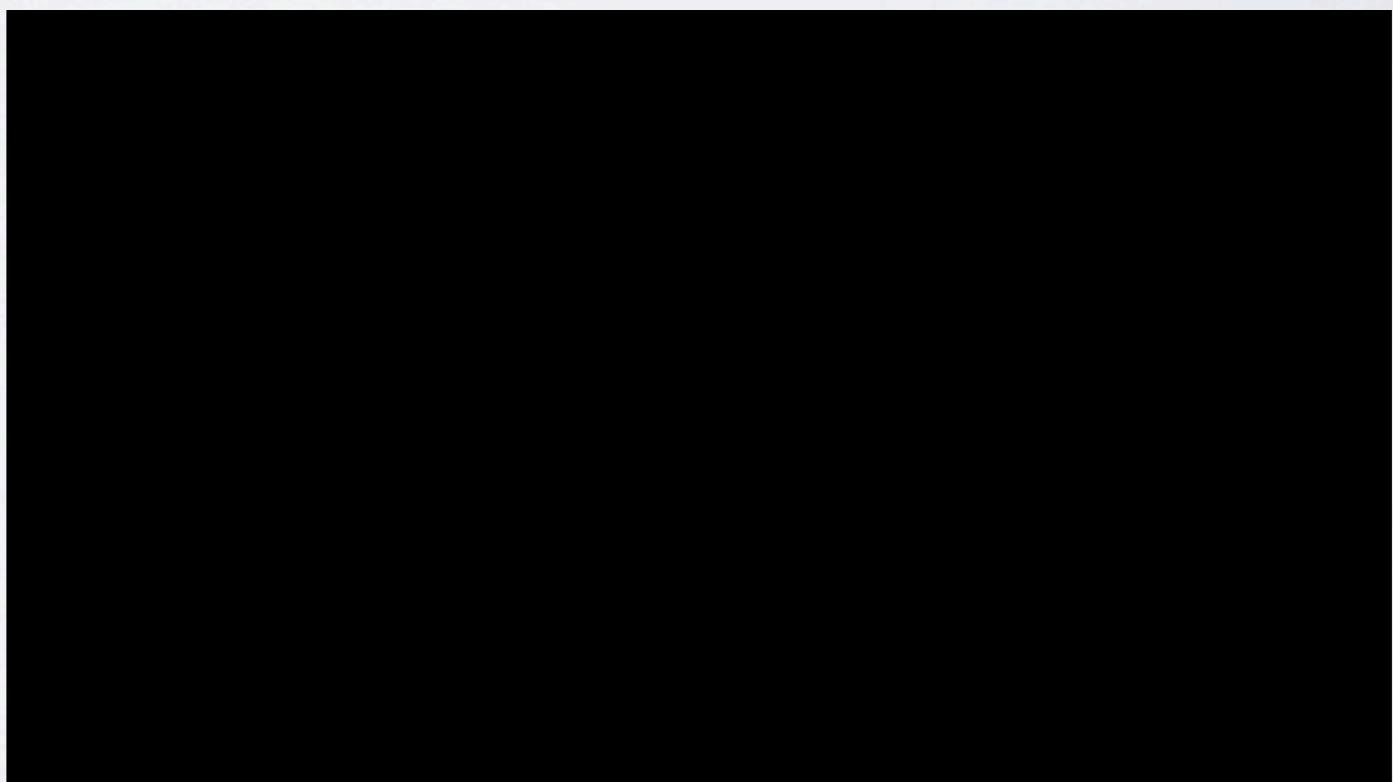
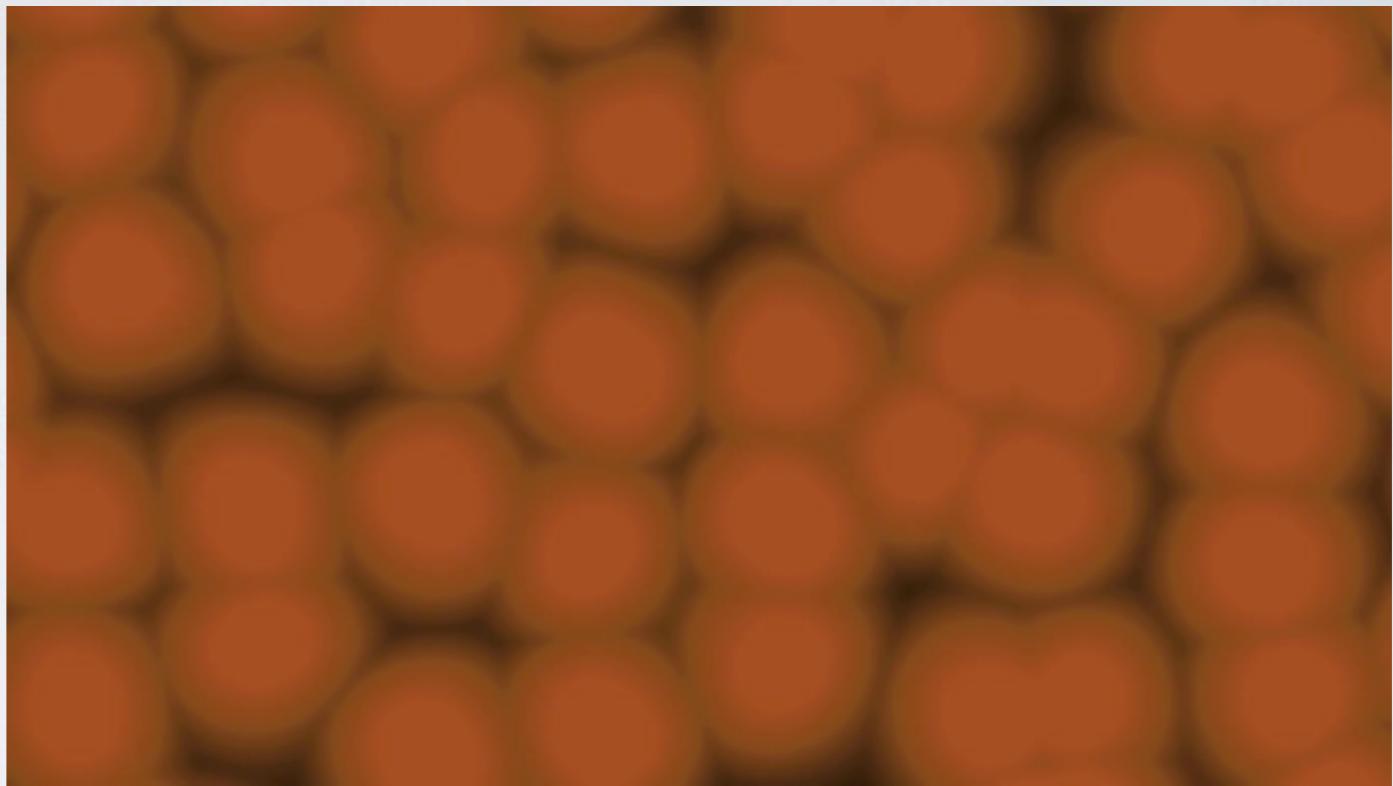
Provides 3D insights;

Indicates interactions  
(morphing between  
conformers, transient  
binding sites);

Displays dynamical  
behaviour (molecular  
ensembles, time-dependent  
events);

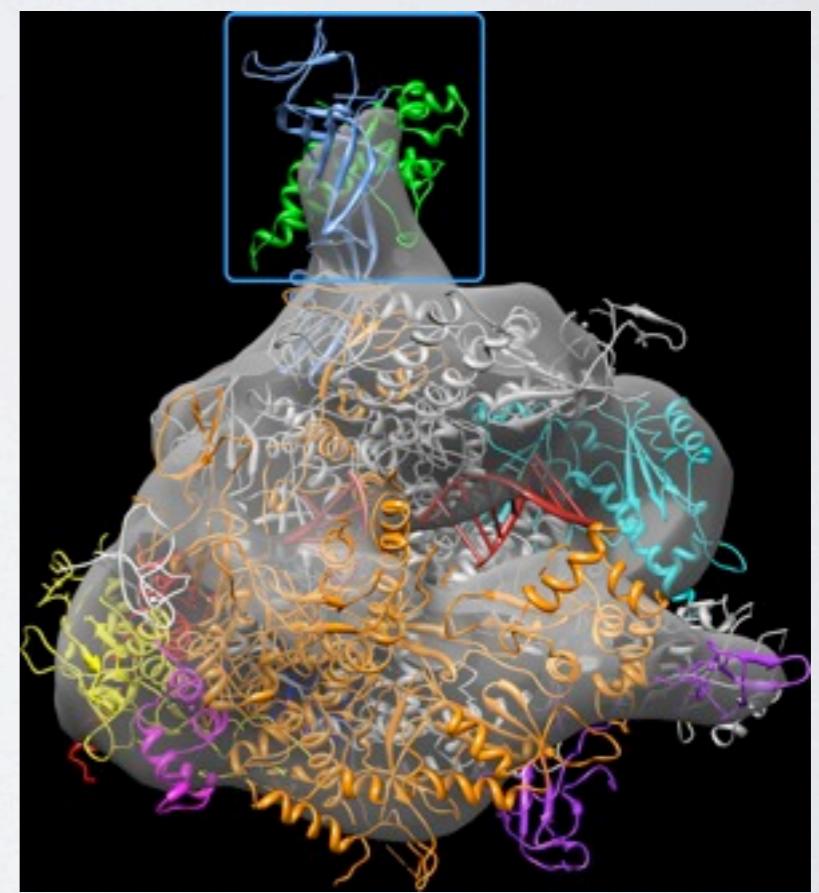
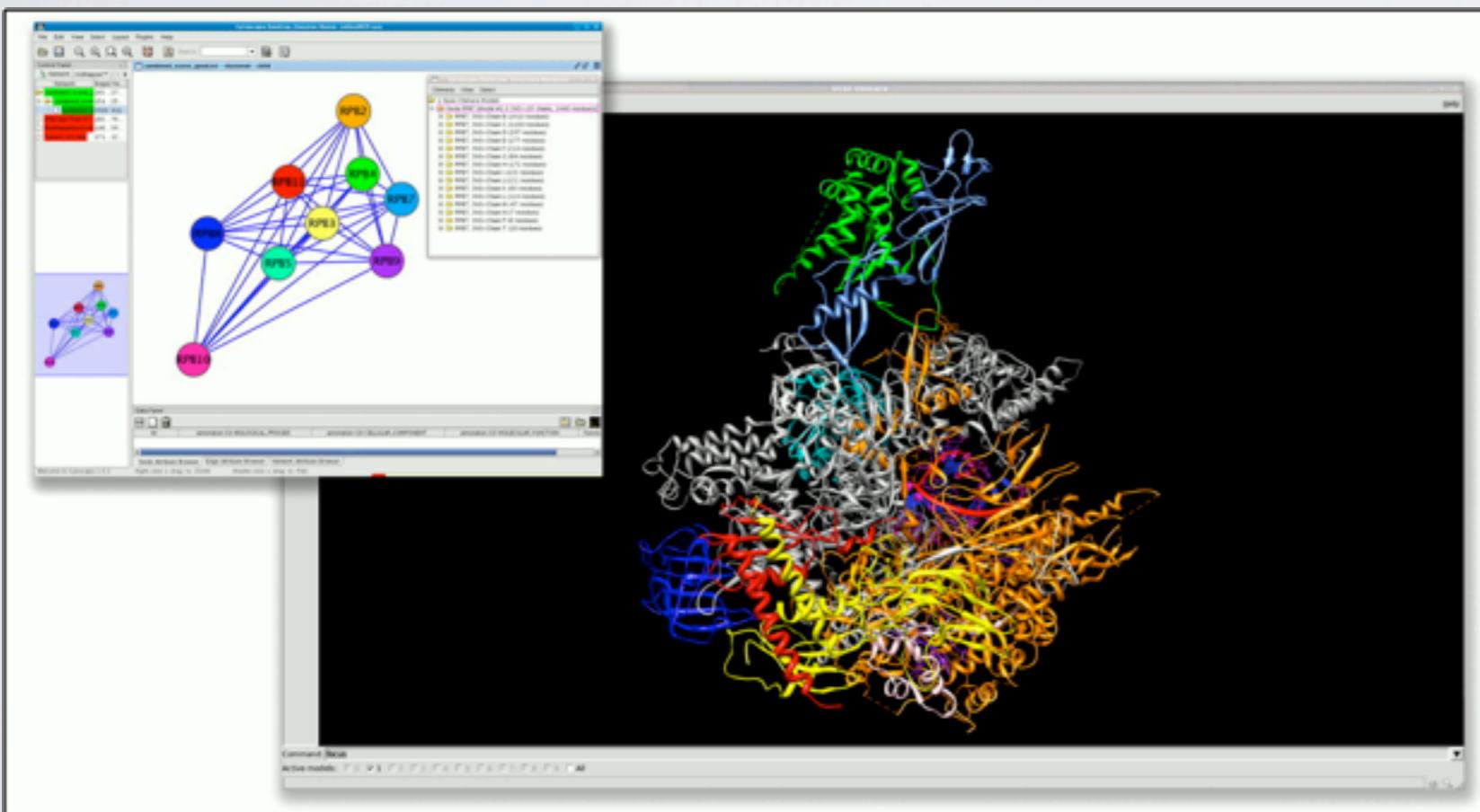
Visualization of molecular  
mechanisms (e.g. kinase  
activation, silk fiber, protein  
unfolding);

Multiscale representations.



# VISUALIZATIONS FOR SYSTEMS BIOLOGY

Example: UCSF Chimera / Cytoscape **structureViz** plugin



Human/Yeast RNA Polymerase II fitting, Morris, Meng & Ferrin, Mol. Cel. Proteomics, 2010

# INSTEAD OF CONCLUSIONS

What can I do for you?

# ACKNOWLEDGEMENTS



**Conrad Huang, John “Scooter” Morris, Darren Weber, Eric Pettersen,  
and Thomas Ferrin**

UCSF Chimera

**Andrew Kramer**  
Video Copilot

**Dave Evans**  
f.r.u. Studio

**Alistair Burleigh, Adam Monk**  
Wrap3

**Wolfgang Müller, Martin Golebiewski**  
HITS

# SOME USEFUL LINKS

**UCSF Chimera** <http://plato.cgl.ucsf.edu/chimera/>

**VMD** <http://www.ks.uiuc.edu/Research/vmd/>

**Maya** <http://usa.autodesk.com/maya/>

**mMaya** <http://www.molecularmovies.com/toolkit/>

**Adobe Suite** <http://www.adobe.com/products/creativesuite.html>

**Video Copilot** <http://www.videocopilot.net/>

**Red Giant** <http://www.redgiantsoftware.com/>

**Wrap3** <http://www.wrap3.co.uk/>

**ZBrush** <http://www.pixologic.com/home.php>