

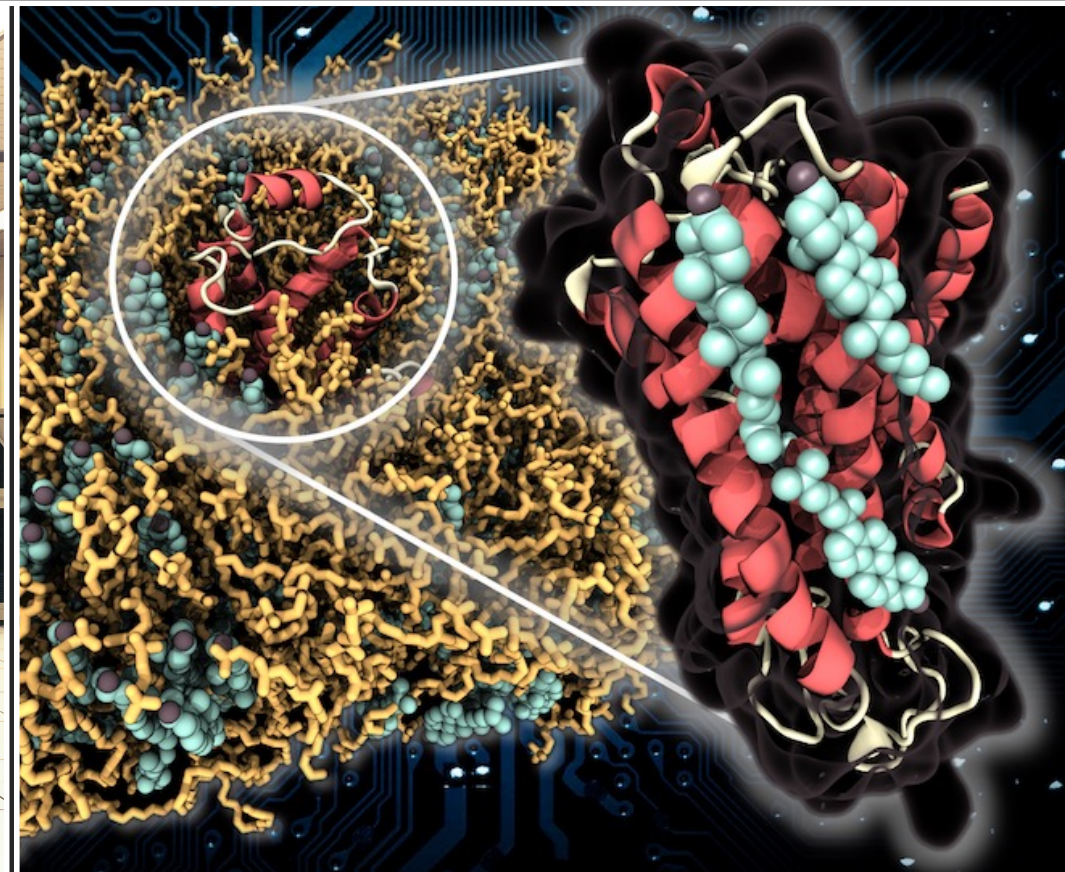
# Physics of Biology – Biomolecular Simulations of Living Systems

Ilpo Vattulainen

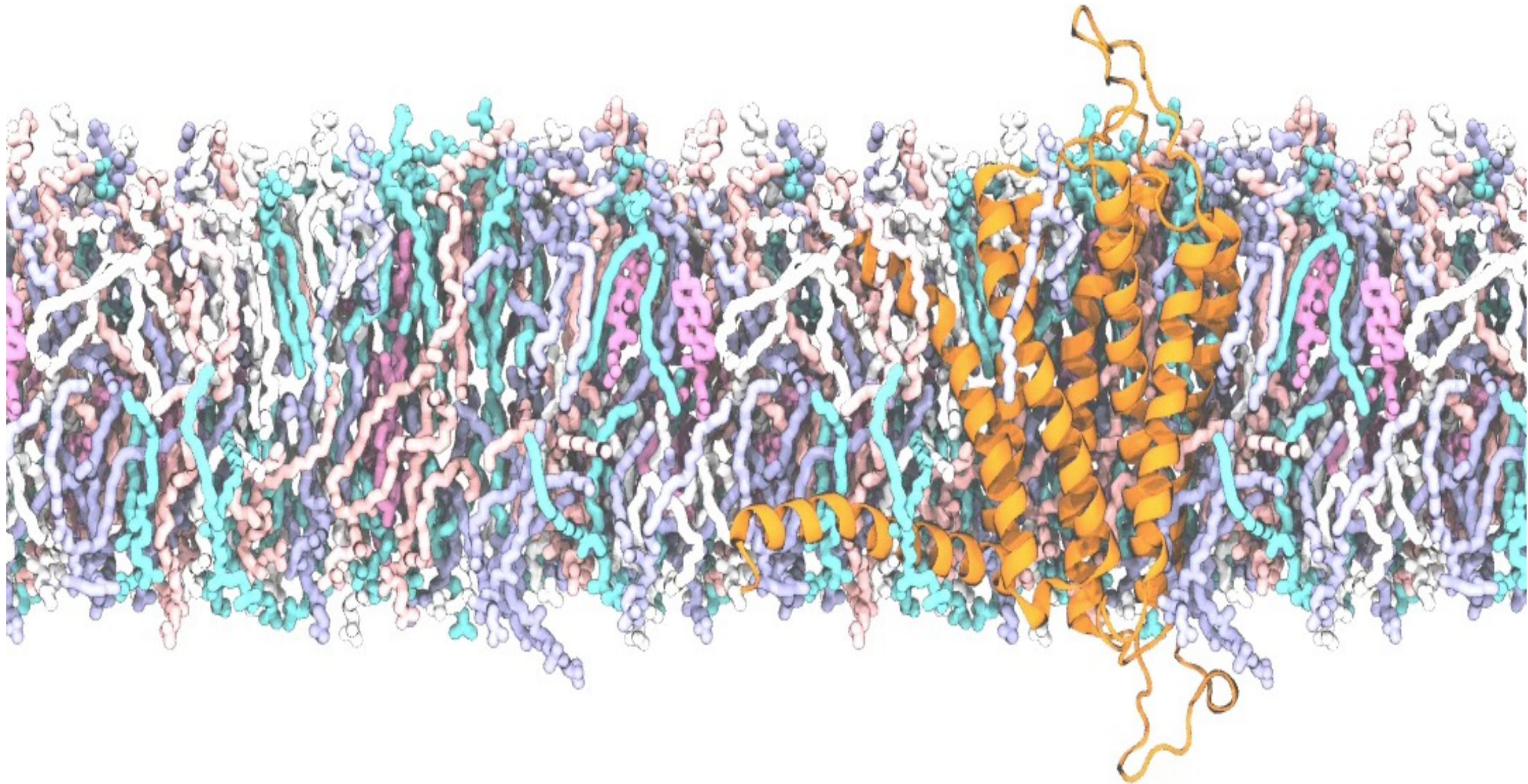
Biological Physics

Dept Physics, Univ of Helsinki, Finland

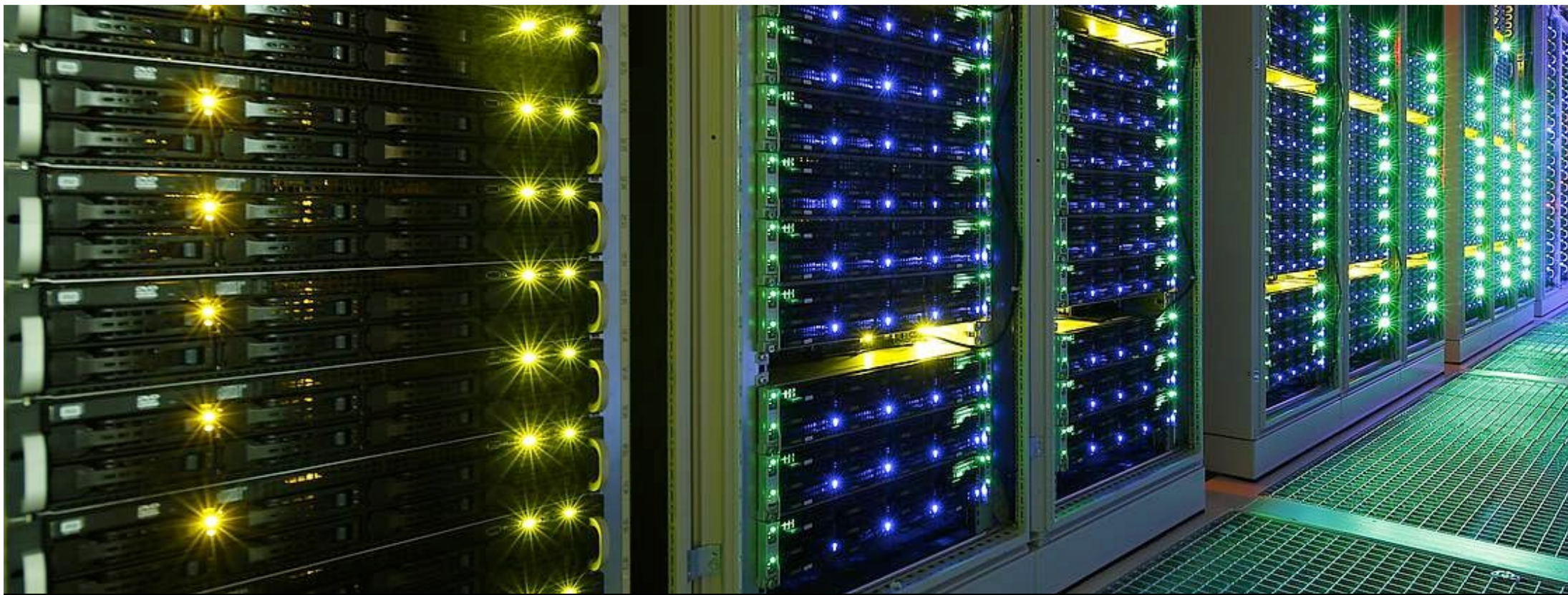
Center of Excellence in Biomembrane Research



# ATOMISTIC & MOLECULAR SIMULATIONS

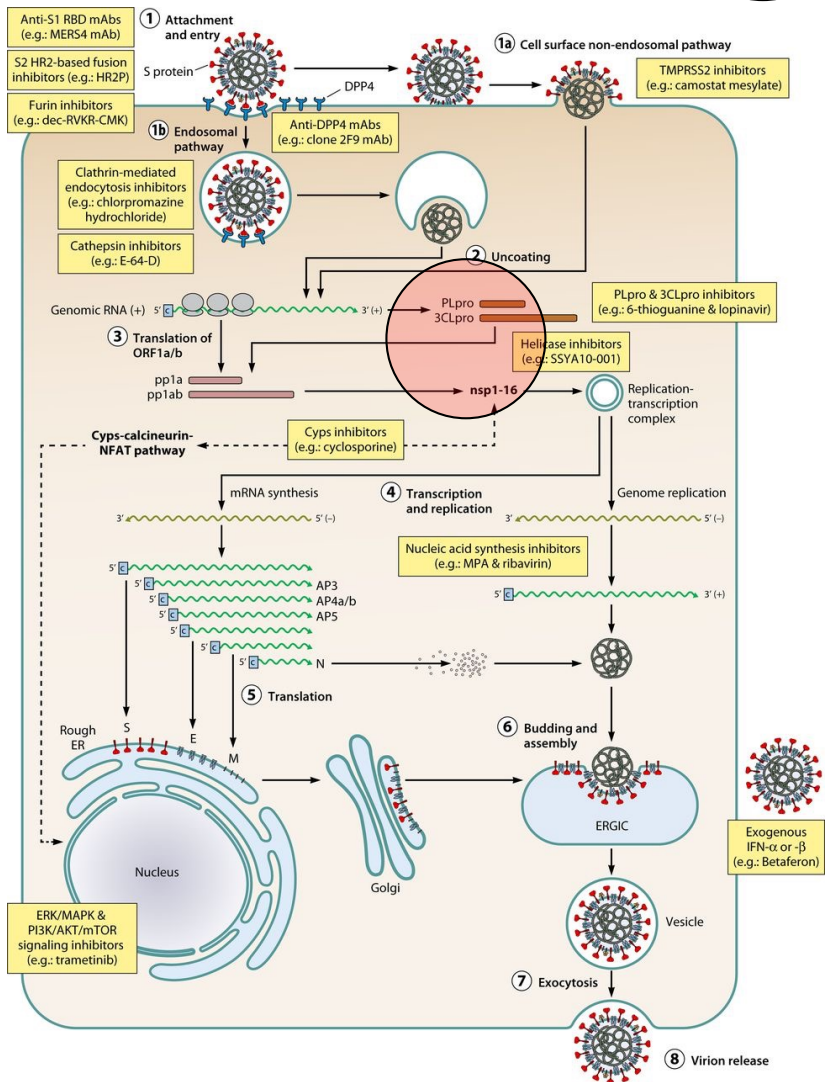
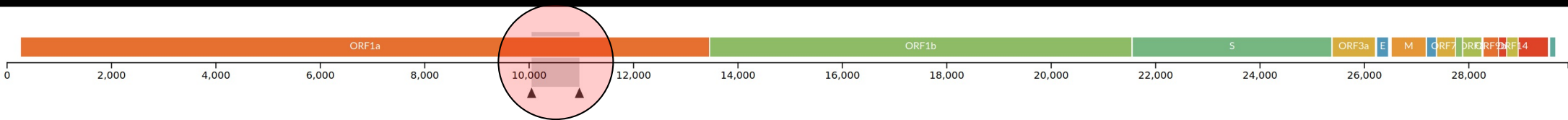


# COMPUTER SIMULATIONS TODAY

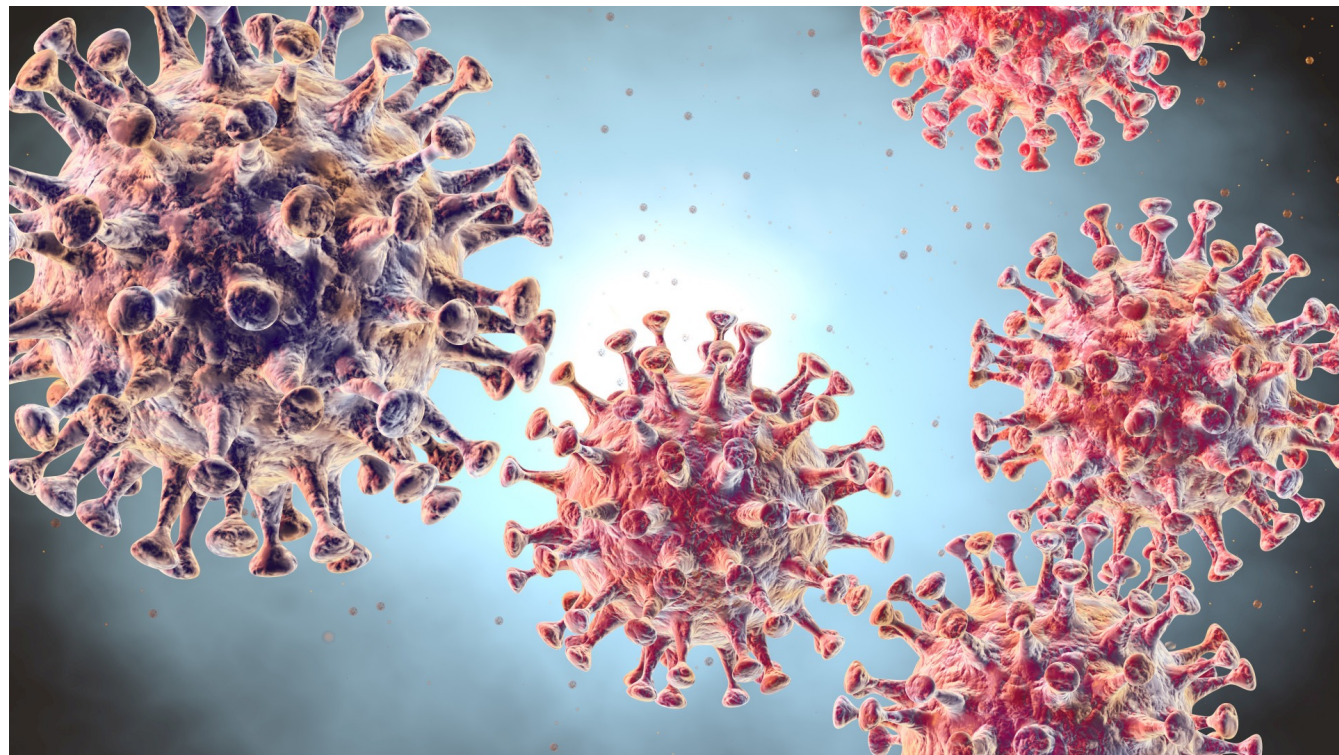


**ENIAC was able to carry out  $\sim 10^4$  operations/second.  
Today, the leading supercomputers do close to  $10^{18}$  operations/second.**

# TIMELY SAMPLE: SARS-COV-2 & ITS MAIN PROTEASE (3CLPRO)



After viral entry, an enzyme known as the main protease of SARS-COV-2 is needed for its replication. If the function of main protease is blocked, the replication of the virus is inhibited.

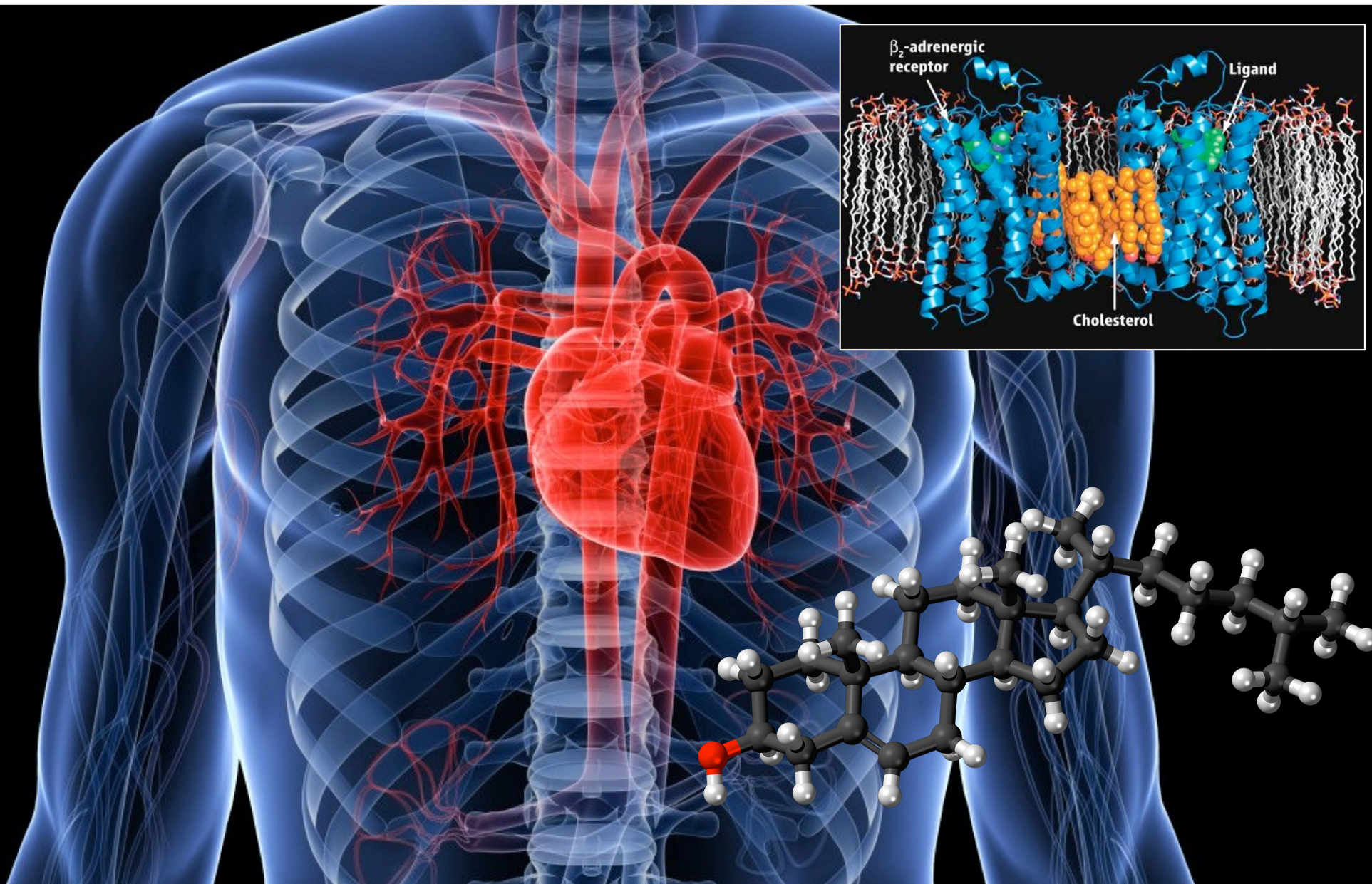


# LEUKEMIA - DIMERIZATION OF CYTOKINE RECEPTORS

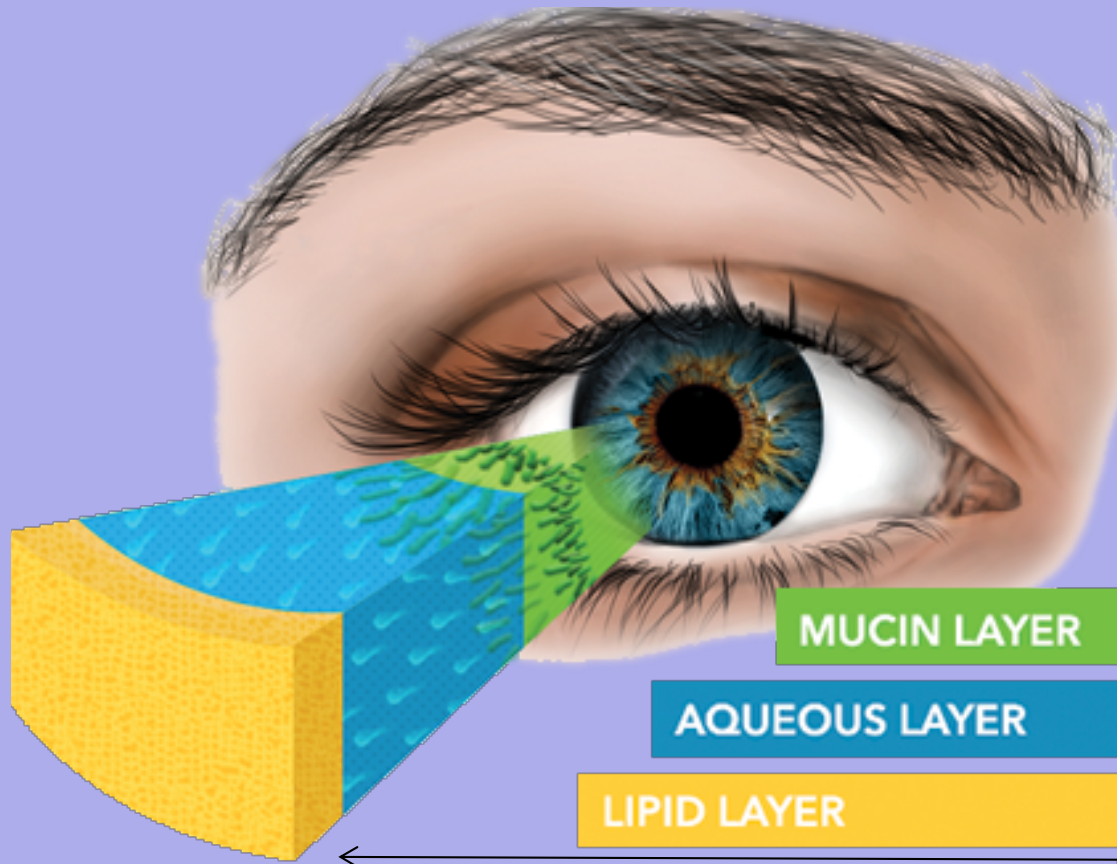


- If these receptors associated with Janus kinases are too active, the outcome can be disease, such as leukemia
- Typical cause are mutations, but the mechanism of action?
- Experiments & simulations showed that the mechanism of activation is the dimerization of two related monomer proteins
- Certain mutations induce dimerization without cytokine binding

# TACHYCARDIA – BETA BLOCKERS AND LIPIDS CONTROL THE BEATING OF THE HEART



# DRY EYE SYNDROME



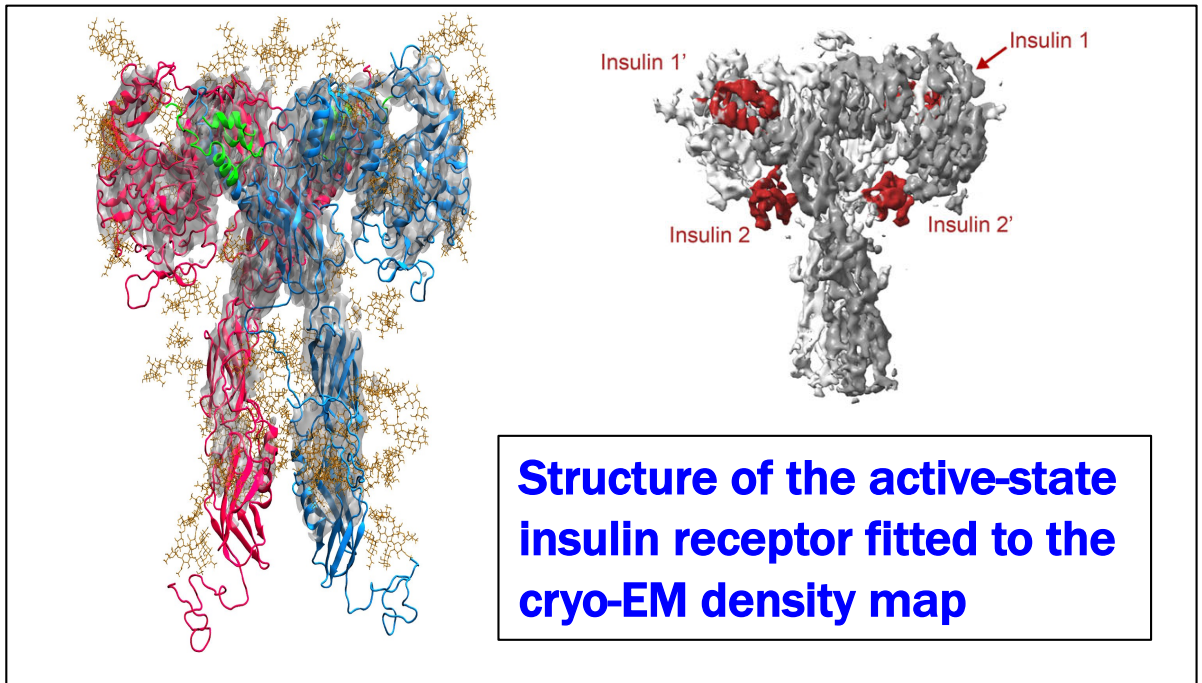
**Tear Fluid Lipid Layer (TFLL):  
~20-100 nm thick**

- **One of the most common ophthalmological diseases**
- **Typically caused by excessive evaporation of tear fluid from the ocular surface**
- **Current eye drop treatments help only a couple of hours – some key content is missing**
- ***Lipidomics data show that DES patients have reduced wax ester profiles in the tear fluid lipid layer***

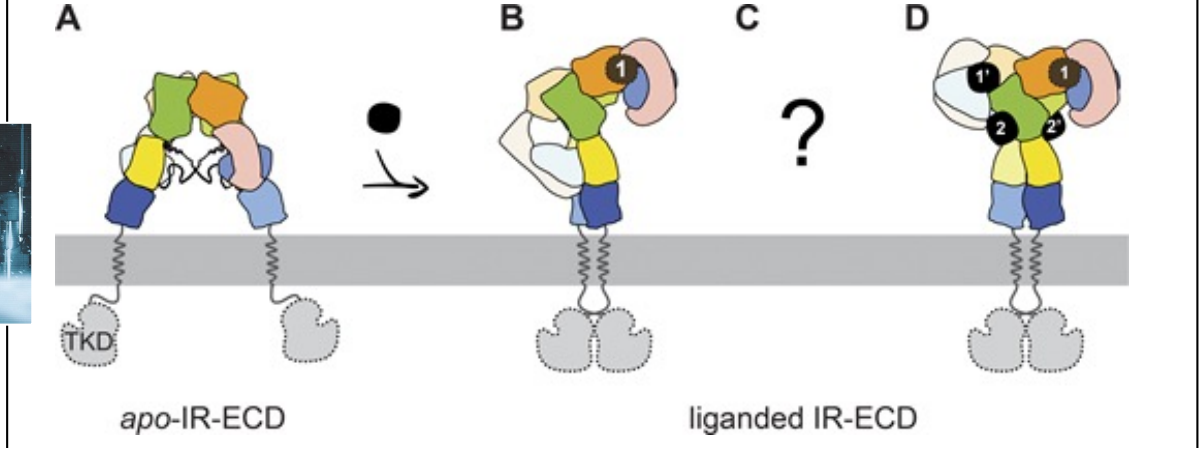
# IMPAIRMENT OF INSULIN RECEPTOR ACTIVATION LEADING TO TYPE 2 DIABETES



Guttman et al., J Cell Biol (2019)



However, activation process of the insulin receptor?





# Biological Physics of Living Systems

<https://www2.helsinki.fi/en/researchgroups/biophysics>

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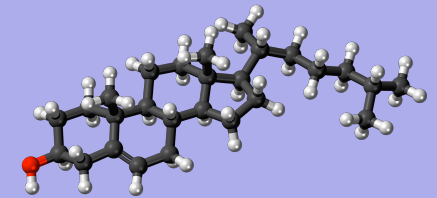
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Kandista Graduun ja Väitökseen...

## Biomolecular Simulations & Artificial Intelligence Contributing to Health

- How biological processes take place in healthy cells?
- And if biological processes are impaired, then how diseases emerge?



### Examples

- Intelligence – where does it arise from? (Memory, recognition, etc.)
- We stay alive due to oxygen pumped by our lungs, but why?
- Type 2 diabetes & cardiovascular diseases (good and bad cholesterol)
- Neurological diseases
- Eye diseases
- Heart diseases, such as tachycardia
- Cancer in its many forms
- Viral infections & immunity
- How cells generate the energy they need for their survival

