

On computational analysis of macromolecules

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Life Sciences
Center



Institute of
Biotechnology

Life on the molecular level

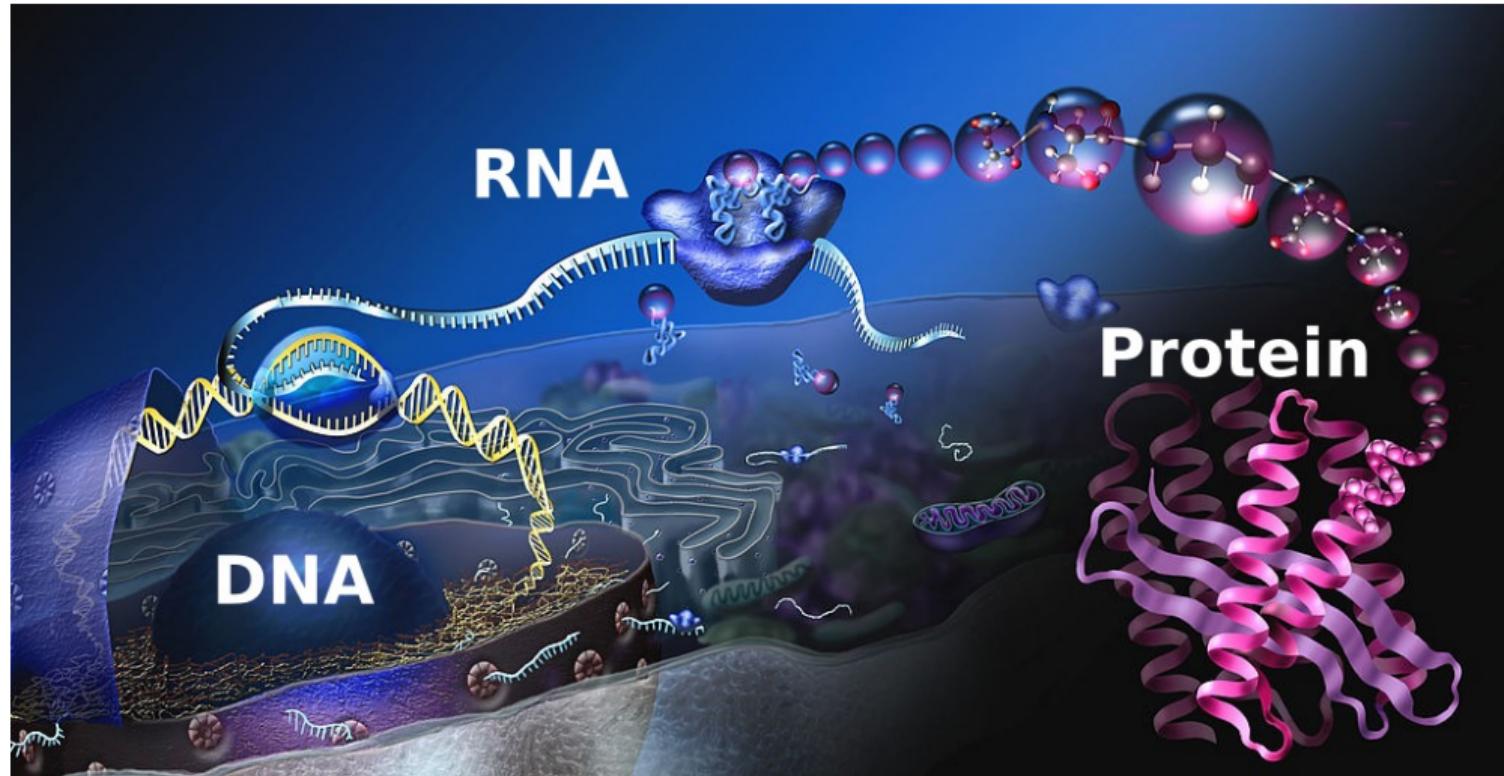
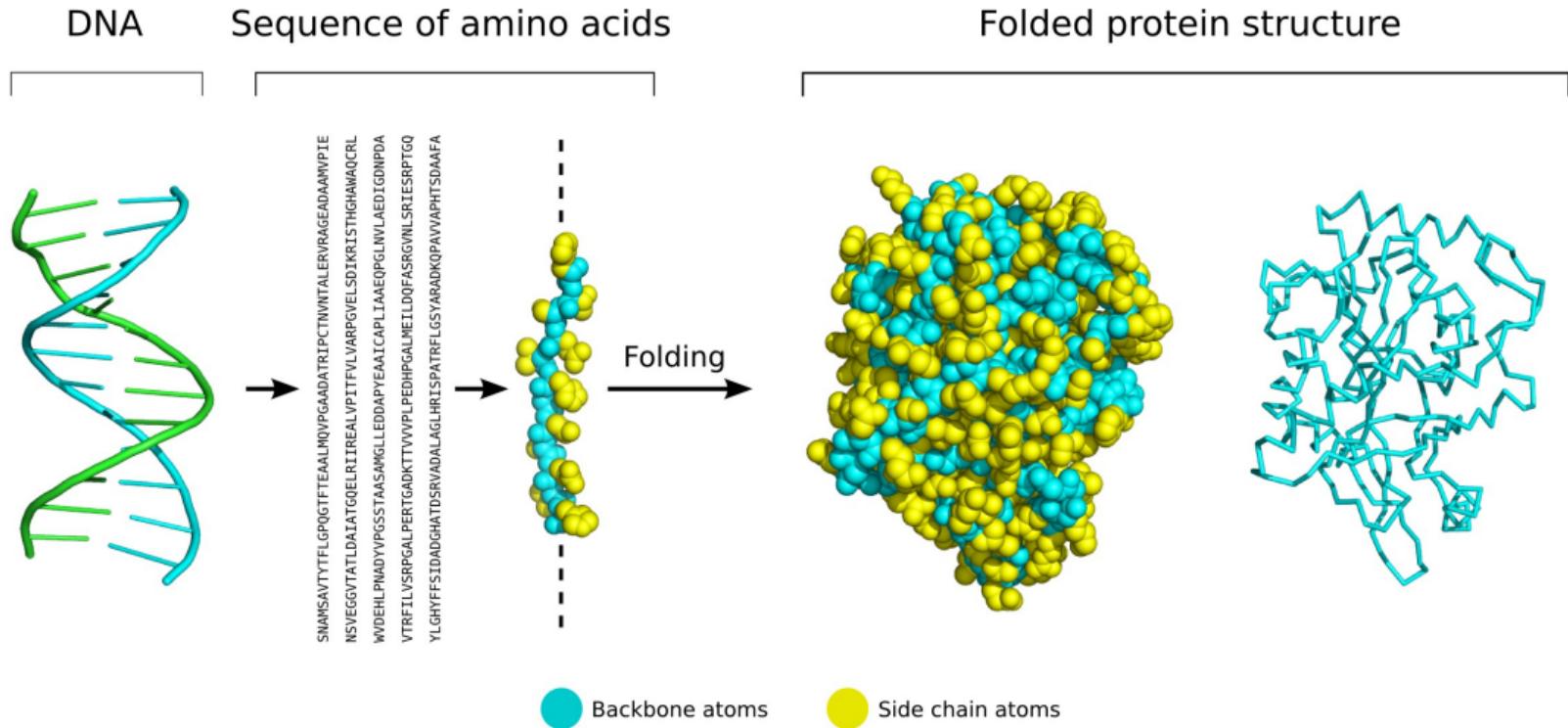
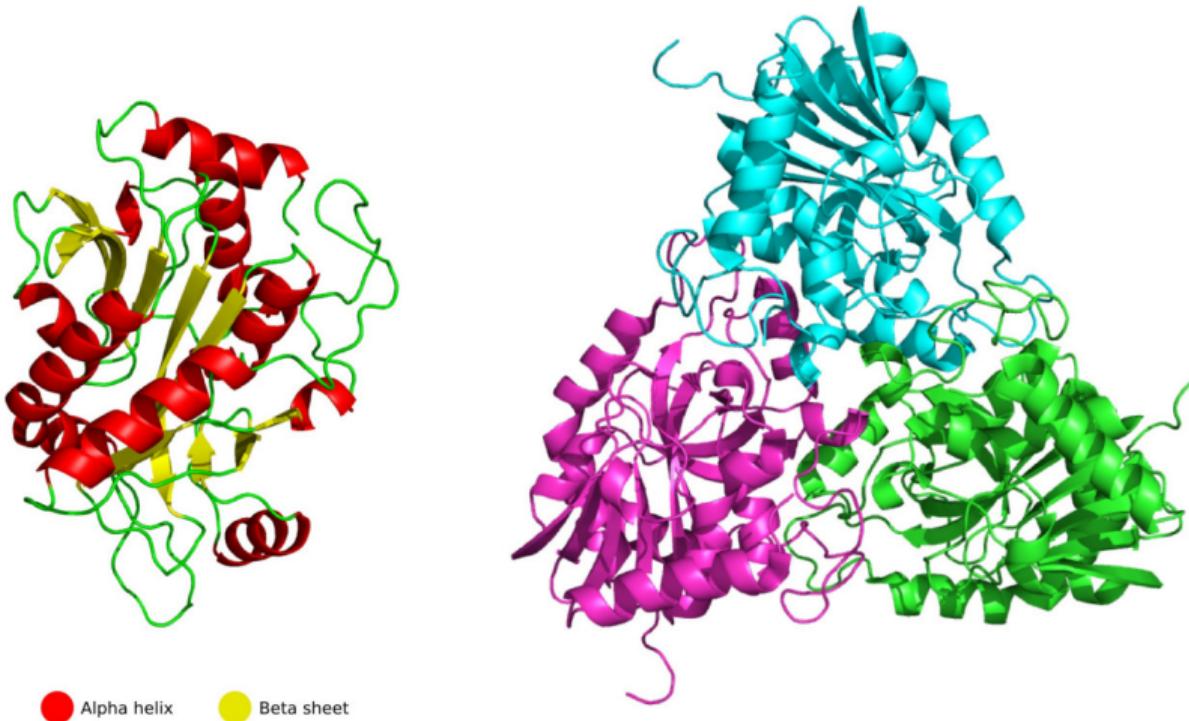


Image source: jonlieffmd.com/blog/new-studies-reveal-higher-levels-of-genetic-complexity

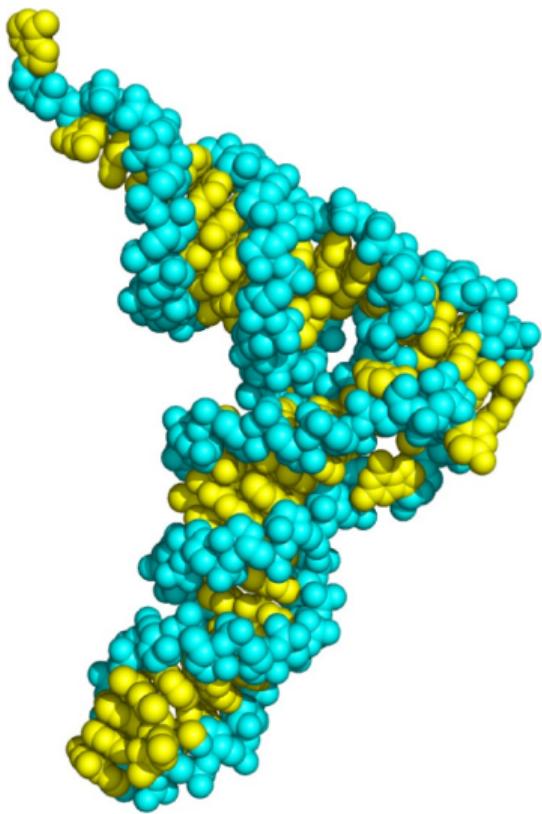
Protein structures



Protein structures



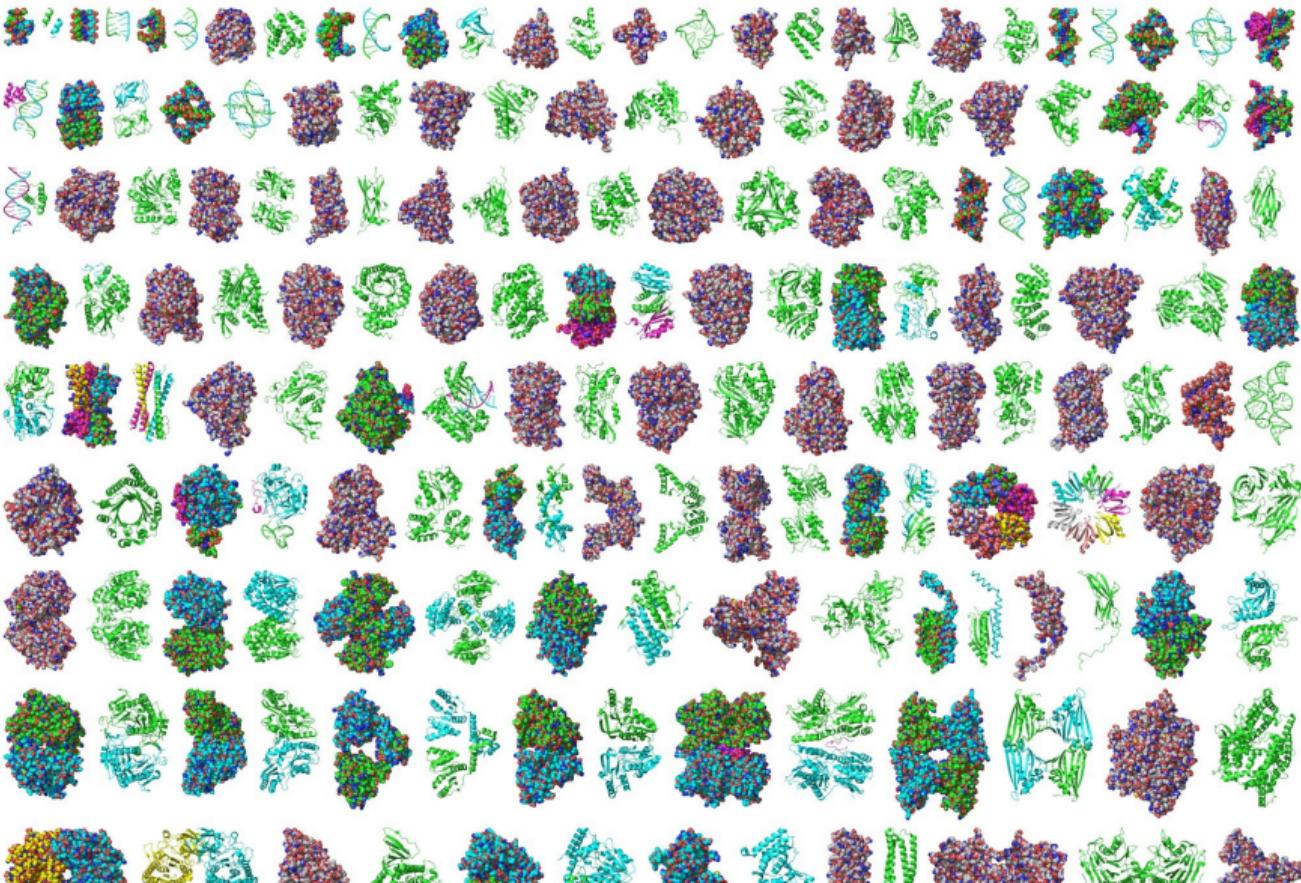
Nucleic acid structures



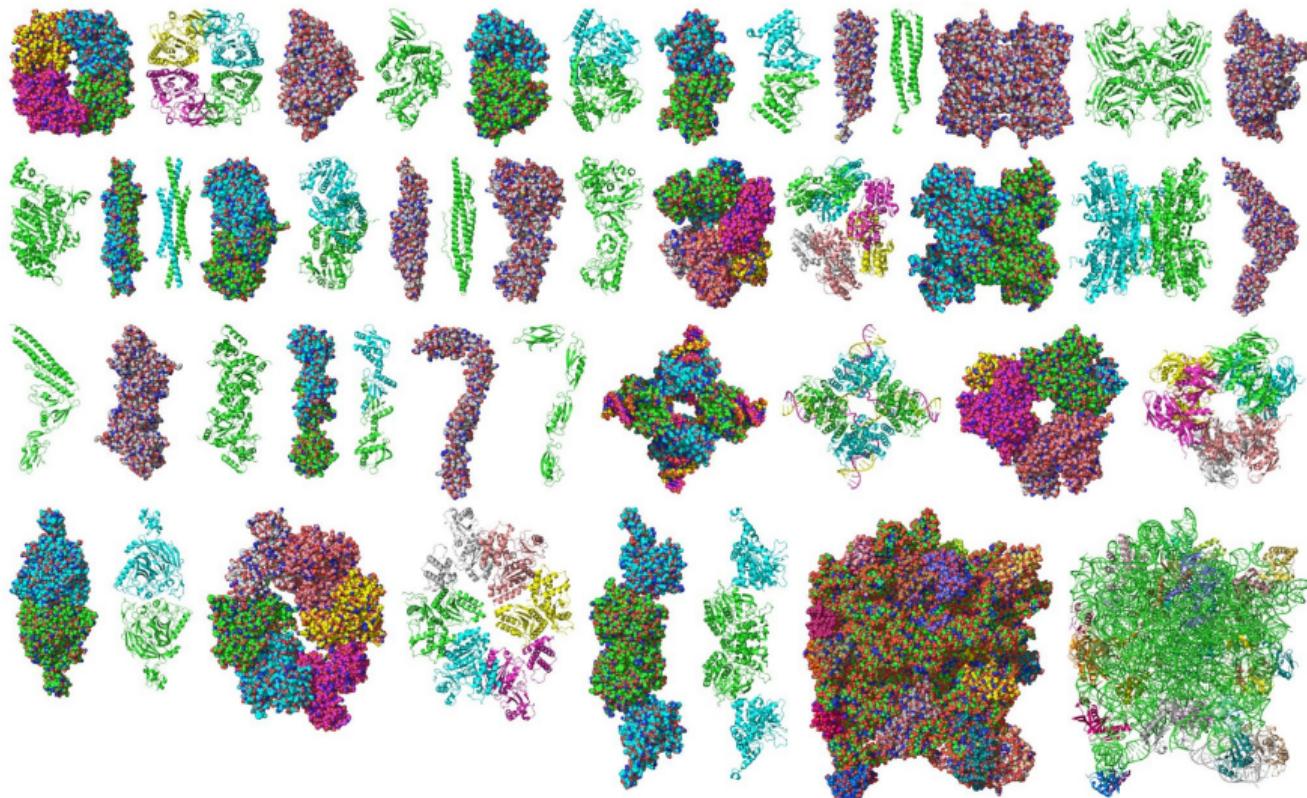
Protein and nucleic acid complexes



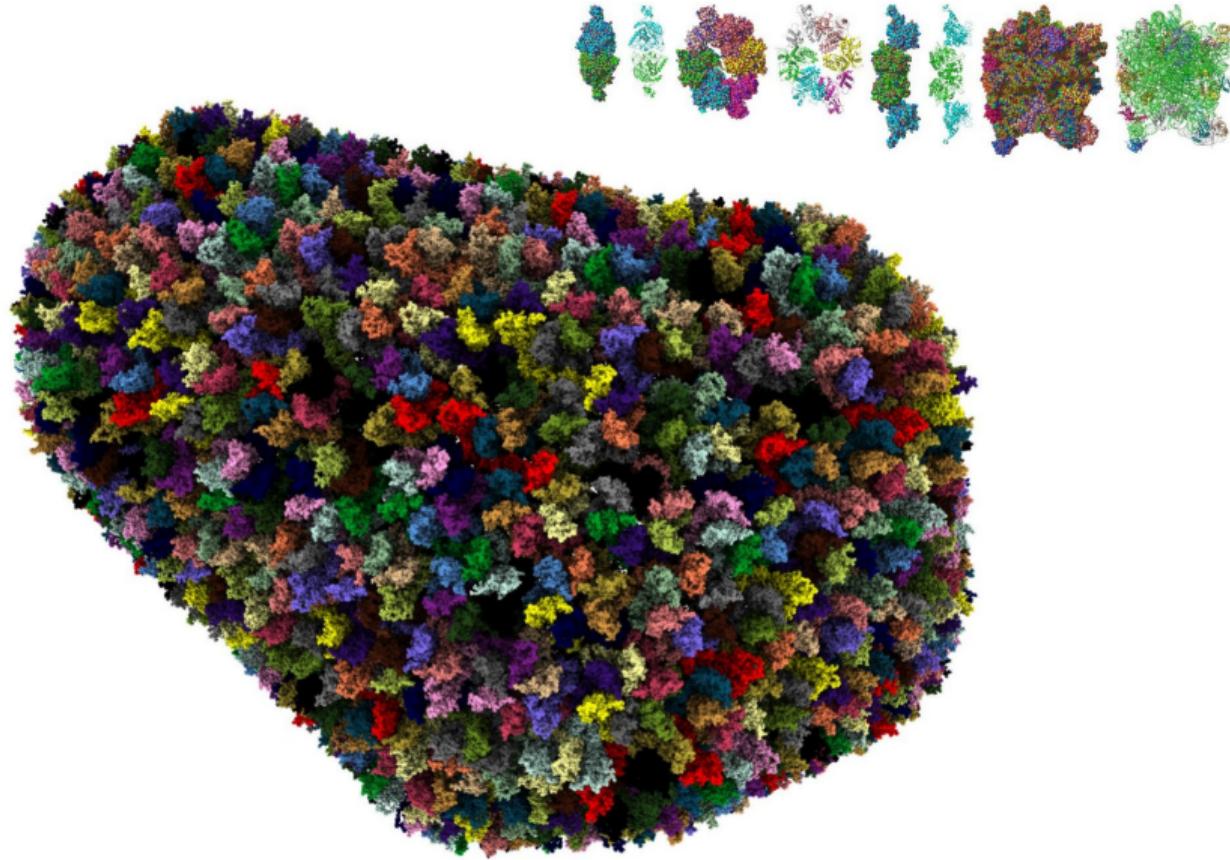
Variety of biomolecular structures

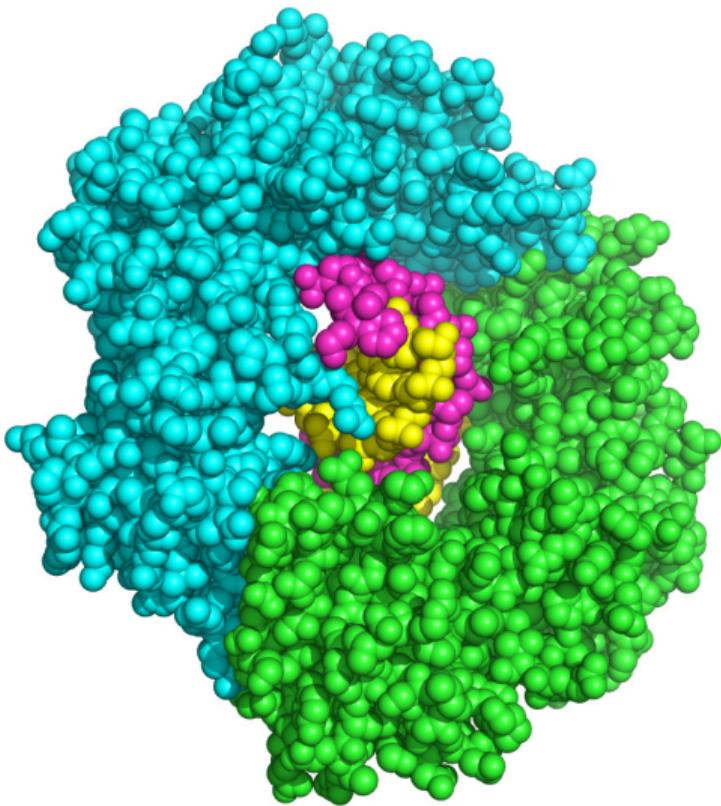


Variety of biomolecular structures



Variety of biomolecular structures





When studying biological macromolecules, some common problems are:

- ▶ analyzing how different parts in a molecule interact
- ▶ selecting the best prediction of a multimeric complex

Some possible solutions involve:

- ▶ computational geometry
- ▶ machine learning using open data
- ▶ developing free software

Let's try things

Go to "<https://www.kliment.lt/current>", open the Voronota-GL viewer.

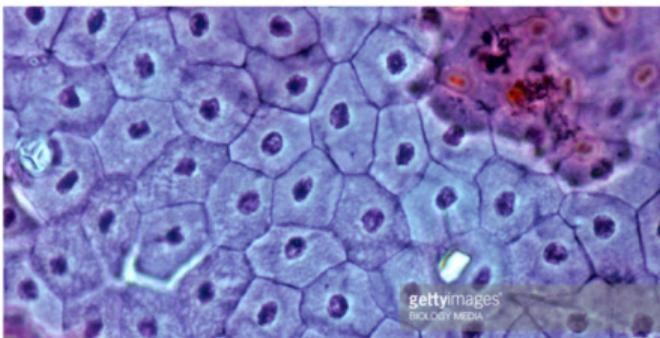
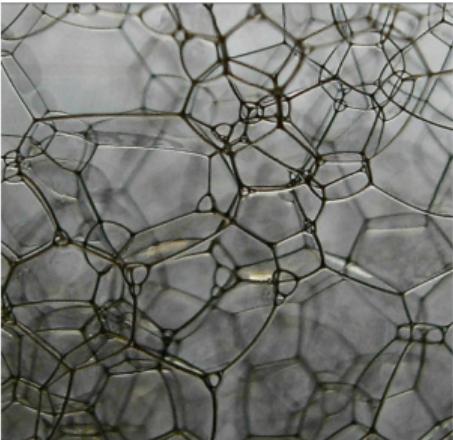
In Voronota-GL, fetch '1azm', let's look at it.

Then fetch '1ca2', '1cam', '1cnw'.

Voronoi diagram intro

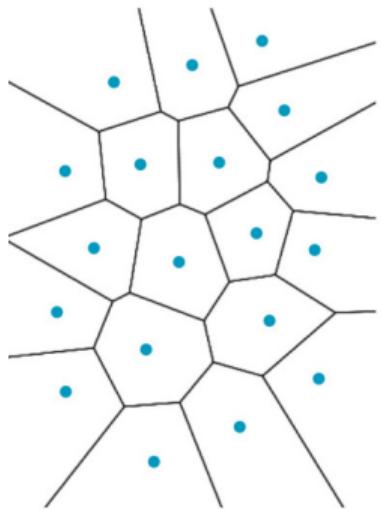
- ▶ "Life and Times of Georgy Voronoi": <https://arxiv.org/abs/0912.3269>
- ▶ Interactive Voronoi diagram demos (in 2D):
 - ▶ <http://alexbeutel.com/webgl/voronoi.html>
 - ▶ <https://nullprogram.com/voronoi-toy/>

Voronoi tessellation examples in nature

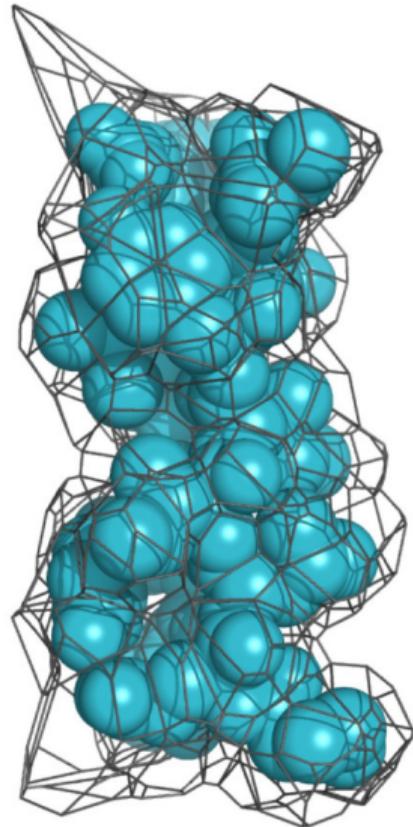
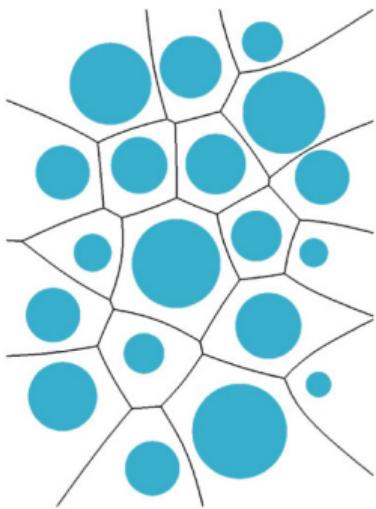


Voronoi diagram of points and balls

"Classic" Voronoi diagram
of points



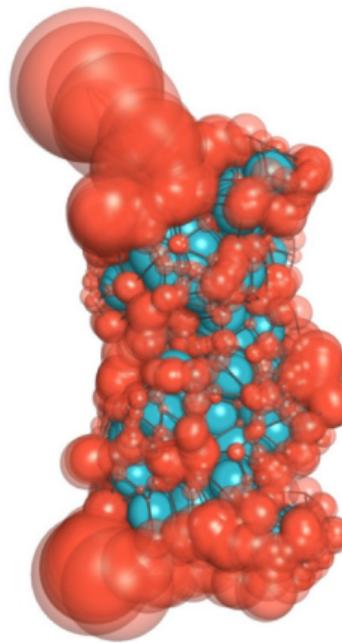
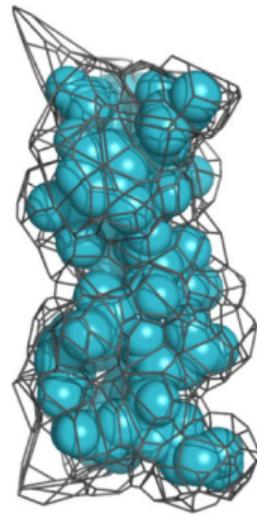
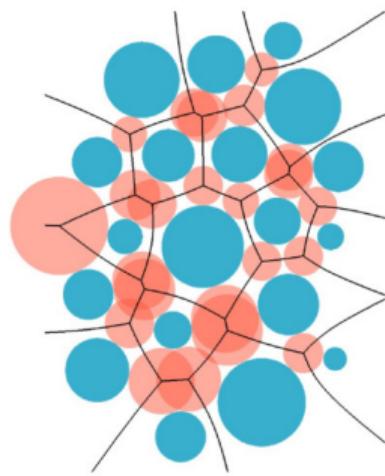
Voronoi diagram
of balls



Voronoi vertices correspond to empty tangent spheres

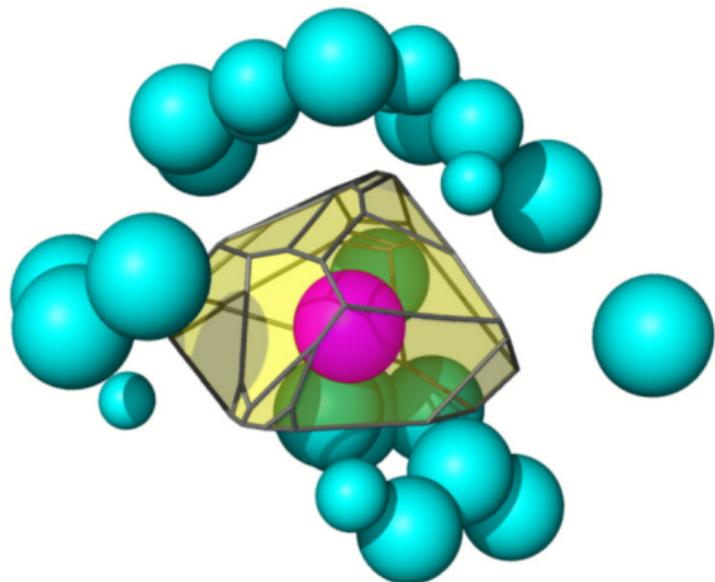
Atomic balls

Empty tangent spheres

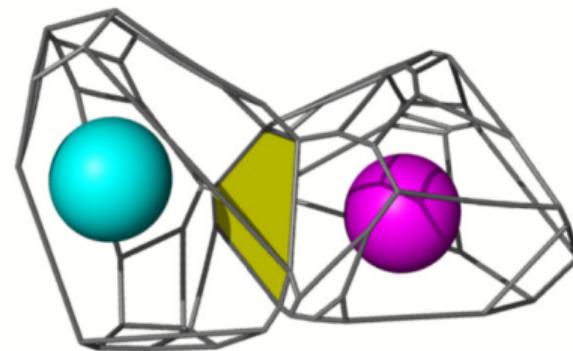


Voronoi tessellation-based analysis of structures

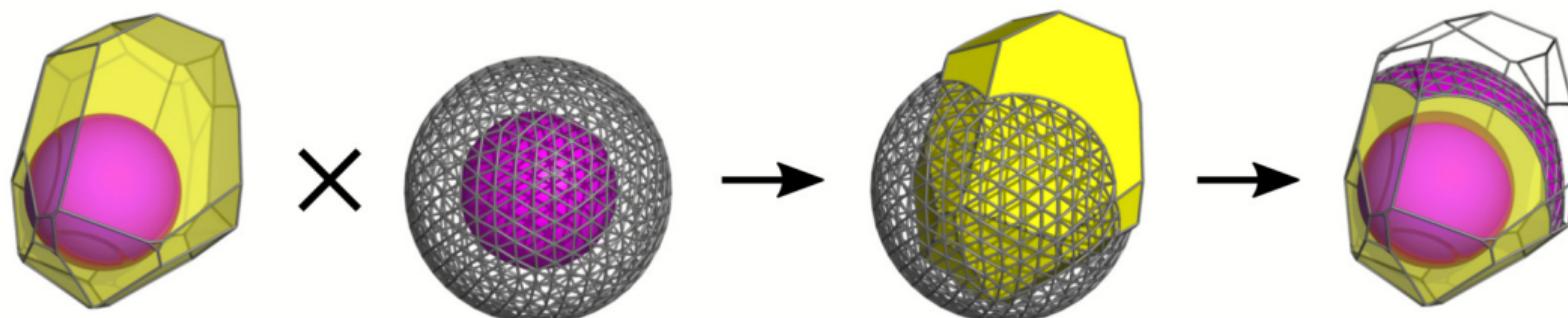
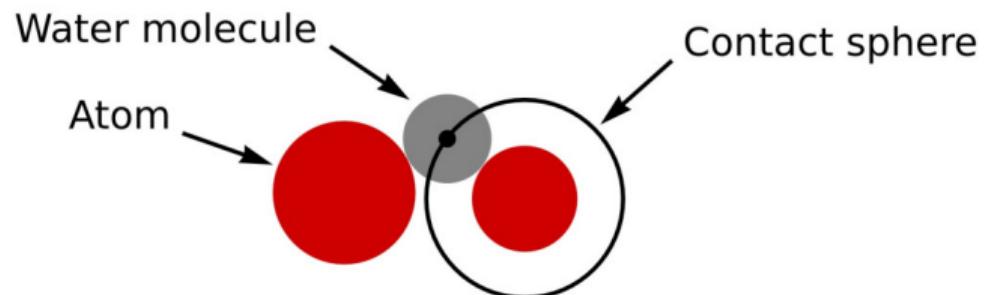
Voronoi cell of an atom surrounded by its neighbors



Atom-atom contact surface defined as the face shared by two adjacent Voronoi cells.

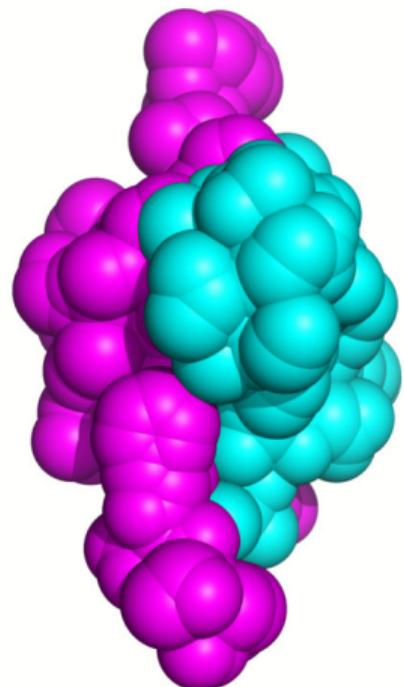


Constrained contacts

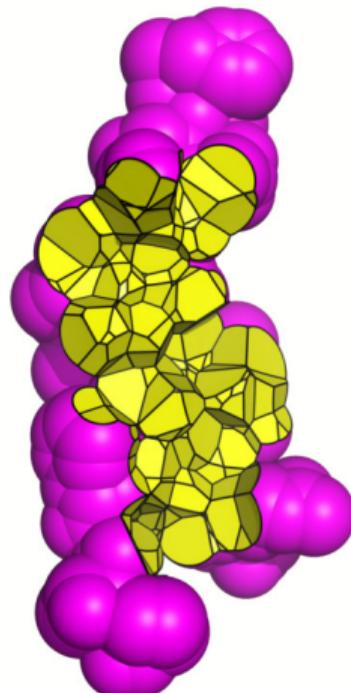


Inter-chain contacts

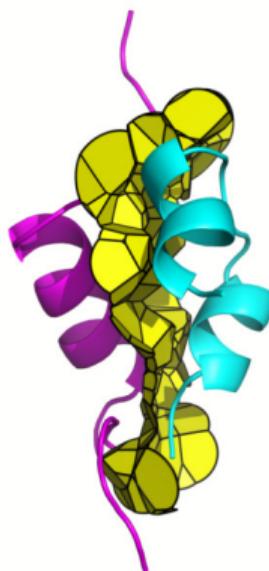
Solvent-accessible surface
of an insulin heterodimer
PDB:4UNG colored by subunit



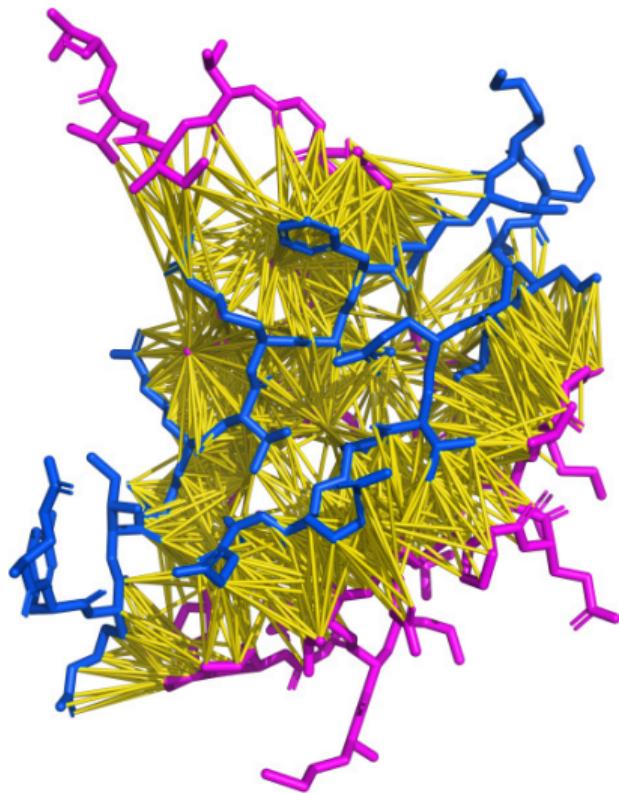
The intersubunit interface
shown together with the
SAS of one subunit



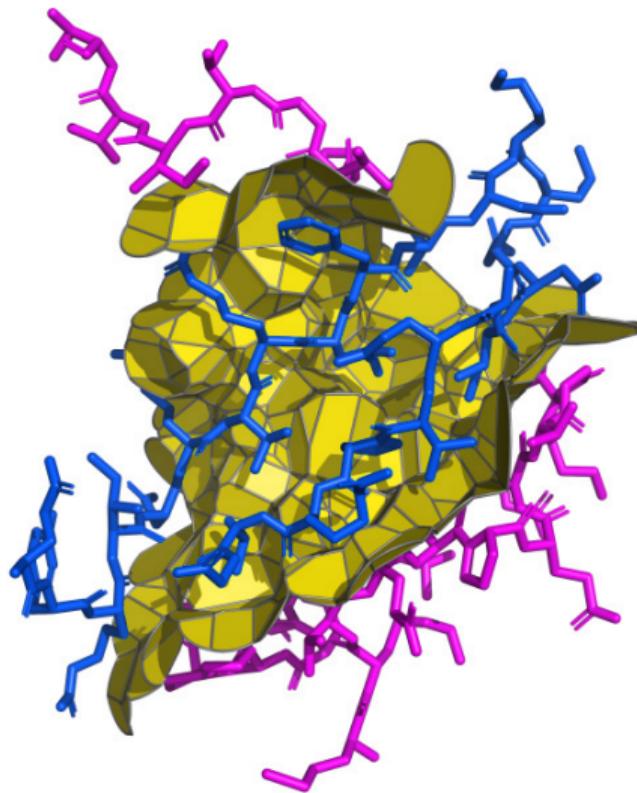
The intersubunit interface
shown together with
both subunits represented
as cartoons



Inter-chain contact areas vs distances



VS



Let's try more things

Go to "<https://www.kliment.lt/current>", open the Voronota-GL viewer.

In Voronota-GL, fetch '1cnw', let's look at it again.

Then fetch '4ung', let's look at the interchain interface (then explore demos, e.g. "score, mutate, rescore" and others).

Let's try more things

Let's start not from a PDB ID, but from the UniProt entry
"<https://www.uniprot.org/uniprotkb/P33038/entry>".

Let's try more things

- ▶ Hemoglobin 2HHB 1HHO (<https://pdb101.rcsb.org/motm/41>).
- ▶ HIV proteases 7HVP 1HSG 1HXB 1HXW (<https://pdb101.rcsb.org/motm/6>).
- ▶ DNA 1BNA (<https://pdb101.rcsb.org/motm/23>)
- ▶ Protein-DNA complex 3BEP
- ▶ RNA 2TRA (<https://pdb101.rcsb.org/motm/15>)
- ▶ Ribosome 4V5C (<https://pdb101.rcsb.org/motm/121>)

Thanks

Thank you!

Useful links:

- ▶ <https://www.kliment.lt>
- ▶ <https://www.bioinformatics.lt>
- ▶ <https://grulab.imag.fr>



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