

Protein representation and structural understanding

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Representing protein molecules

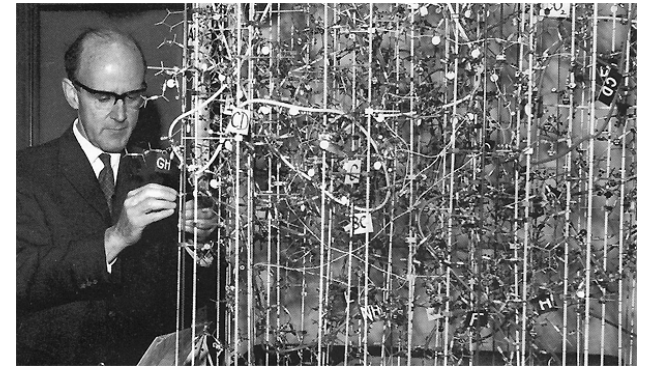
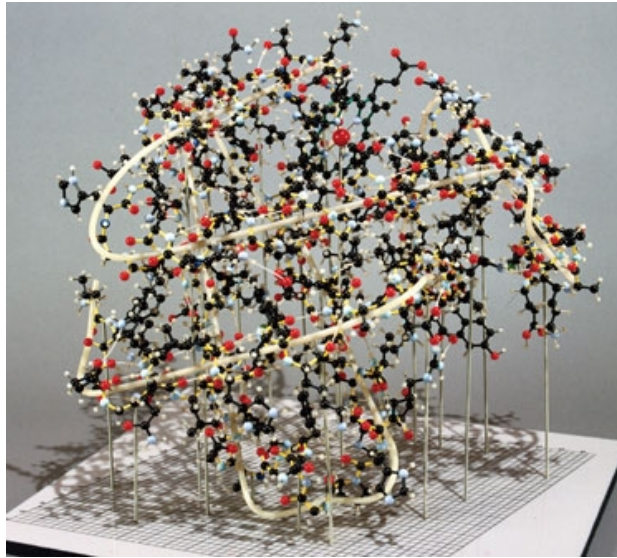
- Proteins have **complex 3D structures** usually characterized by well-defined structural features (secondary, tertiary and quaternary). [But there are also intrinsically disordered proteins.]
- **Protein structure \Rightarrow protein function**
- So, we need ways of representing proteins, in order to **visualize** and **understand** their structural features.
- We need to represent proteins using some kind of **visual model**.
- In this presentation we consider only **static protein structures**, as produced by protein crystallography, structural NMR, etc. But proteins move, as discussed in other classes.

Once upon a time: real physical models built in metal, plastic, etc

- The first models were built in that way, which required **a lot of work!**



Kendrew building myoglobin



Perutz building hemoglobin

- Kendrew and Perutz shared the Nobel Prize with Watson and Crick.
- Nowadays, things are much easier: we can represent proteins in a computer screen and “move” the models with the mouse.
- This presentation introduces some of the most common visual representations for proteins, provided by the program **PyMOL**.

Space-filling or CPK (Corey–Pauling–Koltun) sphere model

Usual colors: white for hydrogen, black for carbon, blue for nitrogen, red for oxygen, yellow for sulfur, etc. (here green for carbon)

Roughly half of the atoms are hydrogens, which are often not displayed.

Ball-and-stick model

Atoms represented as small spheres and bonds as thin sticks.

Stick model

Only bonds are shown as sticks. Like structural chemical formulas, but with colors instead of chemical symbols.

Backbone model / C_α trace

Only main-chain atoms / smoothed tube connecting C_α atoms.

Ribbon or Richardson diagram

Cartoon-like representation highlighting secondary structure elements.

Molecular surface

Continuous surface beyond which solvent cannot penetrate (interior versus exterior). Useful to visualize cavities, channels, etc.

Combining different molecules and representations

Different molecular parts can be contrasted using different representations.

Similar representations can be used for small molecules, nucleic acids, etc.

Feeling creative? You can also do visual arts...

