Using Parallel Computing in Drug Design

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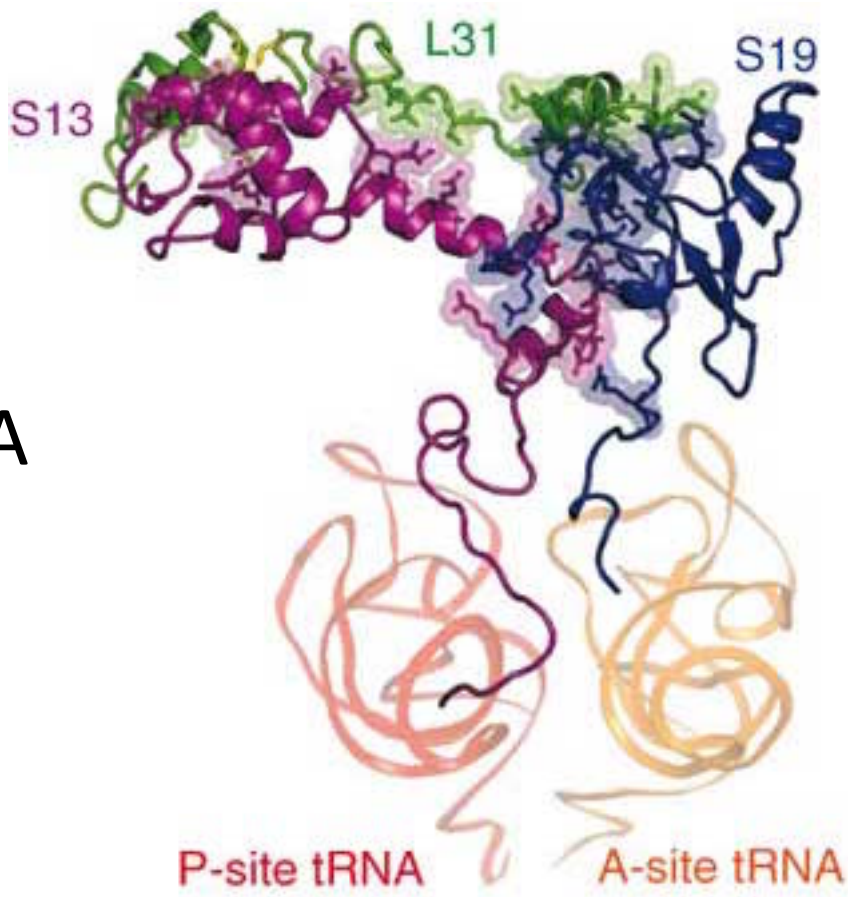
How do pharmaceutical companies design the medicines we use?

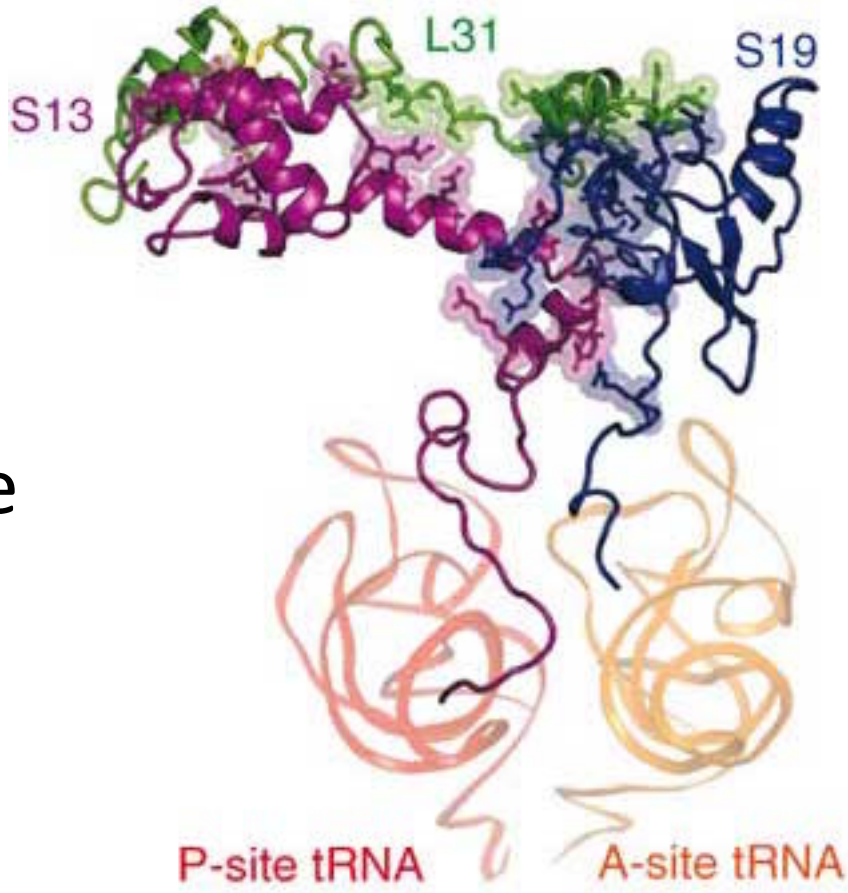
How medicines work

- Our **DNA** is like a book of recipes
- Instead of food, DNA contains the instructions for making **proteins** in our bodies

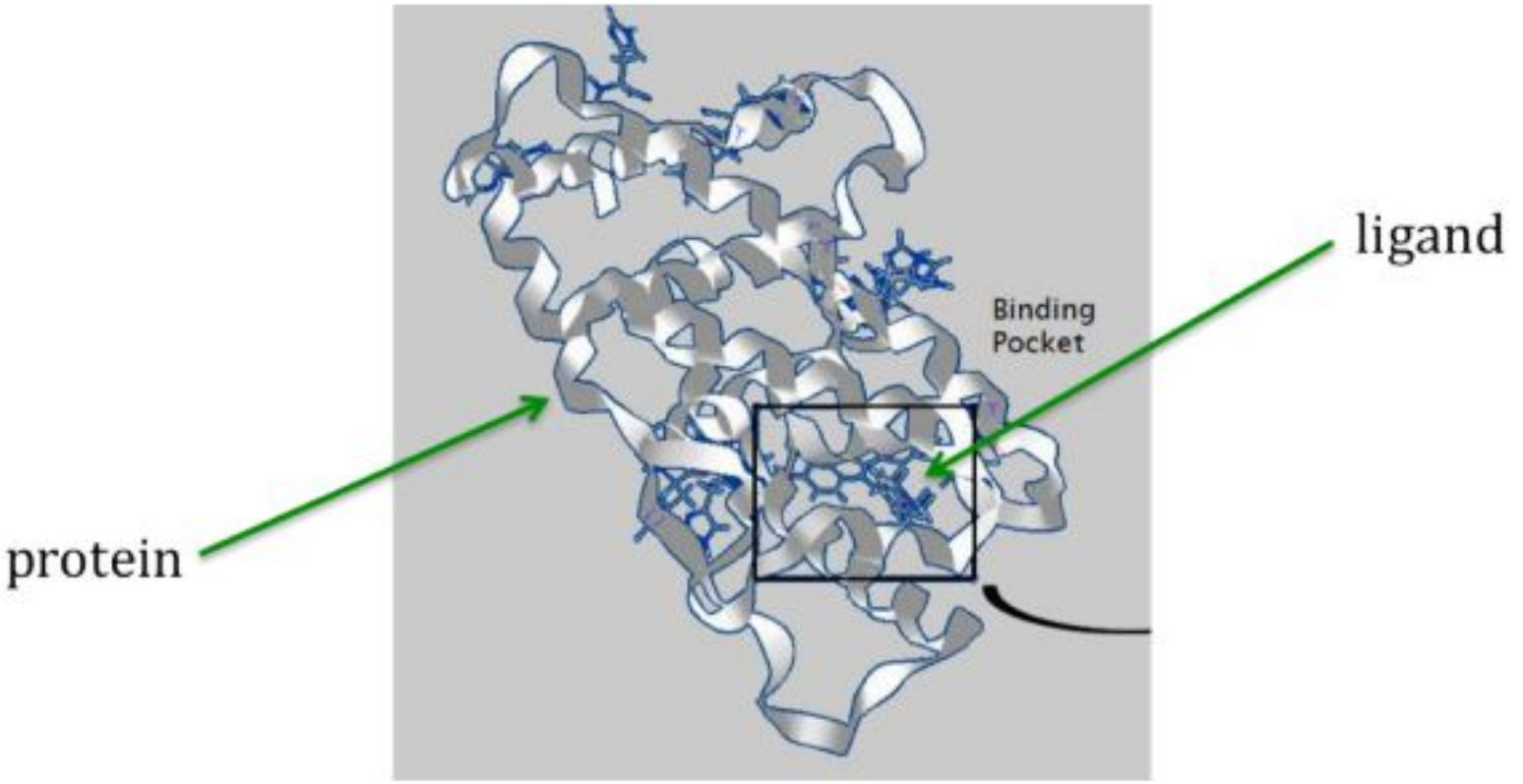


How medicines work

- A **protein's shape** determines the function it performs in a person's body
- To design a drug, we can **find *ligands* (new pieces)** to change a protein's shape



How medicines work



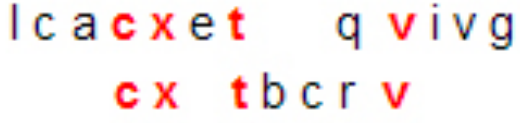
Strategy for drug design software

1. **Generate ligands** to try for particular protein
   - Some ligands will fit, some won't
2. Compute a **score for each ligand** that simulates how well it will:
   - fit that protein; and
   - produce a desired shape change
3. Identify the **highest scoring ligands** for actual synthesis (production) and testing

Drug design exemplar code

A program *structured like* drug design software

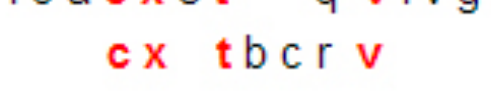
1. **Generate ligands** to try for particular protein
   - Random character *strings* of random lengths
2. Compute a **score for each ligand**
   - Compare for **maximum match** with string representing a protein
   - Insertions and deletions allowed
3. Identify the **highest scoring ligands**



Drug design exemplar code

A program *structured like* drug design software

1. **Generate ligands** to try for particular protein
   - Fast
2. Compute a **score for each ligand**
   - Takes a long time
   - **Parallelize** by using **multiple computation threads** for different ligands



3. Identify the **highest scoring ligands**
   - Fast – just sort and find maximum

Drug design exemplar code

Command-line arguments:

./drugdesign-static ***threads maxlen count***

- ***threads*** is number of simultaneous threads
- ***maxlen*** is *maximum* length of a ligand
  - *Each ligand* has random length up to this max
- ***count*** is number of ligands to score