

Using Parallel Computing in Drug Design

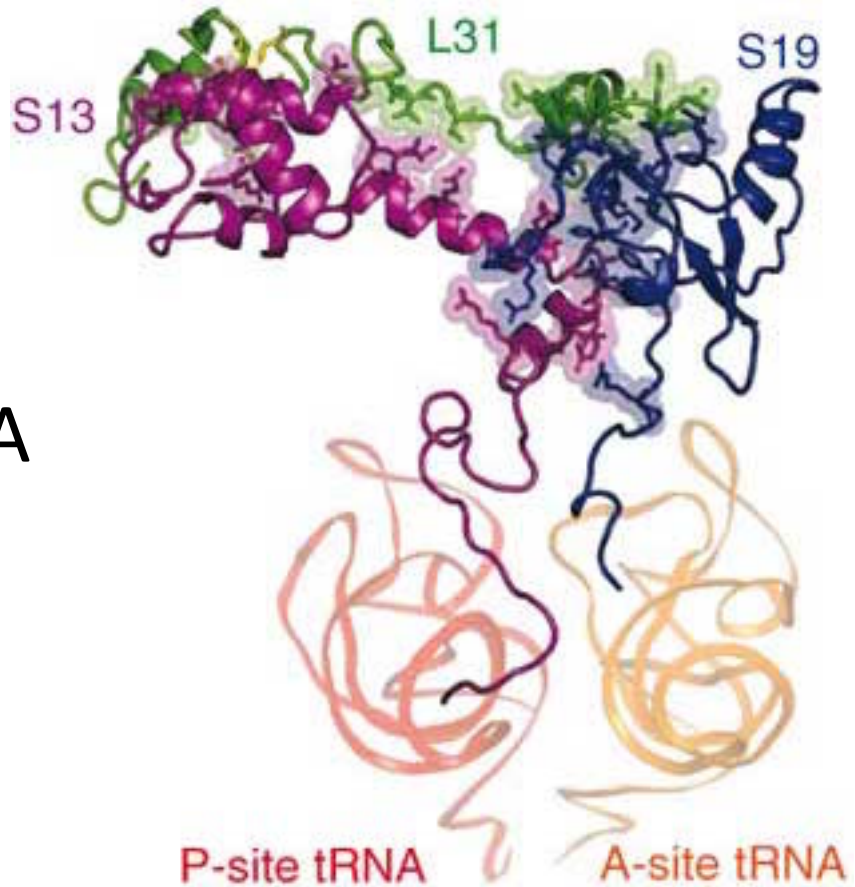
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How do pharmaceutical companies design the medicines we use?



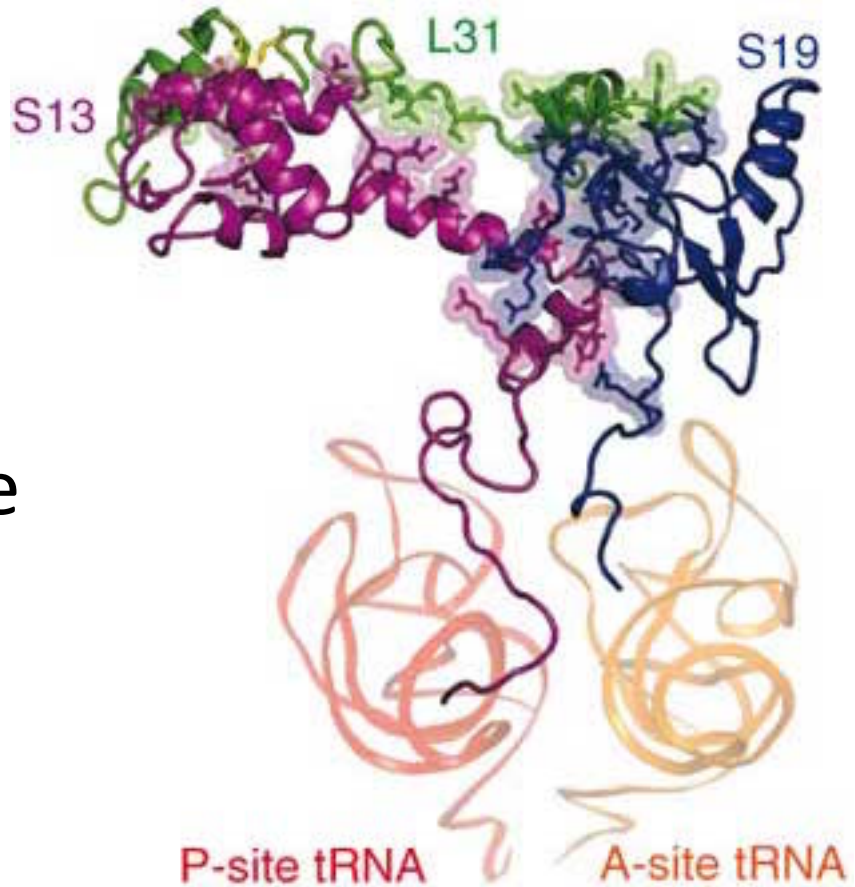
How medicines work

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

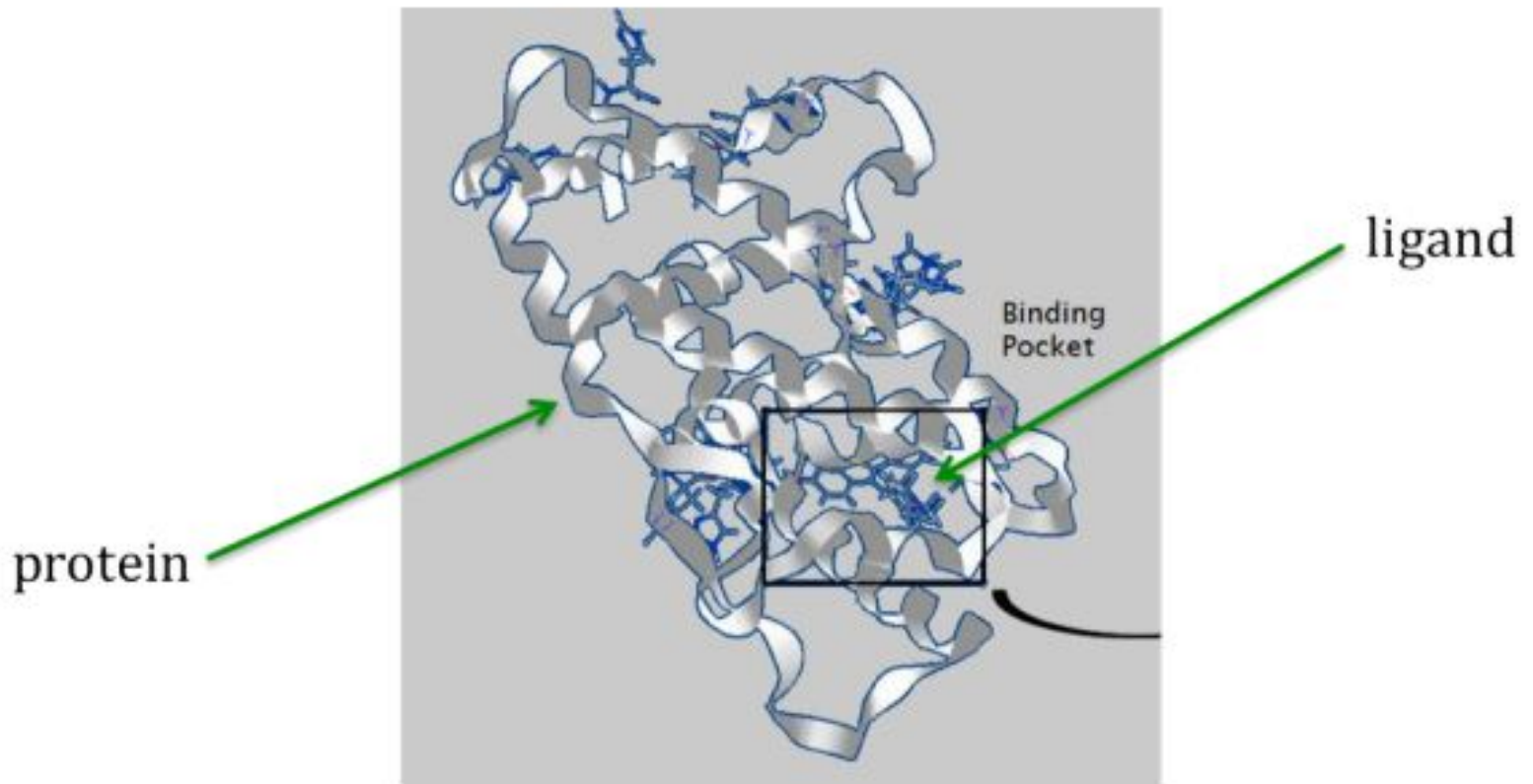


How medicines work

- 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

```
l c a c x e t   q v i v g  
      c x   t b c r v
```

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

lca**cx**et qv**iv**g
cx tbc**r**v

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