QUANTUM COMPUTING AND DRUG DISCOVERY

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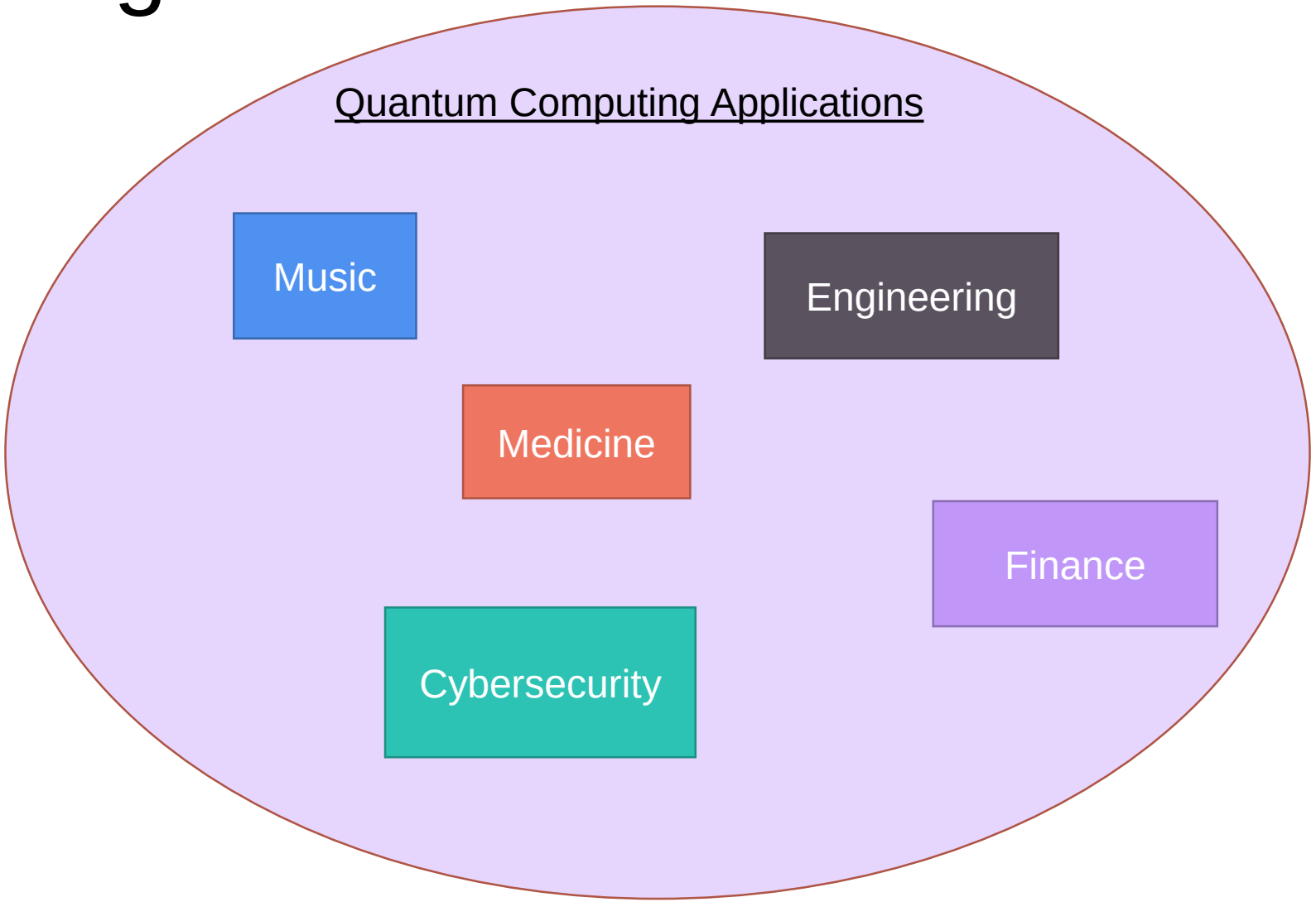
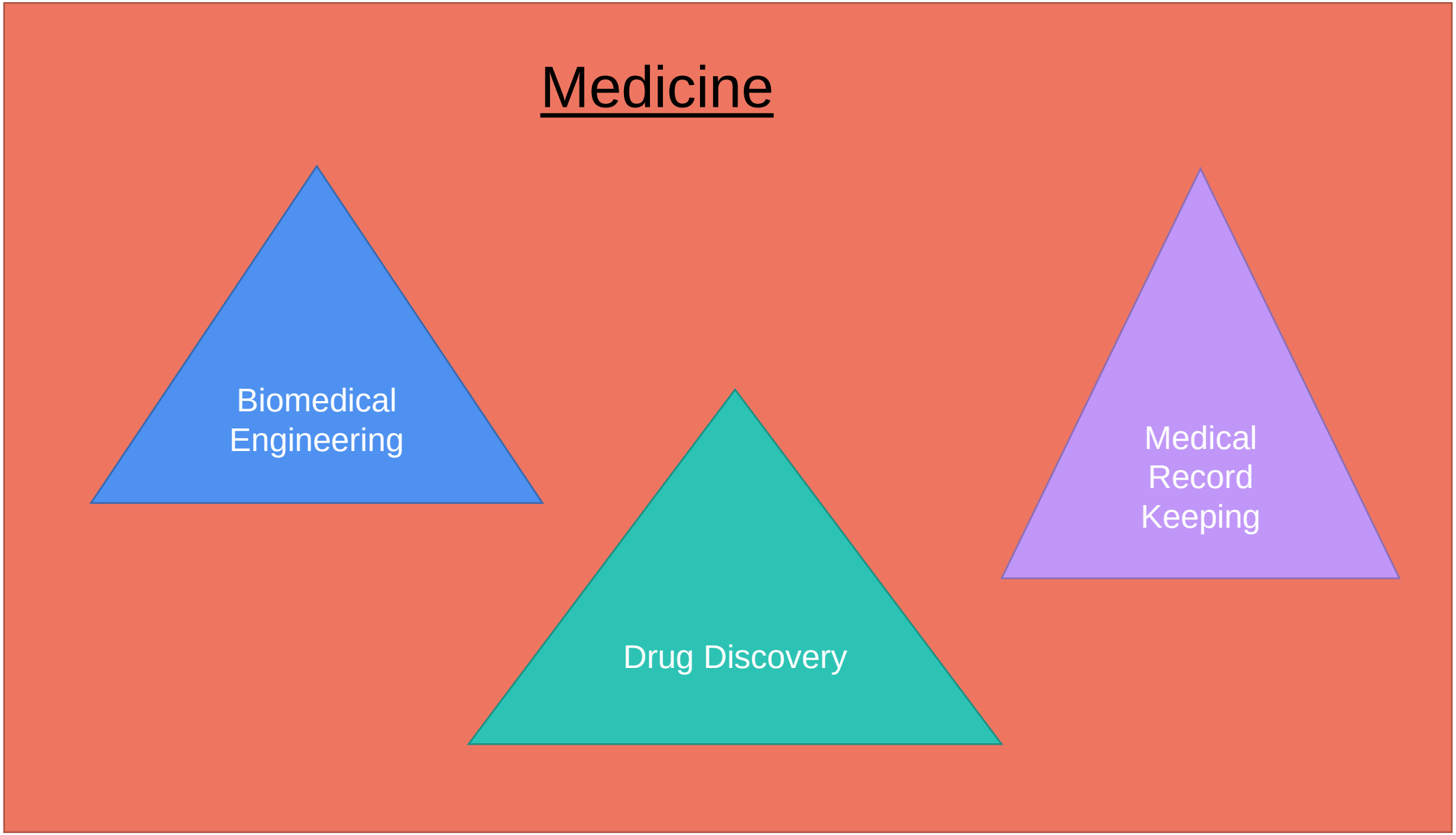
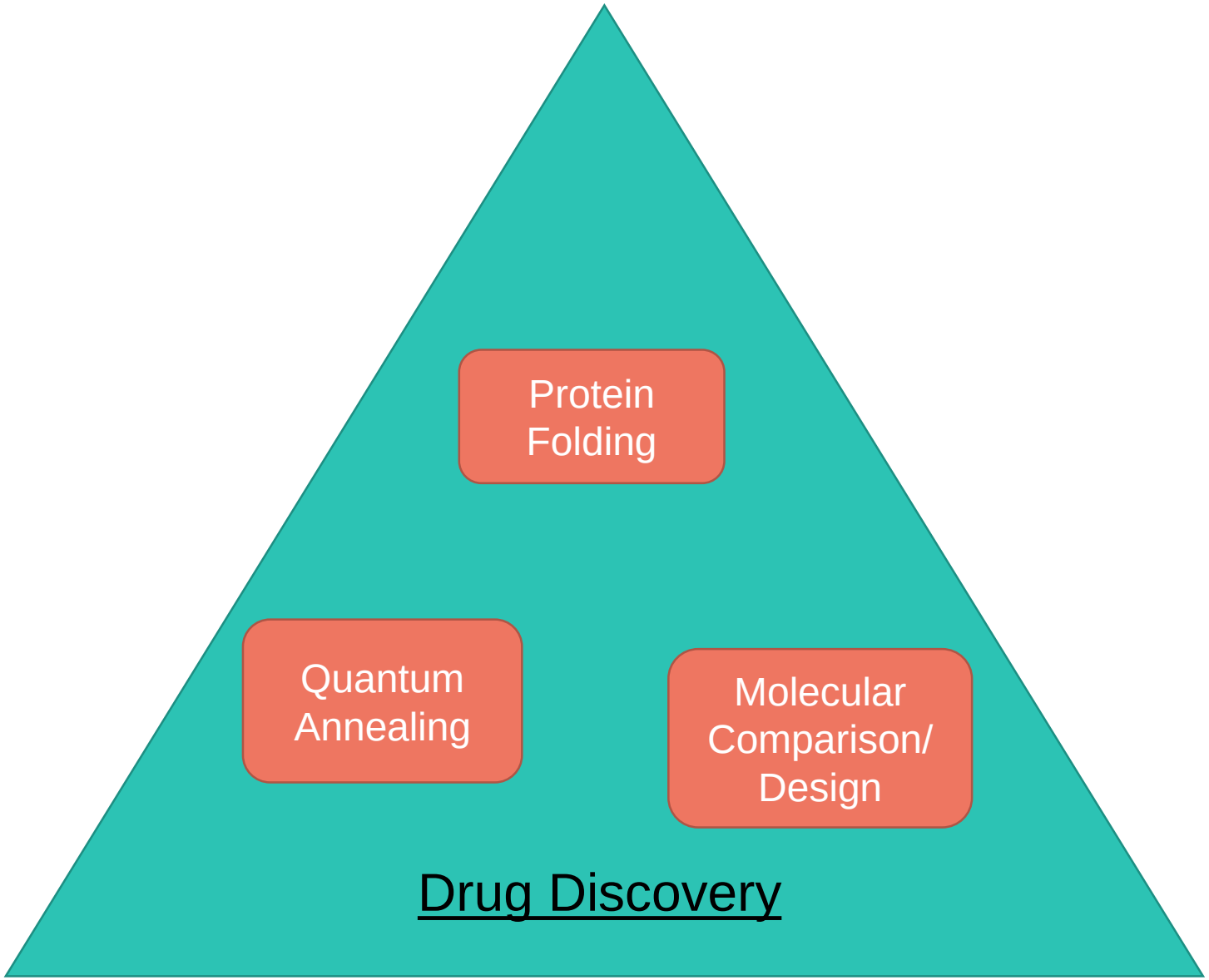
The Big Picture

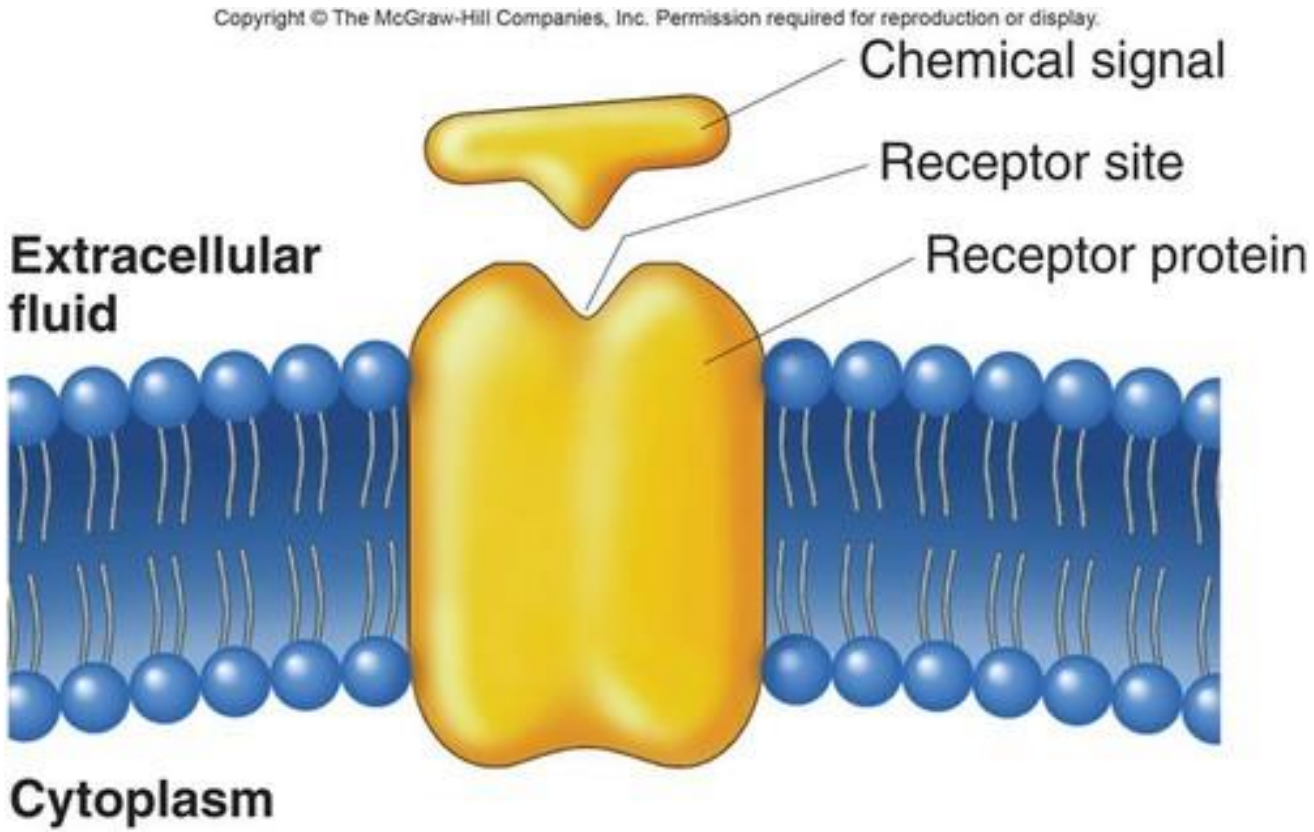



Medicine
Biomedical Engineering
Drug Discovery
Medical Record Keeping


Protein Folding
Quantum Annealing
Molecular Comparison/ Design
Drug Discovery

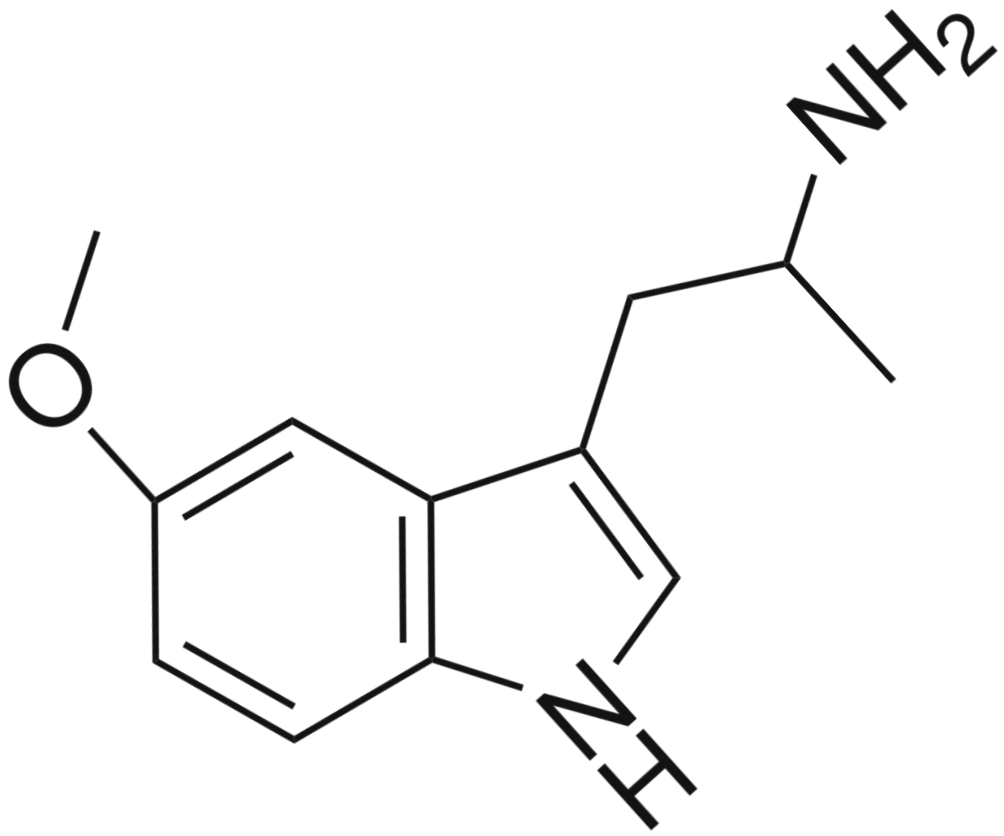
Molecular Comparison

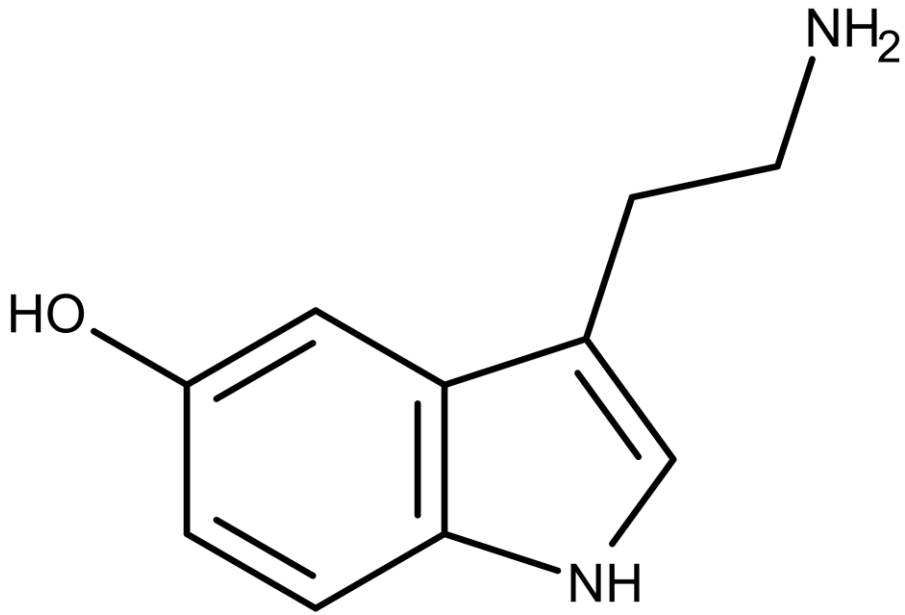
- What is it?



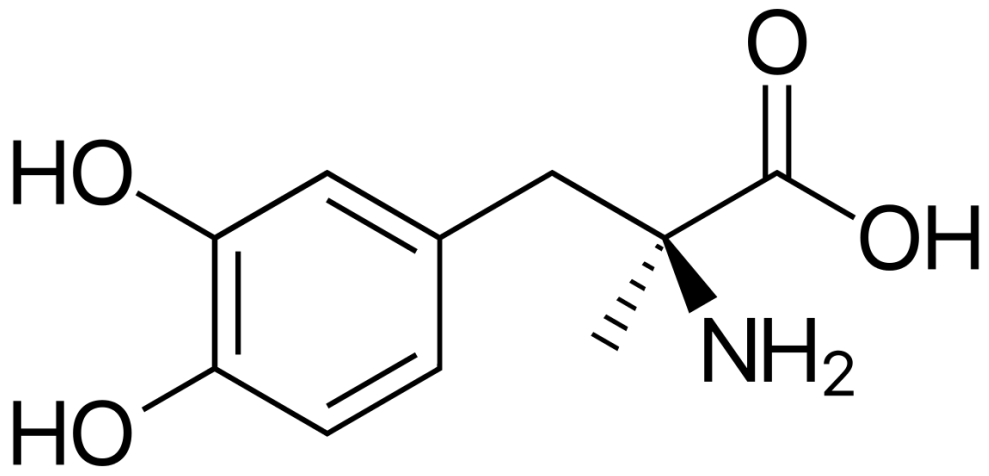
There is a problem…

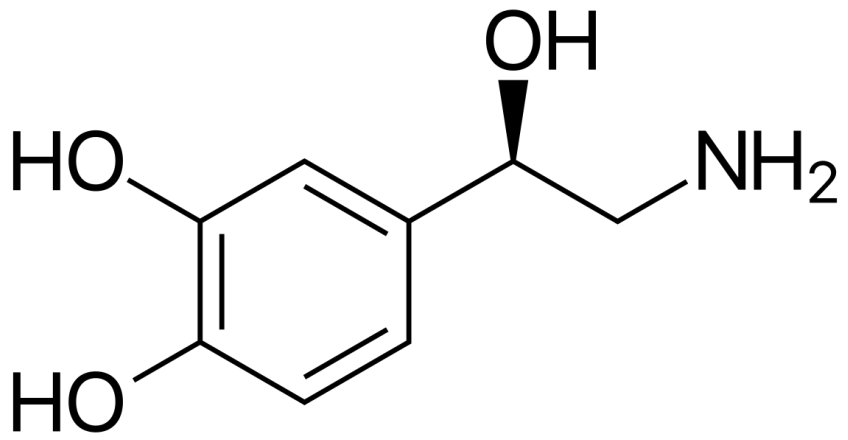
5-MeO-aMT



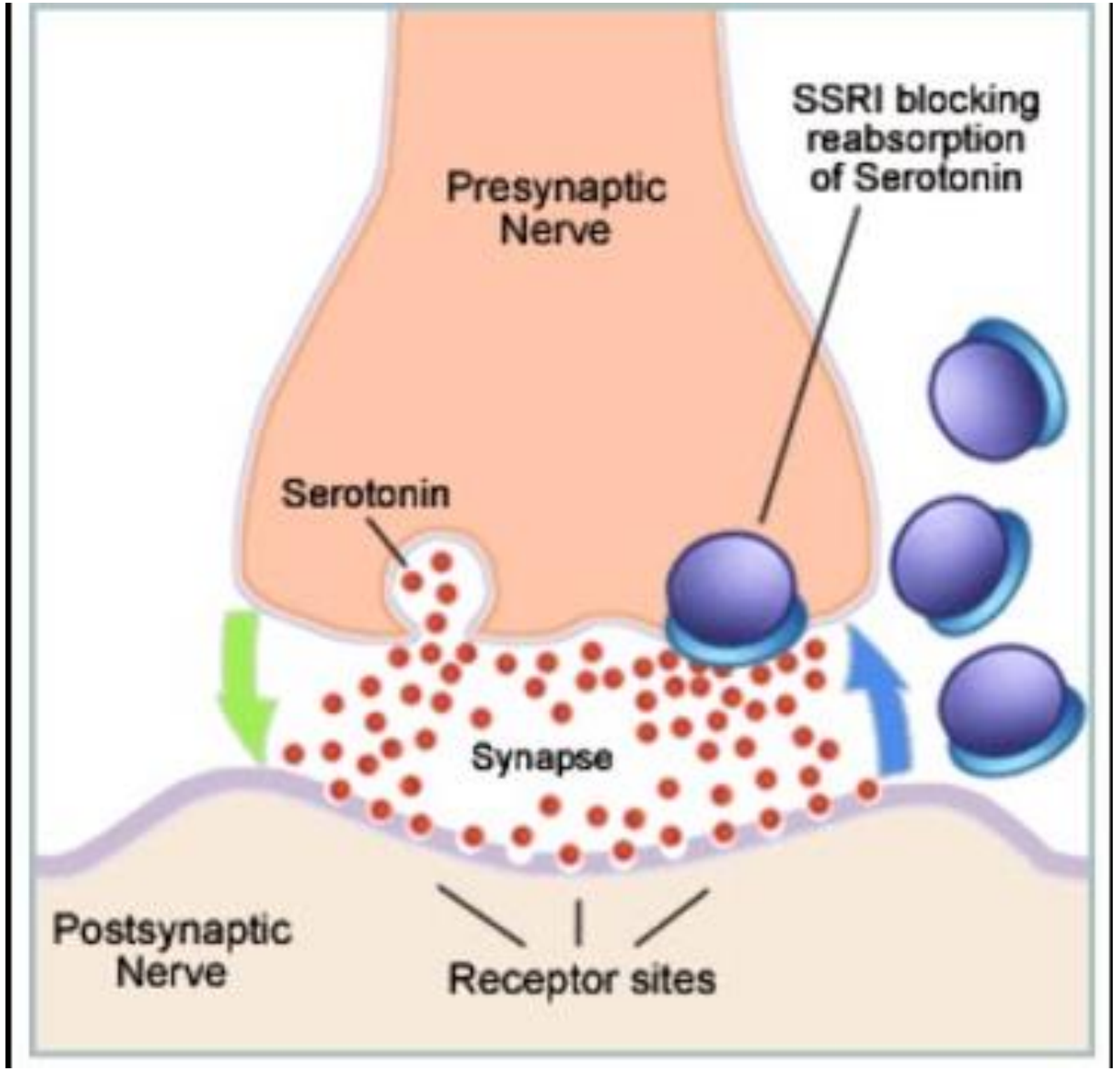


Methyldopa vs. Norepinephrine

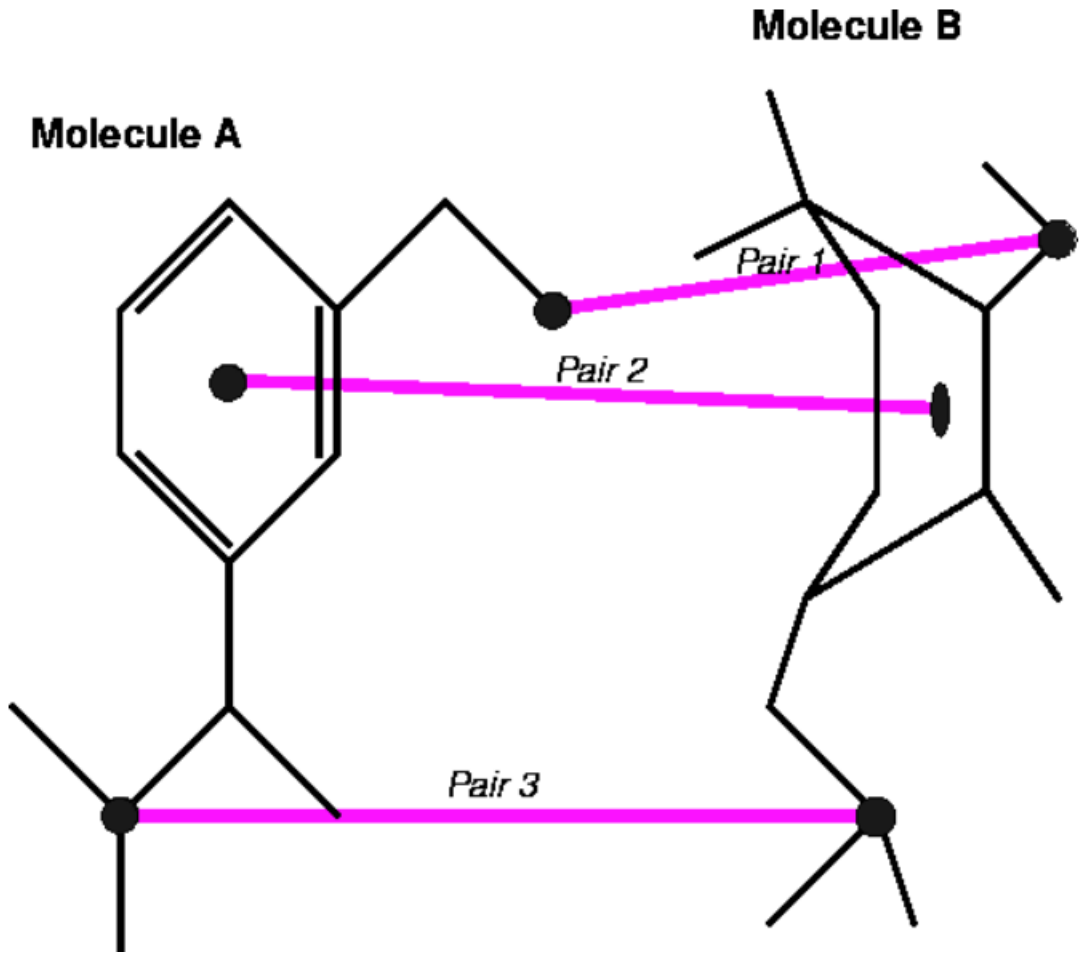




Selective Serotonin Reuptake Inhibitor (SSRI)



How is all of this done?



Quantum Computing

- Classical does it just fine.
- Quantum capitalizes on accuracy, breadth, and depth.

Where is this studied?

Biogen

1QBit

accenture

Quantum Molecular Design

Step 1

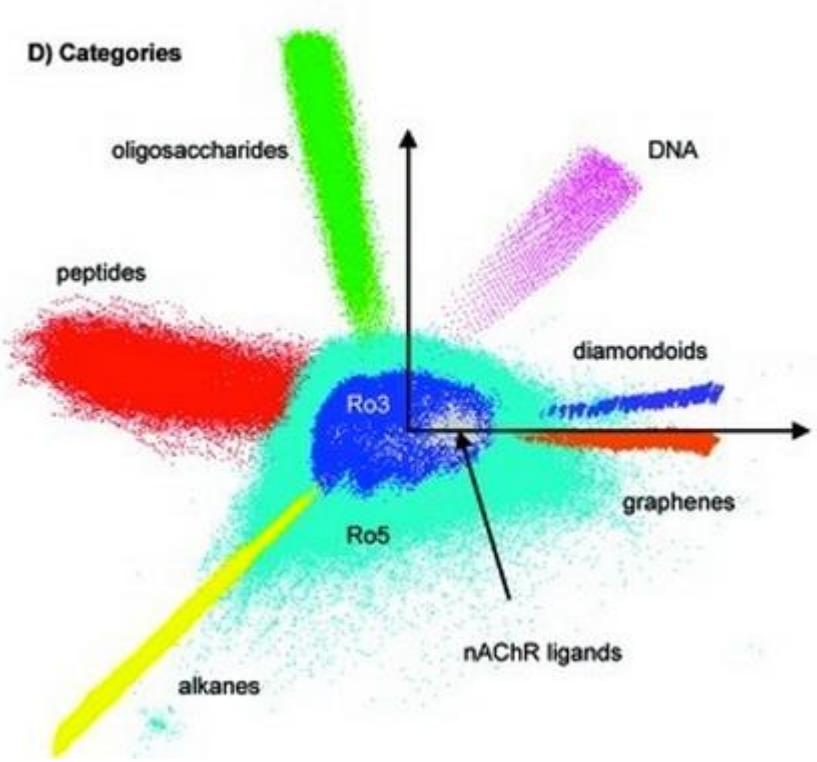
- Extract information from a target.

Step 2

- Search in a larger database.

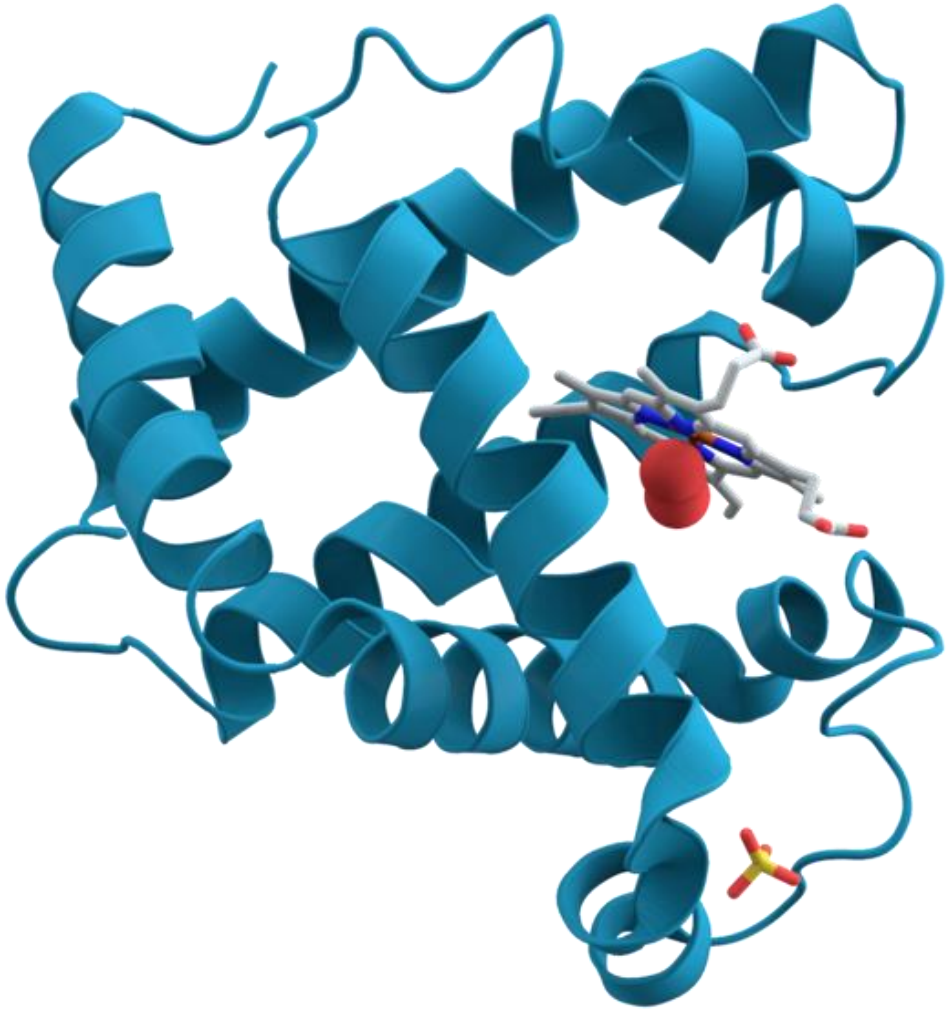
Step 3

- Create a novel chemical space by varying functional groups.

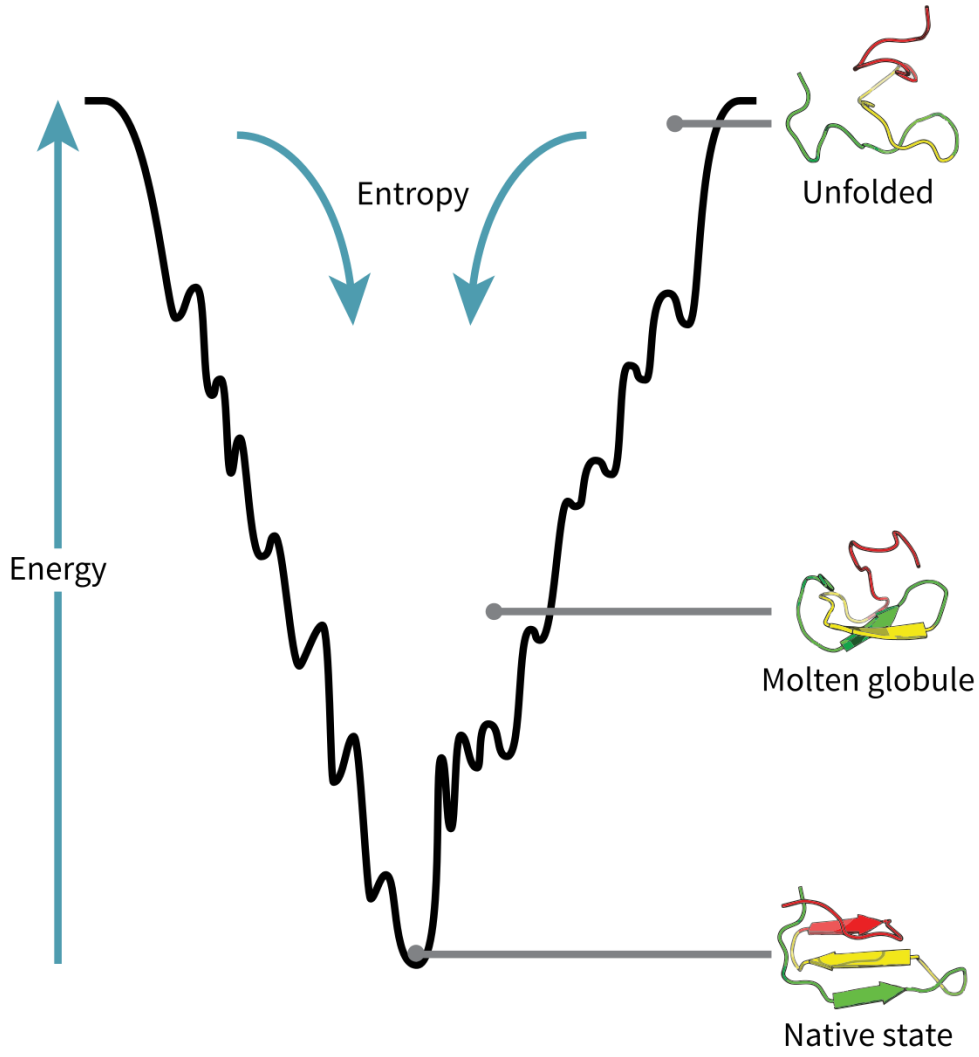


Protein Structure Prediction

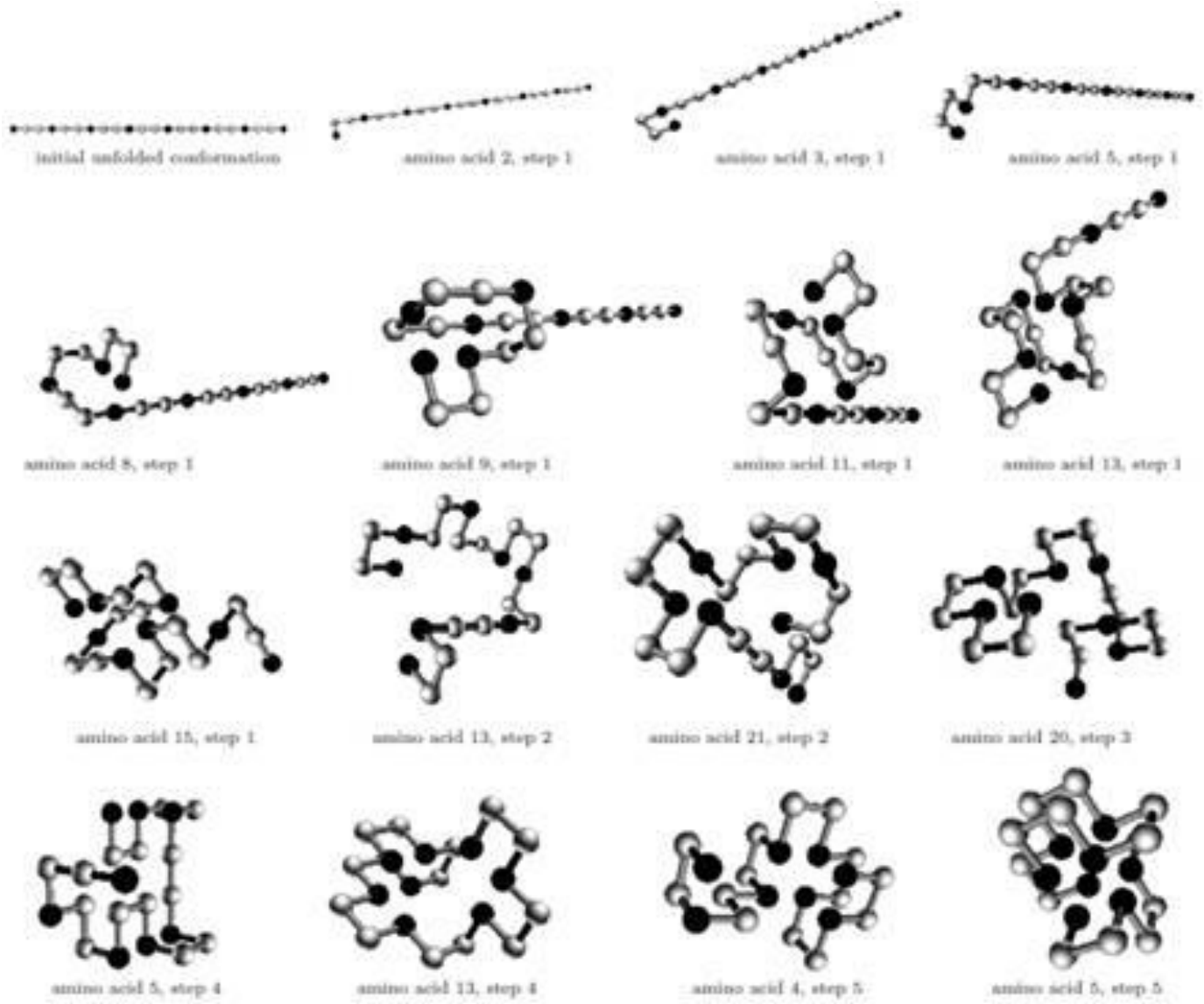
Some background…



Funnel hypothesis



Protein Lattice Model



Diabatic Quantum Computing

- Rapidly changing conditions prevent the system from adapting its configuration during the process, hence the spatial probability density remains unchanged.
- Typically, there is no eigenstate of the final Hamiltonian with the same functional form as the initial state.
- System ends in a linear combination of states that sum to reproduce the initial probability density.

Adiabatic Quantum Computing

- Gradually changing conditions allow the system to adapt its configuration, hence the probability density is modified by the process.
- If the system starts in an eigenstate of the initial Hamiltonian, it will end in the corresponding eigenstate of the final Hamiltonian.

The Problem to Solve

- The less energy, the better.
- It is NP-hard
- Quantum algorithms may have potential…

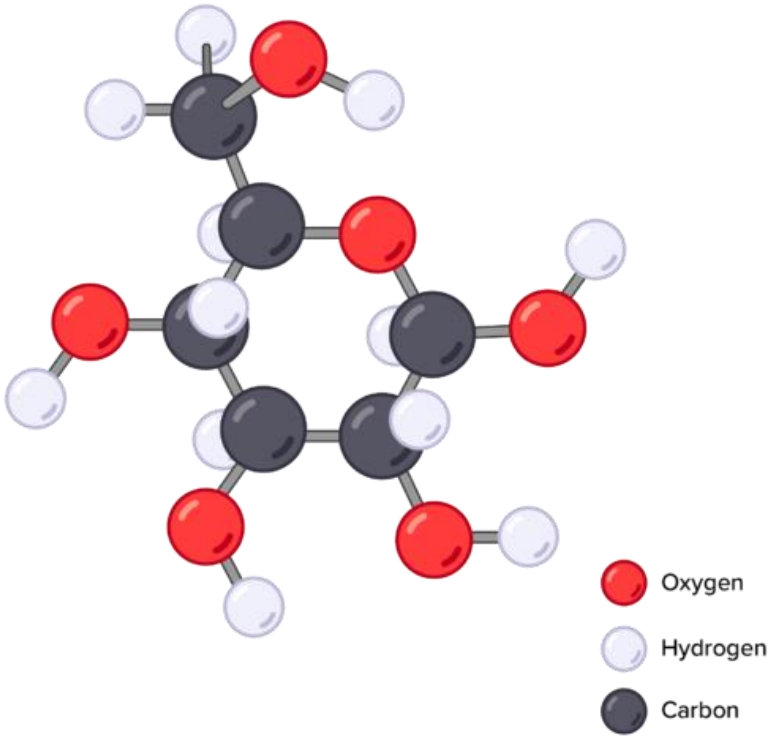
A Possible Solution?

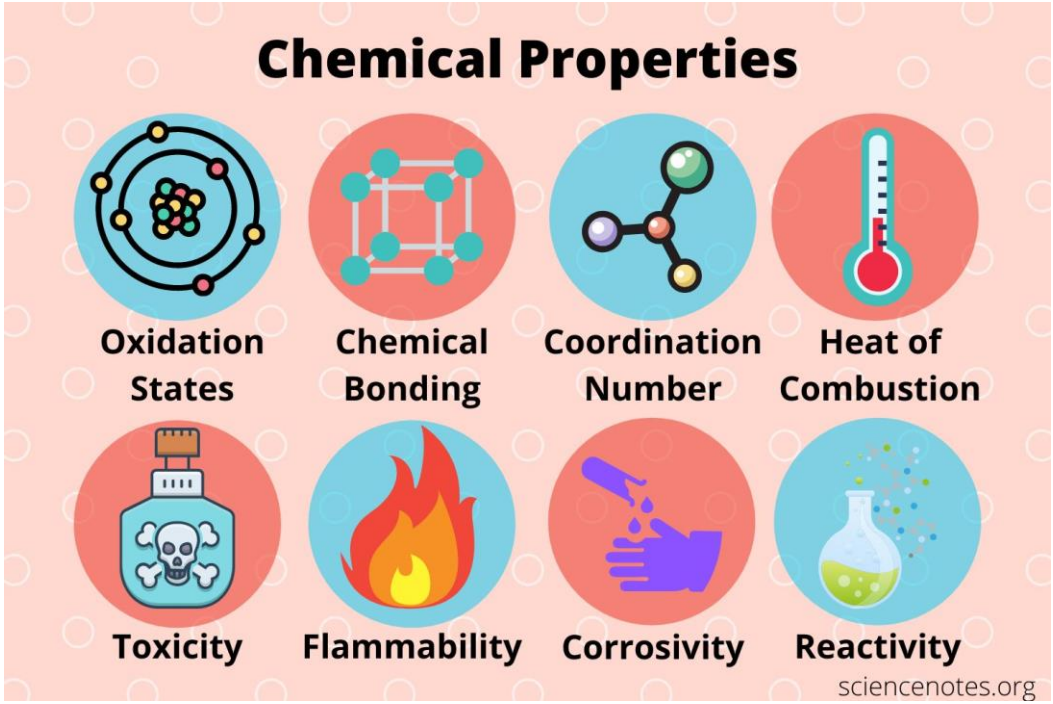
Quantum Annealing

What is it?

- In simple terms, finding the global minimum over a set of candidate solutions.

Uses


Oxygen
Hydrogen
Carbon


Chemical Properties
Oxidation States
Chemical Bonding
Coordination Number
Heat of Combustion
Toxicity
Flammability
Corrosivity
Reactivity
sciencenotes.org

Let’s slow down…

- A useful quantum computer needs to process a set of continuous parameters that is larger than the number of subatomic particles in the universe.

2-Qubits

$$|00\rangle$$
$$|01\rangle$$
$$|10\rangle$$
$$|11\rangle$$

1,000 to 10,000 qubits needed.

↓

$2^{1,000}$ continuous parameters (about 10^{300})

↓

$$3.28 \times 10^{80} \ll 1.0 \times 10^{300}$$

CONCLUSION