



# QuantFold

Simulated Protein Folding with Quantum Annealing on D'Wave's  
Hardware for Drug Discovery Implications

# Quantum Neural Networks Skin Cancer Image Detection

Try Our Demo

# Anaxa - securing the storage & transmission process of health data

<https://anaxa.tech/>

Affiliations:

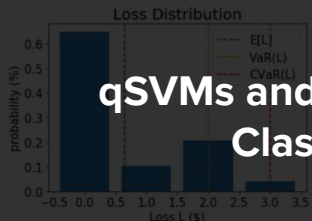


Biomedical Zone

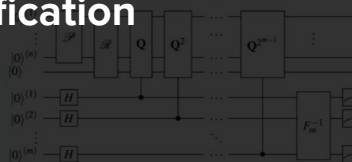


BACE Accelerate

Utilizing the quantum amplitude estimation algorithm to compute the risk measures of a simple 2-asset portfolio



Code  
Medium Article



Expected Loss  $E[L]$ : 0.6409  
Value at Risk  $VaR[L]$ : 2.0000  
 $P[L \leq VaR[L]]$ : 0.9591  
Conditional Value at Risk  $CVaR[L]$ : 3.0000

# qSVMs and Cancerous Cell Classification

Utilizing the quantum support vector machine algorithm to classify breast cancer cells as benign or malignant w/ IBM's Qiskit



```
'predicted_labels': [0 1 0 0 0 0 1 1 1 0 1 1 0 1 1 1 1 1]
'predicted_classes': ['Benign', 'Malignant', 'Benign', 'Benign', 'Benign', 'Benign', 'Malignant', 'Malignant', 'Malignant', 'Benign', 'Malignant', 'Malignant', 'Benign', 'Malignant', 'Malignant', 'Benign', 'Malignant', 'Malignant', 'Benign', 'Malignant', 'Malignant', 'Malignant', 'Malignant', 'Malignant']
```

[Presentation Deck](#)  
[Code](#)  
[Research Proposal](#)  
[Medium Article](#)

**Over 6 million deaths per year due to neurodegenerative disorders**

# The Protein Folding Problem

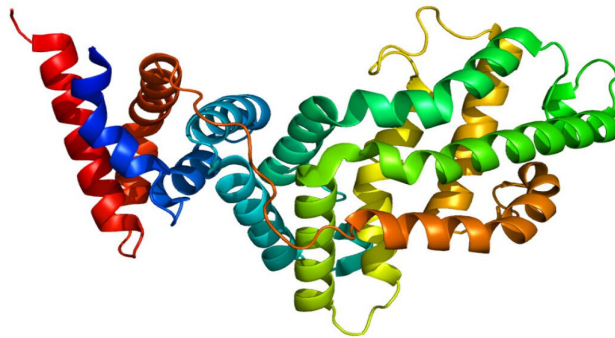
How can a protein's amino acid sequence dictate its three-dimensional atomic structure?

## Sequence

GIAISVGFAYIMINTYFEVLVAF  
WCCACWWFPKQNPKIHKHT  
MIQTAEGQIMNPAGWHWR  
GNIEKVGFAFNFSTCLDICTW  
WIDPETSEYAYNWMVHMDN



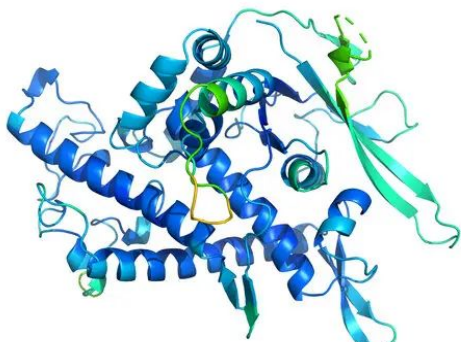
## Structure



# The Protein Folding Problem

How can a protein's amino acid sequence dictate its three-dimensional atomic structure?

**3D-Structure Relationship**



**Computational Drug Design**



**Our current computational methods are  
not efficient enough.**

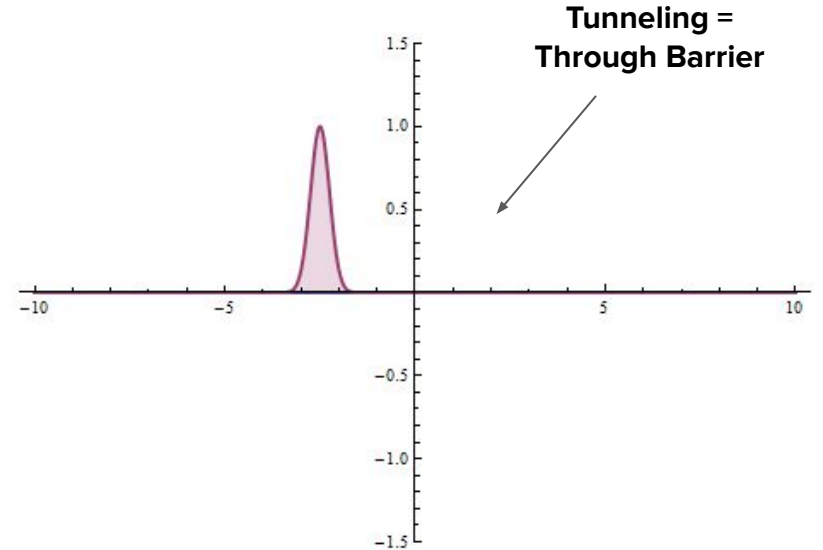
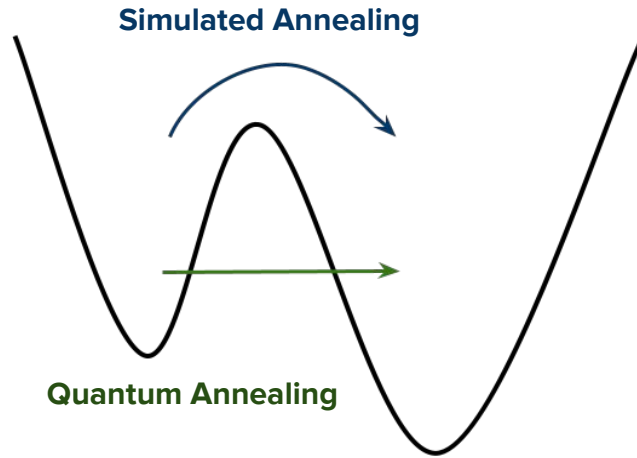
**>150 residues proteins unable to be computed**

**No classical algorithm exists that is able to  
find a protein's minimum energy in  
polynomial time**

# Quantum Tunneling Effect

**Simulated Annealing = Over Energy Barrier = ↑ Expensive**  
**Quantum Annealing = Through Energy Barrier = ↓ Expensive**

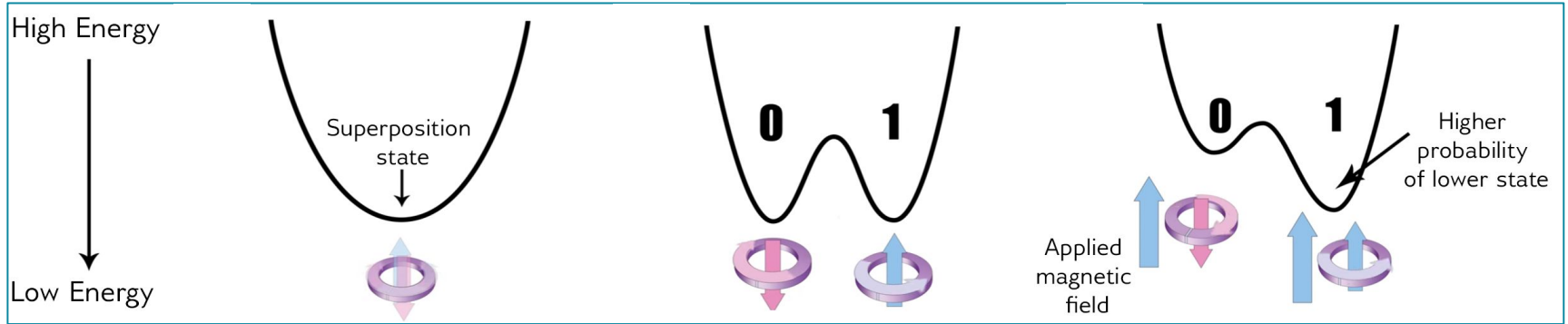
Protein Energy Landscape





# Quantum Annealing

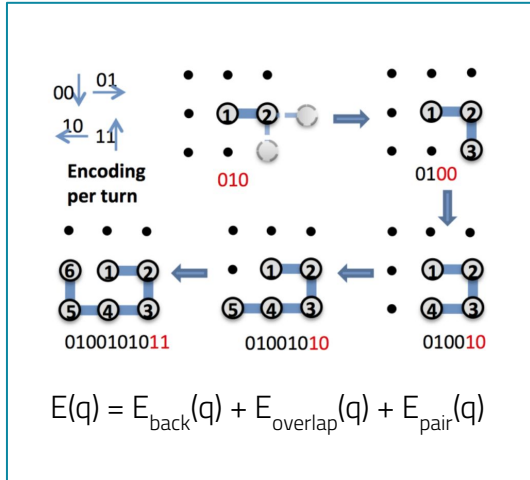
Finds protein's minimum energy with **speedup** from quantum tunneling



- 1 Apply biases and couplers to superpositions of qubits to optimize for annealing
- 2 Energy change computed, step is accepted for each residue
- 3 Energy landscape is defined and energy is minimized to reach native structure

**n qubits =  $2^n$  solutions** able to be run at the same time

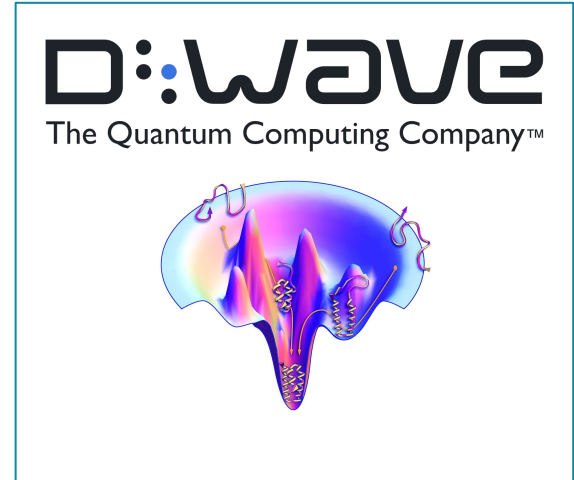
# QuantFold



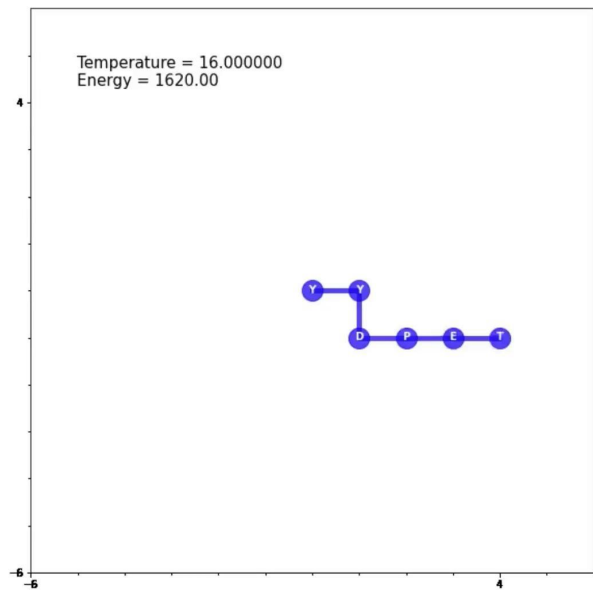
Turn Ancilla Encoding

- ① Define a schedule for annealing temperature  $T$
  - ② Randomly choose  $i^{\text{th}}$  qubit  $q_i$
  - ③ Perform a qubit flip
  - ④ Compute energy change in energy  $\Delta E = E - E'$
  - ⑤ Accept step if  $\exp(-\Delta E/T)$  expresses the probability a state of energy  $E$  relative to the probability of a state of zero energy  $> \text{random.uniform}(0, 1)$ .  
If  $\Delta E \leq 0$ , always accept
- $$\text{Probability} = \frac{1}{1 + e^{-\frac{\Delta E}{T}}}$$
- ⑥ Process repeats as  $T \rightarrow 0$

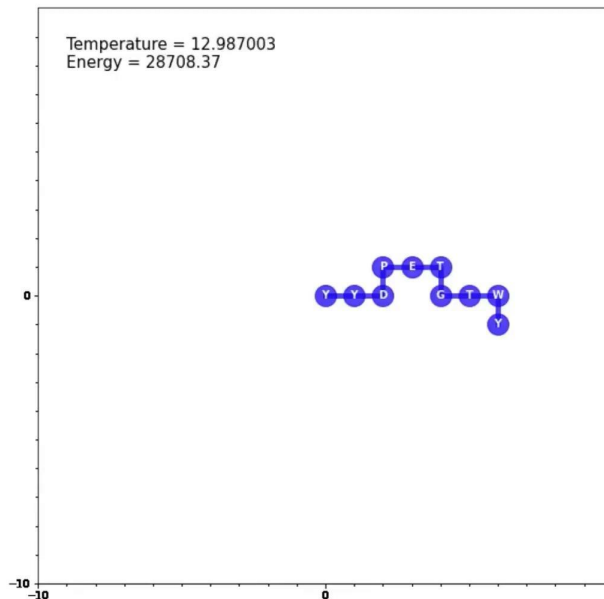
Quantum Annealing



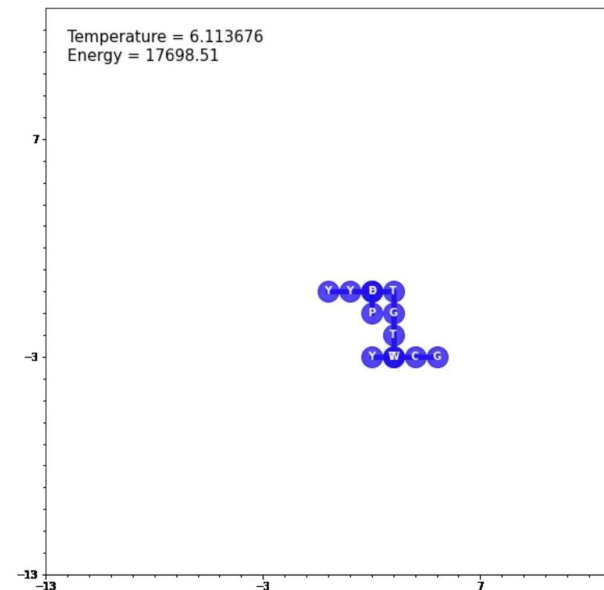
Run on D'Wave Annealer



**6 Residues**



**9 Residues**



**12 Residues**

	6 Residues	9 Residues	12 Residues
Conventional Simulated Annealing	<b>18.6%</b> <b>12.2 s</b>	<b>13.3%</b> <b>25 s</b>	<b>6.1%</b> <b>38.0 s</b>
Quantum Annealing, D'Wave's Annealer	<b>86.6%</b> <b>2.6 s</b>	<b>70.8%</b> <b>8.0 s</b>	<b>61.0%</b> <b>12.0 s</b>

# QuantFold

**Modeling protein structures** -  
energy conformations,  
sequence information



Efficient  
**prediction and classification**  
in protein sequences



Optimized  
generation  
of new  
**computational drug designs**

**Stage 1**

**Stage 2**

**Stage 3**



Let's Connect!

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