

# Does a Simple Lattice Protein Exhibit Self-Organized Criticality?

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## Introduction

There are many unanswered questions when it comes to protein folding. These questions are interesting because the tertiary structure of proteins determines its functionality in living organisms. How do proteins consistently reach their final tertiary structure from the primary sequence of amino acids? What explains the complexity of tertiary structures? Our research uses a simple hydrophobic-polar lattice-bound computational model to investigate self-organized criticality as a possible mechanism for generating complexity in protein folding and protein tertiary structures.

## Self-Organized Criticality (SOC)

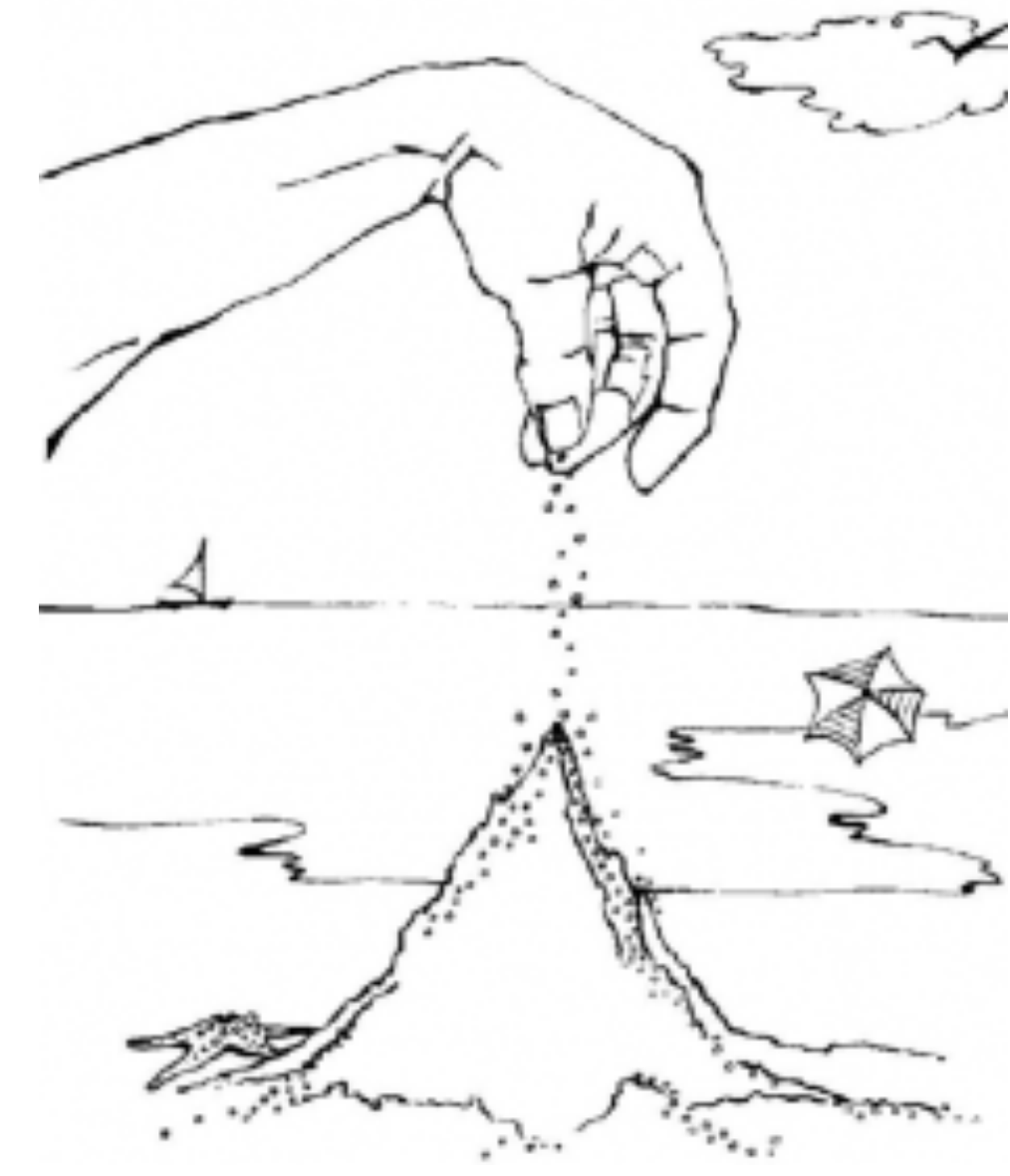


Figure 1  
Representation of sand pile model

- a dynamical system at a critical state
- characterized by power law behavior
- both time and scale invariant

### Sand Pile Model

**Critical Trait:** steepness of slope  
**Critical State:** critical slope is reached  
**Avalanches:** grains of sand falling of steep slopes  
**Avalanche Size:** number of grains falling the distribution of avalanches follows a power law

### Protein Folding Model

**Critical Trait:** minimizing energy  
**Critical State:** non-native structure  
**Avalanches:** rapid changes in structure (due to overcoming energy barriers)  
**Avalanche Size:** number of consecutive folds

The Boltzmann factor, a probability function, allows some folds to occur that don't decrease the energy of the protein.

## Model and Algorithm

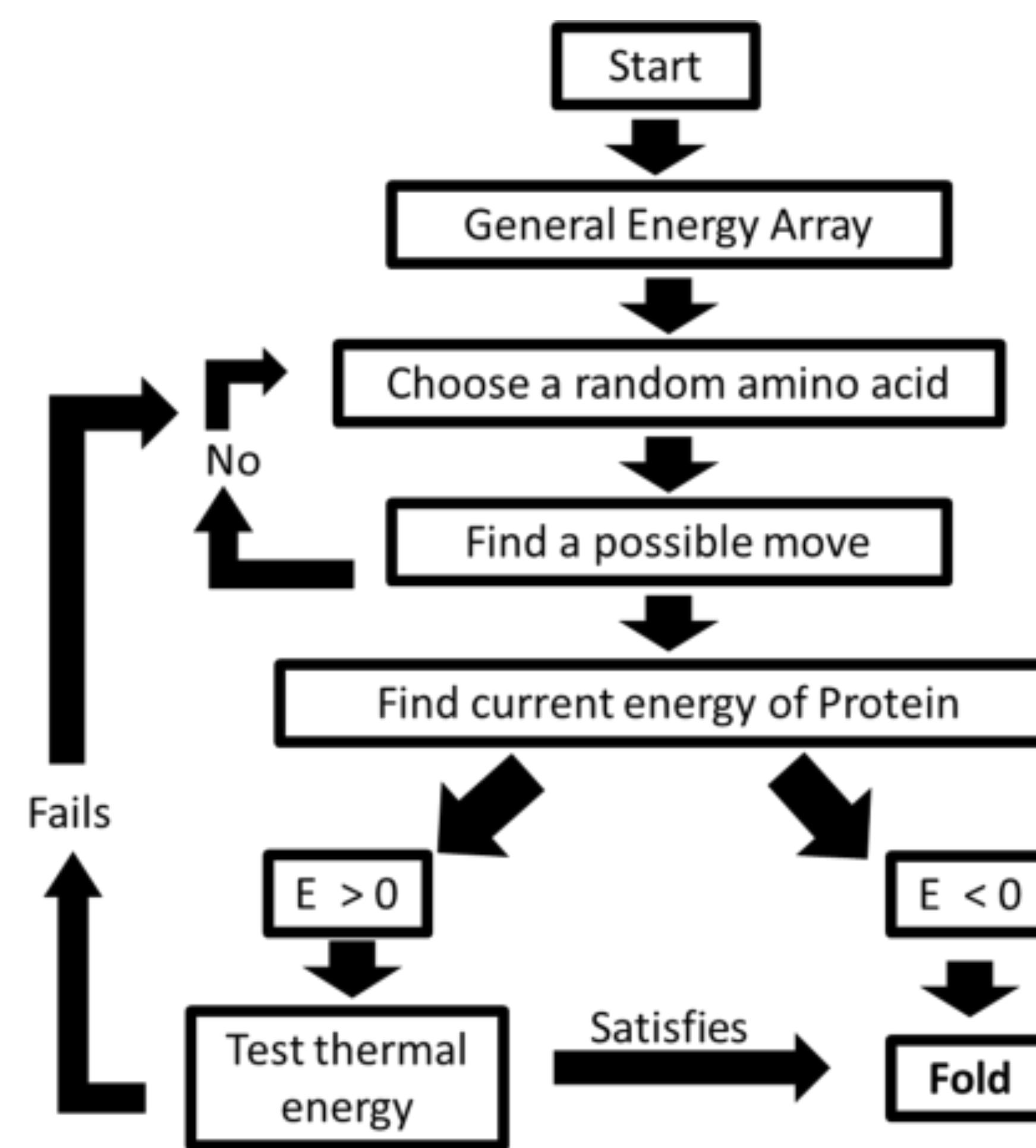


Figure 3  
flow chart for simulation

Model:

- 3D lattice: 1 bond length, no stretching
- HP model: 2 types of amino acids- hydrophobic (H) and polar (P)
- One amino acid moves at a time

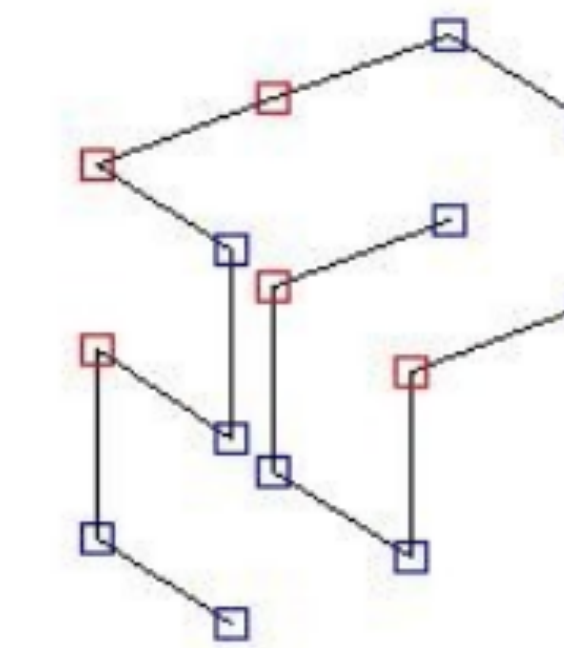


Figure 4  
Sample folded protein

Algorithm:

- The model starts with linear chain made up of a specific sequence of hydrophobic or polar amino acids on a 3D lattice.
- Randomly, an amino acid is chosen for the first move.
- Is there a possible move? No, then a new amino acid is chosen. Yes, move one.
- Current energy of the protein. If  $E < 0$ , fold.
- If  $E > 0$ , then using the Boltzmann factor, the thermal energy is tested. If satisfied a fold occurs.

## Scaled Avalanche Distributions

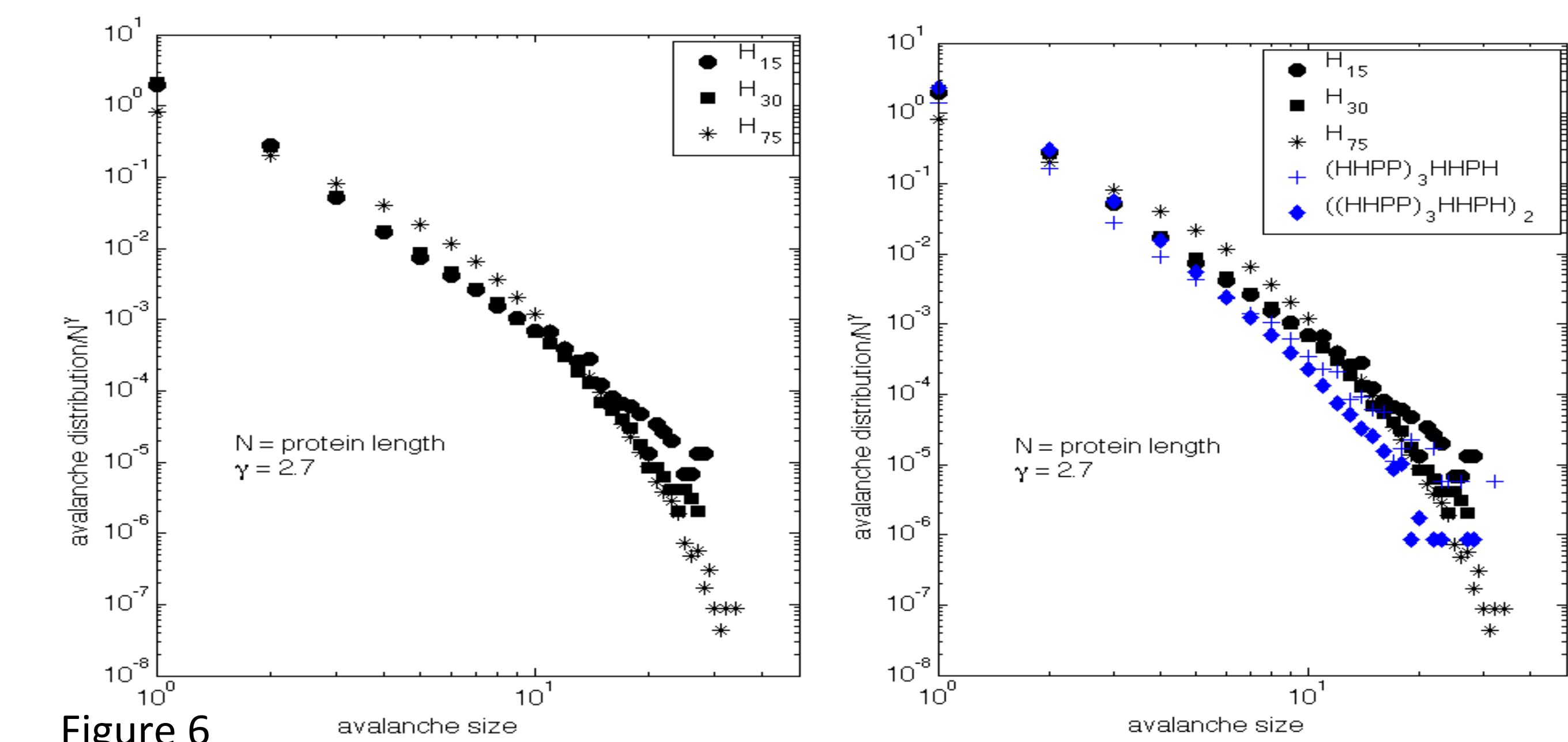


Figure 6  
Scaled avalanche distributions for one sequence type (left) and both sequence types (right)

## Discussion of Results

- Some evidence that specific primary structures exhibit SOC behavior (power law and scaling)
- further analysis needed to establish SOC behavior
  - larger proteins, different primary structures, improved sampling statistics, KS test

## Future Research

- Is SOC connected to tertiary structure?
- How does the ratio of H-P amino acids in the protein affect SOC behavior?
- Do more sophisticated models exhibit SOC?
  - variable bond length
  - alternate avalanche definition
  - molecular dynamics
- Explore contact maps of tertiary structure

## Avalanche Distributions

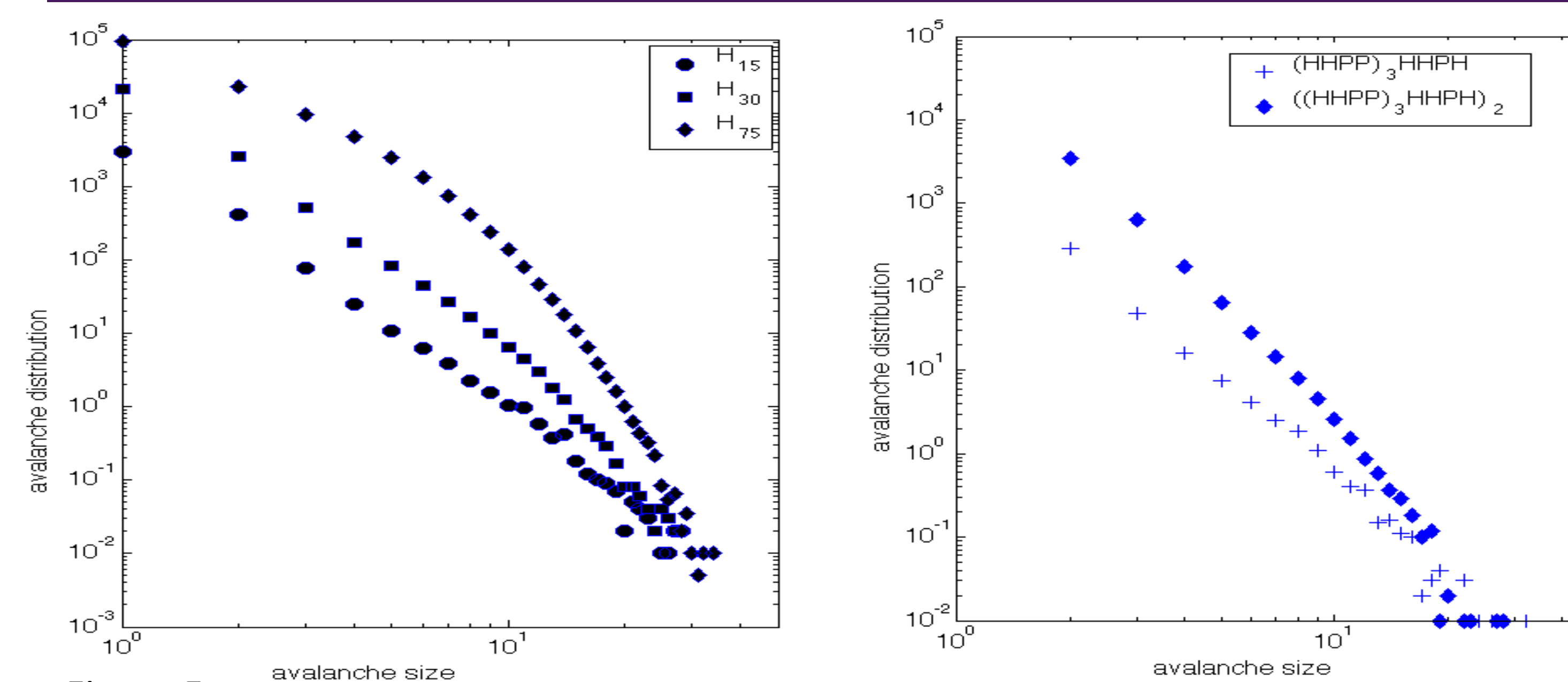


Figure 5  
Avalanche distributions for 2 different primary structure types