



HP Model

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Introduction

HP Model

The Energy ...

3D Version

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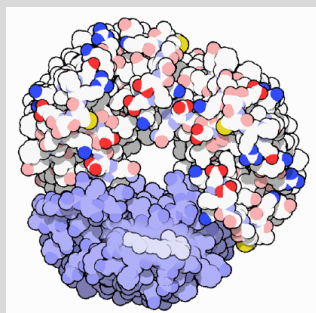
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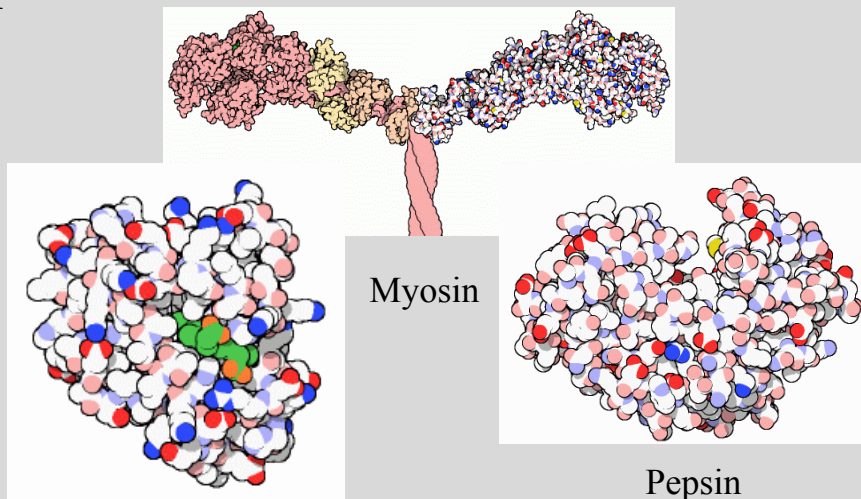
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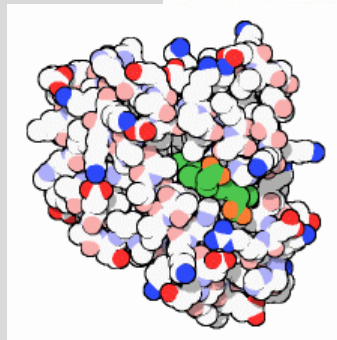


Rhodopsin



Myosin

Pepsin



Hemoglobin

From Protein Data Bank (PDB)

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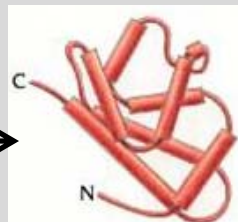
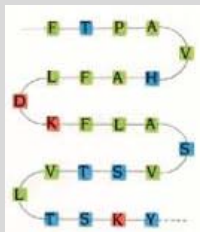
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Genome
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Function



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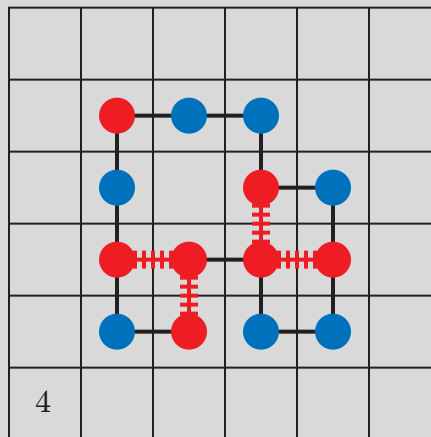
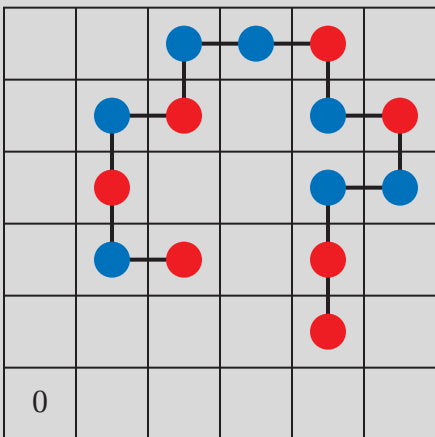
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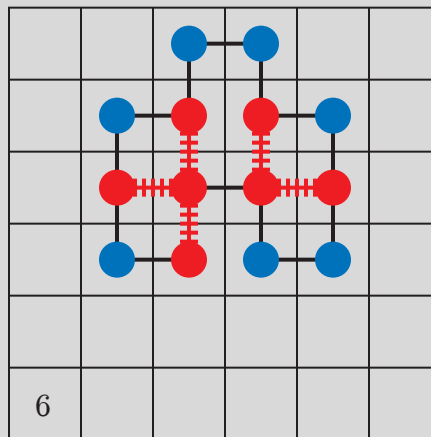
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H ●

P ●





2. HP Model

Protein conformation Self-avoiding chain on a 2D square or 3D cubic lattice.

Energy $E = - \sum n$, where n is number of hydrophobic contacts.

Model The native conformation is the one with minimum energy.

Minimum Energy Conformation An NP complete problem.

Studies on folding HP sequences HZ, CHCC, CI, GA, SA, GTS, EMC, GMC, GSA, PERM, SISPER, ACO, EES, nPERMis, nPERMh.

Opportunities Unsolved problem for sequences with medium length.

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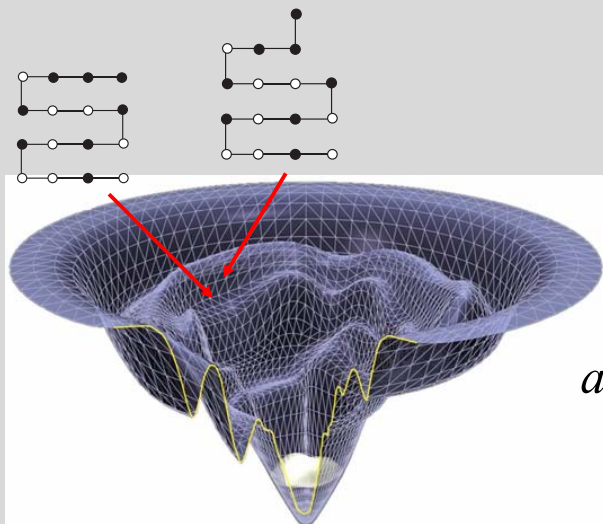
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3. The Energy Landscape



- Start with a conformation x .
- Draw y from $q(x,y) = q(y|x)$.
- Accept the new conformation with probability

$$a(x,y) = \min \left\{ 1, \frac{\pi(y)q(y,x)}{\pi(x)q(x,y)} \right\}$$
$$= \min \left\{ 1, e^{[E(x)-E(y)]/k_B T} \right\}$$



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4. 3D Version

