A Simulating the Folding of Different Sequences Using Monte Carlo

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Much work on hydrophobicity has been done in an attempt to answer the following question: do compact conformations due to hydrophobic collapse help protein folding [1][2]. Many theories have been advanced to study the folding mechanism of polypeptide chains [2]. We are interested to investigate the relationship between protein folding problem and hydrophobic properties. In this work, the HP model and Monte Carlo Method are used to study the effect hydrophobic on the folding problem. We used a cubic lattice and and several chains with distinct sequence . Somes of these sequences are presented in the Table 1. These sequences has different number of hidrophobic residues and proposed by [3]. For each simulation, we measure six parameter and the final geometry of the chain. We measured the:hydrophobic contacts, energy, maximum distance, end-to-end distance, gyration radius, medium energy. We used the language Java to implement the simulation of the chains with monte carlo method and HP model. The simulations were realized in an cubic lattice model varying the number of hydrophobic residues and theirs positions on the chain. In this moment, we are simulating 5 sequences based real molecules (proteins/peptides) presented in the 1. We intended to compare the folding of our model with the folding of the detailed model of these proteins. We are comparing the results obtained with HP model with results generated by Molecular Dynamict. We can observe that the positions of hydrophobic residues is very important to the allows that the chain folding more fast and more easy.

Nº	Hydrophobic Sequence with 27 monomers No-Polar(H)-Polar(P)	Resíduos Hidrofóbicos	Hydrophobic Sequence with 64 monomers No-Polar(H)-Polar(P)
27.1	PHPHPHHHPPHPHPPPPPPPPPPPPHHP	64.1	PPHHHHHPPPHHPPPPPHHPPPHPPPPPPPHPHP PPHPPHPPHPPPPPHPPPPHHPHHPPHPPHP
27.2	PHHPPPPPPPPPPPHHPPHHPPHPPHPH	64.2	PPHPHPPHPPHHHPHHHHPPHHHPPPPHPHPPP HPHPPPHPHPPPPPHPHPPHPHPPPHPPHPP
27.3	HHHHPPPPPHPPPPPHHHPPPPPPPPH	64.3	HPHHPPHHPHPPPPPHHHPHHHHPPHPPHPHHP PPHPHPPHHHPHHPHPPPPPHHHHHHHHPPP
27.4	HHHPPHHHHPPPHPHPPHHPPHPPPHH	64.4	HPPHHPPHPPHPHPPHPPPPHPPPPPPPHPHPHH HPPHPHPPPHPHPPHHPPHPPHPPHPHHHPH
27.5	HHHHPPPPHPHHPPPHHPPPPPPPPPP	64.5	HPPPHHPPHPHPPPHPPPHPHHPPPHHPHPHHP HPPHPPPHPPHPHHHPPHPPHPPHHHPHHHH
27.6	HPPPPPPHPHHHPPHHPPPHPPPPHPH	64.6	HPPHHPHHHHPPPPPPHHPPHPPPPHHPPPHPP HPHHPHPPPPHHPPPPHPPPPPHPPPPHPHH
27.7	HPPHPHHPPPHPPPPPHPHHPHPHPHH	64.7	PPPPHPPPHPPPHHHHPHHPPPPPHPPHPHHPH PHPPPPPHPPPPPPPPPPHHHHPPPPHHPPH
27.8	HPPPPPPPPPPPHPHPPPPPPPPPPHPHH	64.8	PPPHHHPPHPHPPHPPHHPPPHPPHPPHHPHPP PHPPPPPPPPHPHHHPHHHHHPPHHPPPHPPH
27.9	PPPPPPPHHHPPPHPHHPPPHPPHPPP	64.9	HPPHPPHHHPPPPHPHPPPHPHHPHHHHHPPPP HPHPHPPPPHPHPPPHHPHPPPPHPPHHPHP
27.10	PPPPPHHPHPHPHPHPPHHPHHPHPPP	64.10	PPHPPHPPHHHPPPHPHPPHPPHPPPPPPPHPPH HHPPHPPHPPHPHPPPPPPPHHHPPPPPPHPHP

Table 2 – Five sequences based in real molecules (proteins/peptides) [5].

Lenght	Sequence (H- Hydrophobic and P - Hydrophilic)
46	PHHHPHHHPPPHPHHPHHPPHPHHHHPHPPHHHHHPHPHHPPHHP
58	HPHHHHPHHHPPHHPHPHHPHHHPHPHPHHPPHHHPPHPHPPPPHPPHPPHHPPHPPH
103	PHHPPPPPPHHPPHHPHPPHPPPPPPPPHPPPHHPHHPPPPPPPHPPHPHPPHPPPPPHHHPPPPPHHPHHPPPPP PHHPPPPHHHHPHPPPPPPPPPPHHHHHHPPHPP
124	PPHHHPHPPPPHPPPPPHHPPPPHHPPHHPPPPHPPPPHPPHHPPPHHPHHPHHHPPPPHHHPPPPPPPHHPPH PPHPHPPHPPPPPPPPHPPHHHPPPPHPPPHHHHHPPPPHHPHPHPHPH
136	HPPPPPHPPPPHPHHPHHPPPPHPHHHPPPPHPHPHHHHPPPPPPPPPPPPHPPHPPPHPHHPPPHHPPHPPHP HPHPPPPPPPPPPHPPPHHHHHHPPPHHPPHHHPPPHHPHHHHHPPPPPPPPPHPPPPPPHPHPPPP

Figure 1: Tables

References

[1] A.G. Cox, and L. R. Johsnton: Analyzing energy landscapes for folding model proteins. Journal of Chemical Physics, 2006, 124:204714.

[2] C. L. Oliveira, T.H.R. Silva, V. B. Leite and J. Chahine: Frustration and hydrophobicity interplay in protein folding and protein evolution. Journal of Chemical Physics, 2006, 125:084904.

[3] L. TOMA, S. TOMA, Contact Interaction Method: A New Algorithm for Protein Folding Simulations. Protein Science, v. 5, p. 147-153, 1996

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