Plegamiento de Proteínas. El Modelo de Davydov/Scott

Protein Folding and the Davydov/Scott model

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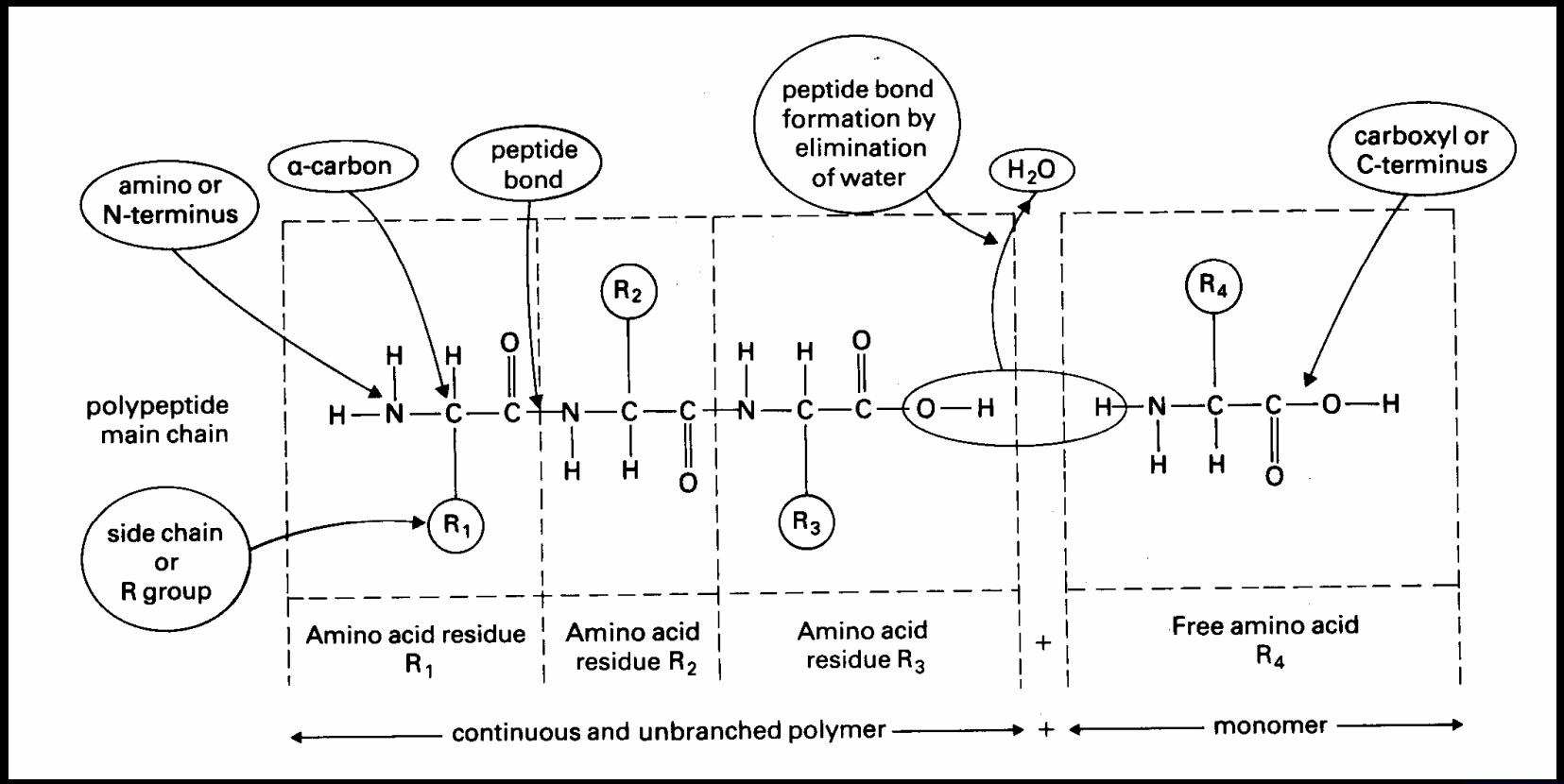
The Primary Structure of Proteins



Amino acid side chains

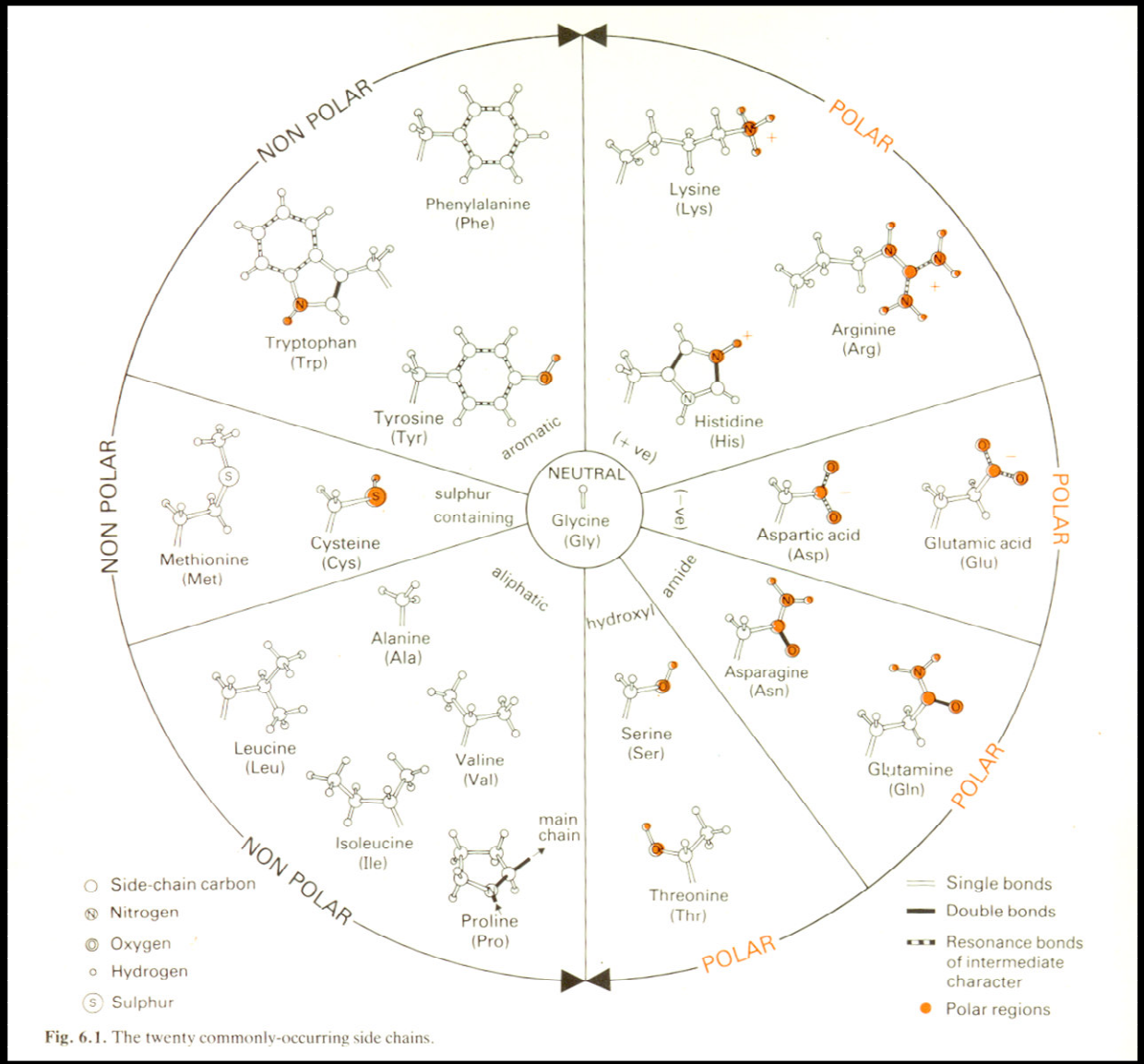


Fig. 6.1. The twenty commonly-occurring side chains.

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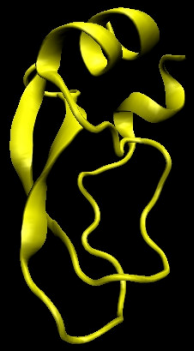
The three-dimensional structure of Proteins

α

β

Unstructured



α/β

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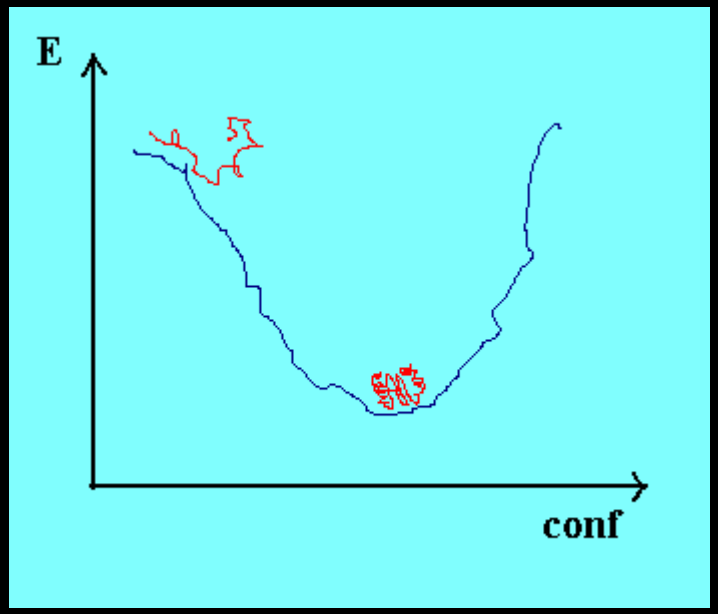
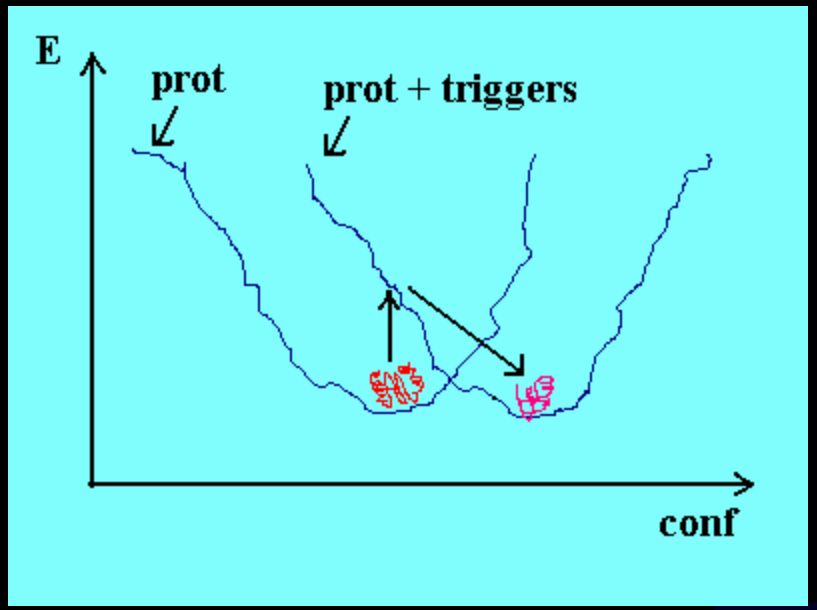
A Funnel energy landscape ?

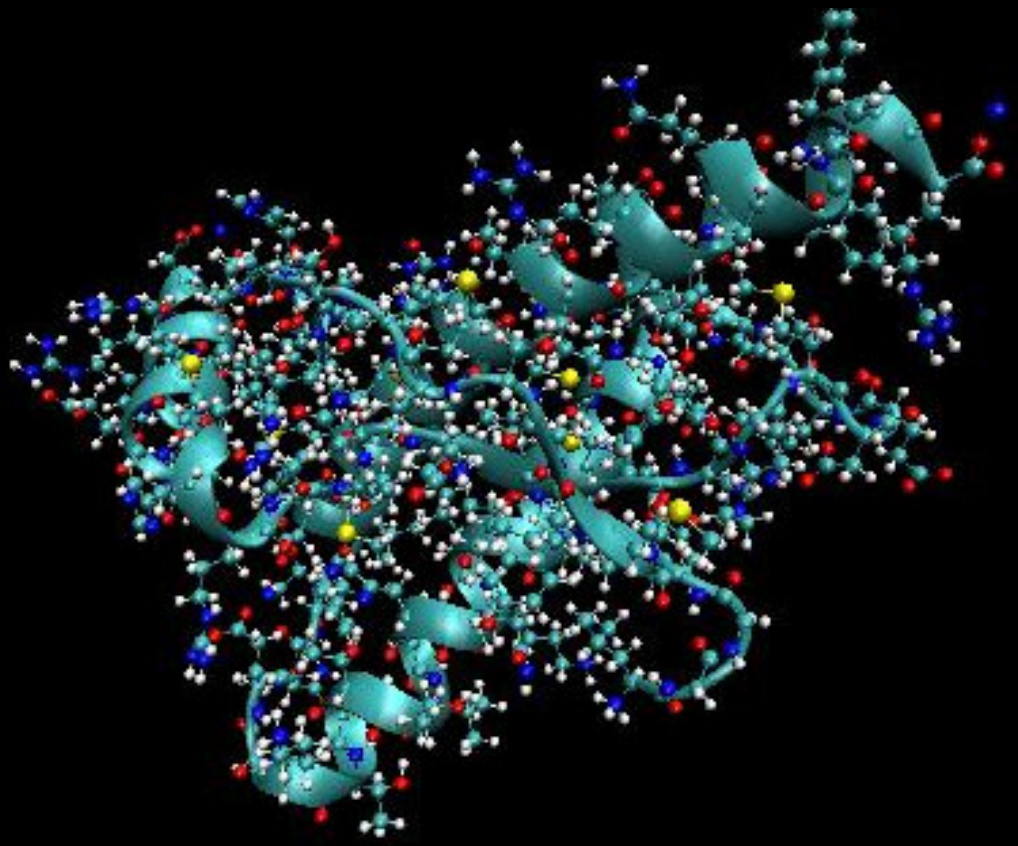
Protein Folding



Conformational Change



The Structure of Proteins



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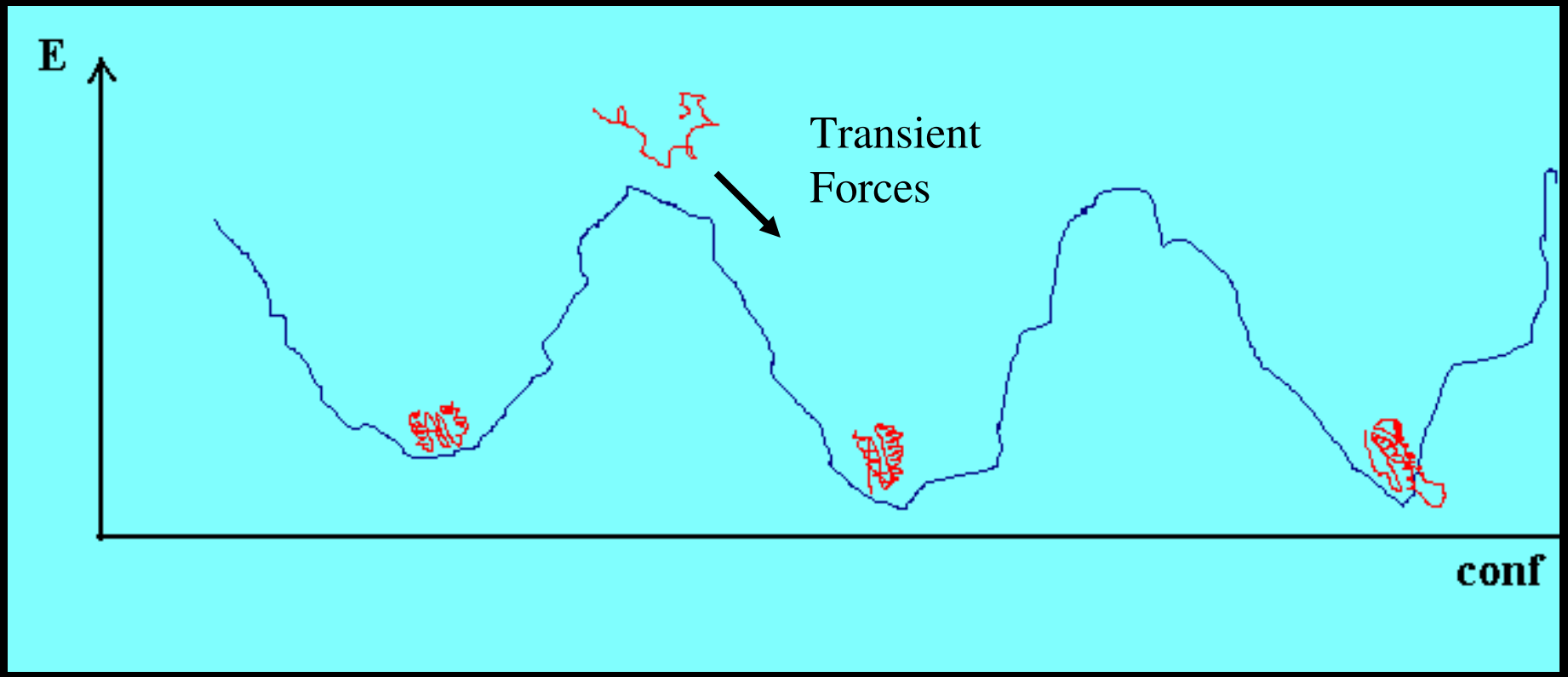
The Classical Potential Energy of Proteins

$$V = \sum_{bonds} K_r \left(r - r_{eq}\right)^2 + \sum_{angles} K_\theta \left(\theta - \theta_{eq}\right)^2 +$$

$$+ \sum_{dihedrals} \frac{E_n}{2}\left[1 + \cos\left(n\varphi - \gamma\right)\right] + \sum_{i<j} \left(\frac{A_{ij}}{R_{ij}^{12}} - \frac{B_{ij}}{R_{ij}^{6}} + \frac{q_i q_j}{\varepsilon R_{ij}} \right)$$

A Multi-funnel energy landscape



Conclusion: classical potentials cannot explain the selection of the native funnel. Other, transient, forces must exist to effect that selection.

The VES Hypothesis

The first step in protein folding and function is the storage of energy in the form of Vibrational Excited States.

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The Davydov/Scott model