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Two complementary views on the protein folding puzzle

The ability of protein chains to fold spontaneously is a long-standing puzzle in molecular biology. Here we describe physical theories estimating (i) protein folding time, as the time of overcoming the free-energy barrier separating the native (N) and unfolded (U) states of protein chains, and (ii) the volume of conformation space, which is to be scanned to find the most stable chain fold. In the theory of folding rates, a special role is played by the mid-point of thermodynamic and kinetic equilibrium between U and N states. Paradoxically, a theoretical estimate of the "U-to-N" folding time is easier to get from consideration of the "N-to-U" unfolding, because it is easier to outline a good unfolding pathway than a good folding pathway, while, after the physical "detailed balance" law applied to the transition mid-point, the "U-to-N" time equals to the "N-to-U" time. The complementary analysis of the volume of conformation space, which is to be scanned going "from U to N" in a search for the most stable fold, performed at the level of formation and assembly of secondary structures, outlines the upper limit of folding times. It is shown that both theories (based on "N-to-U" and "U-to-N" transitions) delineate the observed range of single-domain globular protein folding rates. The first part of this work (study of the "N to U" transitions) has been supported by the grants of the HHMI, RFBR, MCB, and its second part (study of the "U to N" transitions) by the RSF grant 14-24-00157.

Biography

Alexei Finkelstein has done his PhD in biophysics, moscow phystech., 1976, DSc biophysics, Moscow University 1991. Author of >250 scientific papers and books "protein physics", (five russian, two english and two chinese editions), and "physics of protein molecules" (in Russian). citation index by google scholar about 8400, hirsch index about 42. Since 1970, member and since 1999, head of protein physics laboratory at the institute of protein research, RAS. Since 1998, full professor of the Moscow University. Awards from FIRCA, INTAS, CASP, HHMI (3 times), RFBR, RSF, Moscow Grant, etc. State Prize of Russia in Science (1999), elected to the Russian Academy of Sciences (2008).

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