Managing protein folding process with intelligent process parameters adjustment

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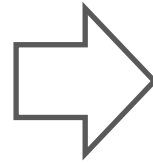Barbara Kalinowska, Zbigniew Baster, Dawid Dułak

INNOVATIVE ECONOMY
NATIONAL COHESION STRATEGY

PL GRID+

We want to simulate how a protein achieves three dimensional structure starting from an amino acid sequence
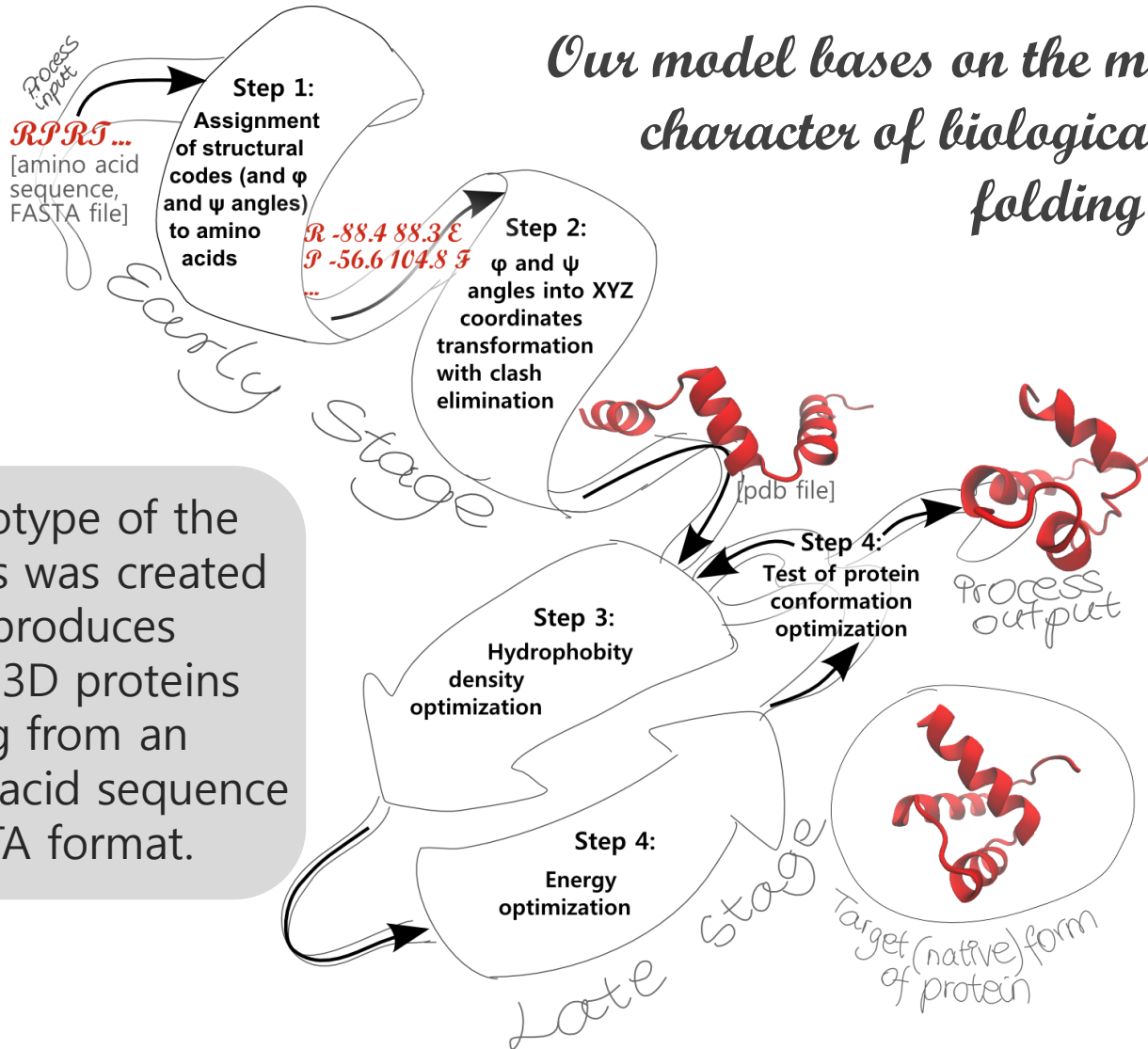
RPRTAFSSEQLARLKREF
NENRYLTERRRQQLSSE
LGLNEAQIKIWFQNKRAKI

Why to simulate folding process?

- The solution of protein structure prediction plays critical role for computer aided drug design.
- The correct recognition of target protein molecule increases the effectiveness of drug efficiency.

Our model bases on the multi-step character of biological protein folding process.

Process input

RPRT...
[amino acid sequence, FASTA file]

Step 1:
Assignment of structural codes (and φ and ψ angles) to amino acids

R -88.4 88.3 E
P -56.6 104.8 F
...

Step 2:
φ and ψ angles into XYZ coordinates transformation with clash elimination

Early Stage

A prototype of the process was created which produces folded 3D proteins starting from an amino acid sequence in FASTA format.

[pdb file]

Step 3:
Hydrophobity density optimization

Step 4:
Test of protein conformation optimization

Process output

Step 4:
Energy optimization

Late stage

Target (native) form of protein