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Tailoring β-peptide foldamers by backbone stereochemistry

Foldamers, the non-natural self-organizing biomimicing systems show similar properties to the proteins, e. g. they have a tendency to fold into the specific periodic compact structures. The most thoroughly studied representatives of this field are the β-peptides consisting of β-amino acids. The prevailing 3D structure of a foldamer is determined by many factors, such as the stereochemistry, the residue type, the side-chain topology and chemistry, etc.

Based on the backbone stereochemistry, binary geometrical descriptors were devised in order to gain a simplified representation of the stereochemical building blocks governing formation of the secondary structure of peptidic foldamers. Analysis of the bitstreams of the known β-, α- and α/β-peptide secondary structures demonstrated clear relationships between the bit pattern and the preferred self-organization type. Data on the *de novo* designed foldamers demonstrate that the helices complying with the rules adopt novel biomimetic helices in solution (Fig. 1).

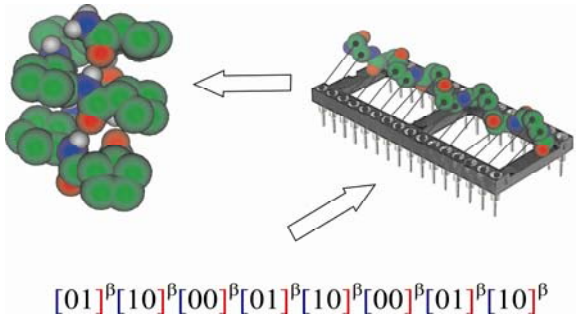

Figure 1. The *de novo* design methodology

Our results nevertheless suggest an interesting analogy: the peptidic foldamer chain acts as an analog computer executing the commands encoding the sequence of stereochemical building blocks. In this way, the proposed binary codes can be regarded as the basic instruction set in the assembly language of the peptidic foldamer sequences as analog computers.