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Application of the experimental methods revealed that proteins, one of the essential components of the cellular machinery, adopt various structural forms. Proteins consist of combined in various ways, interacting with each other, small building blocks. Most proteins comprise different types of building blocks that are mixed to form compact irregular structures. There are, however, proteins in which one type of building block is repeated continuously, one after the other, resulting in highly regular structures. One of the best-studied structures of this type is the so-called α-helical coiled coils. Regularity of their structures has opened the possibility of developing mathematical models that not only allow describing and quantifying their structural parameters, but also designing completely new structures, not yet observed in nature. Although parametric equations, which constitute a mathematical description of coiled-coil structures, were proposed and implemented already by Francis Crick, they are still the basis for studies aimed at designing new coiled coil-based nanostructures of various applications.

The aim of the project described herein is to develop a mathematical model in terms of a set of parameters for two additional classes of repetitive protein structures other than α-helical coiled coils. The first of these types is known as a π-helical coiled coil and is a hypothetical structure, which has not been observed in nature. Its building block, a π-helix, has been studied; however there were no attempts towards amplifying it to obtain a new regular and repetitive structure. The case of the second class of structures, β-helix, is different as many structures of this class have been identified. Development of parametric models for β-helices will enable cataloguing these structures and defining general rules that relate their sequences to structures. This, in turn, will allow designing new β-helix structures, not yet observed in the nature.

Accomplishment of this project will be of high importance for studies on protein structures and will lead to creation of a "molecular toolkit" that can be used in designing and creating new structures with precisely defined parameters. Studies on nature-inspired nanomaterials are also important for another reason - they allow validating our understanding of evolutionary processes, which lead to the emergence of the observable "protein universe".