Bacillus subtilis spores are metabolically inactive and are distinguished by their high resistance to harmful environmental factors. When environmental conditions become more favorable, the spore germination process is initiated, leading to the formation of a vegetative form. The biochemical signal for the initiation of germination may be an increase in the concentration of specific inducers - germinants - in the spore environment. The initiation of the process takes place with the participation of germination receptors.

One of the germination receptors is the GerA receptor, which was the main focus of this research work. The GerA receptor induces the germination process in response to L-alanine and/or L-valine and is built of three subunits: A, B and C. Literature data show that all subunits are essential for the receptor to function properly. The GerA receptor, which is the focus of this dissertation, is located in the inner membrane of the spore and two of its subunits, GerAA and GerAB, are integral membrane proteins. The structure of the receptor and the mechanism of signal transduction initiating the germination process, despite numerous studies, remains unknown.

The main aim of this study was to develop a theoretical model of the GerA receptor and to investigate potential binding sites for germinants initiating the germination process. This model, given the strong relationship between structure and biological function of macromolecules, can be used for further studies aimed at elucidating the mechanism of germination initiation.

In a first step, theoretical models of the receptor subunits (GerAA, GerAB and GerAC proteins) were built. Modelling was performed using homology modelling methods. The obtained models were then used to build receptor models and to determine potential binding sites of germinants. Mutant models of GerAA protein were also investigated and then were used to explain the influence of structure on the phenotype of the mutants.

To predict potential binding sites of germinants, molecular docking methods were used. Since the literature does not mention where exactly the ligand-binding pocket is located and only speaks in general terms of the A and B subunits as potentially binding germinants, global docking was used in this study to provide information on the location of potential binding sites.

Based on the observation of similarities in the clustering process of chemotaxis and germination receptors, as well as the homologues used to model the subunits, it was assumed during the study that the subunits could form homodimers or homotrimers, which then, with the involvement of the GerD protein, cluster into a receptor.

Based on the results obtained during research, two models of the GerA receptor were presented. The first one was built on the basis of monomers of subunits, whereas the second model is built of dimers and thus forms, similarly to chemotaxis receptors, a trimer of dimers. Docking of germinants to the subunits and the receptor complex indicates several potential interaction sites that are responsible for the initiation of the germination process.