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Predictions of the structure of *Bacillus subtilis* GerA germination receptor complex in the membrane model

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Statement of the Problem: Spores of *Bacillus subtilis* are extremely resistant to harsh environmental factors and can survive for years in their dormant state. However when the favorable conditions arise spores can rapidly lose their dormancy and resistance in the process of spore germination. Germination can be triggered by germinants – nutrients, that bind to a specific germination receptor (GR). One of such receptors and the main interest of this study is GerA GR, which is composed of three subunits: GerAA, GerAB and GerAC is located in the spore inner membrane. Subunits A and B are predicted to be integral membrane proteins and responsible for germinants binding. However, till now there is no definitive knowledge describing the 3D structure of this receptors.

Methodology: Models of GerA subunits were predicted using homology modeling approach, using Modeller program. Due to lack of close structural homolog GerAA and GerAB models were predicted using multitemplate modeling approach. Based on protein-protein interaction sites prediction, on biological assembly of templates used in homology modeling and on the similarity in the GRS clustering process to chemotaxis receptors clustering, we proposed that GerA subunits may form homodimers or homotrimers. Homocomplexes were predicted using protein-protein and symmetrical docking methods; using SAM program, ClusPro, ROSIE and GrammX servers. Proposed models of GerA receptor were built based on the protein-protein interaction sites prediction and using two approaches: molecular dynamics simulation in Amber package and a spontaneous proteins aggregation simulations. Models of GerA receptor were embedded into biological membrane model and optimized using the Martini force field.

Findings & Significance: We were able to propose models of GerA germination receptor complex embedded into membrane model. Determination of GerA receptor structure and topology is an important step in study of the relationship of structure and function and mechanism of action of GerA receptor.

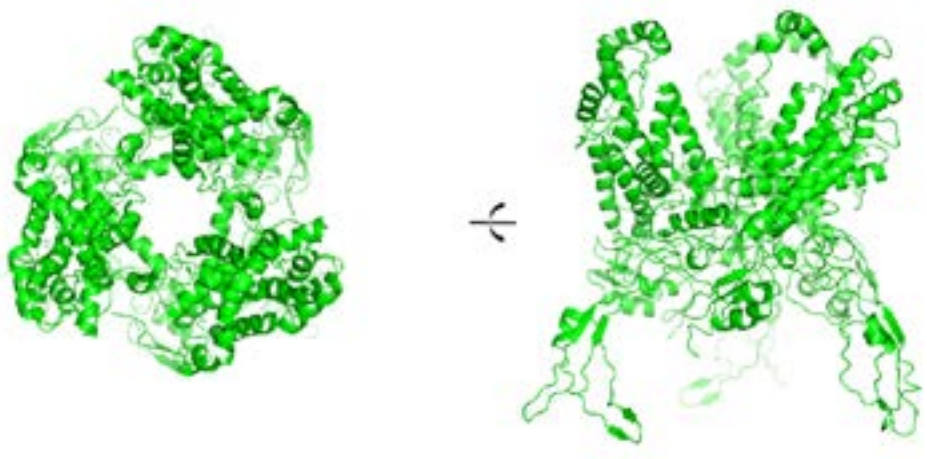

Figure 1: Homotrimer of GerAA subunit model.

Recent Publications:

1. Korza G and Setlow P (2013) topology and accessibility of germination proteins in the *bacillus subtilis* spore inner membrane. Journal of Bacteriology. 195(7):1484-1491.
2. Griffiths K et al. (2011) Germination proteins in the inner membrane of dormant *Bacillus subtilis* spores colocalize in a discrete cluster. Molecular Microbiology. 81(4):1061-1077.
3. Hsu P C et al. (2017) CHARMM-GUI Martini maker for modeling and simulation of complex bacterial membranes with lipopolysaccharides. Journal of Computational Chemistry. 38(27):2354-2363.
4. Li Y et al. (2010) Crystal structure of the GerBC component of a *Bacillus subtilis* spore germinant receptor. J. Mol. Biol. 402(1):8-16.
5. Setlow P (2014) Germination of spores of bacillus species: what we know and do not know. Journal of Bacteriology. 196(7):1297-1305.

Biography

Inga Jamrozek obtained her BA Degree in Bioinformatics and MA Degree in Biotechnology from the University of Gdansk, Poland. She is currently a third year PhD student at the Intercollegiate Faculty of Biotechnology (IFB) of University of Gdansk (UG) and Medical University of Gdansk (MUG), Poland. Her major research interests lies in developing a model of GerA receptor and molecular mechanism of its function. This study is an interdisciplinary research conducted within Laboratory of Molecular Bacteriology at IFB of UG and MUG.

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