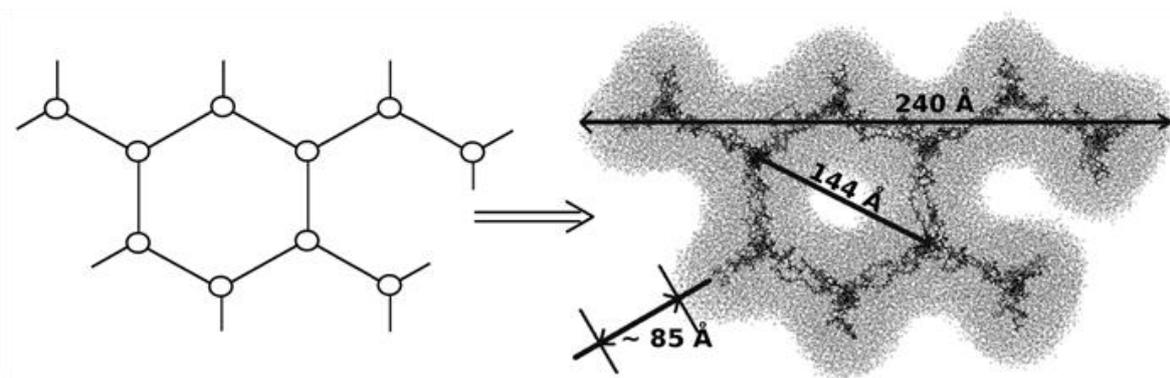


## CONSTRUCTION, MOLECULAR DYNAMICS AND STRUCTURAL ANALYSIS OF THE BACTERIAL CELL WALL PEPTIDOGLYCAN LAYER MODELS

Rafal Slusarz, Monika Szulc, Janusz Madaj

*Faculty of Chemistry, Sugar Chemistry Chair, University of Gdansk, Gdansk, Poland*

The peptidoglycan (PG) and teichoic acids (TA) are a key target for antibacterial treatment in the infections caused by some Gram-positive bacteria. Proper understanding of the mechanisms of binding to the bacterial cell wall seems to be crucial for proper development of new drug candidates effective against these bacteria. The exact three-dimensional structure of the bacterial cell wall PG layer is still unverified because of its complexity and the lack of pure and separate samples, suitable for structural studies. In this work we constructed two different models of Gram-positive bacteria PG layer: the layered model in which the glycan strands run parallel to the cytoplasmic membrane and the scaffold model in which the glycan strands run perpendicular to the membrane. We focused on PG structure and its arrangement in both models. PG conformational changes during geometry optimization, models relaxation and molecular dynamics of fully hydrated PG layer models were described and discussed. We have found that the border surface of both models differ from the surface located away from the edge of models and the chains formed by disaccharide units prefer helix-like conformation. This curling of PG chains strongly affects the shape of antibiotic-accessible surface and thus is crucial for new drug development.



### Acknowledgments:

This work was supported by the European Union within the European Regional Development Fund (grant UDA-POIG.01.01.02-14-102/09/03). The computational time in the Academic Computer Center in Gdansk CI TASK, Poland is acknowledged.