Structure and Dynamics of The Bacterial Cell Wall by Solid-State NMR

S. Hediger[a], M. Giffard[a], A. Gansmüller[b], T. Kern[b], C. Bougault[b], W. Vollmer[c], B. Joris[d], J.-P. Simorre[b]

[a] *Institut Nanosciences et Cryogénie, CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble, France*
[b]*Institut de Biologie Structurale Jean-Pierre Ebel, 41 rue J. Horowitz, 38027 Grenoble, France*
[c]*Institute for Cell and Molecular Biosciences, Newcastle University,NE2 4HH Newcastle Upon Tyne, UK*
[d]*Centre d'ingénierie des protéines, Université de Liège, Sart-Tilman, B4000 Liège, Belgium*
(sabine.hediger@cea.fr)

The cell wall is essential for maintaining viability of bacteria. It gives the bacterial cell its shape and protects it against osmotic pressure, while allowing cell growth and division. It is made up of peptidoglycan (PG), a biopolymer forming a multi-gigadalton bag-like structure, and additionally in Gram-positive bacteria, of covalently linked anionic polymers called wall teichoic acids (WTA). TAs are thought to play important roles in ion trafficking, host-cell adhesion, inflammation and immune activation.

In this contribution, we compare the flexibility and the organization of PG from Gram-negative bacteria with its counterparts from different Gram-positive bacteria using solid-state nuclear magnetic resonance spectroscopy (NMR) under magic-angle sample spinning (MAS). Flexibility of the PG network is found to mainly correlate with its reticulation rate, showing a decrease of dynamics going form *E. coli* to *S. aureus* via *B. subtilis*. We also show that ^{31}P solid-state NMR is particularly well adapted to characterize WTAs on isolated cell walls as well as on intact cells. Complexation of the cell wall with divalent ions (Mg^{2+} and Mn^{2+}) was studied as well. Our results highlight an important structural aspect of Gram-positive cell wall architecture and allow proposing a new model for the interaction of divalent ions with both WTAs and carboxyl groups of peptidoglycan[1]. Interaction of PG with a protein is also presented[2].

References:
2. Kern T., Giffard M., Hediger S., Amoroso A., Giustini C., Bui N.K., Joris B., Bougault C., Vollmer W., Simorre J.-P., *J. Am. Chem. Soc.*, 132, 10911-10919 (2010).
2. Kern T., Hediger S., Müller P., Giustini C., Joris B., Bougault C., Vollmer W., Simorre J.-P., *J. Am. Chem. Soc.*, 130, 5618-5619 (2008).