Different Types of Ca^{2+} binding sites in SiiE

A. Sandmann, H. Sticht

Division of Bioinformatics, Institute for Biochemistry

The adhesion protein SiiE mediates contact between Salmonella enterica and the host cell. It consists of 53 repetitive bacterial immunoglobulin (BIg) domains. It binds two Ca^{2+} ions per domain in two structurally different types of coordination sites. It very likely recruits the Ca^{2+} ions upon secretion from the membrane while passing through the bivalent cation filled bacterial lipopolysaccharide layer (see Griessl et al [1]).

Chelation experiments showed distortion of the straight, rod-like structure in the absence of Ca^{2+} coordination. Infection experiments showed distinct changes of SiiE mediated characteristics upon deactivation of type I versus type II coordination sites.

We used MD simulations to characterize the flexibility of SiiE wild type and mutant proteins. For this we used the X-ray structure of BIg 50-52 (PDB code 2YN5) which contains the typical conserved SiiE domain interface between BIg 51 and 52. Mutants contain either deactivated type I, type II or type I&II coordination sites. The systems show different behavior with respect to domain-domain bending as well as rotation.

We used steered molecular dynamic simulations to estimate the relative binding energies and maximal binding forces for type I versus type II Ca^{2+} binding sites. A larger work was required to remove Ca^{2+} from the type II binding site within BIg 51 compared to the type II binding site between BIg 51 and 52. The maximal required force was comparable for the two binding sites.

[1] M. H. Griessl, B. Schmid, K. Kassler, C. Braunsmann, R. Ritter, B. Barlag, Y. D. Stierhof, K. U. Sturm, C. Danzer, C. Wagner, T. E. Schaffer, H. Sticht, M. Hensel, Y. A. Muller, *Structure* **2013**, *21*, 741-752.