Goldschmidt 2021 Abstract
https://doi.org/10.7185/gold2021.6480

Synchronisation of nanofibrils with $CaCO_3$ crystallisation – Vaterite mineralization by *Megabalanus rosa* cement protein (MrCP) 20.

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Nature has always been astounding instructor and biomineralization is one such tasks that we are striving to learn. It is a quintessential process for shelled organisms like crustaceans. Barnacles are aggressive macrofoulers secured to foreign substratum for its survival and its soft body is enclosed in outer shell radiating from base plate that are calcerous in nature. Its adhesion is established by secretion of multi protein complex called cement from its base plate. The base plate of *Megabalanus rosa* (*M.rosa*), a well-studied acorn barnacle, secretes at least five proteins of varying molecular weight in the cement (MrCPs) and the protein of current interesting study is MrCP20. It is also intriguing to note that CP20 protein is absent in membranous base stalked barnacles.

MrCP20 is found to be rich in cysteine residues and the pattern of Cys-X-X-X-X-X-Cys, Cys-X-X-Cys and Cys-X-Cys is conserved. There were no evidence of intermolecular disulphide bond reported. Our group also published the 3-D solution NMR structure of rMrCP20 to be folded into three structural domains intervened with two dynamic stretches [1]. The structural domains are dominated with antiparallel beta strands that are stabilized by intramolecular disulphide bonds and the beta strands from domain 2 and 3 are enriched with acidic amino acids imparting negative charged core to the structure. MD simulation studies of solution NMR structure described that MrCP20 adopts multiple dynamic conformations hinting at its heterologous functions. Incidentally, we found that MrCP20 forms and stabilizes metastable vaterite polymorph of $CaCO_3$.

An array of spectroscopic studies with ATR-FTIR, Raman, solution and solid state NMR was carried out to understand the vaterite morphogenesis and formation. Interestingly, we found the vaterite formation involves PILP (polymer – protein in this case induced liquid phase) that nucleates crystallisation that in turn promotes fibrillation of protein. Altogether, the mechanism of vaterite formation provides important insight in the regeneration/stabilization of exoskeleton of barnacles thriving in multitude of environment.

References:

[1] Mohanram H et al, (2019) Three-dimensional structure of Megabalanus rosa Cement Protein 20 revealed by multi-dimensional NMR and molecular dynamics simulations. Phil. Trans. R. Soc. B37420190198.