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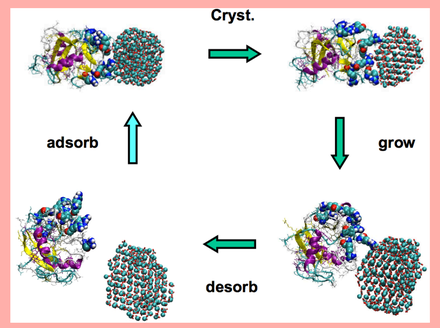
Molecular dynamics simulations of peptide sequences and calcium carbonate

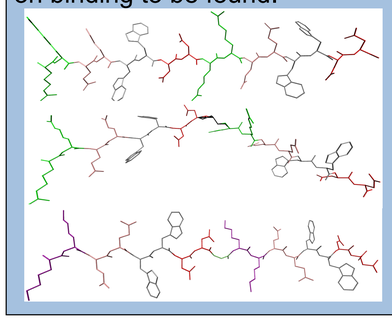
1. Introduction

Calcium carbonate is a common biomineral found in shells, spicules and spines as well as other biological structures. Avian eggshells contain a layer of calcite. In chicken eggshells, it has been found that they also contain a large amount of the protein ovocleidin-17. Previous molecular dynamics simulations have shown that this protein acts as a catalyst in the nucleation of calcium carbonate as shown in the diagram below [1].The aim of this project was to investigate this interaction.



2. Peptides

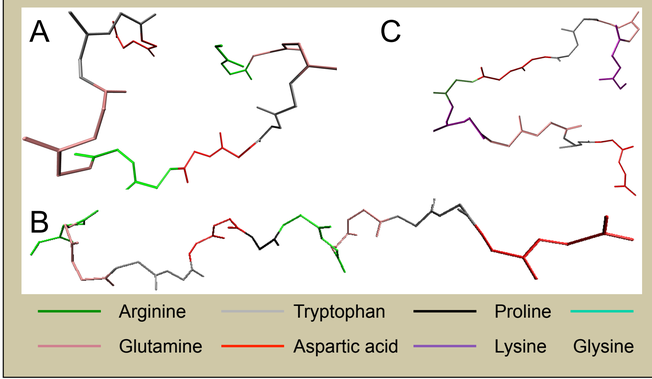
Three model peptides with doublets of charged residues were made, labelled A, B and C. The first two were chosen as they were similar to a protein found in geese eggshells. The introduction of a proline residue in the second peptide is expected to alter the secondary structure. The third peptide has lysine instead of arginine and a glycine residue in the middle. The glycine is expected to alter secondary structure of the peptide and the substitution with lysine will allow the effect of arginine on binding to be found.



\+ -
RREEWWDD
RREEWWDD
RREEWWDDP
RREEWWDD
KKEEWWDDG
KKEEWWDD

3. Peptide conformations

MD simulations of these peptides showed the most energetically favoured conformation of each one. We can see that the proline in the second peptide gives it the most sturdy structure. These conformations were used for further simulations.



5. Conclusions

Each simulation was performed twice with the peptide rotated in a different way. The residues which bound to the calcium carbonate nanoparticle are shown below.

	ARG	ASP	TRP	GLN	GLY
A1	X	X	X		
A2	X	X	X		
B1	X	X	X		
B2	X			X	
C1					X
C2					

We can conclude that arginine is important in binding and that peptides A and B appear to bind more quickly than C. Peptide B binds the quickest, suggesting that a straight secondary structure may be important in binding to $CaCO_3$.

References

[1] Freeman C.L.; Harding J.H.; Quigley D.; Rodger P.M. *J. Phys. Chem.* **2011**, *115*, 8175-8183.
[2] Ajikumar P.K. *et. al. Angew. Chem.* **2005**, *117*, 5612-5615.

4.Simulations with $CaCO_3$

Simulations of each peptide with an amorphous calcium carbonate nanoparticle were performed. In each case the peptide bound to the nanoparticle and changed conformation. The final conformation of each peptide is shown along with it's RMSD over the simulation.