# Application of computational methods to develop materials resistant to bacterial biofilm formation

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The prevention and eradication of bacterial biofilms remains a major unsolved global healthcare challenge. Bacterial biofilms are communities of bacteria that readily form on the surfaces of implanted medical devices such as urinary catheters and endotracheal tubes. Within a biofilm bacteria become up to 1000 times more tolerant to antibiotics and the host's immune defences[1]. To address this problem novel materials are required that are able to prevent biofilm formation. However, there are innumerable possible materials that could be screened and the interactions between bacteria and surfaces are poorly understood[2].

To effectively search for novel materials resistant to bacterial attachment we have used a high throughput screening approach to assess the bacterial-material interaction for hundreds of different polymers in parallel[3]. We then applied computational modelling to develop structure-function relationships between the material properties and their biological performance[4-6]. Such models can be used to screen virtual libraries of materials to identify potential candidate polymers for further experimental screening. Two approaches were taken, in the first we modelled hundreds of diverse polymers that represented a large chemical space[4,5]. Although these models could be broadly applied they were difficult to interpret. Concurrently, we explored correlations between molecular descriptors and a subset of structurally related materials to create a model that more readily enabled the design of new monomers resistant to biofilm formation. Specifically, we have identified a correlation between the molecular rigidity and hydrophobicity of the pendant groups on polyacrylates with bacterial biofilm formation[6].

The further development of computational modelling applied to bacterial-material interactions will lead to the identification of optimised materials with biofilm resistant properties by unravelling the complex structure-function relationships.

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