

## Galactan as a filler to prevent biofilm formation - An *in-silico* approach

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### ABSTRACT

**INTRODUCTION:** Oral biofilm is a virulence factor in many oral infectious diseases, including dental caries, gingivitis, periodontitis, periapical periodontitis, and peri-implantitis. Implanted biomaterials (such as Gutta-percha points) provide a surface for bacterial adhesion and biofilm formation, ultimately leading to biomaterial infections. Galactan is a polysaccharide that is made up of polymerized galactose. They are found in red seaweeds and are commercially important due to their widespread use as gelling and thickening agents in the food industry. Assessment of these polysaccharides as a filler or a sealant in endodontic purposes can be a boon for the dental industry as they have gelation and thickening properties and are derived from a natural source.

**AIM:** This study is to analyse the effects of galactan used as a filler and in the prevention of biofilm formation.

**MATERIALS AND METHODS:**

**RESULTS:**

**DISCUSSION:**

**CONCLUSION:**

**KEYWORDS:** Biofilm, Caries, Galactan,

### INTRODUCTION

Oral biofilm is a virulence factor in many oral infectious diseases, including dental caries, gingivitis, periodontitis, periapical periodontitis, and peri-implantitis. According to definitions, biofilms are oriented collections of microorganisms that are attached to one another or to a surface and covered in extracellular polymeric substance (EPS) that the microorganisms produce on their own. Mature biofilm is composed of approximately 5-25% bacterial cells and 75-95% glycocalyx matrix (1). Biofilms can be observed nearly wherever there is moisture. Biofilms can be found in nature in industrial bioreactors, on rocks in streams, and in animal host environments like the otolaryngologic, vaginal, and gastrointestinal tracts and oral cavity (2). The oral microflora contains over 700 different bacterial species. Most species prefer certain sites over others because of the unique local environment those sites provide, such as the periodontal pocket's anaerobic environment (3). Microflora can be found in both caries-free and periodontitis-free people, as well as caries-affected and periodontitis-affected people, and many clinical studies show that the percentage of certain bacterial species, such as *Streptococcus mutans* or *Porphyromonas gingivalis*, is increased in patients with caries or periodontitis, respectively (4). Biofilm formation is a complex procedure. Each organism has its own way of adhering to surfaces. Attachment via flagella, pili, and polysaccharide adhesins are some of the modes. Bacteria adhere to the surface and progress to biofilm formation.

Implanted biomaterials such as Gutta-percha points provide a surface for bacterial adhesion and biofilm formation, ultimately leading to biomaterial infections. Regardless of how thoroughly the root canal system is cleaned and shaped, complete elimination of microorganisms is not possible, and these microorganisms may remain in dentinal tubules, apical ramifications, and periapical areas (5). One of the most common bacterial species isolated from root canals of failed treatment teeth is *Enterococcus faecalis* (6). *E. faecalis* is known to form biofilm on the Gutta-percha points in the root canal system regardless of the type or technique of sealer application. However, adding disinfectant such as sodium hypochlorite reduces the invasion of such bacteria to a certain level. There is a need to search for a new filler and sealant in which microbes such as *E. faecalis* and *S. mutans* do not adhere to prevent the biofilm formation.

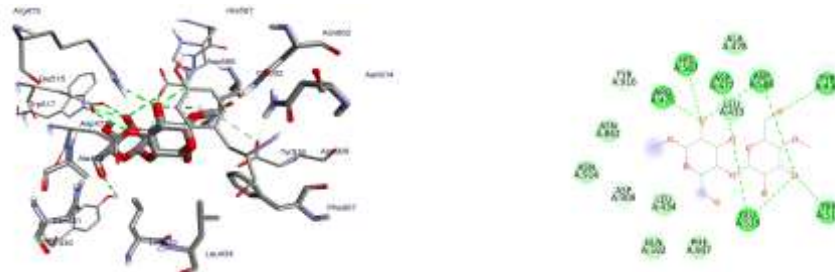
Galactan is a polysaccharide that is made up of polymerized galactose. They are found in red seaweeds and are commercially important due to their widespread use as gelling and thickening agents in the food industry. They are also used in cosmetic and biomedical products. Sulfated galactan has shown antiviral, anti-inflammatory, anti-adhesive, and anti-coagulative properties (7). Agars and carrageenans are galactans derived from red algae cell walls. Carrageenans are

used in emulsion stabilisation, syneresis control, bodying, binding, and dispersion because they gel, thicken, or suspend (8). Agars are used to make primary impressions and food products. These polysaccharides are commonly found in a variety of manufactured products. Assessment of these polysaccharides as a filler or a sealant in endodontic purposes can be a boon for the dental industry as they have gelation and thickening properties and are derived from a natural source. This study is to analyse the effects of galactan used as a filler and in the prevention of biofilm formation.

**MATERIALS AND METHODS**

**RESULTS**

**3AIC with Galactan**



Molecular docking scores and residual amino acid interactions of compounds against Protein (PDB ID: 3AIC).

Ligands	Affinity (kcal/mol)	H-bond	Residual interactions	
			Hydrophobic/Pi-Cation	Vander Waals
Galactan	-7	Arg-475, His-587, Asp-477, Asp-588, Tyr-430, Trp-517, Glu-515	Tyr-916, Asp-909	Ala-478, Leu-433, Phe-907, Gln-592, Leu-434, Asn-914, Asn-862

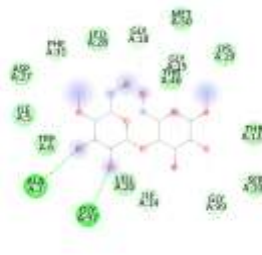
**4RBM with Galactan**



Molecular docking scores and residual amino acid interactions of compounds against Protein (PDB ID: 4RBM).

Ligands	Affinity (kcal/mol)	H-bond	Residual interactions	
			Hydrophobic/Pi-Cation	Vander Waals
Galactan	-5.8	Ala-304, Pro-305, Asp-337, Glu-343, Tyr-295	Val-306, His-234, Leu-237, Leu-299, Arg-243	

**4M7U with Galactan**



Molecular docking scores and residual amino acid interactions of compounds against Protein (PDB ID: 4M7U)

Ligands	Affinity (kcal/mol)	H-bond	Residual interactions	
			Hydrophobic/Pi-Cation	Van dar Waals
Galactan	-7	Ala-7, Gly-97	Phe-31, Gly-18, Gly-15, Gly-99, Ile-14	Asp-27, Leu-28, Thr-46, Met-50, Lys-19, Thr-126, Ser-100, Leu-20, Trp-6, Ile-5

## DISCUSSION

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