IN VITRO AND IN SILICO STUDIES: ANTI-BIOFILM ACTIVITY OF ACTIVATED VIRGIN COCONUT OIL (AVCO) AGAINST CARIOGENIC *Streptococcus mutans*

Ummi Aqilah[1] and Zurainie Abllah[2]

[1]Department of Biotechnology, Kulliyyah of Science, International Islamic University Malaysia, Bandar Indera Mahkota, 25200 Kuantan, Pahang, Malaysia
[2]Department of Paediatric Dentistry and Dental Public Health, Kulliyyah of Dentistry, International Islamic University Malaysia, Bandar Indera Mahkota, 25200 Kuantan, Pahang, Malaysia.

*Corresponding author email: drzura@iium.edu.my

ABSTRACT

The oil of *Cocus nucifera* (Arecaceae) has numerous medicinal values. The fatty acids contents of the oil have been studied and determined to exhibit antimicrobacterial activity. However, the activity of the oil combatting *Streptococcus mutans* (*S. mutans*) biofilm is still not known. Here in this study, we evaluated the antibiofilm activity of AVCO against *S. mutans* biofilm and we studied the binding affinity of the prominent fatty acids (Lauric Acid, Capric Acid, Caprylic Acid, and Myristic Acid) with Quorum Sensing (QS) DNA receptor gene (PDBID: 1NXO) and the *Staphylococcus aureus* LuxR family (PDBID: 3B2N). The minimum biofilm inhibition concentration (MBIC) and the minimum biofilm eradication concentration (MBEC) for antibiofilm activity were determined by serial dilution method, and biofilm thickness on *S. mutans* was quantified by confocal laser scanning microscopy (CLSM). The molecular docking study was performed using AutoDock Vina 1.1.2 program to determine the binding location and the interaction formed between the selected fatty acids and QS DNA receptor and LuxR genes. At the concentration of 15.63 mg/ml of AVCO, it successfully inhibits the development of *S. mutans* biofilm, and AVCO (62.52 mg/ml) eradicate biofilm that was formed by the bacteria. The z-stack images obtained from CLSM allows the construction of 3-D biofilm structure and a significant difference in the thickness of *S. mutans* biofilm pre and post-treatment with AVCO were observed. In silico analysis revealed that these fatty acids could interact efficiently with the bacterial communication quorum-sensing (QS) regulators *Streptococcus* OmpP and *Staphylococcus* Lux proteins. The oil of AVCO possessed dual-function where anti-biofilm agents in AVCO not only inhibit growth but also control the colonization and accumulation of caries-causing *S. mutans*.

Keywords: Antibiofilm, Antiquorum sensing, AVCO, CLSM, Docking Studies,

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