Identification of esters in carious dentine

Staining and chemo-mechanical excavation

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av

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Fakultetsopponent:

Professor Pekka Vallittu

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Avhandlingen baseras på följande delarbeten

I. Almhöjd US, Norén JG, Arvidsson A, Nilsson Å, Lingström P. (2014) Analysis of carious dentine using FTIR and ToF-SIMS. Oral Health Dental Manag 13:735-744.

II. Almhöjd US, Lingström P, Melin L, Nilsson Å, Norén JG. (2015) Staining of carious dentine using dyes with covalent and electrostatic binding properties – an *in-vitro* study. Oral Health Dental Manag 14:194-200.

III. Almhöjd US, Lingström P, Nilsson Å, Norén JG, Siljeström S, Östlund Å, Bernin D. (2017) Molecular insights into covalently stained carious dentine using solid-state NMR and ToF-SIMS. Submitted for publication.

IV. Lai G, Capi CL, Cocco F, Cagetti GM, Lingström P, Almhöjd U, Campus G. (2015) Comparison of Carisolv system vs traditional rotating instruments for caries removal in the primary dentition: A systematic review and meta-analysis. Acta Odontol Scand 73:569–580.

SAHLGRENSKA AKADEMIN
INSTITUTIONEN FÖR ODONTOLOGI

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Identification of esters in carious dentine

Staining and chemo-mechanical excavation

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Abstract

Dental caries is clinically seen as a yellowish-brown discoloration that can be explained by the reactions between proteins and sugars resulting in Maillard products. However, the discoloration of carious dentine is an imprecise indicator of whether or not the dentine is caries free. Other processes might act in concert with the Maillard reactions. This thesis describes how special functional groups formed in the carious process can be used in connection with dyes that selectively stain the carious tissue in order to avoid over excavation.

The initial study aimed to analyse unique functional groups in sound and carious dentine and their presumed reaction with hydrazine derivative using Fourier Transform Infrared Spectroscopy (FTIR) and Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS). The second and third studies focused on the possible formation of covalent bonds between carious dentine and $^{15}N_2$-hydrazine, $^{15}N_2$-labelled Lucifer Yellow, and stains carrying a hydrazine derivative respectively, using ToF-SIMS, solid-state NMR spectroscopy (^{13}C and ^{15}N) and light-microscopic observations. The latter aimed to evaluate the type of binding, electrostatic or covalent, to carious dentine. A systematic review with an adjacent meta-analysis evaluated the ability of a chemically based product in clinical caries excavation.

The results revealed ester groups unique to the carious dentine, with a higher occurrence in the inner layer of carious dentine, which, after reaction with hydrazine derivative, form covalent bonds not seen in sound dentine. This is a selective binding in comparison with dyes with only an electrostatic binding capacity. The systematic review found that the chemo-mechanical excavation technique is as efficient as burs, albeit with a longer treatment time but with enhanced patient comfort**.**

It is concluded that ester functional groups unique to carious dentine can be specifically stained with dyes carrying a hydrazine group, thereby acting selectively in distinguishing between sound and carious dentine. As a result, using a more precise indicator will support the identification of the end-point during clinical caries excavation.

Keywords: Caries removal, Caries detection, Carious dentine, Covalent binding, Dental caries, Electrostatic binding, FTIR, Hydrazine derivative, NMR, Staining, ToF-SIMS

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