# NMR Metabonomic Analyses of Whole Saliva from Children with and without Caries. 

Angeli, R., ${ }^{1}$ Fidalgo, T.K.S., ${ }^{1,2}$ Gonçalves, E., ${ }^{1}$ Souza, I., ${ }^{2}$ Freitas-Fernandes, L. ${ }^{2,3}$ Almeida, F.C.L., ${ }^{1}$ Valente, A.P. ${ }^{1}$

${ }^{1}$ Centro Nacional de Ressonância Magnética Nuclear, Instituto de Bioquímica Médica; ${ }^{2}$ Departamento de Odontopediatria e Ortodontia, Faculdade de Odontologia, Universidade Federal do Rio de Janeiro; ${ }^{3}$ Biothec Consult, Rio de Janeiro, Brazil

Oral biofilms are formed at solid and semi solid surfaces on oral cavity and are known to influence the occurrence of oral disease. The aim of this study was to analyze whole saliva from children with and without caries using NMR methods. Non stimulated whole saliva from 6 years old female children were collected into a plastic tube kept on ice. Whole saliva was centrifuged $10,000 \mathrm{~g}$ at $4^{\circ} \mathrm{C}$ for one hour. We acquired ${ }^{1} \mathrm{H}$ NMR and 1D-NOESY as well as ${ }^{1} \mathrm{H}-{ }^{1} \mathrm{H}$ correlation (TOCSY) and heteronuclear correlation (HSQC) spectra using a Bruker 800 MHz equipped with 5 mm high-resolution probe at $25^{\circ} \mathrm{C}$. The NMR data demonstrated the stability of the whole saliva samples for at least 6 hours. Differences in resonances intensities were observed in the samples of patient with and without cavities. 1D experiment revealed that region $3-4 \mathrm{ppm}$ and $7-9 \mathrm{ppm}$, the resonance intensity was higher in children with caries than without. These differences were better characterized by bidimensional spectra by TOCSY and ${ }^{1} \mathrm{H}^{13} \mathrm{C}$ HSQC. Low molecular weight components of saliva are markers of its metabolic state. This study show that salivary components presented variation among children with and without caries disease since previous studies of our group showed that small variation occur in saliva metabolites among healthy children. It is also possible to conclude that the whole saliva could be analyses by NMR experiments and therefore further investigation could be done with larger group of children.

Key words: NMR, metabonomic and saliva
Suported: IMBEBB, FAPERJ and CNPq

