NMR Metabonomic Analysis of Whole Saliva of 3-12 Years Old Children.

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The characterization of saliva metabolites is an important diagnostic tool for identification of systemic and oral disease. The aim of the present study was to identify metabolites from whole saliva of healthy children and establish a gold standard, using Nuclear Magnetic Ressonance (NMR) spectroscopy. Fifty eight children from 3 to 12 years old, without oral as well as systemic diseases were included in this study. The children were divided by three groups according to the dentition such as deciduous, mixed and permanent. The sample consisted of 3 ml of non stimulated whole saliva that were collected, then was centrifuged ($10,000g$ at 4^0C) and the supernadant was stored at $-80°$C until NMR analyses. ^{31}P and ^{1}H NMR spectra were acquired using a Bruker 400 MHz Advance spectrometer (Bruker Biospin, Germany) equipped with a Bruker 5 mm high-resolution probe, at 25^oC. The intensity of each resonance was analysed using Amix (Bruker) to determine the metabolomic variation within the dentitions. ^{31}P chemical shift was used to pH measurenment. The children with deciduous dentition presented lower pH values while children with permanent dentition and older than 10 years old presented higher pH values and less variation among pacients. ^{1}H resonances were used to analyze metabolites that were identified using TOCSY spectrum. The intensities of lactate, propionate, succinate presented statistic difference ($p<0.005$) among the different dentitions. The results indicate an unique and satisfactory standard of salivar metabolites that could guide futures studies to determination of oral and systemic disease biomarkers.

Key words: metabonomic, NMR, saliva.