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## Metabolic Fingerprint of Latex by $^1\text{H-NMR}$ : Distinction between High and Low Production Clones

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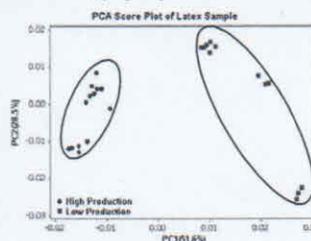
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Latex, natural rubber, is composed for the most part by poly(cis-1,4-isoprene) polymer and minor compounds such as: proteins, carbohydrates, lipids, and minerals. Poly(cis-1,4-isoprene) has peculiar physical-chemistry properties and very often can not be replaced by synthetic rubber (poly(styrene-butadiene)).<sup>1</sup>  $^1\text{H-NMR}$  spectroscopy is an important tool for organic compounds identification and has been applied with successful in the identification of animals and plant metabolites. Since the number of information provided by  $^1\text{H-NMR}$  spectrum is wide the use of statistical tools is essential. Principal Component Analysis (PCA) has been shown positive results at the interpretation of  $^1\text{H-NMR}$  data.<sup>2</sup>

The aim of this work was to evaluate the use of  $^1\text{H-NMR}$  to distinguish between latex samples of *Hevea brasiliensis* which shown high and low production of poly(cis-1,4-isoprene) by using PCA analysis.

The figure shows the PCA score plot of the latex samples. According to this was possible to differentiate samples between high and low production. The PCA loading plot (not shown) shows that the variables responsible for the distinction between the clusters are the compounds: acetate, acetoacetate, succinate, citrate, aconitic acid, choline, betaine, quebrachitol, ascorbate, and formate. The metabolite quebrachitol is a polyol present in high concentration in latex sample from *Hevea* and is related to the biosynthesis of poly(cis-1,4-isoprene).<sup>3</sup>



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## NMR of $\text{Na}^+$ , glycine and HDO in isotropic and anisotropic carrageenan gels

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Chiral gels that become anisotropic when stretched or compressed differ from liquid crystals in that there is a continuum of anisotropy that can be obtained: the transition from isotropic to slightly anisotropic to more anisotropic states can be controlled and reversibly changed. In the last few years we introduced a simple device that achieves this by using gelatine as the chiral alignment gel.<sup>1,2</sup> Recently we described two new polysaccharide based gels that become anisotropic by stretching and can be reversibly adjusted just like gelatin, but at much lower gel concentrations, and can be used at 37 °C.<sup>3</sup> Chemically alike,  $\iota$ - and  $\kappa$ -carrageenan gels yield quite different alignment properties for small chiral and prochiral solutes.<sup>3</sup> This finding implies structural differences for  $\iota$ - and  $\kappa$ -carrageenan gels, and raises the question of the necessary structural elements for (carbohydrate) gels to become anisotropic when stretched. Here we discuss the isotropic and anisotropic states of  $\iota$ - and  $\kappa$ -carrageenan gels as detected by  $\text{Na}^+$  ions, glycine and monodeuterated water and monitored by solution  $^1\text{H}$ ,  $^2\text{H}$ , and  $^{23}\text{Na}$  NMR spectroscopy.<sup>4</sup> Anisotropy was introduced by stretching the polysaccharide gels, and the degree of structural alignment depended on the extent of stretching as well as gel and salt concentration, and the nature of cation and anion. For  $^{23}\text{Na}^+$  ( $\text{NaCl}$ ) a strong binding component of the anisotropy in  $\iota$ - and less in  $\kappa$ -carrageenan gels was found, in contrast to a partial binding of glycine, and a spatial and a gel-concentration-dependent anisotropic effect for deuterated water (HDO). This finding is explained by the electrostatic interactions between  $\text{Na}^+$  and ionic sulphate groups in the carrageenan polymer; HDO probably only interacts via hydrogen bonding; while glycine presumably interacts by both means.<sup>4</sup> The new methodology is ripe for spectral analysis of chiral mixtures.

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