NMR phytometabolomics for chemosensory signatures

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Introduction

The field of NMR has been a continuously expanding area exploring novel applications and resulting in advances in many disciplines like medicine, agriculture and pharmaceutical research. With growing importance of nutrition in healthcare, another new and innovative use of NMR could be in sensory sciences. One of the major factor in nutritional science is the organoleptic property of taste, by which a dieter judges the quality of food. Taste has both subjective and objective components. This study looks at the objective aspect, i.e. chemical sense of taste, in tandem with the objective assessment of the subjective element of taste. A combination of untargeted NMR based phytometabolomics and Electronic tongue based chemometrics have been used to study nutraceutical plants, some of which like *Capsicum annum* have antiobesity property.[1]

Materials and Methods

Samples: Twenty three nutraceutical plants from the category of sweet and pungent were studied: sweet - *Cocos nucifera*, *Cucumis sativus*, *Ananas comosus*, *Annona squamosa*, *Asparagus racemosus*, *Agaricus campestris*, *Mangifera indica*, *Morus alba*, *Musa paradisiaca*, *Myristica fragrans*, *Phaseolus aerous*, *Vitis vinifera*, *Phoenix sylvestris*; pungent - *Capsicum annum*, *Mentha piperata*, *Cinnamomum tamala*, *Prunus amygdalus*, *Brasica campestris*, *Raphanus sativus*, *Trigonella foeneum*, *Cuminum cyminum*, *Piper longum* and *Zingiber officinale*.[2] The samples were prepared in aqueous form.

NMR: Water suppressed 1D proton spectra were acquired using a 700 MHz spectrometer (Agilent, USA) with the following parameters: relaxation delay - 14 sec, spectral width - 11 ppm, 32 scans and 32K data points. Deuterated TSP in a coaxial insert was used as an external reference standard. The data was subjected to Principle Component Analysis (PCA) using MestReC and Unscrambler X10. The spectra for this were binned and bucketed at intervals of 0.04 ppm.

Electronic tongue: Taste was objectively assessed with a 16 autosampler E-Tongue (Alpha MOS, France) using a set of 7 sensors based on Chemical modified Field Effect Transistor (ChemFET) principle[3]. PCA was performed and Euclidean distance analysis was used to determine the correlation between samples and taste standards.

Results and Discussion

Electronic tongue: The samples could be divided into sweet and pungent groups based on the reference data base library developed in the lab. The multivariate analysis also showed the nutraceuticals under sweet category mapping close to each other and the rest (pungent) away from the sweet group.

NMR: Analogous to the PCA on the E-tongue data, the PCA analysis of NMR spectral data also revealed distinct clusters for the sweet and pungent group of plants (Fig. 1a). Although the two PCAs have used data from different techniques, there is general agreement between the two measurements. These results indicate that NMR spectroscopy has the potential to fingerprint different tastes and act as a magnetic tongue. Figure 1b shows representative 1D proton spectra of nutraceutical plants from the two taste categories. Although majority of the phytochemicals from plants are essentially identical (primary and secondary metabolites), there are distinct differences as well (shown highlighted) suggesting that the taste phenotypes could be related to the minor components. The nutraceuticals from sweet category showed high presence of sugars (α-, β-glucose and sucrose) (primary metabolites) and polyphenols (secondary metabolites). On the other hand, pungent plants showed significant presence of non-sweet amino acids such as valine, threonine, methionine, isoleucine and proline. Significant amounts of flavonoids and flavonol glycosides (secondary metabolites) were also seen in pungent category. It is to be noted that pungent taste has been shown to have antiobesity property.[1]

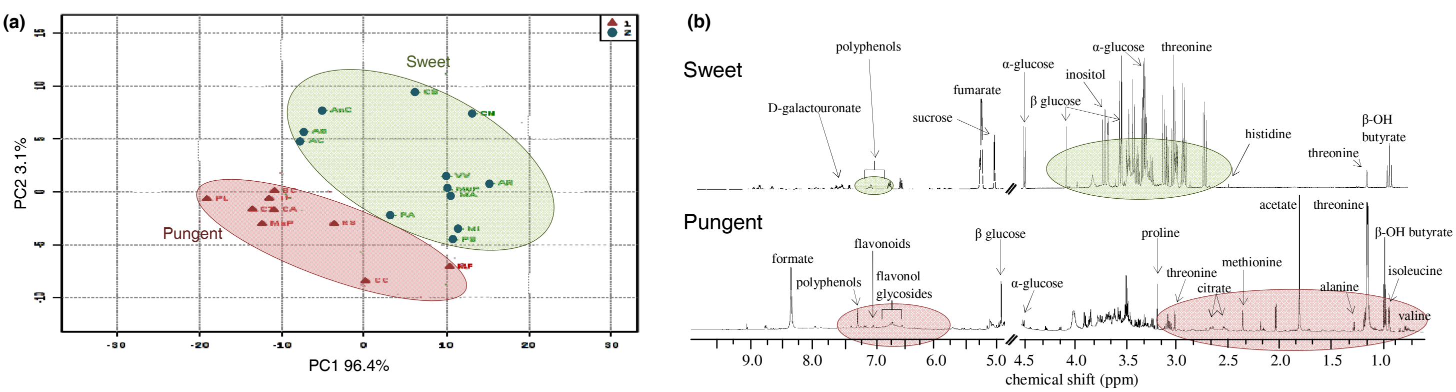

Figure 1: Analysis of nutraceuticals from two taste categories: **(a)** PCA clustering of NMR spectral data **(b)** Representative proton NMR spectra from each group

Conclusion

This study has explored the use of proton NMR as a tool to analyse the organoleptic property of taste, a major parameter in food science. Markers for the sensory descriptors could be identified from the NMR spectra. It is interesting to note the same classification reached independently by PCA of data from two techniques, namely NMR and Etongue. Although it is encouraging to see similarities between the NMR and sensory data, the important question is how well this organoleptic property of taste can be predicted by NMR. Further studies are underway to address this question. This study shows another expanded use of NMR in nutritional healthcare.

References

(1) Clegg ME, Golsorkhi M, Henry CJ: Combined medium-chain triglyceride and chilli feeding increases diet induced thermogenesis in normal-weight humans. Eur J Nutr 2012; 52(6): 1579-1585.
(2) Jayasundar R. Ayurvedic approach to functional food. In: Introduction too functional food science. DM Martirosyan (Ed), Food Science Publisher, USA (in press).
(3) Riul A Jr, Dantas CA, Miyazaki CM, Oliveira ON Jr. Recent advances in electronic tongues. Analyst. 2010; 135(10): 2481-2495.