

## Proton Nuclear Magnetic Resonance Based Metabolomics and <sup>13</sup>C Isotopic Ratio Evaluation to Differentiate Conventional and Organic Soy Sauce

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**Abstract :** Organic food products are becoming increasingly popular in recent years, as consumers have turned more health conscious and environmentally aware. A lot of consumers have understood that the organic foods are healthier than conventionally produced food stuffs. Price difference between conventional and organic foods is very high. So, it is very common to cheat the consumers by mislabeling and adulteration. Our study describes the <sup>1</sup>H NMR based approach to characterize and differentiate soy sauce prepared from organically and conventionally grown raw materials (wheat and soybean). Commercial soy sauce samples fermented from organic and conventional raw materials were purchased from local markets. Principal component analysis showed clear separation among organic and conventional soy sauce samples. Orthogonal partial least squares discriminant analysis showed a significant ( $p < 0.01$ ) separation among two types of soy sauce yielding leucine, isoleucine, ethanol, glutamate, lactate, acetate,  $\beta$ -glucose, sucrose, choline, valine, phenylalanine and tyrosine as important metabolites contributing towards this separation. Abundance ratio of <sup>13</sup>C to <sup>12</sup>C was also evaluated by <sup>1</sup>H NMR spectroscopy which showed an increased ratio of <sup>13</sup>C isotope in organic soy sauce samples indicating the organically grown wheat and soybean used for the preparation of organic soy sauce. Results of the study can be helpful to the end users to select the soy sauce of their choice. This information could also pave the way to further trace and authenticate the raw materials used in production of soy sauce.

**Keywords :** <sup>1</sup>H NMR, multivariate analysis, organic, conventional, <sup>13</sup>C isotopic ratio, soy sauce

**Conference Title :** ICNFS 2017 : International Conference on Nutrition and Food Science

**Conference Location :** Istanbul, Türkiye

**Conference Dates :** October 26-27, 2017