

## Identification of 3-Methylbutanoyl Glycosides in Green *Coffea arabica* Beans as Causative Determinants for the Quality of Coffee Flavors

Keiko Iwasa,<sup>1,\*</sup> Daiki Setoyama,<sup>2</sup> Hiroaki Shimizu,<sup>1</sup> Harumichi Seta,<sup>1</sup> Yoshinori Fujimura,<sup>2</sup> Daisuke Miura,<sup>2</sup> Hiroyuki Wariishi,<sup>2</sup> Chifumi Nagai,<sup>3</sup> Koichi Nakahara<sup>1,\*</sup>

<sup>1</sup>Research Division, Suntory Global Innovation Center Limited (Suntory SIC), 5-2-5 Yamazaki, Shimamoto-cho, Mishima-gun, Osaka 618-0001, Japan

<sup>2</sup>Innovation Center for Medical Redox Navigation, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka 812-8582, Japan

<sup>3</sup>Hawaii Agriculture Research Center, P.O. Box 100, Kunia, HI 96759, United States of America

### Abstract

The quality of coffee green beans is generally evaluated by the sensory cupping-test, rather than by chemical compound-based criteria. In this study, we examined the relationship between metabolites and cupping scores for 36 varieties of beans, using a non-targeted LC-MS based metabolic profiling technique. The cupping score was precisely predicted with the metabolic information measured using LC-MS. Two markers that strongly correlated with high cupping scores were determined to be isomers of 3-methylbutanoyl disaccharides (3MDs; 0.01-0.03 g/kg-of-beans) by spectroscopic analyses after purification and one of them was a novel structure. Further, both the 3MDs were determined to be precursors of 3-methylbutanoic acid that enhances the quality of coffee. The applicability of 3MDs as universal quality-indicators was validated with another sample set. It was concluded that 3MDs are the causative metabolites determining beverage quality and may be utilized for green beans selection and as key compounds for improving the beverage quality.

**Keywords;** *Coffea arabica* green coffee bean, Metabolic profiling, Cupping score, 3-methylbutanoyl disaccharide, LC-MS, NMR, Pyrolysis, GC-MS.