

¹H NMR-Based Metabolomic Approach for Understanding the Fermentation Behaviors of Wine Yeast Strains

Hong-Seok Son,¹ Geum-Sook Hwang,² Ki Myong Kim,¹ Eun-Young Kim,² Frans van den Berg,³
Won-Mok Park,¹ Cherl-Ho Lee,¹ and Young-Shick Hong^{1*}

¹*School of Life Science and Biotechnology, Korea University, 5-1, Anam-dong, Sungbuk-gu, Seoul 136-701*

²*Korea Basic Science Institute, Anam-dong, Sungbuk-gu, Seoul 136-713*

³*Department of Food Sciences, Faculty of Life Sciences, University of Copenhagen, Denmark*

ABSTRACT

¹H NMR spectroscopy coupled with multivariate statistical analysis was used for the first time to investigate metabolic changes in musts during alcoholic fermentation and wines during ageing. Three *Saccharomyces cerevisiae* yeast strains (RC-212, KIV-1116 and KUBY-501) were also evaluated for their impacts on the metabolic changes in must and wine. Pattern recognition (PR) methods, including PCA, PLS-DA and OPLS-DA scores plots, showed clear differences for metabolites among musts or wines for each fermentation stage up to 6 months. Metabolites responsible for the differentiation were identified to valine, 2,3-butanediol (2,3-BD), pyruvate, succinate, proline, citrate, glycerol, malate, tartarate, glucose, *N*-methylnicotinic acid (NMNA), and polyphenol compounds. PCA scores plots showed continuous movements away from days 1 to 8 in all musts for all yeast strains, indicating continuous and active fermentation. During alcoholic fermentation, highest levels of 2,3-BD, succinate and glycerol were found in musts with the KIV-1116 strain, which showed the fastest fermentation or highest fermentative activity of the 3 strains, whereas the KUBY-501 strain showed the slowest fermentative activity. This study highlights the applicability of NMR-based metabolomics for monitoring wine fermentation and evaluating the fermentative characteristics of yeast strains.