Integration of Flux Balance Analysis and GC/MS-Based Flux Analysis through Data Reconciliation

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Metabolic flux analysis has been widely used for quantification of cellular biochemical flux in metabolic engineering field. In this field, a key issue that may arise in the application of flux analysis is more accurate calculation for the various given conditions. However we have a few constraints from experiment that can not guarantee the precisely calculated flux distribution in constraint-based flux analysis. Herein, we carried out isotopomer analysis to determine in vivo flux distribution for central metabolism and performed genome-scale constraints-based flux analysis with in vivo flux distribution as reference flux values for quadratic programming. In addition, we demonstrated the extent of flux variability that could provide reliability of newly calculated flux distribution. Consequently, we had almost credible and global flux distribution of biochemical network through integrated approach which was combined constraint-based flux analysis with in vivo flux distribution from isotopomer analysis. This work was financially supported by the Korean Systems Biology Research program (M10309090000-03B5002-00000) of the Korean Ministry of Science and Technology (MOST), the Brain Korea 21 of the Ministry of Education and LG chemicals Chair Professorship. Hardware for computational analysis supported by the IBM-SUR program.