

Metabolite essentiality of pathogens

김현욱, 김태용, 정광준¹, 김수영¹, 이준행¹, 이상엽*

Dept. of Chemical and Biomolecular Eng., KAIST;

¹전남대학교 의과대학

(ehukim@kaist.ac.kr*)

Vibrio vulnificus is a halophilic and highly human-pathogenic bacterium, showing very high mortality rate when infected. In order to facilitate the drug development process for this, we undertook *in silico* analysis to identify specific drug targets in the genome-scale metabolism of *V. vulnificus*. With a newly sequenced and annotated genome of *V. vulnificus*, we first reconstructed its genome-scale metabolic network consisting of 945 reactions and 764 metabolites. Subsequently, we employed constraints-based flux analysis, which is an optimization-based simulation technique, to identify essential metabolites comprising the metabolic network. Metabolites are considered essential if their removal causes cell death. As a result, we found 107 essential metabolites. Drug targeting using *in silico* methodologies facilitates not only the systems-level analysis of the bacterial metabolism, but also a rational design of experiments applicable to biomedical science. [This work was supported by the Korean Systems Biology Research Project (M10309020000-03B5002-00000) of the Ministry of Education, Science and Technology. Further supports by the LG Chem Chair Professorship, Microsoft, and IBM SUR program are appreciated.]