

In silico Drug Targeting of *Vibrio vulnificus* CMCP6

김현욱, 김태용, 이상엽*
한국과학기술원
(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 technique, to identify essential genes. Enzymatic reactions whose deletions result in the failure of biomass formation were primarily considered as drug targets. This simulation identified 209 enzymatic reactions as primary drug targets. 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 Science and Technology. Further supports by the LG Chem Chair Professorship, Microsoft, and IBM SUR program are appreciated.]