

## Finding Alternative 3-hydroxy Propionic Acid Pathways Using *Generalized Enzyme Function* Method

조아연, 윤홍석, 이상엽, 박선원\*  
한국과학기술원  
(sunwon@kaist.ac.kr\*)

At 2004, U.S. Department Of Energy reported twelve high-value added building blocks which can be yield from biomass and converted to various desirable chemicals subsequently. The building blocks are filtered by several screening steps and then twelve top value added chemicals are selected. Among them, we tried to find out the alternative synthetic route of 3-hydroxy propionic acid, which is existing only the pathway under the patent currently, using our computational framework which adopts *Generalized Enzyme Function* method. Finally we displayed the *Gibbs Free Energy* with *Group Contribution* method. The propanoate metabolism is considered as an original pathway and several alternatives are found; for example, Acetyl-CoA to the 3-HPA through enzyme reactions such as 4.1.1.9, 1.2.1.18, and 1.1.1.59.

### Acknowledgement

This work was supported by Center for Ultramicrochemical Process Systems sponsored by KOSEF and the Korean Systems Biology Research Program of the Ministry of Science and Technology and by the BK21 project. Further supports from LG Chemicals Chair Professorship and IBM-SUR program are greatly appreciated.