

Enzyme Grouping and Profile Analysis for Virtual Enzyme Screening

박지향, 김병기*
서울대학교 화학생물공학부
(byungkim@snu.ac.kr*)

Enzyme screening is a crucial step for biological synthesis of valuable chemicals. Extensively accumulated data on enzyme sequences and specificities make possible to screen enzymes computationally. Such virtual enzyme screening becomes gradually complementary and even competitive to the traditional experimental screening methods. Our approach uses enzyme grouping based on sequence similarity to predict enzyme function and specificity. We made a program, coded in Python, to group aminotransferases fully automatically using the phylogenetic trees from ClustalW. Subgrouping is followed by profile analysis with HMMER.