

Integrative structural and computational biology of phytases for the animal feed industry

ABSTRACT

Resistance to high temperature, acidic pH and proteolytic degradation during the pelleting process and in the digestive tract are important features of phytases as animal feed. The integration of insights from structural and in silico analyses into factors affecting thermostability, acid stability, proteolytic stability, catalytic efficiency and specific activity, as well as N-glycosylation, could improve the limitations of marginal stable biocatalysts with trade-offs between stability and activity. Synergistic mutations give additional benefits to single substitutions. Rigidifying the flexible loops or inter-molecular interactions by reinforcing non-bonded interactions or disulfide bonds, based on structural and root mean square fluctuation (RMSF) analyses, are contributing factors to thermostability. Acid stability is normally achieved by targeting the vicinity residue at the active site or at the neighboring active site loop or the pocket edge adjacent to the active site. Extending the positively charged surface, altering protease cleavage sites and reducing the affinity of protease towards phytase are among the reported contributing factors to improving proteolytic stability. Remodeling the active site and removing steric hindrance could enhance phytase activity. N-glycosylation conferred improved thermostability, proteases degradation and pH activity. Hence, the integration of structural and computational biology paves the way to phytase tailoring to overcome the limitations of marginally stable phytases to be used in animal feeds.

Keyword: Thermostability; Acid stability; Proteolytic stability; Improved activity; Microbial phytases