

# Interplay between quaternary structure and catalytic function: A Molecular Dynamics Study of Mono- and Dimeric Forms of Alkaline Phosphatase

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## Abstract

The enzyme *Escherichia Coli* (*E. Coli*) Alkaline Phosphatase (AP) has a homo-dimeric quaternary structure. Although each subunit of the enzyme is equipped with its own catalytic site, a monomeric AP does not exist in nature and the engineered mutants have significantly reduced activity. We will perform a comparative analysis based on Molecular Dynamics (MD) simulations of dimeric and monomeric forms of AP so as to reveal which structural and dynamic features enable the native dimer to be catalytically functional whereas the monomeric enzyme is not. Special attention will be paid to the stabilisation provided by the interface of the two subunits in the dimeric form of AP and its interplay, e.g. via a hydrogen bonding network, with the structures of the active sites and the coordination sphere of the catalytically essential metal ions.