

# Dances with enzymes: Coarse-grained simulation of glycolytic enzyme assembly formation

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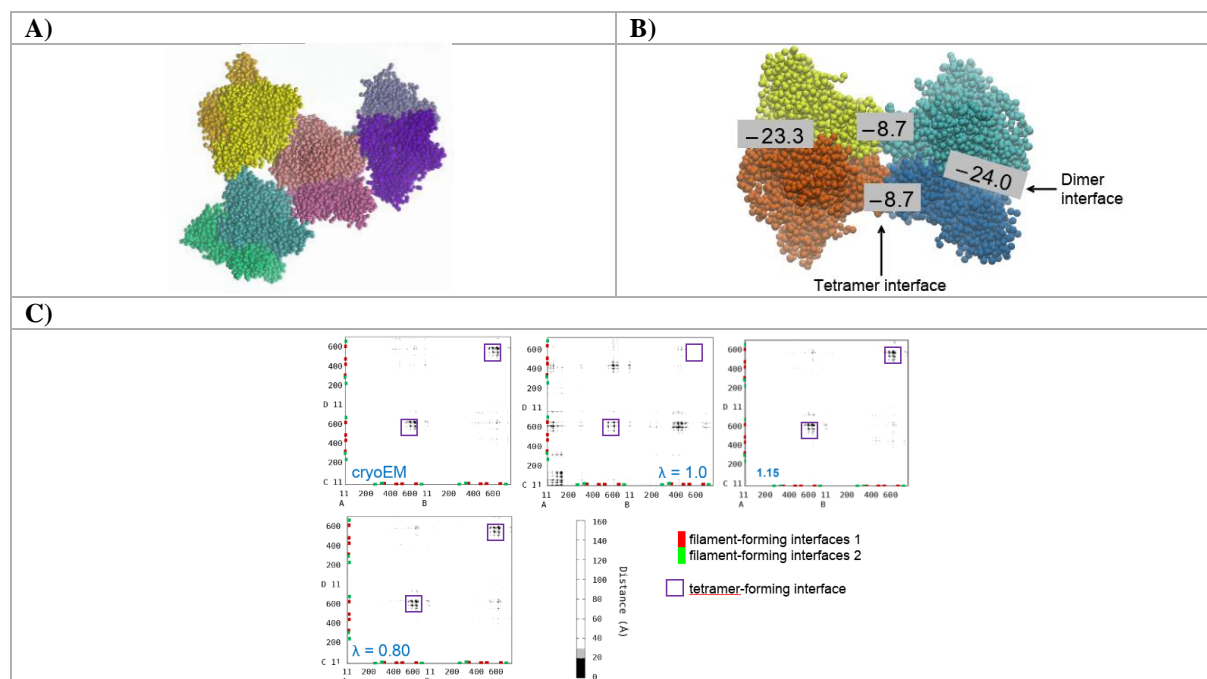
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Various enzymes are able to interact with each other to form dynamic assemblies in cells. In particular, the human liver phosphofructokinase 1 (PFKL) has been identified as a prominent member of glycolytic enzyme assemblies and shown to form filaments<sup>1,2</sup>. However, the mechanism of the formation of these structures and their physiological roles remain poorly understood.

This work uses coarse-grained MD simulations to describe the assembly formation by PFKL. We investigate the stability of the PFKL tetramer and characterize the interactions between PFKL dimers using the Martini 3 force field and some rescaling factors<sup>3,4</sup>. Our results provide a starting point for a comprehensive description of the behavior of PFKL in glycolytic enzyme assemblies.

Figure 1. A) Tetramer and filament interfaces captured by Martini 3 are consistent with experimental data, but their relative stability is not accurate. B) Predicted binding affinities (kcal/mol) predicted by PRODIGY show a weak stability of PFKL tetramer interface which is not captured by Martini3, C) except when using a rescaling factor.



**Keywords:** glycolytic enzyme, enzyme assembly, coarse-grained simulation, force field rescaling

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