Solvation Effect around Firefly Luciferase: Computational Perspective

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Abstract

Firefly bioluminescence has been intensively studied with both experiments and computations. However, there are still lingering questions regarding its chemical details. During this presentation, we will first discuss the pH dependent behavior of the firefly bioluminescence primarily based on molecular dynamics simulations. We will see that the overall protein structure is generally resilient to pH variations but the nature of the pocket changes noticeably especially with the water content around the luciferase active site. The possibility of color modulation depending on the water content will be inspected. We then will move on to see whether this micro-solvation effect can change the chemical nature of the enzymatic system. In the end, we will observe that water is indeed a key element that can even decide the chemical balance between different emitting species. Different aspects originating from "different water" will be revealed, showing the yet-fascinating nature of this prototypical bioluminescent system.

Keywords: oxyluciferin, solvation, molecular dynamics, simulation, dynamics

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