Uncovering the Origin and Evolution of the Firefly Bioluminescence Storage Protein

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Bioluminescence is present in a diverse range of organisms. One of the most studied luminous organisms is the firefly, a member of the Lampyridae family. Firefly bioluminescence is produced when the luciferase protein oxidizes a small molecule called luciferin. The luciferin substrate is an unstable molecule and easily oxidized. While beneficial in light production, this becomes problematic when luciferin is non-specifically oxidized, which wastes resources. In response, some luminous organisms, such as fireflies, evolved mechanisms to store luciferin using the luciferin sulfotransferase protein (LST). Previous research has concentrated on the origin and evolution of luciferase, while the storage protein has remained relatively unexplored. We investigate how the luciferin storage mechanism originated using a novel application of molecular modeling and docking to characterize the structure and binding affinities of extant and ancestral LST sequences. By analyzing phylogenetic trees of the evolution of LST in eight species of fireflies, we identified the point of origin. Utilizing HADDOCK to compare the protein structures of ancestral LST, we determined a hypothesized pathway of evolution for LST function through a promiscuous enzyme. Our results further our knowledge of how bioluminescence evolved and more broadly, how functionally specialized proteins evolve. This study demonstrates that modeling and docking tools are invaluable tools to advance the future of evolutionary biology study.

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