Examining Chromophore Formation in GFP-like structures

Amanda Amoh, Danielle L'Heureux, Marc Zimmer
Chemistry Department, Connecticut College, New London CT 06320

Abstract

Green fluorescent proteins were first discovered in jellyfish in the mid-1950s. A few years later, Osamu Shimomura began studying the proteins at Princeton University. Shimomura became the first to study, isolate, and identify key features of GFP, including characterization of the chromophore in 1979. In 2008 Shimomura, Chalfie, and Tsien won the Nobel Prize for their work with GFP. Since the initial discovery of GFP, scientists have discovered many more naturally occurring proteins, as well as produced genetically modified versions of the wild-types that also fluoresce. Today, the RCSB Protein Data Bank (PDB) contains crystal structures for 297 green fluorescent proteins (GPFs) and GFP-like proteins. Fluorescent proteins (FPs) contain eleven beta sheets and a central alpha helix, which contains the chromophore (Figure 1). It has been proposed that there is a break in the hydrogen bonding of the alpha helix in the immature form of the fluorescent proteins, Figure 2 left. This break forms a kink in the neatly folded amino acid sequence, easily allowing for autocatalytic chromophore formation (Figure 2), without having to break any hydrogen bonds. We have computationally generated the immature form of the all the wild-type FPs in the pdb. A conformational search was then conducted on the FPs in their immature forms . We will be examining the hydrogen bonding networks in the alpha helices of all mature and immature FPs to find the important ones that are conserved in all wild type structures.

Figure 1.

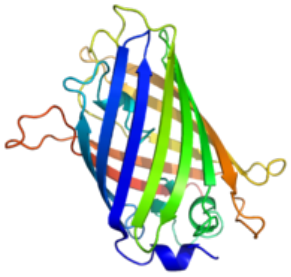

Figure 2.