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Structural dynamics of flavin-proteins with magnetic field sensitivity: potential for magnetic imaging and control of biological pathways

Magnetic fields offer a noninvasive means of probing and potentially controlling biological processes through spin-dependent photochemistry. Understanding how protein structure and dynamics govern these effects is essential for developing genetically encoded reporters and actuators that respond to magnetic fields. Recently we have demonstrated control of spin-correlated radical pair (SCRPs) dynamics in systems involving red fluorescence proteins (RFP) using magnetic resonance in a live transgenic animal. The emission of various RFPs, in the presence of a flavin cofactor, can be modified by a combination of static and radio-frequency (RF) magnetic fields applied near the electron spin resonance frequency. This effect was measured at room temperature both in vitro and in the nematode *C. elegans*, genetically modified to express the RFP mScarlet (Burd et al. Nature 2026).

To further understand the mechanism for the development of genetically encoded protein biomarkers we have investigated the structure and dynamics of magnetic field effects (MFE) positive proteins. Using static and light-activation crystallography, we identified a binding pocket for the oxidized FMN in RFP, and showed that it escapes upon photoactivation. We further applied molecular dynamics methods to link these observations mechanistically to the photochemical pathway that generates SCRPs and gives rise to magnetic-field-dependent behavior of these radicals. The role of the FMN binding pocket was further investigated through photoreduction of FMN in various binding pocket mutants. Finally, I will discuss possible directions on using structural dynamics of engineered LOV-domain proteins for magnetic control of protein conformation and downstream biological functions using magnetic field.

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