

Oxygen Reactivity in Flavoenzymes

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Our presentation will summarize our efforts towards a more in-depth understanding of the ability of flavoenzymes to differentially react with oxygen (1-6). We have investigated different types of monooxygenases and oxidases, which are capable of activating molecular oxygen through the stabilization of a flavin-(hydro)peroxide intermediate. Most remarkably, in flavin-containing monooxygenases flavin-hydroperoxide formation directly involves the NADP⁺ ligand, which, therefore, appears to play the dual function of reducing the flavin and stabilizing a critical catalytic intermediate. We have also been performing molecular dynamics simulations to visualize the pathways for oxygen diffusion across the protein matrix. We are using a combination of site directed mutagenesis and molecular dynamics to investigate the role of residues surrounding the flavin in tuning oxygen reactivity.

References

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