

Mechanism for Antibody Catalysis of the Oxidation of Water by Singlet Dioxygen

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It was recently reported that antibodies, regardless of source or antigenic specificity, generate hydrogen peroxide (H_2O_2) in a photo-oxidative process involving singlet molecular oxygen (1O_2). Quantum mechanics (QM) methods were used (B3LYP Density Functional Theory) to delineate the plausible mechanisms for this efficient conversion of water to HOOH. We have studied the catalysis of some of the more probable mechanisms proposed from QM, by antibodies. We then used the QM structures for products and transition states with the Hier-Dock method to search for sites in the antibody that would stabilize the reaction intermediates. Indeed, we find such sites in the barrel-like interface of light and heavy chains of the antibody and TCR, a structure unique to these systems.

