Microwave-catalyzed Mechanism of Enzymes

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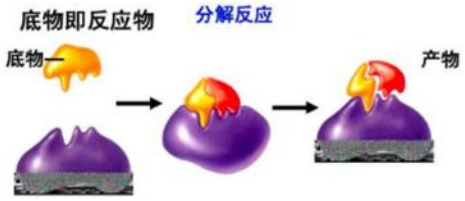
Summary

Traditionally, the mechanism of enzymatic catalysis has often been explained by the "induced fit" model, but this model struggles to fully account for its exponential catalytic efficiency. This paper proposes a new mechanism: proteases can be viewed as a kind of molecular nuclear magnetic resonance system, where H^+ or metal ions reversibly coordinate with amino groups, generating an induced electric field, which in turn triggers the formation of an alternating electromagnetic field in the α-helix structure and interacts with the static magnetic field produced by the β-sheet structure. At specific carboxyl groups (with bond characteristics), nuclear magnetic resonance of hydrogen atoms or electrons is excited, thereby generating microwave radiation locally. This microwave promotes the dissociation of substrates into highly reactive free radicals or ions, greatly accelerating the reaction rate. This paper combines quantum tunneling effects with microwave catalysis theory to provide a new physical explanation for the high efficiency of enzyme-catalyzed reactions.π_4^4

1. Introduction

Enzyme-catalyzed reactions are a crucial class of biochemical reactions in living systems. Under non-catalytic conditions, the rates of many biochemical reactions are extremely low, so the catalytic action of enzymes is vital for cellular functions. Traditional catalytic theory posits that enzymes enhance reaction rates by stabilizing the transition state and reducing activation energy (Ea). The widely accepted "induced fit" model emphasizes the conformational adjustments that occur when enzymes bind to substrates, thereby improving recognition and catalytic efficiency.



However, the model fails to fundamentally explain why the rate of enzyme catalysis can reach 10^8–10^13 times that of non-catalytic reactions. In the 1980s, Judith Klinman and others discovered through isotope substitution experiments that alcohol dehydrogenase exhibits significant kinetic isotope effects during catalysis, suggesting that quantum tunneling (especially proton tunneling) plays a crucial role in enzyme catalysis [1,2]. Nonetheless, whether the tunneling effect is the primary catalytic force remains controversial.

In recent years, microwaves have demonstrated tremendous potential as an efficient catalytic means in organic synthesis. They achieve energy transfer through the rotation of polar molecules and ion migration, significantly enhancing the reaction rate. Inspired by this, this paper explores whether protein enzymes utilize the microwave resonance mechanism for efficient catalysis at the molecular scale.

2. Basic principle of microwave catalysis

Microwaves are electromagnetic waves with frequencies ranging from 300 MHz to 300 GHz. Since Gedye et al. first applied microwaves to organic synthesis in 1986, numerous studies have

shown that microwaves can greatly enhance reaction rates and yields. The main mechanisms of its action include:

· Polar molecule rotation: The microwave electric field causes high-speed turning of polar molecules, leading to instantaneous polarization and bond rotation of molecules;

· Ion migration: Charged particles move rapidly in an alternating electric field, generating collisions and frictional heat;

· Energy absorption and conversion: Polar substances (such as water, proteins, nucleic acids, etc.) absorb microwave energy and convert it into molecular vibration and rotation energy, thereby reducing the reaction activation energy.

In fact, it should be that the microwave frequency matches the resonance energy level of electron spin, which can excite electron energy level transitions. For polar molecules, the "dipole moment" formed by the internal electron cloud offset rotates in the microwave field, generating high temperatures; if the dipole moment is a branch of a large molecule, it is not easy to rotate, which further induces chemical bond breaking, producing free radicals or ions, greatly enhancing the reaction activity.

Therefore, high temperatures together with ionization and free radicals are the true nature of microwave chemical reactions!

3. Structure of Protease and Formation Mechanism of Electromagnetic Field

3.1 The secondary structure of protein and electron behavior

The secondary structure of proteins mainly includes α-helices and β-folds. Studies have shown that the hydrogen bond network in the peptide chain can support the migration of electrons between amino acid residues through the quantum tunneling effect [4].

3.2 Electric field induction and electromagnetic field generation

In the enzyme active center, H^+ or metal ions reversibly coordinate with amino groups, triggering a dynamic induction effect. This electric field is transmitted to the carboxyl end through the σ-π and σ-p hyperconjugation systems.

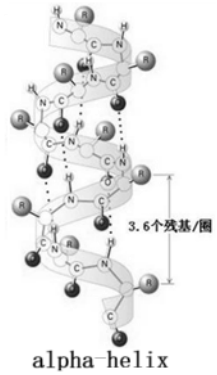
· In the α-helix structure, electrons flow in phase within the three-stranded helix, forming an alternating current, which in turn generates an alternating magnetic field B_o;

In the β-sheet structure, electrons move in a single direction in a circular motion to form a stable static magnetic field B_1. If the α-helix is perpendicular to the β-sheet structure, and the active carboxyl group is located at the junction of the two, it forms an orthogonal combination of alternating and static magnetic fields, meeting the basic conditions for nuclear magnetic resonance.

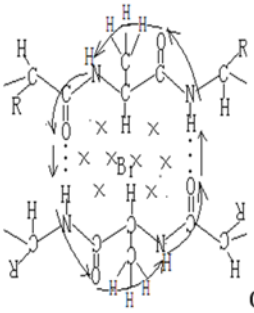
3.3 Resonance Characteristics of Carboxyl Groups

The p-orbital of the hydroxyl oxygen in the carboxyl group forms a p-π conjugate structure with the carbonyl π bond. Under the influence of the induced electric field, the hydrogen atom or electron in the carboxyl group oscillates between the two oxygens, forming a dynamic structure similar to a bond. Experiments show that the two C–O bond lengths in formic acid and

other carboxylic acids are equal, supporting this resonance model.π_4^4



alpha-helix



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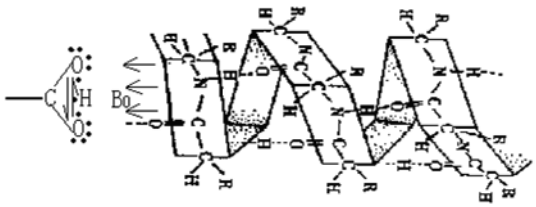

Carboxyl π_4^4 bond

Alternating magnetic field

α-helix structure β-folding enzyme microwave catalysis mechanism (NMR) diagram

4. Catalytic mechanism of enzymes as molecular NMR machines

Under the influence of the orthogonal magnetic field described above, hydrogen atoms in the carboxyl group (or electrons, or dissociated H^+ protons) undergo spin resonance, leading to spin energy level transitions. After recovery, microwave radiation is released locally. When this microwave is absorbed by the substrate, it causes covalent bond vibrations, distortions, and eventually homolytic cleavage, producing two highly reactive radicals (for non-polar substrates) or ions (for polar substrates). Since the microwave energy can directly act on chemical bonds, the reaction barrier is significantly reduced, resulting in an exponential increase in reaction rate. This mechanism also provides a reasonable explanation for the kinetic isotope effect observed in Klinman's experiments: when the hydrogen in the substrate is replaced by deuterium or tritium, its resonance frequency does not match the microwave frequency produced by the enzyme, leading to an inability to effectively excite bond breaking and a sharp decrease in reaction rate.

5. Conclusion

This paper proposes that protease is essentially a molecular nuclear magnetic resonance system. It constructs orthogonal electromagnetic fields through α-helix and β-fold structures, excites hydrogen or electron spin resonance at carboxyl sites, generates local microwaves, and efficiently catalyzes the conversion of substrates to active intermediates. This model integrates quantum tunneling, electromagnetic resonance, and microwave catalysis theories, providing a new mechanism explanation for the ultra-high catalytic efficiency of enzymes and offering a theoretical basis for the design of artificial enzyme catalysts.

References

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