

On the special specificity of Glyoxalase I, a Metalloenzyme that accepts both enantiomers of its chiral substrate but converts them to only the S-D enantiomer of lactoylglutathione



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Abstract

Glyoxalase I (GlxI) is a member of the glyoxalase system, which is important in cell detoxification and converts hemithioacetals of methylglyoxal (a cytotoxic byproduct of sugar metabolism) and glutathione into D-lactate. GlxI accepts both S and R enantiomers of hemithioacetal, but converts them to only the S-D enantiomer of lactoylglutathione. Interestingly, the enzyme shows this unusual specificity with a rather symmetric active site (a Zn ion coordinated to two glutamate residues; Glu-99 and Glu-172). Recently, we have studied different aspects of the GlxI reaction in four separate works using computational chemistry methods [1–4]. Our Molecular dynamics simulations and hybrid quantum mechanics/molecular mechanics calculations show that Glu-172 is more flexible and basic than Glu-99 in the catalytic reaction of GlxI and is much closer to flexible loops inside the protein. In addition, the higher basicity and flexibility of Glu-172 may explain the special stereospecificity of GlxI.

3. “Can a Quantum Mechanical Cluster Model Explain the Special Stereospecificity of Glyoxalase I?/ Computational and Theoretical Chemistry Vol 1188 (2020) .
4. Quantum Mechanics/Molecular Mechanics Study of the Reaction Mechanism of Glyoxalase I/ Inorganic Chemistry/ Vol 59 Issue 4(2020).
5. Selective aerobic photocatalytic oxidation of benzyl alcohol over spherical structured WO₃/TiO₂ nanocomposite under visible light irradiation/ Journal of Sol-Gel Science and Technology/ Vol 87 Issue 1(2018) .

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Biography:

MEHDI IRANI has completed his PhD at the age of 25 years from Sharif University of Technology. Now, he works at University of Kurdistan as an assistant professor. Mehdi is a theoretical chemist working mainly on enzymatic reactions.

Speaker Publications:

1. “Amino Acid Oxidation of Candida antarctica Lipase B Studied by Molecular Dynamics Simulations and Site-Directed Mutagenesis / Biochemistry (2013) Vol 52, Issue 7
2. “Catalytic mechanism of human glyoxalase I studied by quantum-mechanical cluster calculations / Journal of Molecular Catalysis B Enzymatic Vol 13 (2016)