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Abstract

The Reactivity of Purine and its derivatives at Xanthine Oxidase active site

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Abstract:

Enzymes that possess molybdenum in their active sites catalyze biological processes that are essential to the organism for survival. One of the most studied of the molybdenum-containing enzymes is xanthine oxidoreductase. Xanthine oxidoreductase catalyzes the purine degradation, taking hypoxanthine to xanthine and then xanthine to uric acid at the C2 and C8 positions of the molecule, respectively. The activities and rates of reactions determined using the substrates revealed that hypoxanthine was by far the most reactive and the substrates with –CH3 group such as 6-Methyl purine were shown to be less reactive for XOR enzymes. The reactivity of xanthine oxidoreductase enzyme with a range of substrates could be described using steady state enzyme kinetic constant, Michaelis constant (km). The Mulliken atomic charges on the locus of interaction sites were computed to characterize the electrophilicity of the interaction sites of the respective substrates. In addition to the Mulliken atomic charges, the constituent chemical fragments were performed using AOMix software program. Purine is considered as the least electrophile (qc = 0.009193) of all purine derivatives and hypoxanthine keto is considered as the most electrophile (qc = 0.161378) of all purine derivatives. This indicates that hypoxanthine keto can undergo the fastest rate of reaction with the active site at its C2 position whereas purine could undergo the slowest rate of reaction with the active site at its C6 position. Finally, we clearly show that % contribution for Cs-HOMO (for Pu-C6) is the highest in comparing to the other two interaction sites of Pu-C2 and Pu-C8. The value of Km reflects a good agreement with the Mulliken atomic charges of the optimized structures of the free substrates in an increasing order of their electrophilicity (purine = 0.009193, Xanthine = 0.152253 and Hypoxanthine = 0.161378).

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