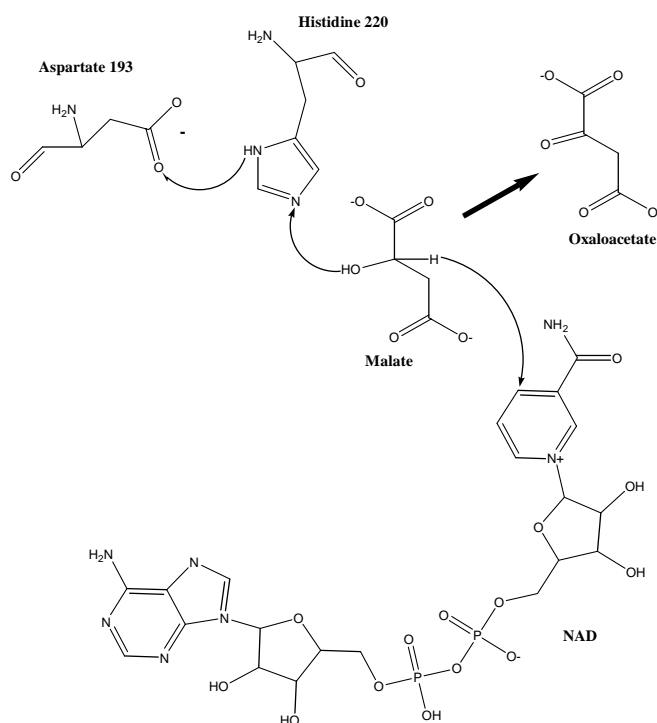


# A Conformational Analysis of Nicotinamide-Adenine-Dinucleotide as it relates to a QM/MM Study of Glyoxysomal Malate Dehydrogenase

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Malate Dehydrogenase (MDH) catalyzes the interconversion of malate (an ionized form of malic acid found in fruit) into oxaloacetate, a molecule important in the metabolism of carbohydrates and in the synthesis of amino acids.



MDH exists in multiple forms but the focus of this study was on watermelon Glyoxysomal Malate Dehydrogenase as its crystal structure has been solved to a resolution of 2.5Å. The goal of this work was to understand the process by which gMDH is able to catalyze malate to oxaloacetate conversion. Results center around a conformational search done on Nicotinamide-Adenine-Dinucleotide, a molecule which binds to the active site of glyoxysomal Malate Dehydrogenase preceding the conversion of malate to oxaloacetate. These results are necessary for future work which will use QM/MM to study electronic and energetic properties of the reaction catalyzed by the gMDH enzyme.