UTEP Bioinformatics

Integrating Bioinformatics and Computational Chemistry Computations with Experiment and Structure to Understand the Aldehyde Dehydrogenases

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A comprehensive bioinformatics analysis of the Aldehyde Dehydrogenase enzyme superfamily is used to identify the sequence and structural elements that are essential to the functioning of all of the enzymes in the superfamily as well as those sequence and structural elements critical to individual families. These essential and critical elements are described and integrated with structural and experimental information which serves as the basis for mixed molecular and quantum mechanical calculations that serve to define the geometry of substrate binding and elucidate the steps in the catalytic mechanism. These calculations show a unique role for the protein backbone during this catalysis which will be described. These calculations indicate that distinct genetic diseases involving different mutations in different Aldehyde Dehydrogenases may have the same mechanistic basis.

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