**Computational Investigation of the Mechanism of Oxalate Decarboxylase**

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Oxalate decarboxylase (OxDC) is a manganese-dependent enzyme that catalyzes the breakdown of oxalate to carbon dioxide and formate in the presence of oxygen. The mechanism by which C-C bond cleavage occurs is poorly understood, but the reaction is thought to proceed via a metal-bound oxalate radical anion, based on mutagenesis studies, heavy atom isotope effect measurements and EPR data (*1-3*). This poster will detail the results of recent computational studies that have employed active site models to explore how oxalate coordination and metal oxidation state might affect the energetics of C-C bond cleavage. Our results suggest that current mechanistic proposals for the catalytic mechanism may need substantial revision.

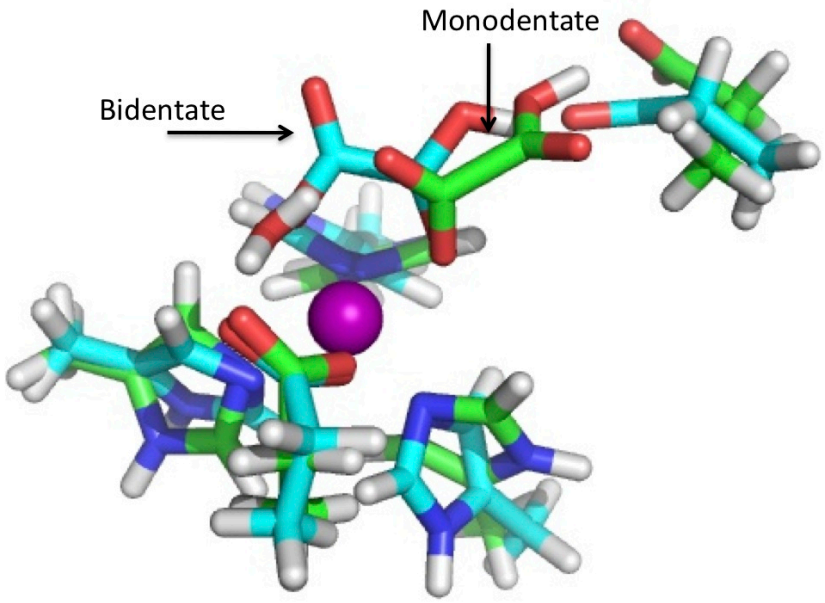


Figure: Active site model structures showing how oxalate might interact with the catalytically active Mn(II) center in a monodentate and bidentate fashion.

**References**

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