

# Computational Investigations of Enzyme Mechanisms: An Application to the B<sub>12</sub>-Independent Glycerol Dehydratase

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The biological dehydration of 1,2-diols has been traditionally thought to be exclusively dependent on Coenzyme B<sub>12</sub>, in a non-REDOX process. Recently, however, a B<sub>12</sub>-independent enzyme system has been discovered in which glycerol is dehydrated with the assistance of an Fe-S cluster that effects the reductive cleavage of S-adenosylmethionine (SAM) [1,2]. In this contribution, results from a computational investigation of the mechanistic aspects of this reaction will be presented. Particular focus will be placed on the substrate transformation and its comparison to the B<sub>12</sub>-dependent system. The significance of the similarities and differences between the two biological dehydration strategies will be discussed.

- [1] C. Raynaud, P. Sarcabal, I. Meynial-Salles, C. Croux, P. Soucaille, *Proc. Natl. Acad. Sci. USA*, **2003**, *100*, 5010.
- [2] J. R. O'Brien, C. Raynaud, C. Croux, L. Girbal, P. Soucaille, W.N. Lanzilotta, *Biochemistry*, **2004**, *43*, 4635.