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Single vs Multi Conformational QM/MM approach for enzymatic catalysis: The case of study of the HBP Sdesulfinase from the 4S pathway

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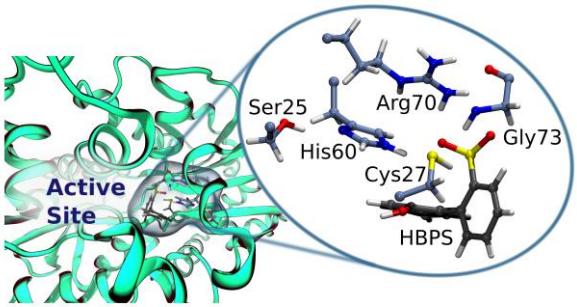
Graphical Abstract



Abstract.

Sulfur oxides emission is one of the major causes for the formation of acid rain and other noxious atmospheric pollutants. Fossil fuels have sulfur containing molecules that, upon combustion, are degraded producing sulfur oxides. Conventional methods become unprofitable in order to achieve the level of desulfurization required by legislation. One alternative is the use of sulfur metabolizing bacteria that possess enzymatic machinery capable of removing sulfur, without degrading the calorific content of the molecule. Rhodococcus erythropolis is capable of performing such task using four different enzymes: DszA, DszB, DszC and DszD. DszD is an HBPS desulfinase which ultimately cleaves the carbon-sulfur bond. The way DszB performs this reaction is still an object of discussion. Different mutagenesis studies have revealed key aminoacid residues for the reaction to occur of which can be named Cys27, His60 and Arg70[1, 2]. Through the use of MD we obtain different conformations of the active site which are then used to elaborate QM/MM models in order to study of the desulfination reaction of DszB [3, 4]. Our results assure the importance of Cys27, His60 and Arg70 for the reactivity of the enzyme, as well as re vealing other important residues such as Gly73, which functions as a stabilizer of Cys27.

Introduction *(optional)*

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Materials and Methods *(optional)*

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Results and Discussion *(optional)*

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Conclusions *(optional)*

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References *(mandatory)*

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4. Sousa, S.F., et al., *Improving the Biodesulfurization of Crude Oil and Derivatives: A QM/MM Investigation of the Catalytic Mechanism of NADH-FMN Oxidoreductase (DszD).* J Phys Chem A, 2016. **120**(27): p. 5300-6.