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Computational chemistry strategies for Bioremediation

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Bioremediation can be defined as the field of knowledge related to the use of microorganisms consortia and processes for the degradation and detoxification of environmental contaminants. As examples of the potential of bioremediation, we mention the use of enzymes such as DFPase and OpdA, respectively found in the squid *Loligo vulgaris* and in the bacterium *Agrobacterium radiobacter*, which have been studied due to their performances in the degradation of organophosphorus compounds (used as agricultural defensive agents and chemical warfare agents). Computational Chemistry, in turn, is an important branch of Chemistry that uses computational methods to understand

and predict the behavior of molecular systems. Since 2016, the Computational Chemistry Group from the Federal University of Lavras (UFLA, Brazil) has been contributing to the field of bioremediation through research papers focusing on the enzymatic degradation of warfare agents and pesticides. By means of a brief summary of the state-of-the-art of these two fields of knowledge, we intend to present some contributions from our group to the field of bioremediation and to present some possible trends for the future of this field based on possible molecular targets and on the literature available so far.

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