The contribution of structural computational biology to the engineering of enzymes and the development of novel synthetic reactions

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Enzymes are powerful catalysts, which can be used for a wide range of innovative, efficient and eco-compatible processes that can open the way to many biotechnological applications. However, enzymes available in nature have evolved to operate under physiological conditions on a narrow range of substrates and they often do not display the physico-chemical properties compatible with their use in extreme conditions required in industrial-scale biocatalytic processes. With the potential offered nowadays by enzyme engineering techniques, we have seen in recent years numerous examples of successful computer-aided protein design that enabled tremendous improvements of enzyme properties for various applications, including the catalysis of novel synthetic reactions. Nonetheless, progress in this field, in particular with computational techniques, remains to be done in order to fasten structure-based enzyme design and accelerate the generation of efficient biocatalysts.

This lecture will discuss recent developments of our laboratory in three areas: (i) development of computational methods for multi-scale modeling and protein design; (ii) structure/knowledge-based enzyme engineering; and (iii) the development of chemo-enzymatic synthesis processes. These developments will be presented through specific research projects ongoing in our laboratory and emphasis will be placed on the contribution of structural computational methods in our approaches.