



Research Doctorate (Ph.D.) in Chemical Sciences
32nd Cycle – Academic Year 2016/2017

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Project Information

1 - Title

De novo designed oxygen-activating metalloenzymes

2 - Key words

metalloenzymes, *de novo* design, peptide synthesis, coordination chemistry, catalysis

3 - Abstract

The development of peptide-based catalysts that match or even exceed catalytic properties of natural counterparts is remarkable for their possible industrial and biotechnological applications. This project aims at developing artificial oxygen-activating metalloenzymes, based on *de novo* design scaffolds, able to promote selective oxidation with high efficiency. Our attention will be devoted to enzymes that employ non-heme iron or copper centers as cofactors for dioxygen activation. Starting from the *de novo* DF (*Due Ferri*) proteins, with four-helix bundle structure, a careful design process will be carried out to reproduce the dinuclear type 3 copper center of tyrosinases. To get insights into the factors that rule the chemistry of the metal center, several models will be synthesized and screened. Moreover, the possibility of engineering a metal site that is not natively found in helical bundles will be explored. The mononuclear iron center of α KG dependent oxygenases, which is housed in a β -sheet structural motifs, will be engineered in a *de novo* coiled coil.

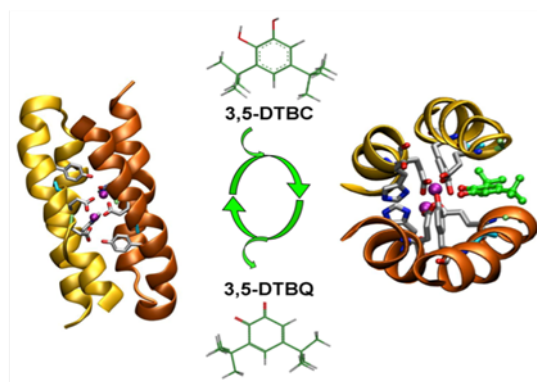


Figure 1. di-Zn(II)-DF3 (PDB ID:2KIK) catalyzes the oxidation of 3,5-DTBC to the corresponding quinone (3,5-DTBQ).