In silico redesign of oxidoreductases.

Emanuele Monza

[1]*Zymvol Biomodeling SL, C/ Roc Boronat 117 2nd floor module 6, 08018 Barcelona, Spain*

emonza@zymvol.com

Oxidoreductases are among the most challenging enzymes to redesign in silico. They contain complex cofactors and the mechanism often does not involve bond breaking and forming. Therefore, catalytic contact analysis, transition state theory and semi-empirical approaches are not always a viable way and alternative tools must be adopted.
We present the principles of our approach to this class of enzymes, with a special focus on laccases. Our methodology combines classical mechanics approaches to enzyme-substrate recognition with fast reactivity scoring approaches [1]. This range from simply electron donor-acceptor distances to “smart” quantum chemical approaches.
Successful case stories are presented [2,3,4], followed by preliminary results of new challenges that are currently being tackled in our company.

References

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3. Giacobelli et al, *Catal. Sci. Technol.*, 7, 515-523, **2017**
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