IN SILICO ENZYME ENGINEERING – SUCCESSFUL STORIES AND FUTURE OUTLOOK

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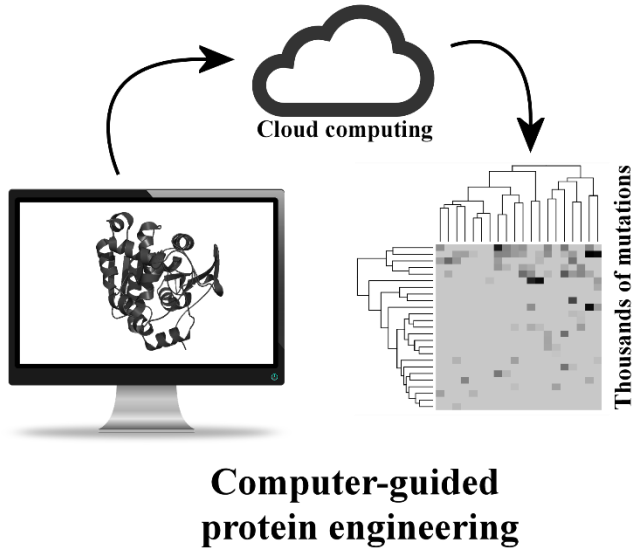
Part of the goals of the multi-partner INDOX European project (indoxproject.eu) was to identify, select and tailor oxidoreductases to obtain *ad hoc* industrial biocatalysts with optimized properties. Thanks to the combined effort of experimental and computational researchers we have successfully improved a variety of enzymatic processes including the industrial synthesis of: 1-naphthol[1], 25-hydroxyvitamin D3[2], and conductive polyaniline[3]. The computational methodologies employed, in some design efforts, will be presented and the importance of fast and accurate computer-guided protein engineering solutions[4,5] discussed.



Due to the outstanding accomplishments obtained during the last 3 years, we have recently funded an *in silico* protein engineering company – ZYMVOL. Our goal is to democratize the use of computer simulations in protein engineering processes and create consumer awareness to the importance of enzymatic applications in many industrial fields. We employ state of the art, open source software making our in silico solutions truly cost-effective thou capable of predicting the effect of thousands of mutations in days. Furthermore, thanks to cloud computing architecture, universities, SMEs and large industrial protein producers will have access to on-demand computer simulations that will considerably reduce the lab to market time for new industrial proteins.

Figure 1 – Our in silico approach allows scientists to probe their protein of interest for thousands of point mutations in days. The use of open source software and cloud based-computing makes our solutions affordable for a widespread use of computer simulations in protein engineering processes.

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