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#ICMolTalks

Victor Guallar

Barcelona Supercomputing Center. Barcelona (Spain)

January, 31th

16:30h Assembly Hall

Bioprospecting Active Sites for Industrial Biochemistry

Abstract

Optimization through engineering of enzymes is becoming a routinary action in Industrial Biochemistry. The generation of large amounts of sequence data allows building smarter mutant libraries which, combined with robotics and directed evolution approaches, often lead to new variants with optimal performance. In addition, computational modeling using molecular mechanics or artificial intelligence approaches is becoming highly predictive. Modeling offers a faster and a cheaper approach, introducing important enrichment factors in the experimental validation. In this talk we will summarize recent efforts in our lab (as well as in our spin off) for the bioprospecting and engineering of enzymes. We will focus on examples developed or with high interest for Industrial purposes, introducing, for example, our recent PluriZyme designs, where we added alternative catalytic active sites into enzymes. PluriZymes allow to combine two different biochemistries into a single enzyme scaffold, introducing one-pot cascade reactions combining transaminase and esterase activities. Moreover, following similar approaches, we have been able to transform a pore protein into a PET-nanoparticle chewing enzyme, reaching activities 10x higher than best PTases and LCCs.

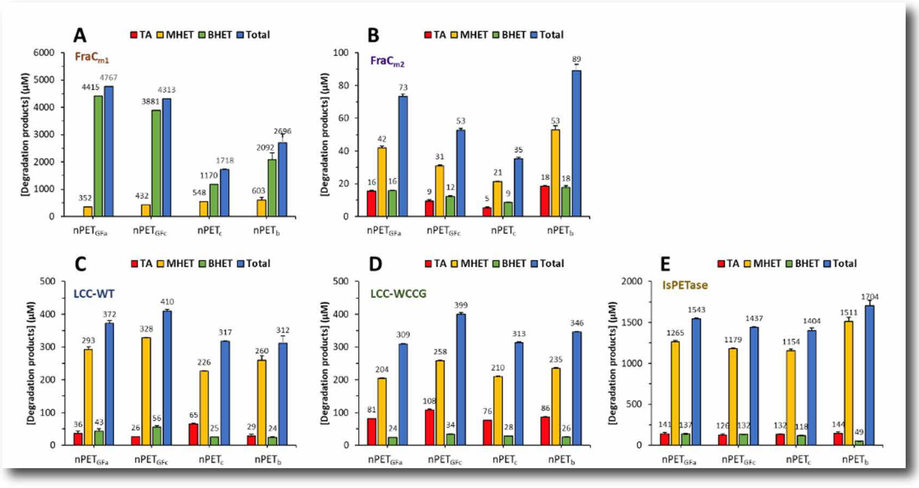

Figure. PET nanoparticle degradation by our engineered pore proteins, and comparison to best performing PETases.

Biography

An ICREA Professor at the Barcelona Supercomputing Center (BSC), Dr. Guallar completed his PhD in theoretical chemistry between University Autonomous of Barcelona (Spain) and UC Berkeley (USA) (January 2000). After three years as a postdoctoral researcher at Columbia University (USA), he was appointed assistant professor at Washington University School of Medicine (USA), before moving his group to BSC in 2006. His laboratory has grown considerably since developing important contributions in computational biophysics, such as the protein-ligand modeling software PELE, and biochemistry, including computational algorithms for enzyme engineering and the introduction of the first PluriZyme (enzyme with multiple actives sites).

Prof. Guallar has been awarded several important research projects, including the award of a prestigious advanced ERC grant. His lab has produced over 200 papers in international journals and completed 18 PhD thesis. In addition to algorithms development and application, the group recently placed importance in adding interdisciplinary fields, such as visualization techniques, data mining and machine learning.

Prof. Guallar is founder of BSC's first spin off, Nostrum Biodiscovery, a biotech enterprise created in 2016 which aims to collaborate with companies for the development of drugs and molecules of biotechnological interest, with clients in North America, Europe, Asia and Oceania.