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Disruptive mixed *in vitro-in silico* approach for protein engineering and screening

We present a strategy that combines wet-lab experimentation and computational protein design for engineering polypeptide chains. The protein sequences were numerically coded and then processed using Fourier Transform (FT). Fourier coefficients were used to calculate the energy spectra called "protein spectrum". We use the protein spectrum to model the biological activity/fitness of protein from sequence data. We assume that the protein fitness (catalytic efficacy, thermostabilty, binding affinity, aggregation, stability) is not purely local, but globally distributed over the linear sequence of the protein. Our patented method does not require any protein 3D structure information and find patterns that correlate with changes in protein activity (or fitness) upon amino acids residue substitutions. A minimal wet lab data sampled from mutation libraries (single or multiple points mutations) were used as learning data sets in heuristic approaches that were applied to build predictive models. We show the performance of the approach on designed libraries for 3 examples: Enantioselectivity, thermostability and binding affinity. We can screen up to 1 billion protein variants (10^9).

Biography

Frederic CADET is Vice President in Research & Development of the company Peaccel. He has a PhD in Protein Engineering, Data mining and Biosimulation. From 2004 to 2008, as an Executive School, University & Research Commissioner, he managed a budget of 1.3 billion Euros and was responsible for 32,000 employees. He is Former Chairman of the ERA Nets (European Research Area Networks) NetBIOME. He has developed pioneering research activities in bioinformatics. He is author of over 70 publications and Referee for 17 international scientific journals. He is Organizing Committee Member for 2nd International Conference on Genetic and Protein Engineering, November 14-16, 2016 Atlanta, USA.

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