Pharmaceut Reg Affairs 2012, 1:4
http://dx.doi.org/10.4172/2167-7689.S1.008

OMICS Group Conferences
Accelerating Scientific Discovery

2nd International Conference and Exhibition on
Pharmaceutical Regulatory Affairs

November 23-24, 2012 Hyderabad International Convention Centre, India

Strategies in enzyme engineering - significance, advances and exploiting the benefits of computational approaches

Naveen Kulkarni
Polyclone Bioservices Pvt. Ltd., India

Designer Enzymes and *Proteins* mimicking evolution on a laboratory timescale can be used to modulate and optimize challenging bimolecular properties such as activity, selectivity, stability, resistance to proteolytic degradation, solubility, etc,. Engineering enzymes and turning them into molecular machineries for producing pharmaceutical product is a billion dollar market. Therefore, the understanding of enzyme-substrate (E-S) relationship and studying the thermodynamics of protein folding is critical for both drug discovery, development and in their production. Rational redesign and directed evolution approach are the two major ways of exploring new properties of a given biomolecule. These approaches are time and resource consuming, shown to produce higher failure rate than success rate, sometimes becomes an iterative process without reasoning. To intervene with greater impact at this point is the use of computational biology which is used not only to predict novel properties of biomolecules but also as a tool to reason and explore the atomic level details responsible for a specific change. The pitfalls of using computational tools are mainly due to inappropriate selection of algorithms and even unreasonable use of such techniques would lead to false positive prediction, meaning just by misinterpreting the output of a docking or a simulation experiment, will yield results that repeatedly fail to deliver in the lab. Unifying different computational techniques, we have developed a framework and experimented on some commercially important proteins. The *in silico* framework called as enzyme engineering framework (eEF) used for enzyme/protein engineering is a step beyond the SBDD and virtual screening. The framework works sequentially to identify hot spots in enzymes, generate more than a hundred thousand mutations, filter for the most appropriate E-S mutations and simulate E-S reaction to predict the kinetics, activation energies and rate limiting steps of the potential enzyme/protein mutants.

Biography

Naveen Kulkarni is the CEO and founder of Polyclone Bioservices Pvt. Ltd. India. He comes with over 15 years of experience covering a broad range of scientific, entrepreneurial and innovation strategies with markets spanning Europe, USA, Australia and India. Prior to this, he served as the Director of Business Development at Philips Research, where he has successfully developed and managed a portfolio of opportunities for New Business Creation across Healthcare and Energy relevant for India, emerging markets and globally. He has conceptualized and developed novel solutions for accelerating drug discovery and directed teams consisting of experts from different domains including chemistry, proteomics and systems biology. He has been instrumental in conceiving new ideas and has several patents to his credit and has presented in various national and international conferences.

naveen.k@polyclonebio.com