

Title: "Using computer simulations and natural diversity to design more efficient biocatalysts"

Abstract:

Novozymes is the world market leader in bio-innovation with its core business centered on industrial enzymes, microorganisms, and biopharmaceutical ingredients. With over 700 products used in 130 countries, Novozymes' bio-innovations improve industrial performance and safeguard the world's resources by offering superior and sustainable solutions for tomorrow's ever-changing marketplace. Novozymes' natural solutions enhance and promote everything, from removing trans fats in food to advancing biofuels to power the world tomorrow. The *Candida antarctica* lipase B (CALB) has found very extensive use in biocatalysis reactions. Long molecular dynamics simulations of CALB in explicit aqueous solvent confirmed the high mobility of the regions lining the channel that leads into the active site, in particular, of helices $\alpha 5$ and $\alpha 10$. The simulation also confirmed the function of helix $\alpha 5$ as a lid of the lipase. Replacing it with corresponding lid regions from CALB homologues resulted in two new CALB mutants. Characterization of these revealed substantially improved catalytic properties. In this talk these results will be discussed in detail. The research process leading to the improved CALB variants exemplifies clearly how does computational chemistry support the enzyme optimization tasks within a leading biotech company.