THE UNIVERSITY OF TEXAS AT AUSTIN
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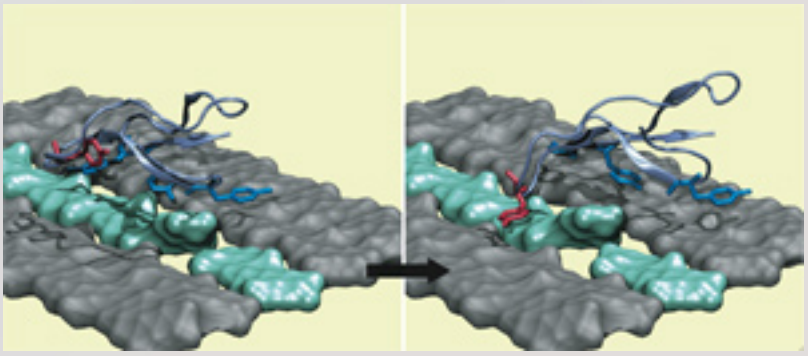
Productive Waste

National Renewable Energy Laboratory researchers use Ranger to extract ethanol from biomass

As the world's reserve of fossil fuels diminishes, scientists are racing to discover viable alternative energy sources. Among the most near-term solutions is biomass—organic matter that can be converted into ethanol. Whether in the form of crop and forestry by-products like corn stover, wheat straw, switch-grass or sawdust, biomass is plentiful, low-cost, and sustainable.

The current process of making ethanol from biomass costs an estimated $2.61 a gallon. "We'd like to reduce that cost to $1.49 a gallon," said Mark Nimlos, senior scientist at NREL in Golden, Colorado. "The research we're doing on Ranger at the Texas Advanced Computing Center involves making enzymes work faster to break down cellulose. If we could do that, biomass ethanol would be cost competitive with other sources of transportation fuel."



This image shows the binding module of this enzyme on a flat (1,0,0) crystalline surface of cellulose. Molecular dynamics simulations show that this domain undergoes a rearrangement when introduced to the cellulose surface. This indicates that the domain has a mechanism for recognizing cellulose surfaces.

Plants have cellulose walls that are difficult to digest, making them an unattractive food and energy source to most organisms. And while some bacteria and fungi secrete enzymes that are capable of turning cellulose into energy, Nimlos says the process of breaking down biomass is expensive because these enzymes aren't efficient enough.

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Using Ranger, Nimlos is performing molecular simulations that imitate the behavior of cellulase enzymes. The results are fed to the experimental group at NREL, who alter the amino acid sequence of the proteins through selective mutation. "We do the computation and another group does an experiment to validate our results. It's a very powerful approach to making improvements to the enzymes."

By fully understanding the hydrolysis process, it may be possible to engineer super-efficient enzymes that can create a substantial amount of energy from agricultural waste products. "We have a milestone for the program to make some predictions that lead to an improvement in the next year or two," Nimlos said.

By 2030, the Department of Energy expects to derive 30 percent of transportation fuel from biomass, and high performance computing is playing a significant role in determining our energy future.

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