27 January 2016

**Use of Nanostructure-initiator Mass Spectrometry (NIMS) to deduce selectivity of reaction in glycoside hydrolases**

Improving the annotation of glycoside hydrolase (GH) phylogenetic trees.

**The Science**

The enzymatic hydrolysis of plant cell wall material is a formidable task due to its complexity. Enzyme cocktails containing multiple classes of polysaccharide-degrading enzymes are used in several existing cellulosic ethanol plants to hydrolyze plant biomass into fermentable sugars. These enzymes are classified into families in the carbohydrate active enzyme (CAZy) database, and they include glycoside hydrolases (GHs), pectic lyases (PLs), carbohydrate esterases (CEs), and others. Due to several experimental limitations, only a small fraction of the enzymes included in CAZy have a function assigned by biochemical analysis.

**The Impact**

Improving the annotation of glycoside hydrolases (GH) phylogenetic trees can help understand the function, synergy, and stability of enzymes and improve the creation of biomass degrading enzymatic cocktails.

**Summary**

In collaboration with researchers at the Joint BioEnergy Institute, researchers in the Great Lakes Bioenergy Research Center used chemically synthesized nanostructure-initiator mass spectrometry (NIMS) probes derivatized with tetrasaccharides to study the reactivity of several enzymes representative of GH function. Patterns of reactivity identified by using these NIMS probes provide a diagnostic approach to assess reaction selectivity as well as comparative apparent rate information. Their results show diagnostic patterns for reactions of a-glucosidase, relaxed but varied specificity of several endoglucanases, and high specificity of a cellobiohydrolase with the model substrate. They also modeled time-dependent reactions of these enzymes by numerical integration, providing a quantitative basis to make functional distinctions among reactive properties, thus providing a new approach to enhance the annotation of GH phylogenetic trees with functional measurements.

**Contacts (BER PM)**

N. Kent Peters  
Program Manager, Office of Biological and Environmental Research  
[kent.peters@science.doe.gov](mailto:kent.peters@science.doe.gov), 301-903-5549

**(PI Contact)**

Brian Fox  
University of Wisconsin – Madison  
bgfox@biochem.wisc.edu

**Funding**

The DOE Great Lakes Bioenergy Research Center and DOE Joint BioEnergy Institute are supported by the US Department of Energy, Office of Science, Office of Biological and Environmental Research, through contract DE-FC02-07ER64494 and through contract DE-AC02-05CH11231, respectively.

**Publications**

Deng K, Takasuka TE, Bianchetti CM, Bergeman LF, Adams PD, Northen TR, Fox BG. “Use of nanostructure-initiator mass spectrometry to deduce selectivity of reaction in glycoside hydrolases”. *Frontiers in Bioengineering and Biotechnology* **290**, 19, pp. 11819 (2015) [DOI: 10.3389/fbioe.2015.00165]

**Related Links**

[include optional related links, one per line]

**PM Recommendation for SC Web Publication**

[Yes or No]