STRUCTURE-FUNCTIONAL STUDIES OF GLYCOSIDE HYDROLASES

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Development of better enzymes for biomass depolymerization and biotransformation has been hindered by the paucity of our knowledge about structure and function of enzymes active on lignocellulosic biomass. According to CAZy out of 159 274 sequences of GHs available in the database in September 2013, 9221 (or 5.7%) were functionally characterized and 817 (or 0.52%) were had their 3D structures determined and made available in the Protein Data Base (PDB). The current situation only got even more challenging as a consequence of the massive amount of data generated by the next-generation sequencing and worldwide (meta)genomics and (meta)transcriptomics projects. In attempt to at least partially bridge the gap between abundance of genomic information and lack of structural and functional data, we determined X-ray structures of several enzymes from GH families 1, 2, 3, 5, 7, 12 and 45, characterized their enzymatic activity (Lima et al., 2013a&b; Textor, et al., 2012; Prates et al., 2013; Nascimento et al., 2014). We also conducted their computational molecular dynamics studies in the attempt to shed more light on their function in the context of the process of plant biomass degradation. In our presentation we will discuss these structures and their relationships with the enzymes activities and specificities.

References:
Lima, L.H.F., et al., Cellulose (2013b) 20: 1573-1585