Glycoside hydrolases planning resistant pretreating biomass with ionic liquids through modeling Comparative and Molecular Dynamics

Fonseca,T.S.[1]; Pascutti,P.G.[1,2]; Gomes, D.E.B.[1]

[1]Instituto Nacional de Metrologia-INMETRO,RJ , [2] Instituto de Biofísica Carlos Chagas Filho-UFRJ, RJ;

The biomass consists of cellulose chains, polysaccharides composed of β-1,4-glycosidic links joined together by hydrogen bonds, insoluble in water and in most organic solvents due to the recalcitrance and its crystallinity. The pretreatment step is essential for promoting the fractionation and increase the chemical accessibility of its main components.

The pretreatment with ionic liquids (ILs) is characterized as a promising solution for biomass recalcirance due to low vapor pressure, thermal stability, and adjustable properties such as polarity, hydrophobicity and miscibility as solventes.

The IL 1-Ethyl-3-methylimidazolium acetate (EMIM-Ac) has been seen as promising solvent. However, interfering with enzymatic activity, due to high ionic strength of the solution, which causes enzime's inactivation. So, planning enzymes resistant to ILs represent an important technological advance making it possible to reuse and reduce costs associated with its production.

In this study we investigated which are the structural characteristics and the effect of pretreatment with ILs on enzyme activity and how EMIM-Ac affects the structure and solvatation of the celulose fibers through dynamics simulations (MD), aiming the understanding of how the IL process the solvatation and embasement to project new IL and enzyme combinations.

The ILs are parameterized using calculations for force field CHARMM 36 using FF-toolkit in MP2 / 6-31G *basis set for geometry optimization and HF / 6-31G* for bias and optimization. The simulation was subjected to energy minimization with the method of conjugate gradient using 100000 steps. MD simulations are being carried out by 50 ns,the NPT set at 313K,1 atm and using electrostatic PME.

Is being built 3D models for planning hydrolases glycoside and a mapping of the conformational space in order to check the effect of hydrolases glycoside after pretreatment with EMIM-Ac and possible resistance enzymes using molecular dynamics simulations and techniques comparative modeling.

Palavra chave: biofuel, molecular dynamic, ionic liquid
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