MOL2NET, International Conference Series on Multidisciplinary Sciences

PREDICTIVE LIGNIN DEGRADATION STATISTICAL MODEL

Abigail Copca Granados abigail2497@hotmail.com

Technology Institute of Pachuca, Hidalgo, Mexico

Abstract:

Lignin is a very abundant biopolymer, which is found in the cell wall of plants along with cellulose and hemicellulose, its structure is very complex and difficult to degrade since it´s composed of phenolic polymers which makes it very resistant, this It´s the main problem in some industries, for example on the production of paper and fuels. Therefore, we intend to develop a prediction model for simulations with lignin and different organisms, with a database obtained from different platforms such as Pumbed, the National Biotechnology Information Center (NCBI), PROTEIN DATA BANK (PDB), etc. Working with the database it was found that the most common enzyme is peroxidase that is present in a type of bacteria called *Pseudonocardia autotrophica*, For this reason, we will work with this enzyme to be able to make the model and do the required simulations.

Keywords: Lignin, degradation, enzymes

1. Introduction

In the paper industry, lignin is not degraded some of the susceptible material is no longer used, which means that it is often not profitable or has significant economic losses. In of research, a predictive statistical model was developed to degrade lignin more easily and thus be able to use it in some other process, seeking to make the compounds linked to lignin being more pure. The research is qualitative and quantitative type, first we perform qualitative research to know the important aspects of lignin, the organisms where it is present, its structure and the properties to be able to determine the reason of why it is so difficult to treat degradation.

Continue with the quantitative research in different platforms such as Punmed National Center for Biotechnology Information (NCBI), PROTEIN DATA BANK (PDB), CHEMBL, to determine the lignolitic enzymes and the most common organisms. A database was made with the main characteristics, taking into account the data bank from which the information was extracted, the code of the enzyme, etc. It was necessary to determine the amount of proteins present in each organism, also to use the PseAAC platform to predict the lignin in a specific protein and determine the Shannon entropy. With the obtained values, work is being done to develop the statistical model in which the most efficient enzyme will be found in order to disintegrate lignin in a way that does not affect cellulose or hemicellulose. It was found that the most common enzyme is peroxidase that is present in a bacteria kind called Pseudonocardia autotrophica, with this discover the statistical model will be performed, which is expected to be effective and sustainable. Because if so, it will be very beneficial in industries, The biggest advantage will be in the economic aspect. The prediction model will help us experiment with different properties of lignin and types of organisms. In order to later find the most efficient organism for the degradation and to be able to put it into practice at the laboratory level and later at the industrial level, which will bring a great benefits.

2. Results and Discussion

The enzyme peroxidase is present in a species of bacterium called Pseudonocardia autotrophica will be our basis to start with the model since it is the most abundant in all data, the statistical program will be used to do it, the research will continue to work until you get the model and start the simulations.

4. Conclusions

The lignin is a biopolymer formed by polymer chains of phenols. Which are rigid and are joined by links C-H. what makes it very resistant to any form of degradation. It is the third main compound of wood, the first two are the cellulose and hemicellulose. In the industry of the paper much is burned as energy recovery, and only a small part is to make different products such as cresols and vanilla. With different methods but all have a high cost, it is important to find a way to easy to degrade is make more easy use, this research aims to find a statistic model to determine which enzyme is most effective and where we could find it. For example bacterium called Pseudonocardia autotrophica is the most likely to work, this bacterium is found in products from easily obtaining.

Notes

1. Chávez-Sifontes & Domine Lignin, structure and applications: depolymerization methods for obtaining aromatic derivatives of industrial interest Avances en Ciencias e Ingeniería - ISSN: 0718-8706 Av. cien. ing.: 4(4), 15-46 (Octubre/Diciembre, 2013)) Universidad Politécnica de Valencia, Instituto de Tecnología Química, ITQ (UPV - CSIC) 2. A. Guliérrez, A.T. Martínez Mecanismo de biodegradación de la lignina. Revista Iberoamericana de Micología 1996; 13: 18-23. 3. Tien M. Propertíes 01 ligninase Irom Phanerocha/e chrysosporium and their possible applieations. CRC Cri! Rev Microbiol1987; 15: 141-168.. 4. BAI Y, Xiaoping Q, WEN X.Effects of culture conditions on ligninolytic enzymes and protease productionbyPhanerochaetechrysosporium in air. Journal of Environmental Sciences 2008; 20, 94–100 p. 5. Shimada M, Higuchi T. Microbial, Enzymatic and Biomimetic Degradation 01 Lignrn. En: Hon DN-S, Shiraiski N (eds) Wood and Cellulosic Chemistry 1991; 557-619,