

Application of chem. Sketch in the field of molecular formulation

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Abstract

In order to energize my research, I have chosen computer software to develop molecular formula of the product formed by the distillation of pretreated biomass, which is obtained from *parthenium hysterophorus*, during course of my research; I have drawn the formula of number of chemicals. This paper deals with the computational analysis of distillate obtained after the distillation of the pretreatment of the raw material. The software chem. sketch is used for molecular modeling and molecular formulation.

Key words; Parthenium hysterophorus, Polymers, Ethanol, chem. Sketch, molecular formulation.

Introduction

Objectives of the study

Most of the biomass contain Lignocellulose, that is a renewable source and in large quantities available with great latent for bioconversion to value-added bio-products. General name of Parthenium hysterophorus is gazer ghass, which is used as potential for the production of bio-polythene.

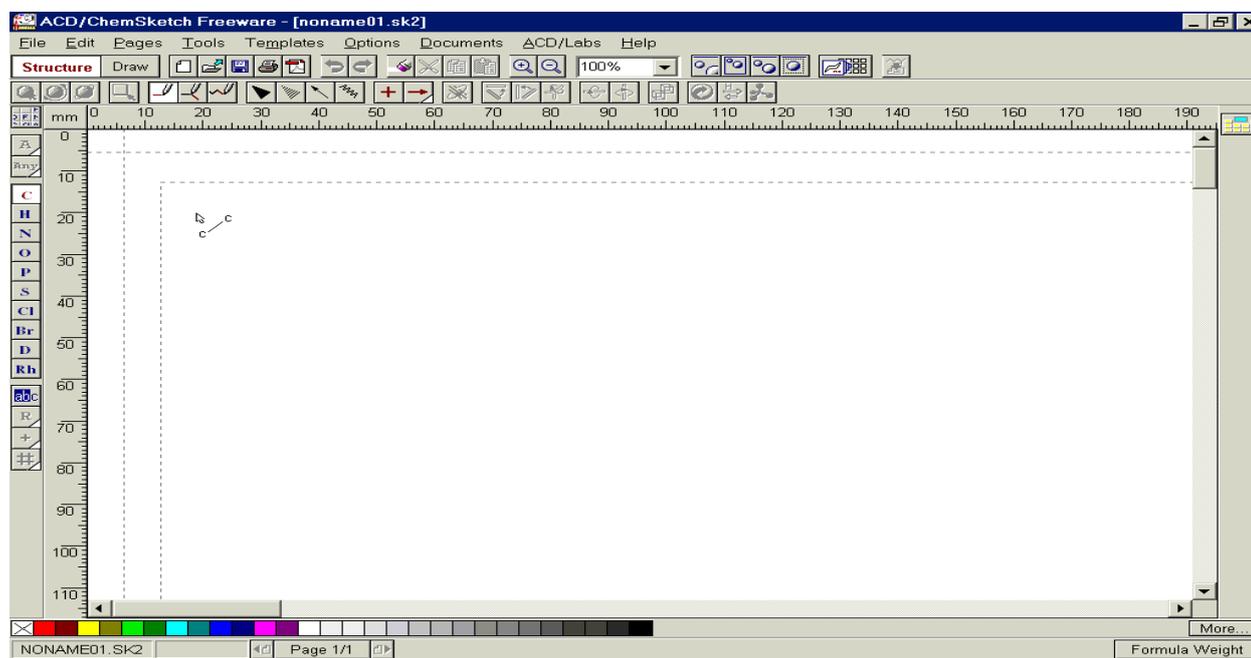
The objectives of the study are as follows:

1. Collection of sample from field and its preparation for the extraction of lignocelluloses biomass.
2. Pretreatment of raw materials.
3. Saccharification of lignocelluloses biomass.
4. Use of computational software (Chem. sketch) computational analysis of distillate, obtained after the distillation of the pretreatment of the raw material.
5. The software chem. sketches is used for molecular modeling and molecular formulation.

Molecular Modeling and Molecular Formulation

Forming a three dimensional mental image from a two dimensional drawing is an advantage for scientists with the help of ChemSketch. When we open this, it is ready to draw carbon by default and places the appropriate number of hydrogen needed on the carbons.

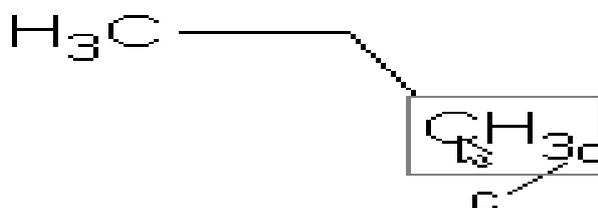
The three default functions are indicated in the picture (next slide). If we place the cursor over a button on the toolbar, its function will appear. Comments and reactions can be added to the screen. A number of common drawing tools are available if we click on "Draw" on the toolbar. As we toggle between the "Structure" and "Draw" modes, we will notice that the toolbars change.



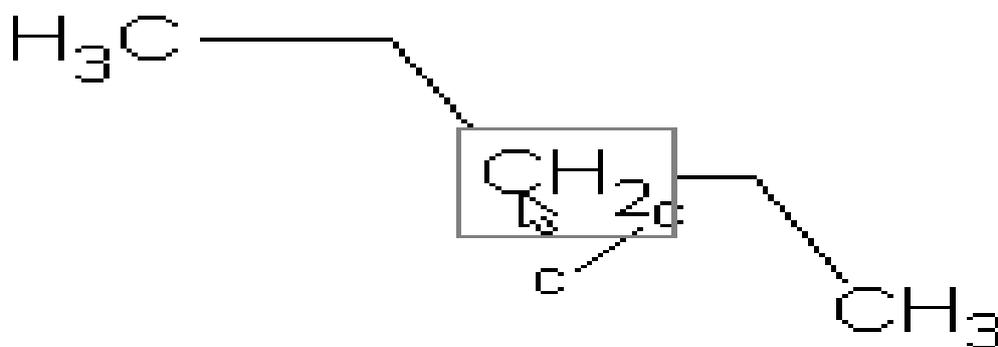
Drawing Chemical Structures

To begin sketch, just click the pointer and a CH₄ appears on the screen. If we tick on this first CH₄ another carbon will add to it. The subsequently carbon added will be at the carbon that is painted with the box.

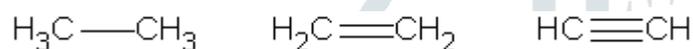
We can position the pointer at any of the carbons to form branches or side chains. The program defaults to demonstrate hydrogen only on the terminal carbons (at the end of the chain). Where the lines gather (or corners), there are carbon atoms with added hydrogen (unless four lines meet).



If we place the cursor over a “corner” in the chain we will see the –CH₂– group appear highlighted in a box as shown below. The number of hydrogen on each carbon adjusts automatically as multiple bonds form or as side chains are added to a structure. The carbon atoms in a molecule must forever have FOUR bonds.



Now if we want to add a double or triple bond, we select the bond position with the cursor. A box will highlight, and then click it once for a double; click it again for a triple bond, and again to go back to a single bond.



One click

two clicks

If we want to insert an atom other than carbon. The easiest way to do this is to add a carbon at the site where we want the other atom and then substitute the new atom for the carbon. Build the two carbon chain. Then go to the carbon and click on it again to add the $-\text{CH}_3$ side chain. Now go to the menu bar on the side and click on O, then Place cursor on the carbon of the side chain and click. The carbon becomes $-\text{OH}$ and the hydrogen are adjusted appropriately.

Conclusion

By making use of chem.sketch, we have drawn the structure of ethanol, likewise we are trying to draw the structure of various others chemical compound present in the distillate .so that the chemical composition of the parthenium hysterophorus can be completely identify and thus justify. Lignocellulosic biomass like Parthenium hysterophorus could be a good source of ethanol that could be used for further production of bioethelene.This then polymerises to polythene. By the production of biopolythene,environment could be protected ,as it eradicate the harmful gagger grass from farmer field as well as easily decomposed to save soil fertility.

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- Get ChemSketch at: <http://www.acdlabs.com/download>.

