
Sybyl: Building DNAs and Minimizing their Energy

Lab 6

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Objectives

In this lab you will become acquainted with Sybyl. This program allows you to draw simple molecules, DNA's and Proteins, perform molecular mechanics, molecular dynamics, and quantum mechanics calculations - and this is just for starters.

The purpose of this lab is to become familiar with Sybyl's graphical user interface and to learn to draw simple structures. The outline for this lab is as follows:

- 1) Setup your .cshrc file for Sybyl
- 2) Review the attached materials
- 3) Do the Sybyl Tutorial

Setup - .cshrc file

You need to modify your .cshrc file so that when you login in you user environment will be set up to run Sybyl. This is fairly easy to do, all you need to do is to add a few lines to your .cshrc file. Start up jot and load your .cshrc file

```
jot .cshrc
```

Add the following lines to this file.

```
alias s `sybyl6.5`  
  
# Set path to trigo so Sybyl can be run by typing s  
set path ($path /usr/people/trigo)  
  
# If Sybyl's license daemon isn't running, start it  
trigo -shell sybyl6.5  
$TA_ROOT/bin/unix/StartLicenseDaemon
```

Note, the location of the lines is not of major importance. However, for ease of debugging it is best to organize things. Aliases are usually put near the top of the file, the rest can be put at the bottom. When your done, click on 'File/save' and then exit. Source your .cshrc file

```
source .cshrc
```

and now when you type 's' Sybyl should start up.

Sybyl

After you modify your .cshrc file, review the attached materials. Then, turn to the Tutorial in the Sybyl manual titled Tutorial and work through it.