Assignment 4 – Molecule Viewer Website

Version 1.00 (last update: Mar. 24, 12:00)
Changes highlighted in yellow
Due date: Tue, April 5, 9:00 AM

Summary and Purpose

For this assignment, you will be creating a webserver that allows users to upload and display molecules.

Deliverables

You will submit all of your work via git to the School's `gitlab` server. This will be used the determine the completion date.

Demo

Grading will be done by demonstration. You will make an appointment with one of the teaching assistants. During your appointment time you will, clone your repo from the gitlab server, demonstrate your code to the TA, and then allow the TA to user your code.

Functionality

Your program should have the following functionality.

Add/remove elements from the system. Design an interface that allows users to add and remove elements from the system. Users should be able to specify the element number, element code, element name, 3 colour values, and radius of an element. It is not required to be able to edit element values, you can always remove one and replace it with a new one. There should be a default set of colours and radius for any elements contained in molecules that do not have an entry in the system. It should not be possible for the user to enter malicious parameters for the element that can damage the system.

Upload `sdf` files to the system. Design an interface that allows users to upload `sdf` files to the system. Invalid `sdf` files should be detected, and an error message generated. It should not be possible to damage the system with a malicious `sdf` file. Upon uploading an `sdf` file, the user should be informed of success. The user should be able to assign the molecule contained in the `sdf` file a name (a malicious name should not be able to damage the system).

Select from a list of molecules. Design an interface that allows users to select one of the molecules that is in the system. Inform the user of the number of atoms and bonds that are in the molecule before they select it.

Display a selected molecule. Display a selected molecule showing all the atoms as shaded spheres according to the element table. Implement a method to change the angle of the molecule (without reloading the entire web-page page).

Navigate between pages. Design a method to navigate between the different functions listed above.

Ask Questions

The instructions above are intended to be as complete and clear as possible. However, it is YOUR responsibility to resolve any ambiguities or confusion about the instructions by asking questions in class, via the discussion forums, or by e-mailing the course e-mail.

Nightmare mode

In addition to everything you did in the previous nightmare modes, add the ability to animate a rotation of the molecule. The molecule should appear to spin smoothly around 360 degrees along each of the cardinal (x,y,z) axes (one axis at a time).

Academic Integrity

Throughout the entire time that you are working on this assignment. You must not look at another student's code, nor allow your code to be accessible to any other student. You can share additional test cases (beyond those supplied by the instructor) or discuss what the correct outputs of the test programs should be, but do not share ANY code with your classmates.

Also, do your own work, do not hire someone to do the work for you.

Grading Rubric

Ability to add/remove elements	5
Ability to upload sdf files	5
Molecule selection	5
Molecule display	10
Molecule rotation	10
Visual presentation	5
Intuitiveness of use	5
Clarity of information presented	5
Total	50