1. Abstract

Grappa is a tool to build molecules and use them for other purposes after building them. This tool is only available via the command line, so therefore not in a user-friendly environment. Building a web application that makes this program interactive is a way to make a tool usable for a broader audience. There are a lot of biologists who don't know how to use the command line properly and this tool would be appealing for those people. This is the reason why this web application is important: to create interest for our target group.

The goal of this project is to make a user-friendly web application that uses the Grappa tool, displays a molecule derived from the input, and save them in a database for further use. The molecule needs to be drawn while your typing the sequence and must be interactive.

This web application is built with different programming languages, such as Java 10, Python, JavaScript and HTML. A few tools are used to organize and build this project, such as Servlets, SQlite databases, Tomcat and JSNetworkx to draw the molecule on the webpage.

The result is a single webpage where the user can enter their sequence for the molecule and the website draws the molecular structure while the user is entering the molecular representation. If the user is done with creating the molecule, it can be saved in a database for later use. It's also possible to zoom in and out of the molecule and an autocomplete feature that utilizes the database to complete the molecule. To help new users on how to make a molecule, there is a help page that describes everything in simple terms.

The conclusion of this project is that it is possible to make a user-friendly web page for biologists to make a molecule with a certain sequence. The communication with the client was an important part, because the product needs to be approved by our target audience.

In the future, this web application can be used by biologists to make a visual representation of a molecule in a user-friendly environment using a sequence. The application works completely.

2. Materials & Methods

2.1 Java SE 10

Java 10 is a programming language that is general-purpose used. It is an object-oriented language that can be used on all platforms. Java SE 10 was released in 2018 and this is the newest version. Java is used in this project for the database interaction, the interaction with the python program and for servlets. [1]

2.2 Servlet

A servlet is a program written in java to communicate with the client on the website. Servlets are used on all platforms and it is used to build a web-based application. In this project Servlet is used to process a form among other things. [2][3]

2.3 Python 3.5

Python 3.5 is a programming language that can be used on many platforms. In python, readability and indentation is important. In this project, python is used for our implementation of the Grappa tool. [4]

2.4 SQlite database

SQlite is a database management system that uses the SQL language to communicate. In this project, the database is used to save molecules. [5][6]

2.5 Apache Tomcat

Tomcat is a server that is used to run web applications. Tomcat supports servlets and JSP files and it takes care of the interaction between JSP pages and the webserver. In this project, Tomcat is used as server to host our Grappa web application. [7][8]

2.6 Grappa

Grappa is a program, written in python 3.5, that translates a linear sequence of tokens to a molecule with nodes and edges. Grappa is used in this project to translate the sequence in a visual molecule on the website. [9]

2.7 Gradle

Gradle is a Java plugin build tool. With Gradle, you can build almost every implementation in your build script. Gradle doesn't do anything unless you add code to the build script. [10]

2.8 JavaScript

JavaScript is a programming language for websites to make things interactive on a page. JavaScript is one of the three main languages to learn for a webdeveloper. JavaScript is often abbreviated as JS and almost every website use JavaScript. In this project, JavaScript is, for example, used to draw the molecule in a interactive way. [11][12]

2.8.1   JQuery

JQuery is a library for JavaScript that simplifies and extends programming in JavaScript. It is a free and open-source library. [15]

2.9 HTML

HTML is the markup language to create web pages. The abbreviation stands for Hyper Text Markup Language. The elements used in HTML are the building blocks for a web page and is made up of so called tags. In this project, HTML is used to create the structure of the web page where you can fill in the sequence for the molecule, and where the drawing tool makes the molecule interactively. [13][14]

2.10   JSNetworkx (drawing tool)

JSNetworkx is a software package written in python to create complex networks. To create a network, the package use nodes and edges. In this project, JSNetworkx is used to draw the molecule on the web page. It takes nodes and edges as input and the output is a molecule. [16]

2.11 Bootstrap (CSS)

Bootstrap is a free CSS framework for developing web applications. It is an open-source toolkit to create and design web pages. In this project, all the CSS is done with the Bootstrap toolkit [17]

Sources

[1] Wikipedia (2019, Jan 15). Java (Programming language). Retrieved from: https://en.wikipedia.org/wiki/Java_(programming_language)

[2] Wikipedia (2014, mart 9). Servlet. Retrieved from: https://nl.wikipedia.org/wiki/Servlet

[3] Oracle (2013). The Java EE 6 Tutorial. Retrieved from: https://docs.oracle.com/javaee/6/tutorial/doc/bnafe.html

[4] Wikipedia (2019, Jan 15). Python (programming language). Retrieved from: https://en.wikipedia.org/wiki/Python_(programming_language)

[5] Wikipedia (2018, Dec 26). Sqlite. Retrieved from: https://nl.wikipedia.org/wiki/SQLite

[6] Sqlite (2019). What is Sqlite? Retrieved from: https://www.sqlite.org/index.html

[7] The apache software foundation (2018). Apache Tomcat. Retrieved from: http://tomcat.apache.org/

[8] Wikipedia (2018, Dec 21). Apache Tomcat. Retrieved from: https://nl.wikipedia.org/wiki/Apache_Tomcat

[9] University of Groningen (2018). Vermouth-Martinize. Retrieved from: https://github.com/marrink-lab/vermouth-martinize

[10] Gradle Inc (2019). Java Quickstart. Retrieved from: https://docs.gradle.org/current/userguide/tutorial_java_projects.html

[11] W3Schools (2019). JavaScript tutorial. Retrieved from: https://www.w3schools.com/js/

[12] Wikipedia (2019, Jan 15). JavaScript. Retrieved from: https://en.wikipedia.org/wiki/JavaScript

[13] W3Schools (2019). HTML introduction. Retrieved from: https://www.w3schools.com/html/html_intro.asp

[14] Wikipedia (2019, Jan 3). HTML. Retrieved from: https://en.wikipedia.org/wiki/HTML

[15] W3Schools (2019). jQuery Tutorial. Retrieved from: https://www.w3schools.com/jquery/

[16] JSNetworkx (2019). JSNetworkx: A javascript port of the NetworkX graph library. Retrieved from: http://jsnetworkx.org/

[17] Bootstrap (2019). Bootstrap. Retrieved from: https://getbootstrap.com/