Tayla Isensee Dr. Anna Ritz Introduction to Computational Biology 7 May 2018

Final Project Report

Motivation

In this project, I wanted to implement a program that sequences cyclic peptides like antibiotics. Because of their unique structure and their absence from the coding genome of the organisms that synthesize them, sequencing cyclic peptides requires the use of mass spectrometry rather than analysis of DNA. This alternative sequencing technique really intrigued me, as did the biological importance of knowing the structure and sequence of antibiotics. Using mass spectrometry to sequence antibiotics was a chapter in our textbook, which also drew me to this project as the textbook and its companion website provided explanations, datasets, and pseudocode that helped further this project.

Data Formatting

The datasets that I obtained came either from the textbook, *Bioinformatics Algorithms*, or from its companion website Rosalind. Most of the larger datasets came from Rosalind, while smaller and toy examples came from the textbook. The only manipulation of datasets was turning sets into lists so that they fit well into my program.

High-Level Steps

My program can: generate both theoretical linear & cyclic spectrums of a given peptide and provide a possible mass sequence for a cyclic peptide, given ideal experimental data.

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bound algorithm structure, could be used to sequence other peptides and sequence-able elements of an organism that are not found in the genome.