Cyclopeptide Sequencing

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The Problem:

Cyclopeptide Sequencing

- Relies on a “branching and bounding algorithm”
    - Every time the while loop runs, each peptide grows in length by one amino acid
    - Then the spectrum each peptide in the list is be compared to the spectrum of the mystery peptide. If it contains a peak value that is not in the spectrum, it is removed from the list
    - This continues until the peptide whose spectrum exactly matches the given spectrum is identified
- Pros:
    - Faster than a brute force algorithm
- Cons:
    - Still very slow
    - Only worked if the given spectrum was perfect and didn’t have any missing or extraneous peaks.
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Leaderboard w/ Spectral Convolution

- Spectral convolution narrows down the number of amino acids that are added to the peptides each time.
  - Calculate the difference between each peak in the spectrum
  - Based on the numbers between 57 a«

References

1. Compeau, P., & Pevzner, P. (2015). *BIOINFORMATICS ALGORITHMS: An active learning approach* (Vol. 1). S.l.: ACTIVE LEARNING.
2. “Tyrocidine.” *Wikipedia*, Wikimedia Foundation, 30 Apr. 2018, en.wikipedia.org/wiki/Tyrocidine. [Source of Image on 2nd Slide]