

Python Lab

A Complex Example Using Control Statements

Proteomics Informatics, Spring 2014

Week 5

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Last week's HW Assignment

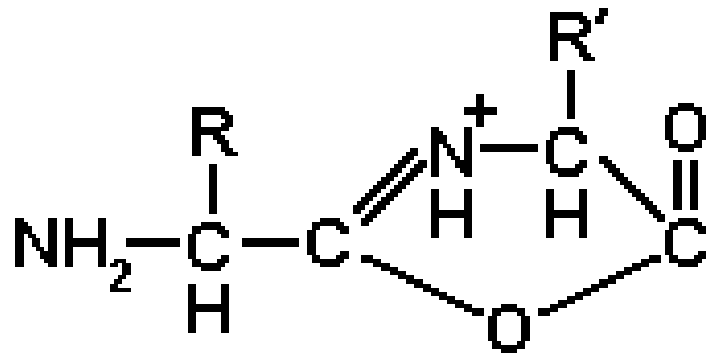
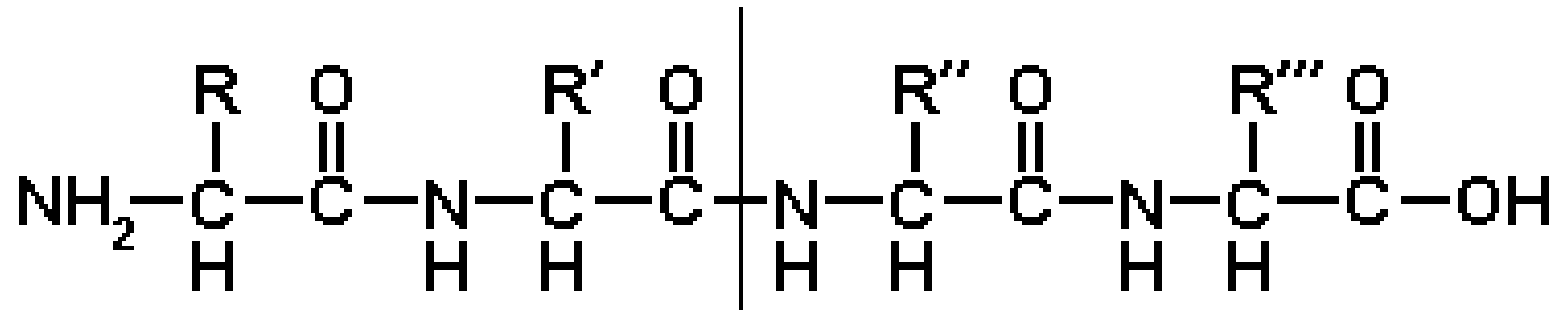
Recap

- Control statements
- if/else branching operation
- for loops and access patterns

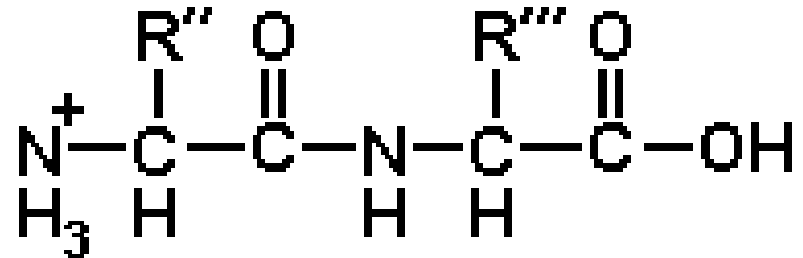
Today

- More complex example:
 - **Compute Peptide Fragment Ions**
- **Problem:** Given a peptide sequence and charge state, compute m/z of various b- & y-ions

First, hand calculations



B ion



Y ion

HW Assignment

- Add remaining neutral losses
 - b-nh3
 - y-h2o
 - y-nh3
- Add remaining multiply-charged fragments
 - y+

Next Class

- Functions