#!/usr/bin/perl -w

# This simple script sums or subtracts all possible amino acid residues
# from a mono charged m/z peak in a MS/MS spectrum and shows results on
# screen to assist de novo sequencing of peptides
#
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#
$i = 1;

while ($i) {
  # Peak m/z
  print "m/z peak:";
  my $frag = <STDIN>;
  print "sum or subtraction: ('+' or '-'): ";
  my $oper = <STDIN>;
  chomp $frag;
  chomp $oper;
  # Monoisotopic amino acid's mass
  if ($oper eq '+') {
    $mass_G = 57.02+$frag;
    $mass_A = 71.04+$frag;
    $mass_S = 87.03+$frag;
    $mass_P = 97.05+$frag;
    $mass_V = 99.07+$frag;
    $mass_T = 101.04+$frag;
    $mass_C = 103.01+$frag;
    $mass_I = 113.08+$frag;
    $mass_L = 113.08+$frag;
    $mass_N = 114.04+$frag;
    $mass_D = 115.03+$frag;
    $mass_Q = 128.06+$frag;
    $mass_K = 128.09+$frag;
    $mass_E = 129.04+$frag;
    $mass_M = 131.04+$frag;
    $mass_H = 137.06+$frag;
    $mass_F = 147.07+$frag;
    $mass_R = 156.10+$frag;
    $mass_Y = 163.06+$frag;
    $mass_W = 186.08+$frag;
  } else {
    $mass_G = $frag-57.02;
    $mass_A = $frag-71.04;
    $mass_S = $frag-87.03;
    $mass_P = $frag-97.05;
    $mass_V = $frag-99.07;
    $mass_T = $frag-101.04;
    $mass_C = $frag-103.01;
    $mass_I = $frag-113.08;
$mass_L = $frag-113.08;
$mass_N = $frag-114.04;
$mass_D = $frag-115.03;
$mass_Q = $frag-128.06;
$mass_K = $frag-128.09;
$mass_E = $frag-129.04;
$mass_M = $frag-131.04;
$mass_H = $frag-137.06;
$mass_F = $frag-147.07;
$mass_R = $frag-156.10;
$mass_Y = $frag-163.06;
$mass_W = $frag-186.08;

# Print the results
print "G = $mass_G\n";
print "A = $mass_A\n";
print "S = $mass_S\n";
print "P = $mass_P\n";
print "V = $mass_V\n";
print "T = $mass_T\n";
print "C = $mass_C\n";
print "I = $mass_I\n";
print "L = $mass_L\n";
print "N = $mass_N\n";
print "D = $mass_D\n";
print "Q = $mass_Q\n";
print "K = $mass_K\n";
print "E = $mass_E\n";
print "M = $mass_M\n";
print "H = $mass_H\n";
print "F = $mass_F\n";
print "R = $mass_R\n";
print "Y = $mass_Y\n";
print "W = $mass_W\n";
print "\n";
}

# Exit the program
exit;
Supplementary information: Screenshot of perl script denovo.pl used to assist de novo sequencing of a peptide from MS/MS spectra.