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#!/usr/local/bin/perl

#####
# Hydropathy-Analyis: (C) Ulrich Krauss(2012)
#
# Reads in txt-file in fasta format containing unaligned amino acid sequences
# Assigns a hydropathy "value" according to the Kyte-Doolittle scale to each
# amino acid and writes a "out-file.txt" that contains an ordered space
# separated list of hydropathy values for each sequence in the fasta file
#
# The outfile can easily be imported into any data analysis software such as
# MS excel, Origin, GraphPadprism
#
# FASTA FORMAT:
# >Sequence 1
# AAAAAAAAAAAAAAAA
#
# >Sequence 2
# CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
#####
# NOTE:Supply a gap-free sequence alignment in fasta format to allow easy
# plotting and visualization
#
# NOTE:Input Fasta file has to be located in the same directory as the script
#
# SYNTAX: HPLOT_v1.pl fasta-input-file.txt
#
#####

$/ = '\777'; # entire input to be read in one slurp
$seqs = <>; # read input, assigning to single string

while ($seqs =~ m/^(>[^>]+)/mg) { # match indiv. sequences by '>'s = Fasta Format
    push(@seqs,$1); # and store in array
}

for (@seqs) {
# only allow characters A-Z,a-z,0-9,'_','-' , and '.' in names;
    /> *([\w\-\.]+)/ && ($seq_name = $1);

    if ($seq_name) {

        my $seqI = $_;
        $seqI =~ s/^>.*\n//; # remove FASTA header
        $seqI =~ s/\n//g; # remove endlines

        my $value = '';
        my $codon = '';

        for (my $i=0; $i < (length($seqI)) ; $i +=1) {
            $codon = substr($seqI,$i,1);
            $value .= seq2value ($codon);
        }
    }
}

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# write out-file
    open (MYFILE, '>>out-file.txt');
    printf MYFILE ('%1$6s %2$6s %3$6s', $seq_name, $seqI, $value);
    print MYFILE "\n";
    close (MYFILE);

# on-screen output
print " \n\n$seq_name $value\n\n";

}

else {
    warn "couldn't recognise the sequence name in \n$_";
}
}

exit;

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#sub hydropathy-scale - kyte-doolittle
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sub seq2value {

my($codon) = @_;
$codon = uc $codon;

my(%scale) = (

'A' => '1.80 ',
'R' => '-4.50 ',
'N' => '-3.50 ',
'C' => '2.50 ',
'D' => '-3.50 ',
'E' => '-3.50 ',
'F' => '2.80 ',
'G' => '-0.40 ',
'H' => '-3.29 ',
'I' => '4.50 ',
'K' => '-3.90 ',
'L' => '3.80 ',
'M' => '1.90 ',
'P' => '-1.60 ',
'Q' => '-3.50 ',
'S' => '-0.80 ',
'T' => '-0.70 ',
'V' => '4.20 ',
'W' => '-0.90 ',
'Y' => '-130 ',

);
if (exists $scale{$codon}) {
return $scale{$codon};
} else {
    print STDERR "bad amino acid ";
    exit;
}

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}\n}\nexit;
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