

```

class ProteinParam :
# These tables are for calculating:
#   molecular weight (aa2mw), along with the mol. weight of H2O (mwH20)
#   absorbance at 280 nm (aa2abs280)
#   pKa of positively charged Amino Acids (aa2chargePos)
#   pKa of negatively charged Amino acids (aa2chargeNeg)
#   and the constants aaNterm and aaCterm for pKa of the respective termini
# Feel free to move these to appropriate methods as you like

# As written, these are accessed as class attributes, for example:
# ProteinParam.aa2mw['A'] or ProteinParam.mwH20

aa2mw = {
    'A': 89.093, 'G': 75.067, 'M': 149.211, 'S': 105.093, 'C': 121.158,
    'H': 155.155, 'N': 132.118, 'T': 119.119, 'D': 133.103, 'I': 131.173,
    'P': 115.131, 'V': 117.146, 'E': 147.129, 'K': 146.188, 'Q': 146.145,
    'W': 204.225, 'F': 165.189, 'L': 131.173, 'R': 174.201, 'Y': 181.189
}

mwH2O = 18.015
aa2abs280= {'Y':1490, 'W': 5500, 'C': 125}

aa2chargePos = {'K': 10.5, 'R':12.4, 'H':6}
aa2chargeNeg = {'D': 3.86, 'E': 4.25, 'C': 8.33, 'Y': 10}
aaNterm = 9.69
aaCterm = 2.34

def __init__ (self, protein):
    protein=protein.upper()
    self.protein=''.join([aa for aa in protein if aa in ProteinParam.aa2mw])
    #protein will convert to uppercase
    self.proteinDict={aa: self.protein.count(aa) for aa in ProteinParam.aa2mw}
    #cleans the input string to include only valid amino acids and stores a
    count dictionary of each of them
    pass

def aaCount (self):
    #return the total number of valid amino acids in the input sequence
    return sum(self.proteinDict.values())
    pass

def pI (self):
    #search for pH value with a net charge of approximately 0 using binary
    search and using it to calculate the isoelectric point rounded to two decimal
    places
    low=0.0
    high=14.0
    while (high-low)>0.01:
        mid=(high+low)/2
        if self._charge_(mid)>0:
            low=mid
        else:
            high=mid
    return round((high+low)/2,2)
    pass

def aaComposition (self) :
    #Return the composition that we already calculated in init
    return self.proteinDict

```

```

    pass

def _charge_(self, pH):
    #return the net charge of the protein at a specific pH
    #calculates it by using the pKa values of charged amino acids and terminal
groups
    pos_charge=0.0
    neg_charge=0.0
    for aa, pKa in self.aa2chargePos.items():
        pos_charge+=self.proteinDict[aa]*(10**pKa)/(10**pKa+10**pH)
    for aa, pKa in self.aa2chargeNeg.items():
        neg_charge+=self.proteinDict[aa]*(10**pH)/(10**pKa+10**pH)
    #add terminal charges
    pos_charge+=(10**self.aaNterm)/(10**self.aaNterm+10**pH)
    neg_charge+=(10**pH)/(10**self.aaCterm+10**pH)
    return pos_charge-neg_charge
    pass

def molarExtinction (self, cystine=True):
    #calculate and return the molar extinction coefficient using Y, W, and C if
cystine is true
    extinction=self.proteinDict['Y']*self.aa2abs280['Y']+\
                self.proteinDict['W']*self.aa2abs280['W']
    if cystine:
        extinction+=self.proteinDict['C']*self.aa2abs280['C']
    return extinction
    pass

def massExtinction (self):
    #return the mass extinction coefficient which is molar extinction divided
by molecular Weight, and returns 0.0 if the molecular weight is 0
    myMW = self.molecularWeight()
    return self.molarExtinction() / myMW if myMW else 0.0

def molecularWeight (self):
    #return the total molecular weight of the sequence and accounts for water
loss
    total_mass=sum(self.aa2mw[aa]*count for aa, count in
self.proteinDict.items())
    num_peptide_bonds=self.aaCount()-1
    return total_mass-(num_peptide_bonds*self.mwH2O) if self.aaCount()>0 else
0.0
    pass

# Please do not modify any of the following. This will produce a standard output
that can be parsed

import sys
def main():
    inString = input('protein sequence?')
    while inString :
        myParamMaker = ProteinParam(inString)
        myAANumber = myParamMaker.aaCount()
        print ("Number of Amino Acids: {aaNum}".format(aaNum = myAANumber))
        print ("Molecular Weight: {:.1f}".format(myParamMaker.molecularWeight()))
        print ("molar Extinction coefficient:
{:.2f}".format(myParamMaker.molarExtinction()))
        print ("mass Extinction coefficient:
{:.2f}".format(myParamMaker.massExtinction()))

```

```

print ("Theoretical pI: {:.2f}".format(myParamMaker.pI()))
print ("Amino acid composition:")

if myAAnumber == 0 : myAAnumber = 1 # handles the case where no AA are
present

for aa,n in sorted(myParamMaker.aaComposition().items(),
key= lambda item:item[0]):
    print ("\t{} = {:.2%}".format(aa, n/myAAnumber))

inString = input('protein sequence?')

if __name__ == "__main__":
    main()

class NucParams:
    rnaCodonTable = {
        # RNA codon table
        # U
        'UUU': 'F', 'UCU': 'S', 'UAU': 'Y', 'UGU': 'C', # UXU
        'UUC': 'F', 'UCC': 'S', 'UAC': 'Y', 'UGC': 'C', # UXC
        'UUA': 'L', 'UCA': 'S', 'UAA': '-', 'UGA': '-', # UXA
        'UUG': 'L', 'UCG': 'S', 'UAG': '-', 'UGG': 'W', # UXG
        # C
        'CUU': 'L', 'CCU': 'P', 'CAU': 'H', 'CGU': 'R', # CXU
        'CUC': 'L', 'CCC': 'P', 'CAC': 'H', 'CGC': 'R', # CXC
        'CUA': 'L', 'CCA': 'P', 'CAA': 'Q', 'CGA': 'R', # CXA
        'CUG': 'L', 'CCG': 'P', 'CAG': 'Q', 'CGG': 'R', # CXG
        # A
        'AUU': 'I', 'ACU': 'T', 'AAU': 'N', 'AGU': 'S', # AxU
        'AUC': 'I', 'ACC': 'T', 'AAC': 'N', 'AGC': 'S', # AxC
        'AUA': 'I', 'ACA': 'T', 'AAA': 'K', 'AGA': 'R', # AXA
        'AUG': 'M', 'ACG': 'T', 'AAG': 'K', 'AGG': 'R', # AXG
        # G
        'GUU': 'V', 'GCU': 'A', 'GAU': 'D', 'GGU': 'G', # GxU
        'GUC': 'V', 'GCC': 'A', 'GAC': 'D', 'GGC': 'G', # GxC
        'GUA': 'V', 'GCA': 'A', 'GAA': 'E', 'GGA': 'G', # GxA
        'GUG': 'V', 'GCG': 'A', 'GAG': 'E', 'GGG': 'G' # GxG
    }
    dnaCodonTable = {key.replace('U', 'T'):value for key, value in
rnaCodonTable.items()}

    def __init__(self, inString=''):
        self.nucComp={}
        self.codonComp={}
        self.aaComp={}
        if inString: #if string is given, call addSequence method
            inString=inString.upper().strip() #removes white space and capitalizes
all input
            self.addSequence(inString)
            pass

    def addSequence (self, inSeq):
        nucString=''.join(inSeq.upper().split()) #removes white spaces and
capitalizes all input
        rnaString=nucString.replace('T', 'U') #replaces all 'T' with 'U' for RNA
string

```

```

        for nuc in nucString: #initializes nucleotide counts
            if nuc in 'ACGTU':
                self.nucComp[nuc]=self.nucComp.get(nuc, 0)+1

        #iterating from position 0 to end of rnaString
        for index in range(0, len(rnaString)-2, 3):
            codon=rnaString[index:index+3]

            #sets codon to 3 letter increments
            if 'N' in codon or len(codon)!=3:
                continue
            #codon counts
            self.codonComp[codon]=self.codonComp.get(codon, 0)+1
            #amino acid counts
            aa=self.rnaCodonTable.get(codon, '-')
            self.aaComp[aa]=self.aaComp.get(aa, 0)+1
            pass
        def aaComposition(self):
            return self.aaComp
        def nucComposition(self):
            return self.nucComp
        def codonComposition(self):
            return self.codonComp
        def nucCount(self):
            return sum(self.nucComp.values())

import sys
class FastAreader :
    """
    Define objects to read FastA files.

    instantiation:
    thisReader = FastAreader ('testTiny.fa')
    usage:
    for head, seq in thisReader.readFasta():
        print (head,seq)
    """

    def __init__ (self, fname=None):
        '''constructor: saves attribute fname '''
        self.fname = fname

    def doOpen (self):
        ''' Handle file opens, allowing STDIN.'''
        if self.fname is None:
            return sys.stdin
        else:
            return open(self.fname)

    def readFasta (self):
        ''' Read an entire FastA record and return the sequence header/sequence'''
        header = ''
        sequence = ''

        with self.doOpen() as fileH:

            header = ''
            sequence = ''

```

```
# skip to first fasta header
line = fileH.readline()
while not line.startswith('>') :
    line = fileH.readline()
header = line[1:].rstrip()

for line in fileH:
    if line.startswith ('>'):
        yield header,sequence
        header = line[1:].rstrip()
        sequence = ''
    else :
        sequence += ''.join(line.rstrip().split()).upper()

yield header,sequence
```