Pfeature Manual

Table of Contents

1.0 Composition

In this section, we have described python functions developed for amino acid composition based feature generation. These modules can be used for feature generation for protein sequences to apply machine learning techniques for further analysis.

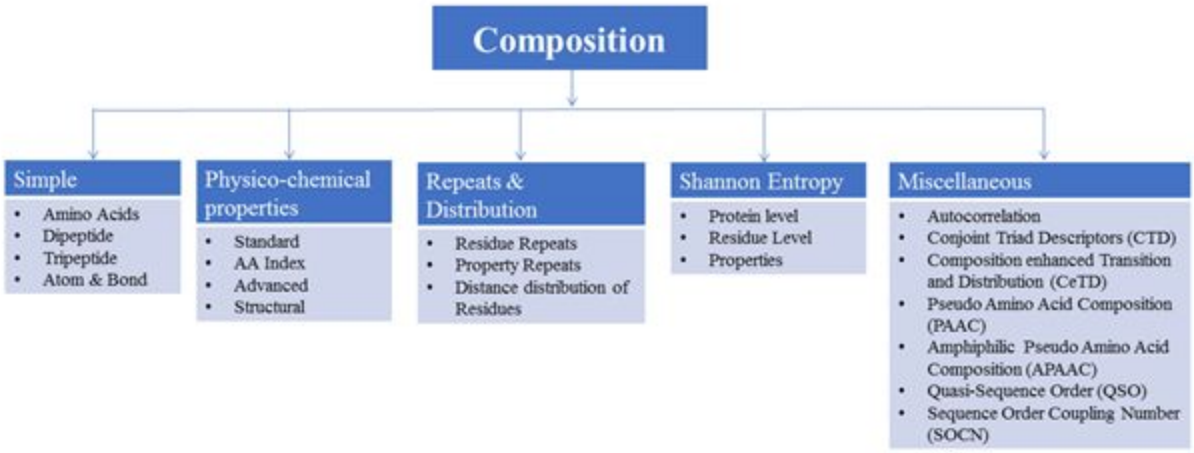


Figure 1: This flowchart shows different menus/submenus for computing different type of composition-based features of protein/peptide composition.

1.1 Simple: This module describes python programs to generate simple composition based feature from a protein. This module is called simple composition as obvious composition has been computed like amino acid composition (20 features), dipeptide composition (400 features) tripeptide composition (8000 features). Pfeature web site provides dynamic web web page to compute these features, our python module have following functions to compute these features.

Function Title	Description
AAC	To calculate Amino acid composition of a peptide
AAC_NT	To calculate Amino acid composition of N-terminal residues defined by user
AAC_CT	To calculate Amino acid composition of C-terminal residues defined by user

AAC_rest	To calculate Amino acid composition of remaining residue from N-Terminal and C-Terminal Residues defined by user
AAC_split	To calculate Amino acid composition by splitting peptide into fragments defined by user
DPC	To calculate Dipeptide composition of a peptide
DPC_NT	To calculate Dipeptide composition of N-terminal residues defined by user
DPC_CT	To calculate Dipeptide composition of C-terminal residues defined by user
DPC_rest	To calculate Dipeptide composition of remaining residue from N-Terminal and C-Terminal Residues defined by user
DPC_split	To calculate Dipeptide composition by splitting a peptide into fragments defined by user
TPC	To calculate Tripeptide composition of a peptide
ATC	To calculate Atomic composition (% of Carbon, Hydrogen, Nitrogen, Oxygen, Sulphur content) of a peptide
ATC_NT	To calculate Atomic composition of N-terminal residues defined by user
ATC_CT	To calculate Atomic composition of C-terminal residues defined by user
ATC_rest	To calculate Atomic composition of remaining residue from N-Terminal and C-Terminal Residues defined by user
ATC_split	To calculate Atomic composition by splitting a peptide into fragments defined by user
BTC	To calculate Bond composition (% of Carbon, Hydrogen, Nitrogen, Oxygen, Sulphur content) of a peptide

BTC_NT	To calculate Bond composition of N-terminal residues defined by user
BTC_CT	To calculate Bond composition of C-terminal residues defined by user
BTC_rest	To calculate Bond composition of remaining residue from N-Terminal and C-Terminal Residues defined by user
BTC_split	To calculate Bond composition by splitting a peptide into fragments defined by user

1.1.1 Amino Acids

Description: This is a simplest feature, which is heavily used in literature for predicting function or structure of a protein. It computes the amino acid composition of each type of residue of a protein sequence. The compositions of all 20 natural amino acids were calculated using the following formula:

$$AAC_i = \frac{R_i}{L} \quad (1)$$

where $\boldsymbol{AAC_i}$ is amino acid composition of residue type $\boldsymbol{i}$; $\boldsymbol{R_i}$ and $\boldsymbol{L}$ number of residues of type $\boldsymbol{i}$ and length of sequence.

In order to compute amino acid composition of different portions of an amino acid sequence, we have developed number of python function (brief description is given below). In web server user may select portion of sequence for calculating protein features.

- **AAC**: Usage: aac_comp(input_filename)
  Description: This function will compute amino acid composition from whole sequence of a protein using Eq. 1.
- **AAC_NT**: Usage: aac_nt (input_filename, n)
  Description: This function computes the amino acid composition of residues selected from N-terminal using Eq.1, user need to provide number of N-terminal residues ***n*** to be used for calculating.
- **AAC_CT**: Usage: aac_ct (input_filename, m)
  Description: This function computes the amino acid composition of residue selected from C-terminal using Eq.1, user need to provide number of C-terminal residues ***m*** to be used for calculating.
- **AAC_REST**: Usage: aac_rest (input_filename, n, m)

Description: This function computes the amino acid composition of remaining residues of a sequence after cleaving ***n*** residues from N-Terminal and ***m*** residues from C-Terminal using Eq.1.

- **AAC_SPLIT:** Usage: aac_split (input_filename, s)
  Description: This function computes the amino acid composition of each portion after splitting sequence in ***s*** portions using Eq.1. This function is important to compute amino acid composition of different portion of a protein.

1.1.2 Dipeptide

Amino acid composition provides only number of different type of residues, no information about order of residues. Dipeptide composition is used to encapsulate the global information about each sequence, which gives a fixed pattern length of 400 (20 X 20). This representation encompassed the information about amino acid composition along local order of amino acid. Traditionally a dipeptide is made of consecutive residues (residue ***i*** and ***i+1***), In 2005, dipeptide of higher order were introduced (**J Biol Chem. 2005; 280:14427-32**). In case of higher order dipeptides, a dipeptide is made of ***i*** and ***i+2*** or ***i+3*** or ***i+4*** etc. instead of consecutive residues (See Figure 1, adapted from **J Biol Chem. 2005; 280:14427-32**).

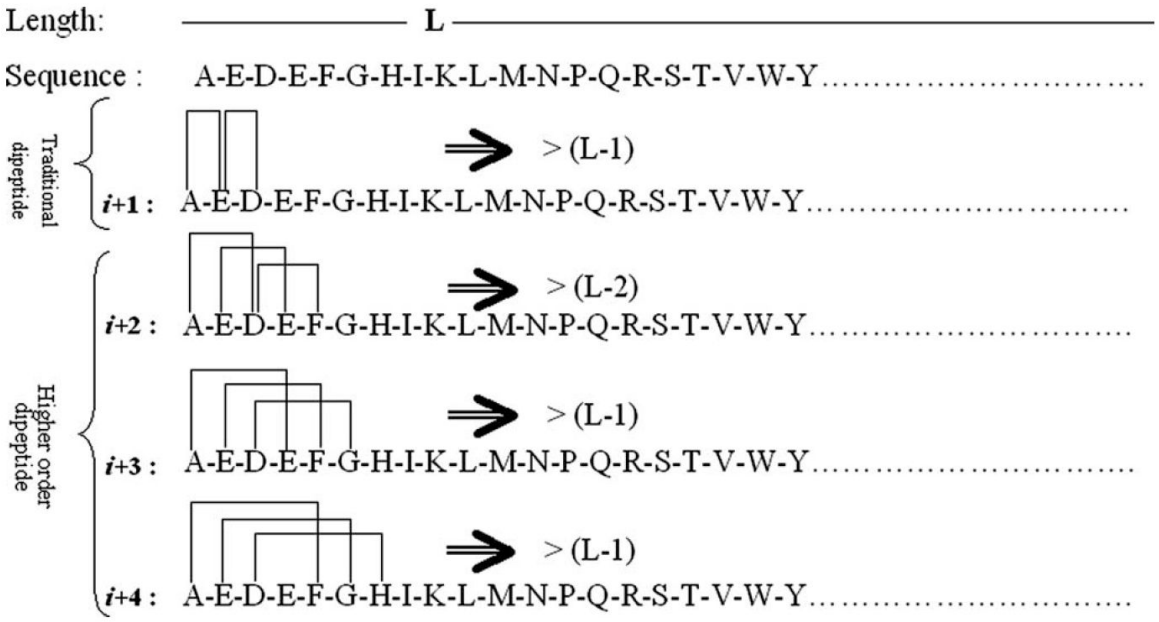


Figure 1: Graphical representation of traditional peptides and higher order dipeptides, figure is adapted from **J Biol Chem. 2005; 280:14427-32.**

In order to compute traditional dipeptide composition from a protein sequence following equation is used

$$DPC_i^j = \frac{D_i^j}{L - j} \quad (2)$$

Where DPC_i^j is the fraction or composition of dipeptide of type ***i*** for jth order. D_i^j and ***L*** are the number of dipeptides of type ***i*** and length of a protein. Here higher order dipeptide D_i^j is made of residue R_i and R_{i+j} where value of ***j*** is 2 or more. In case ***j*** is equal to 1 then dipeptide is called traditional dipeptide.

We have developed number of python functions to compute traditional and higher order dipeptide composition in different portions of an amino acid sequence, we have developed number of python function. In web server user may select portion of sequence for calculating protein features. Following is brief description of these python functions.

- **DPC**: Usage: dpc (input_filename, j):
  Description: This function compute dipeptide in a sequence (input_filename), j is order or dipeptide using Eq. 2.
- **DPC_NT**: Usage: dpc_nt (input_filename, j, n)
  Description: This function computes the dipeptide composition of residues selected from N-terminal using Eq.2, user need to provide order of dipeptide ***j*** and ***n*** number of N-terminal residues.
- **DPC_CT:** Usage: dpc_ct (input_filename, j, m)
  Description: This function computes the dipeptide composition of residues selected from C-terminal using Eq.2, user need to provide order of dipeptide ***j*** and ***m*** number of C-terminal residues.
- **DPC_REST**: Usage: dpc_rest (input_filename, j, n, m)
  Description: This function computes the dipeptide composition of order ***j*** of rest of sequence after removing ***n*** residues from N-Terminal and ***m*** residues from C-Terminal using Eq.2.
- **DPC_SPLIT**: Usage: dpc_split (input_filename, j, s)
  Description: This function computes the dipeptide composition of each portion after splitting sequence in ***s*** portions using Eq.2. This function is important to compute dipeptide composition of order ***j*** of different portion of a protein.

1.1.3 Tripeptide

Three consecutive amino acids form a tripeptide which provide local order in addition to simple composition. Both previous and next residues are used to form a tripeptide. There are total 800 (20*20*20) possible tripeptides from by 20 type of natural residue.

$$TPC_i = \frac{T_i}{L - 2} \quad (3)$$

where TPC_i is tripeptide composition of type i, out of possible 800 tripeptides. T_i and L are number of tripeptides of type i and length of a protein sequence. In order to compute tripeptide composition in a sequence, following functions has been developed.

- **TPC**: Usage: tpc_comp(Input_filename)
  Description: This function computes the tripeptide composition of a sequence using Eq.3.

1.1.4 Atom & Bond

All amino acids are made of atoms and bonds. In this module, we compute different type atom and bond composition. Atomic composition is fraction of Carbon, Hydrogen, Nitrogen, Oxygen and Sulphur atoms present in a protein sequence. For bond composition four types of bonds are considered total number of bonds (including aromatic), hydrogen bond, single bond and double bond. The number of values for each kind of bond is provided as bonds.csv file.

$$ATC_i = \frac{A_i}{N} \tag{4}$$

$$BTCi = \frac{Bi}{N} \tag{5}$$

where ATC_i is atomic composition of type i, A_i and N are number of atoms of type i and number of atoms in a protein. Where BTC_i is atomic composition of type i, B_i and N are number of atoms of type i and number of atoms in a protein.In order to compute atomic composition in a sequence, following functions has been developed.

Atomic Composition	Bond Composition
Carbon Atom	Total Bonds
Hydrogen Atom	Hydrogen Bond
Nitrogen Atom	Single Bond
Oxygen Atom	Double Bond
Sulphur Atom	

Table1: List of Atoms and Bonds included in ATC & BTC Pfeature programs.

- **ATC**: Usage: atc (input_filename)
  Description: This function computes the atomic composition of each amino acid residue of the peptide sequence using Eq.4.

- **ATC_NT:** Usage: atc_nt (input_filename, n)
  Description: This function computes the atomic composition of each amino acid residue selected from N-terminal using Eq. 4, user can give peptide sequence and the value of ***n*** number of N-terminal residues.
- **ATC_CT:** Usage: atc_ct (input_filename, m)
  Description: This function computes the atomic composition of each amino acid residue selected from C- terminal using Eq. 4, user can give peptide sequence and the value of ***m*** number of C-terminal residues.
- **ATC_REST:** Usage: atc_rest (input_filename, n, m)
  Description: This function computes the atomic composition of each amino acid composition of remaining peptide residues cleaved from both N-Terminal and C-Terminal ends using Eq.4, user can give peptide sequence and the value of ***n*** (position from N-Terminal) and ***m*** (position from C-Terminal).
- **ATC_SPLIT:** Usage: atc_split (input_filename, s)
  Description: This function computes the atomic composition of each portion after splitting sequence in ***s*** portions using Eq.4.
- **BTC**: Usage: btc (input_filename)
  Description: This function computes the bond composition of each amino acid residue of the peptide sequence using Eq.5.
- **BTC_NT:** Usage: btc_nt (input_filename, n)
  Description: This function computes the bond composition of each amino acid residue selected from N-terminal using Eq.5, user need to provide number of N-terminal residues ***n*** to be used for calculating.
- **BTC_CT**: Usage: btc_ct (input_filename, m)
  Description: This function computes the bond composition of each amino acid residue selected from C- terminal using Eq.5, user need to provide number of C-terminal residues ***m*** to be used for calculating.
- **BTC_REST:** Usage: btc_rest (input_filename, n, m)
  Description: This function computes the bond composition of each amino acid composition of remaining peptide residues cleaved from both N-Terminal and C-Terminal ends using Eq.5, user can give peptide sequence and the value of ***n*** (position from N-Terminal) and ***m*** (position from C-Terminal).
- **BTC_SPLIT:** Usage: btc_split (input_filename, s)
  Description: This function computes the bond composition of each portion after splitting sequence in ***s*** portions using Eq.5.

Atom & Bond also considered together with the above given operations (NT, CT, REST, SPLIT).

1.2 Physico-Chemical properties

The physico-chemical properties were used to represent a protein. The values of each physico-chemical property for all 20 amino acids were normalized between 0 and 1 using the standard conversion formula. The input vector has scalar values, each representing the average value of a distinct physico-chemical property of protein (**Nucleic Acids Res. 2004; 32:W414-9**).

1.2.1 Standard physico-chemical properties

This function calculates the fraction of each standard physico-chemical property in given sequences. Following properties have been incorporated in Pfeature for calculating compositional features

Table 2: List of physico-chemical properties included in Pfeature for computing features

Positively Charged	Aromaticity	Hydroxylic
Negatively Charged	Acidity	Sulphur Content
Neutral Charge	Basicity	Tiny
Polarity in residues	Neutral (pH)	Small
Non-polarity in residues	Hydrophobicity	Large
Aliphaticity	Hydrophilicity	
Cyclicity	Neutral towards water	

We used following formula to calculate these features

$$PCP_i = \frac{P_i}{L} \tag{6}$$

where $\boldsymbol{PCP_i}$ is physico-chemical properties composition of residue type $\boldsymbol{i}$; $\boldsymbol{P_i}$ and $\boldsymbol{L}$ are sum of property of type $\boldsymbol{i}$ and length of sequence. In order to compute composition of standard properties for different portions of an amino acid sequence, we have developed number of python function (brief description is given below). In web server user may select portion of sequence and type of properties for calculating protein features.

- **PCP**: Usage: pcp_comp(input_filename)
  Description: This function will compute property composition from whole sequence of a protein using Eq. 5.
- **PCP_NT**: Usage: pcp_nt (input_filename, n)
  Description: This function computes the properties composition of residues selected from N-terminal, user need to provide number of N-terminal residues $\boldsymbol{n}$ to be used for calculating.

- **PCP_CT**: Usage: pcp_ct (input_filename, m)
  Description: This function computes the properties composition of residue selected from C-terminal, user need to provide number of C-terminal residues ***m*** to be used for calculating.
- **PCP_REST**: Usage: ppc_rest (input_filename, n, m)
  Description: This function computes the properties composition of remaining residues of a sequence after cleaving ***n*** residues from N-Terminal and ***m*** residues from C-Terminal.
- **PCP_SPLIT:** Usage: pcp_split (input_filename, s)
  Description: This function computes the properties composition of each portion after splitting sequence in ***s*** portions. This function is important to properties composition of different portion of a protein.

1.2.2 Amino Acid index (AAindex)

AAindex is a database of amino acid indices, where AAindex is a set of 20 numerical values representing various physico-chemical and biochemical properties of amino acids. Current version 9.0 of database have total 566 AA indices (https://www.genome.jp/dbget/AAindex/list_of_indices). Pfeature allow user to compute composition of selected AA index via web interface or python function, using following equation

$$AAIC_i = \frac{AAI_i}{L} \tag{7}$$

where $\boldsymbol{AAIC_i}$ is AA index composition of residue type ***i***; $\boldsymbol{AAI_i}$ and ***L*** are sum of AA index value of type ***i*** and length of sequence. In order to compute composition of AA index values for different portions of an amino acid sequence, we have developed number of python function (brief description is given below). In web server user may select portion of sequence and type of properties for calculating protein features.

- **AAIC**: Usage: aaic_comp(input_filename,a)
  Description: This function will compute AA index composition of ***a*** indices from whole sequence of a protein using Eq. 7.
- **AAIC_NT**: Usage: aaic_nt (input_filename, n,a)
  Description: This function computes AA index composition of ***a*** indices from N-terminal, user need to provide number of N-terminal residues ***n*** and list of AA indices ***a*** to be used for calculating.
- **AAIC_CT**: Usage: aaic_ct (input_filename, m,a)
  Description: This function computes AA index composition of ***a*** indices from C-terminal, user need to provide number of C-terminal residues ***m*** and list of AA indices ***a*** to be used for calculating.
- **AAIC_REST**: Usage: aaic_rest (input_filename, n, m,a)

Description: This function computes AA index composition of ***a*** indices of remaining residues of a sequence after cleaving ***n*** residues from N-Terminal and ***m*** residues from C-Terminal.

- **AAIC_SPLIT:** Usage: aaic_split (input_filename, s,a)
  Description: This function computes AA index composition of ***a*** indices of each portion after splitting sequence in ***s*** portions. This function is important to properties composition of different portion of a protein.

1.2.3 Advanced properties

This module allow to compute composition of advanced properties like z1, z2, z3, z4 and z5 of a protein sequence. This "**Advanced**" module is similar to "**Standard**" module of computing physico-chemical properties.

1.2.4 Structural Properties

This module allow to compute composition of advanced properties like secondary structure and surface accessibility of a protein sequence. This "**Structural**" module is similar to "**Standard**" module of computing physico-chemical properties.

1.3 Repeats & Distribution

Most of composition modules describes above measures fraction of particular type of residue or residue property. One of the problem with existing features is that they do not measure repeat of particular type of residue or distribution. In this study, we introduced new features, which compute repeats of amino acids and distribution of amino acids.

Function Title	Description
RRI	To compute Repetitive Residue Information of amino acid of protein sequences.
RRI_NT	To compute Repetitive Residue Information of N-terminal residues defined by user.
RRI_CT	To compute Repetitive Residue Information of C-terminal residues defined by user.
RRI_rest	To compute Repetitive Residue Information of remaining residue from N-Terminal and C-Terminal residues of defined by user

RRI_split	To compute Repetitive Residue Information of amino acid by splitting peptide into fragments defined by user
DDOR	To compute Distance Distribution of residue (DDOR) of protein sequences.

1.3.1 Residue Repeats

This function calculates the Repetitive Residue Information (RRI) for a peptide/protein sequence. RRI measures number of continuous runs of a residue type in a sequence, it can be calculated using following formula.

$$RRI_i = \frac{\sum_{j=1}^{N} (R_j)^2}{\sum_{j=1}^{N} R_j} \tag{8}$$

where $\boldsymbol{RRI_i}$ **,** $\boldsymbol{N}$ and $\boldsymbol{R_j}$ are residue repeat information, maximum number of occurance and number of runs/repeats in occurrence $\boldsymbol{j}$ respectively for residue type $\boldsymbol{i}$.

Example: If a residue is a residue type occurs once at time then value of RRI will be one. For example amino acid alanine ***A*** occurs four times in following sequence "G**A**R**A**GRG**A**RDE**A**RT**A**G"; each time single run. It means ***N*** will be 5, RRI for A can be calculated using following formula

$$RRI_A = \frac{(1)^2+(1)^2+(1)^2+(1)^2+(1)^2}{1+1+1+1+1} = \frac{5}{5} = 1$$

In following sequence "G**AA**RGRG**AAA**RDERTG" amino acid ***A*** occurs two times, first time two runs and second time three runs. It means $\boldsymbol{N=2, R_1=2}$ and $\boldsymbol{R_2=3}$, ***RRI*** for ***A*** can be calculated using following equation

$$RRI_A = \frac{(2)^2+(3)^2}{2+3} = \frac{4+9}{5} = 2.6$$

In following sequence "GRGRGAA**AAA**RDERTG" amino acid ***A*** occurs once with 5 runs. It means $\boldsymbol{N=1,}$ and $\boldsymbol{R_1=5;}$ ***RRI*** for ***A*** can be calculated using following equation

$$RRI_A = \frac{(5)^2}{5} = \frac{25}{5} = 5$$

This means for a given residue type, minimum RRI will be 1 and maximum will be total number of that type of residues in sequence. This value measures multiple runs of a residue in a sequence.

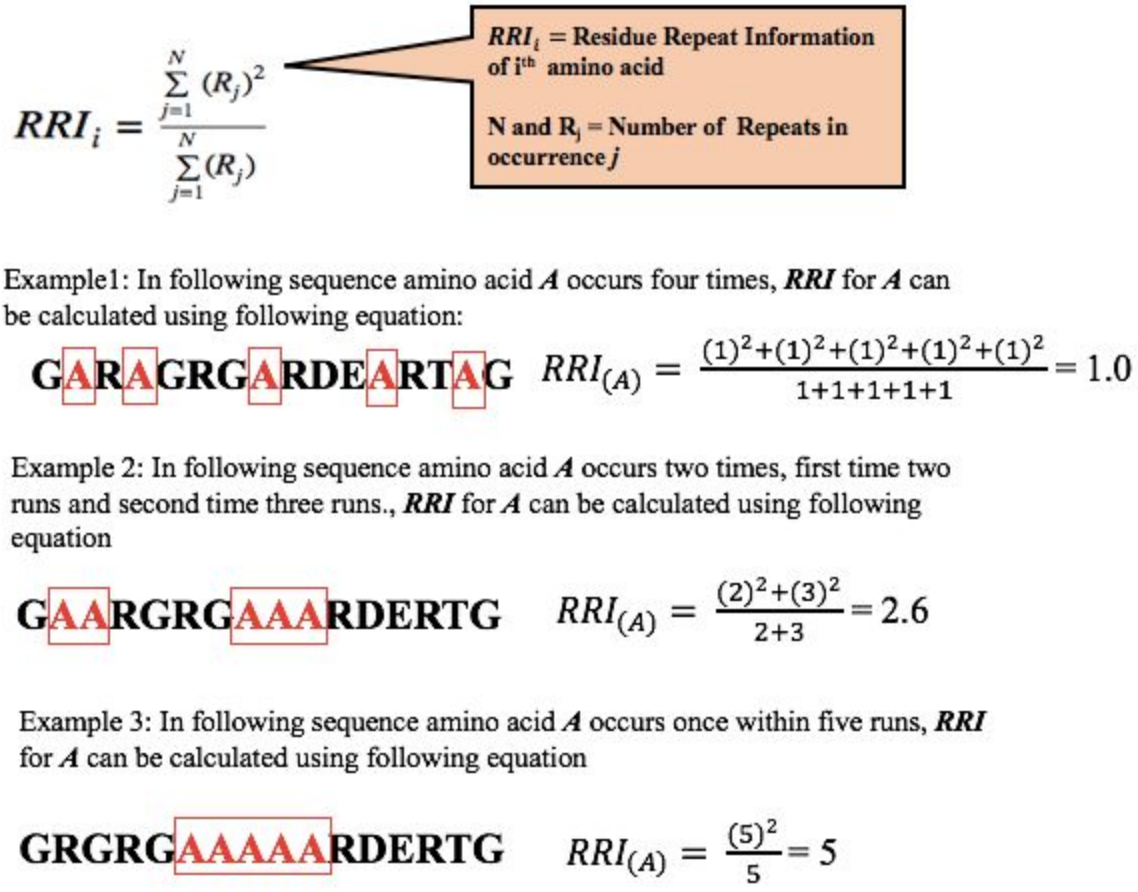


Figure 2: Calculation of Repetitive Residue Information (RRI) for a peptide/protein sequence.

In order to compute repetitive residue information of different portions of an amino acid sequence, we have developed number of python function (brief description is given below). In web server user may select portion of sequence for calculating protein features.

- **RRI**: Usage: rri (input_filename)
  Description: This function will compute repetitive residue information from whole sequence of a protein using Eq. 8.
- **RRI_NT**: Usage: rri_nt (input_filename, n)
  Description: This function computes the repetitive residue information of residues selected from N-terminal using Eq.8, user need to provide number of N-terminal residues ***n*** to be used for calculating.
- **RRI_CT**: Usage: rri_ct (input_filename, m)

Description: This function computes the repetitive residue information of residue selected from C-terminal using Eq.8, user need to provide number of C-terminal residues ***m*** to be used for calculating.

- **RRI_REST**: Usage: rri_rest (input_filename, n, m)
  Description: This function computes the repetitive residue information of remaining residues of a sequence after cleaving ***n*** residues from N-Terminal and ***m*** residues from C-Terminal using Eq.1.
- **RRI_SPLIT:** Usage: rri_split (input_filename, s)
  Description: This function computes the amino acid composition of each portion after splitting sequence in ***s*** portions using Eq.8. This function is important to compute amino acid composition of different portion of a protein.

1.3.2 Property Repeats

This function calculates property repeat information (PRI) which gives the information of repetitiveness of each physicochemical property within a peptide/ protein sequence.

$$PRI_i = \frac{\sum_{j=1}^{N} (P_j)^2}{\sum_{j=1}^{N} P_j} \tag{9}$$

where $\boldsymbol{PRI_i}$ **,** $\boldsymbol{N}$ and $\boldsymbol{P_j}$ are property repeat information, maximum number of occurance and number of runs/repeats in occurrence ***j*** respectively for property type ***i***.

1.3.3 Distance distribution of Residues

This function distance distribution of residues (DDOR) computes the distribution of residue on the basis of distance from N-terminal, C-terminal and inter-distances between same residue within the given peptide/protein sequence.

$$DDOR_i = \frac{(R_{NT})^2 + \sum_{j=1}^{N} (R_j)^2 + (R_{CT})^2}{(L - F_i) + 1} \tag{10}$$

where, $\boldsymbol{DDOR_i}$ is distance distribution of residue type ***i,*** ***N*** is total number of inter-residue distances for type ***i.***

R_{NT} = Residue distance from N-terminal

R_j = Inter-distance between residue type ***i***

R_{CT} = Residue distance from C-terminal

L = Total length of protein sequence

F_i = Frequency of residue type ***i***

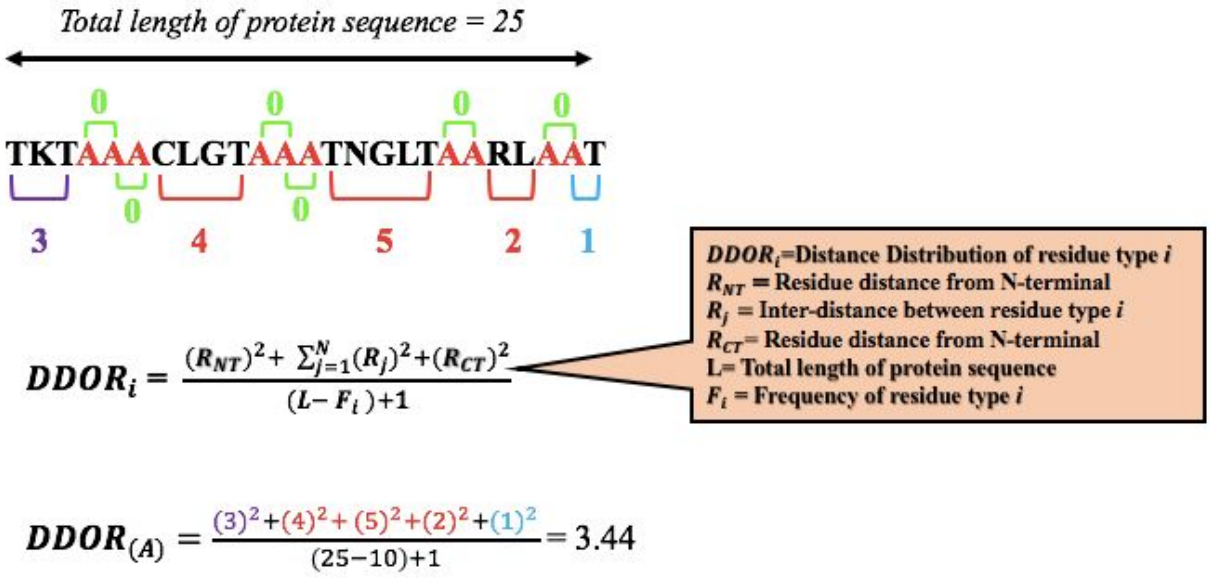


Figure 3: Calculation of Distance Distribution of Residue (DDOR) for peptide/protein sequence.

1.4 Shannon Entropy

1.4.1 Protein Level

Shannon entropy for a protein/peptide sequence can be computed by the standard expression:

$$H(X) = -\sum_{i=1}^{20} p_i \log_2 p_i \qquad (11)$$

Where i is the amino acid in the sequence (i=A, C, D, … ,Y) and X is any protein/peptide sequence. See figure below for more details.

Function Title	Description
SE	To compute Shannon Entropy of protein/ peptide sequences.
SE_NT	To compute Shannon Entropy of N-terminal residues defined by user.
SE_CT	To compute Shannon Entropy of C-terminal residues defined by user.
SE_REST	To compute Shannon Entropy of remaining residue from N-Terminal and C-Terminal residues as defined by user.
SE_SPLIT	To compute Shannon Entropy of sub-sequences by splitting protein/ peptide into fragments as defined by user.

- **SE:** Usage: SE (input_filename)
  Description: This function computes the shannon entropy of a protein sequence. Shannon entropy of all sequences were calculated using the Eq. 11
- **SE_NT:** Usage: SE_NT (input_filename, n)
  Description: This function computes the shannon entropy of the N-terminal of a protein sequence, where n is number of N-terminal residues.
- **SE_CT:** Usage: SE_CT (input_filename, m)
  Description: This function computes the shannon entropy of the C-terminal of a protein sequence, m is number of C-terminal terminal residues.
- **SE_REST:** Usage: SE_REST (input_filename, n, m)
  Description: This function computes the shannon entropy of a protein sequence by removing the n and m residues from N- and C-terminal respectively.
- **SE_SPLIT:** Usage: SE_SPLIT(input_filename, s)
  Description: This function computes the shannon entropy of the subsequences of a protein sequence after splitting sequence in s segments.

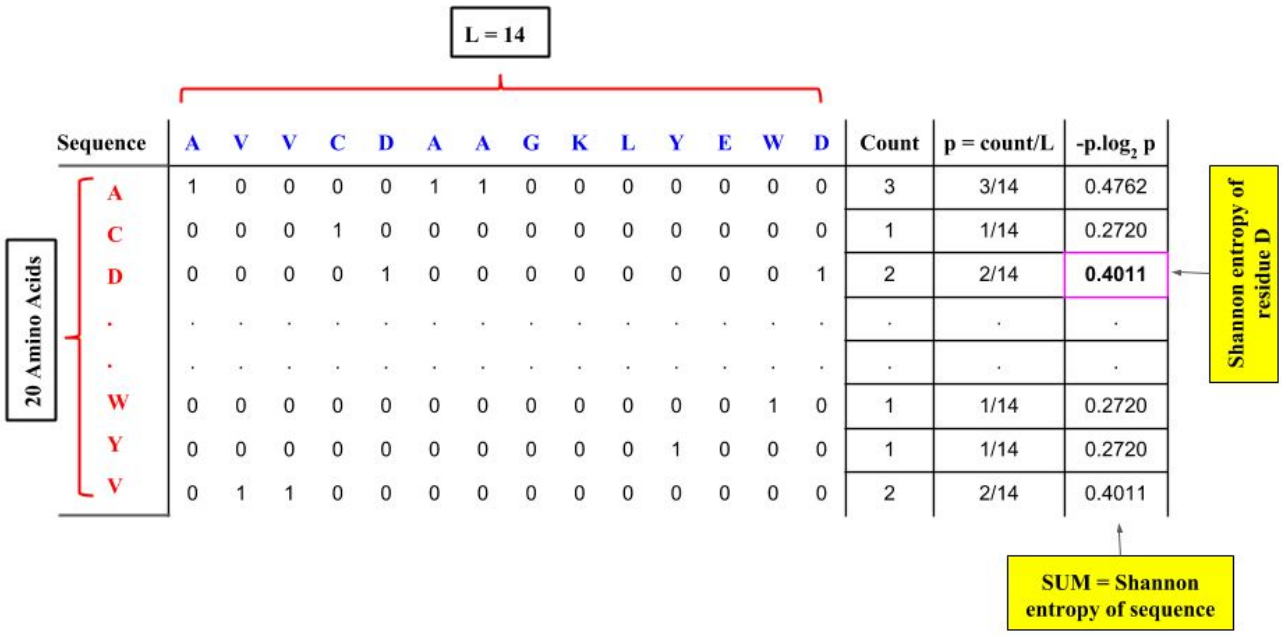


Figure 5 : Calculation of shannon entropy for a protein/ peptide sequence or sub-sequence at protein and residue levels.

1.4.2 Residue Level

- **SER:** Usage: SER (input_filename)
  Description: This function computes the shannon entropy of the residues of the peptide/ protein sequence. Here, user can input a list of sequences for which shannon entropy for every residue can be computed separately for each sequence.
  Shannon entropy of all sequences were calculated using the following formula:

$$H(X) = - p_i \log_2 p_i \qquad (12)$$

  In the above shannon entropy equation, p_i is the probability of a given amino acid in the sequence. [NOTE: Replace all residues except under investigation to zero and calculate entropy iteratively for each of them.]

Function Title	Description
SER	To compute Shannon Entropy of all amino acids of protein/ peptide sequences.

SER_NT	To compute Shannon Entropy of all amino acids of N-terminal residues defined by user.
SER_CT	To compute Shannon Entropy of all amino acids of C-terminal residues defined by user.
SER_REST	To compute Shannon Entropy of all amino acids of remaining residue from N-Terminal and C-Terminal residues as defined by user.
SER_SPLIT	To compute Shannon Entropy of all amino acids of sub-sequences by splitting protein/ peptide into fragments as defined by user.

- **SER_NT:** Usage: SER_NT (input_filename, n)
  Description: This function computes the shannon entropy of the residues of the N-terminal of the peptide/ protein sequence. Here, user can input a list of sequences and N-terminal length for which shannon entropy of the residues can be computed separately.

- **SER_CT:** Usage: SER_CT (input_filename, m)
  Description: This function computes the shannon entropy of the residues of the C-terminal of the peptide/ protein sequence. Here, user can input a list of sequences and C-terminal length for which shannon entropy of the residues can be computed separately.

- **SER_REST:** Usage: SER_REST (input_filename, n, m)
  Description: This function computes the shannon entropy of the residues of peptide/ protein sequence by removing the N- and C-terminal of the sequence. Here, input to the function is the file having all the sequences and the size of N-terminal and C-terminal.

- **SER_SPLIT:** Usage: SER_SPLIT(input_filename, s)
  Description: This function computes the shannon entropy of the residues of subsequences of peptide/ protein sequence. Here, input to the function is the file having all the sequences and the number of splits. The output of the function is shannon entropy for residues corresponding to every split.

1.4.3 **Properties**

This function calculates the Shannon Entropy of a particular Physicochemical property in a sequence. Let the sequence be of length 'l' and has r_i instances of a property present in the

sequence, then the Shannon Entropy $H_i(x)$ of a particular physicochemical property is calculated using the following formula:

$$H_i = -p_i \log(p_i) - (1 - p_i)\log(1 - pi) \quad (13)$$

where p_i is r_i/l

Function Title	Description
SHANNON_all	To compute the Shannon Entropy of an entire protein/ peptide sequence for a physicochemical property defined by user.
SHANNON_NT	To compute the Shannon Entropy of N-terminal residues of protein/ peptide sequence for a physicochemical property defined by user.
SHANNON_CT	To compute the Shannon Entropy of C-terminal residues of protein/ peptide sequence for a physicochemical property defined by user.
SHANNON_REST	To compute Shannon Entropy of remaining residue from N-Terminal and C-Terminal residues of protein/ peptide sequence for a physicochemical property defined by user.
SHANNON_SPLIT	To compute Shannon Entropy of sub-sequences by splitting protein/ peptide into fragments for a physicochemical property as defined by user.

- **SHANNON_all**: Usage: shannon_all(input_filename,featureNum)
  Description: This function gives the Shannon Entropy of an entire sequence for a physicochemical property represented by a number. The user can input the file having all the sequences and a feature number for which the entropy needs to be calculated.

- **SHANNON_NT:** Usage: shannon_NT(input_filename, featureNum, n)
  Description: This function calculates Shannon Entropy of a physicochemical property of a residues from N terminal. User can input the file containing these sequences, featureNumber and the number of n terminal residues.

- **SHANNON_CT:** Usage: shannon_CT(input_filename, featureNum, n)

Description: This function calculates Shannon Entropy of a physicochemical property of a residues from C terminal. User can input the file containing these sequences, featureNumber and the number of C terminal residues.

- **SHANNON_REST:** Usage: shannon_rest(input_filename, featureNum, m,n)
  Description: This function calculates Shannon Entropy of a physicochemical property by removing 'm' N-terminal residues and 'n' C-terminal residues. User can input the file containing these sequences, featureNumber, number of N terminal residues and number of C terminal residues.

- **SHANNON_SPLIT:** Usage: shannon_split(input_filename, featureNum, SPLIT)
  Description: This function calculates the Shannon Entropy of a physicochemical property by splitting the entire sequence into SPLIT parts and then doing the calculation iteratively over each split part. The user can input a file containing the sequences, desired physicochemical property and number of splits to be made in each sequence.

1.5 **Miscellaneous**

Function Title	**Description**
Autocorr	To compute all three autocorrelation descriptors for the protein/ peptide sequences for the AAindex accession numbers given in 'aaindex_file', at a specific value of d given in 'dval' defined by the user.
Autocorr_NT	To compute all three autocorrelation descriptors for the protein/ peptide sequences for the AAindex accession numbers given in 'aaindex_file', at a specific value of d given in 'dval' of N-terminal residues defined by user.
Autocorr_CT	To compute all three autocorrelation descriptors for the protein/ peptide sequences for the AAindex accession numbers given in 'aaindex_file', at a specific value of d given in 'dval' of C-terminal residues defined by user.

Autocorr_REST	To compute all three autocorrelation descriptors for the protein/ peptide sequences for the AAindex accession numbers given in 'aaindex_file', at a specific value of d given in 'dval' as defined by user.
Autocorr_SPLIT	To compute all three autocorrelation descriptors for the protein/ peptide sequences for the AAindex accession numbers given in 'aaindex_file', at a specific value of d given in 'dval' of sub-sequences by splitting protein/ peptide into fragments as defined by user.
CTC	The Conjoint Triad Calculation of the Descriptors of protein/ peptide sequences.
CTC_NT	The Conjoint Triad Calculation of the Descriptors of N-terminal residues defined by user.
CTC_CT	The Conjoint Triad Calculation of the Descriptors of C-terminal residues defined by user.
CTC_REST	The Conjoint Triad Calculation of the Descriptors of remaining residue from N-Terminal and C-Terminal residues as defined by user.
CTC_SPLIT	The Conjoint Triad Calculation of the Descriptors of sub-sequences by splitting protein/ peptide into fragments as defined by user.
CeTD	To compute Composition enhanced Transition Distribution of a peptide
CeTD_NT	To compute Composition enhanced Transition Distribution of N-terminal residues defined by user
CeTD_CT	To compute Composition enhanced Transition Distribution of C-terminal residues defined by user
CeTD_rest	To compute Composition enhanced Transition Distribution of remaining residue from N-Terminal and C-Terminal Residues defined by user

CeTD_split	To compute Composition enhanced Transition Distribution by splitting peptide into fragments defined by user
PAAC	To compute Pseudo Amino acid composition of a peptide
PAAC_NT	To compute Pseudo Amino acid composition of N-terminal residues defined by user
PAAC_CT	To compute Pseudo Amino acid composition of C-terminal residues defined by user
PAAC_rest	To compute Pseudo Amino acid composition of remaining residue from N-Terminal and C-Terminal Residues defined by user
PAAC_split	To compute Pseudo Amino acid composition by splitting a peptide into fragments defined by user
APAAC	To compute Amphiphilic pseudo amino acid composition of a peptide
APAAC_NT	To compute Amphiphilic pseudo amino acid composition of N-terminal residues defined by user
APAAC_CT	To compute Amphiphilic pseudo amino acid composition of C-terminal residues defined by user
APAAC_rest	To compute Amphiphilic pseudo amino acid composition of remaining residue from N-Terminal and C-Terminal Residues defined by user
APAAC_split	To compute Amphiphilic pseudo amino acid composition by splitting a peptide into fragments defined by user
QSO	To compute Quasi-Sequence Order of a peptide
QSO_NT	To compute Quasi-Sequence Order of N-terminal residues defined by user
QSO_CT	To compute Quasi-Sequence Order of C-terminal residues defined by user

QSO_rest	To compute Quasi-Sequence Order of remaining residue from N-Terminal and C-Terminal Residues defined by user
QSO_split	To compute Quasi-Sequence Order by splitting a peptide into fragments defined by user
SOCN	To compute Sequence Order Coupling Number of a peptide
SOCN_NT	To compute Sequence Order Coupling Number of N-terminal residues defined by user
SOCN_CT	To compute Sequence Order Coupling Number of C-terminal residues defined by user
SOCN_rest	To compute Sequence Order Coupling Number of remaining residue from N-Terminal and C-Terminal Residues defined by user
SOCN_split	To compute Sequence Order Coupling Number by splitting a peptide into fragments defined by user

1.5.1 **Autocorrelation**

Autocorrelation descriptors are defined based on the distribution of amino acid properties along the sequence. The amino acid properties used here are various types of amino acid indices (http://www.genome.ad.jp/dbget/aaindex.html). Three type of autocorrelation descriptors are used here viz. Normalized Moreau-Broto, Moran and Geary autocorrelation descriptors as implemented in (**Dong, Jie, et al. *Journal of cheminformatics* 10.1 (2018): 16.**)

The python functions for calculation of these descriptors are described below:

- **Autocorr:** usage: autocorr_aa(seq_file, aaindex_file, dval)
  Description: This function computes all three autocorrelation descriptors for the sequences given in 'seq_file' for the AAindex accession numbers given in 'aaindex_file', at a specific value of d given in 'dval'.
- **Autocorr_NT:** usage: autocorr_aa_n(seq_file, aaindex_file, dval, n)
  Description: This function computes all three autocorrelation descriptors for the N-terminal of sequences given in 'seq_file' for the AAindex accession numbers given in 'aaindex_file', at a specific value of d given in 'dval'. User has to mention length of N-terminal in 'n'.
- **Autocorr_CT:** usage: autocorr_aa_c(seq_file, aaindex_file, dval, m)
  Description: This function computes all three autocorrelation descriptors for the C-terminal of sequences given in 'seq_file' for the AAindex accession numbers given in

'aaindex_file', at a specific value of d given in 'dval'. User has to mention length of C-terminal in 'm'.

- **Autocorr_REST:** usage: autocorr_aa_rest(seq_file, aaindex_file, dval, n, m)
  Description: This function computes all three autocorrelation descriptors for the remainder of sequences given in 'seq_file' when N-terminal and C-terminal are not considered, for the AAindex accession numbers given in 'aaindex_file', at a specific value of d given in 'dval'. User has to mention length of both N-terminal and C-terminal in 'n' and 'm' variables respectively.
- **Autocorr_SPLIT:** usage: autocorr_aa_split(seq_file, aaindex_file, dval, s)
  Description: This function computes all three autocorrelation descriptors for the split parts of the sequences given in 'seq_file' for the AAindex accession numbers given in 'aaindex_file', at a specific value of d given in 'dval'. User has to mention number of split parts in 's'.

  Conditions: dval<=min(L-1, 30) where L is the length of the sequence/ sub-sequence for which autocorrelation descriptors have to be calculated. Seq_file should be a new-line separated .csv file. aaindex_file should be a comma separated .csv file.

1.5.2 Conjoint Triad Descriptors (CTD)

Conjoint triad descriptors are proposed by J.W. Shen et.al. These descriptors explains the features of protein pairs based on the classification of amino acids. The 20 amino acids were clustered into several classes according to their dipoles and volumes of the side chains in the following manner (**Dong, Jie, et al. *Journal of cheminformatics* 10.1 (2018): 16.**):-

Group 1: A, G, V
Group 2: I, L, F, P
Group 3: Y, M, T, S
Group 4: H, N, Q, W
Group 5: R, K
Group 6: D, E
Group 7: C

The conjoint triad descriptors considers the property of amino acid along with its adjacent amino acids as one single unit of three amino acids. Triad of three amino acids belonging to same group are identical in nature, such as RCE and KCD are identical in nature. Protein sequence can be represented as a binary space (V, F) where, V is the vector space of the sequence features, and each feature v_i represents a triad type; F is the frequency vector corresponding to V, and f_i is the frequency of type v_i appearing in the protein sequence. For the amino acids that have been catalogued into seven classes, the size of V should be 7×7×7; thus i = 1,2, ..., 343. Long protein

would have a large value of f_i as compared to small sequences thus creating problem while comparing two heterogeneous proteins. Thus, we will normalize f_i in following manner:-

$$f\_norm_i = (f_i - \min(f_1, f_2, f_3 \ldots\ldots f_{343})) / \max(f_1, f_2, f_3 \ldots\ldots f_{343})$$

The python functions for conjoint triad calculation of these descriptors are described below:

- **CTC whole sequence:** CTC(input_filename)
  Description: This function computes the descriptor value f_i corresponding to each triad group as explained above(Group 1, 2....343 ----111, 112….777) in the protein sequence.

- **CTC_NT:** CTC_NT(input_filename, n)
  Description: This function computes the descriptor value f_i corresponding to each triad group as explained above(Group 1, 2....343 ----111, 112….777) in the N-terminal of the protein sequence. N-terminal value has to be submitted by the user.

- **CTC_CT:** CTC_CT(input_filename, m)
  Description: This function computes the descriptor value f_i corresponding to each triad group as explained above(Group 1, 2....343 ----111, 112….777) in the C-terminal of the protein sequence. C-terminal value has to be submitted by the user.

- **CTC_REST:** CTC_REST(input_filename, n, m)
  Description: This function computes the descriptor value f_i corresponding to each triad group as explained above(Group 1, 2....343 ----111, 112….777) in the remaining sequence after removing N- and C-terminal of the protein sequence. N- and C-terminal values have to be submitted by the user.

- **CTC_SPLIT:** CTC_SPLIT(input_filename, s)
  Description: This function computes the descriptor value f_i corresponding to each triad group as explained above(Group 1, 2....343 ----111, 112….777) in the sub-sequence of the protein sequence. Split value has to be submitted by the user and will generate equivalent sub-sequences from main sequence in continuous manner..

1.5.3 Composition enhanced Transition and Distribution (CeTD): First step is to encode(convert) the peptide/protein sequence on the basis of their group value. All the values are present in aa_aatr_group.csv file. Then occurrence (composition) of each residue within should be calculated using formula:

$$Composition = \frac{Frequency\ of\ same\ Residue * 100}{Length\ of\ peptide\ sequence} \quad (14)$$

attr	1	2	3
hydrophobicity	R,K,E,D,Q,N	G,A,S,T,P,H,Y	C,L,V,I,M,F,W
normalized vander Waals volume	G,A,S,T,P,D	N,V,E,Q,I,L	M,H,K,F,R,Y,W
polarity	L,I,F,W,C,M,V,Y	P,A,T,G,S	H,Q,R,K,N,E,D
polarizability	G,A,S,D,T	C,P,N,V,E,Q,I,L	K,M,H,F,R,Y,W
charge	K,R	A,N,C,Q,G,H,I,L,M,F,P,S,T,W,Y,V	D,E
secondary structure	E,A,L,M,Q,K,R,H	V,I,Y,C,W,F,T	G,N,P,S,D
solvent accessibility	A,L,F,C,G,I,V,W	R,K,Q,E,N,D	M,S P,T,H,Y

There are 9- possibilities that two residues lying next to each other. This is called enhanced transition (E-Transition). 11,12,13,21,22,23,31,32,33 are the 9 possibilities.

Distribution is the measure of presence of particular residue in 5 quartile (0%, 25%, 50%, 75%, 100%) of the peptide sequence.

- **CeTD:** Usage: ctd(input_filename)
  Description: This function will compute the atomic composition of each amino acid residue from whole sequence of a protein using Eq.14
- **CeTD_NT**: Usage: ctd_nt(input_filename, n)
  Description: This function computes the atomic composition of each amino acid residue selected from N-terminal using Eq.14, user need to provide number of N-terminal residues ***n*** to be used for calculating.
- **CeTD_CT**: Usage: ctd_ct(input_filename, m)
  Description: This function computes the atomic composition of each amino acid residue selected from C-terminal using Eq.14, user need to provide number of N-terminal residues ***m*** to be used for calculating.
- **CeTD_REST**: Usage: ctd_rest (input_filename, n, m)
  Description: This function computes the atomic composition of remaining residues of a sequence after cleaving ***n*** residues from N-Terminal and ***m*** residues from C-Terminal using Eq.14.
- **CeTD_SPLIT** : Usage: aac_split (input_filename, s)
  Description: This function computes the atomic composition of each portion after splitting sequence in ***s*** portions using Eq.14. This function is important to compute amino acid composition of different portion of a protein.

1.5.4 Pseudo Amino Acid Composition (PAAC): This group of descriptors has been proposed by K.C. Chou. Let $H_1^o(i)$be hydrophobicity values for i = 1,2,3,.....20, $H_2^o(i)$ be the hydrophilicity values for i = 1,2,3,.....20, and $M^o(i)$ be the side chain masses of the 20 natural amino acids. They are converted to the following quantities by a standard conversion:

$$H_1(i) = \frac{H_1^o(i) - \frac{1}{20}\sum_{i=1}^{20} H_1^o(i)}{\sqrt{\frac{\sum_{i=1}^{20} [H_1^o(i) - \frac{1}{20}\sum_{i=1}^{20} H_1^o(i)]^2}{20}}} \quad (15)$$

Where, $H_2^o(i)$ and $M^o(i)$ are normalized as$H_2(i)$ and $M(i)$ in the same manner.

1.5.5 Amphiphilic Pseudo Amino Acid Composition (APAAC): Amphiphilic Pseudo-Amino Acid Composition (APAAC) is described as:

$$P_c = \frac{f_c}{\sum_{r=1}^{20} f_r + w\sum_{j=1}^{2\lambda} \tau_j} \quad (1 < c < 20) \quad (16(i))$$

$$P_c = \frac{\omega\tau_u}{\sum_{r=1}^{20} f_r + w\sum_{j=1}^{2\lambda} \tau_j} \quad (21 < u < 20+2\lambda) \quad (16(ii))$$

where w is the weighting factor which is set as (w= 0.5),as described in Chou's work (Chou, 2001).

1.5.6 Quasi-Sequence Order (QSO): The quasi-sequence-order descriptors are proposed by K.C. Chou, et.al. Quasi-sequence-order Descriptors obtained from the distance matrix between the 20 amino acids. Schneider-Wrede physicochemical distance matrix (Schneider and Wrede, 1994) and the chemical distance matrix by Grantham (Grantham, 1974) are used by Kuo-Chen Chou.

For each type of amino acid, a quasi-sequence-order descriptor can be described as:

$$X_r = \frac{f_r}{\sum_{r=1}^{20} f_r + w\sum_{d=1}^{nlag} \tau_d} \quad r = 1,2,....20 \quad (17)$$

where *fr* is the normalized occurrence of amino acid type *r,*and *w* is a weighting factor (*w* = 0.1), *nlag* and $\tau_d$is the same which was described above. These are the first 20 quasi-sequence-order descriptors. The other 30 quasi-sequence-order descriptors are defined as:

$$X_d = \frac{w\tau_d - 20}{\sum_{r=1}^{20} f_r + w \sum_{d=1}^{nlag} \tau_d} \quad d = 21,22,....30 + nlag \tag{18}$$

1.5.7 Sequence Order Coupling Number (SOCN): The *d*-th rank sequence-order-coupling number is described as:

$$\tau_d = \sum_{i=1}^{N-d} (d_{i,\, i+d})^2 \quad d = 1,2,3,.....,nlag \tag{19}$$

where *d i,i+d* is the number in a given distance matrix explaining a distance between the two amino acids *i*and *i+d*, nlag is the maximum value of the lag, and N denotes the length of a protein or peptide sequence.

Note: The length of the protein or peptide sequence must be not less than the maximum value of *nlag*.

2.0 Binary Profiles

Figure 2: This flowchart shows different types of protein/peptide Binary profiles based features.

Function Title	Description
AABP	To calculate Amino acid Binary Profile of a peptide
AABP_NT	To calculate Amino acid Binary Profile of N-terminal residues defined by user
AABP_CT	To calculate Amino acid Binary Profile of C-terminal residues defined by user
AABP_rest	To calculate Amino acid Binary Profile of remaining residue from N-Terminal and C-Terminal Residues defined by user
AABP_split	To calculate Amino acid Binary Profile by splitting peptide into fragments defined by user
DPBP	To calculate Dipeptide Binary Profile of a peptide
DPBP_NT	To calculate Dipeptide Binary Profile of N-terminal residues defined by user
DPBP_CT	To calculate Dipeptide Binary Profile of C-terminal residues defined by user
DPBP_rest	To calculate Dipeptide Binary Profile of remaining residue from N-Terminal and C-Terminal Residues defined by user

DPBP_split	To calculate Dipeptide Binary Profile by splitting a peptide into fragments defined by user
ATBP	To calculate Atomic Binary Profile (% of Carbon, Hydrogen, Nitrogen, Oxygen, Sulphur content) of a peptide
ATBP_NT	To calculate Atomic Binary Profile of N-terminal residues defined by user
ATBP_CT	To calculate Atomic Binary Profile of C-terminal residues defined by user
ATBP_rest	To calculate Atomic Binary Profile of remaining residue from N-Terminal and C-Terminal Residues defined by user
ATBP_split	To calculate Atomic Binary Profile by splitting a peptide into fragments defined by user
BTBP	To calculate Bond Binary Profile (% of Carbon, Hydrogen, Nitrogen, Oxygen, Sulphur content) of a peptide
BTBP_NT	To calculate Bond Binary Profile of N-terminal residues defined by user
BTBP_CT	To calculate Bond Binary Profile of C-terminal residues defined by user
BTBP_rest	To calculate Bond Binary Profile of remaining residue from N-Terminal and C-Terminal Residues defined by user
BTBP_split	To calculate Bond Binary Profile by splitting a peptide into fragments defined by user

2.1 Amino Acids

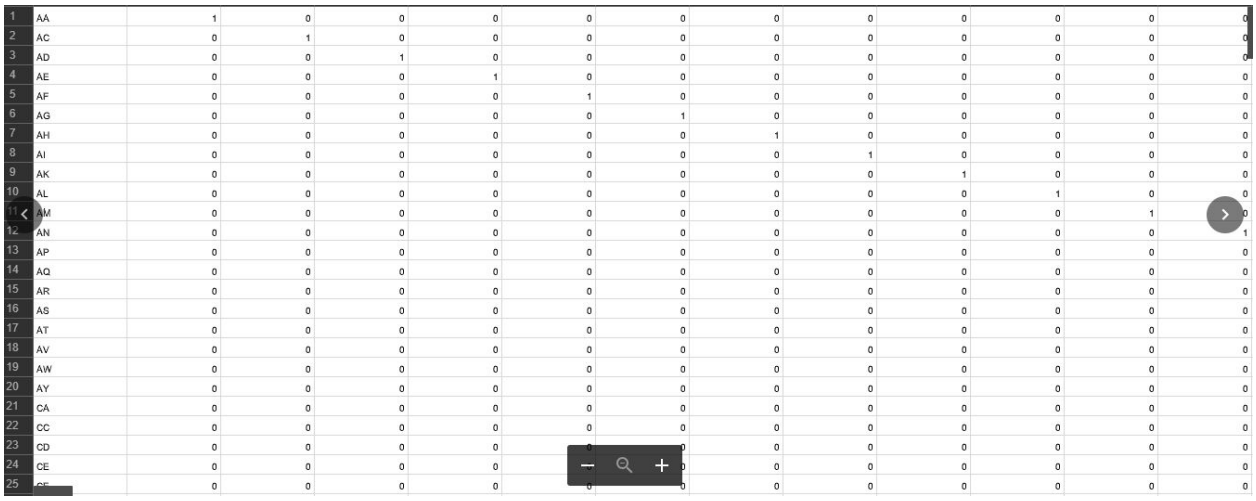
This function generates binary equivalent of each residues. The following table consists of 20-vector binary profile for each residue. Peptide/protein sequences are replaced by their equivalent binary profile.

```
A : 1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
C : 0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
D : 0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
E : 0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
F : 0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
G : 0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0
H : 0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0
I : 0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0
K : 0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0
L : 0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0
M : 0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0
N : 0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0
P : 0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0
Q : 0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0
R : 0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0
S : 0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0
T : 0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0
V : 0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0
W : 0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0
Y : 0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1
X : 0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
```

- **AABP**: Usage: aabp (input_filename)
  Description: This function generates binary profile for residues from whole sequence of a protein.
- **AABP_NT**: Usage: aabp_nt (input_filename, n)
  Description: This function generates binary profile for residues selected from N-terminal, user need to provide number of N-terminal residues ***n*** to be used for calculating.
- **AABP_CT**: Usage: aabp_ct (input_filename, m)
  Description: This function generates binary profile for residues selected from C-terminal, user need to provide number of N-terminal residues ***m*** to be used for calculating.
- **AABP_REST**: Usage: aabp_rest (input_filename, n, m)
  Description: This function generates binary profile of remaining residues of a sequence after cleaving ***n*** residues from N-Terminal and ***m*** residues from C-Terminal.
- **AABP_SPLIT**: Usage: aabp_split (input_filename, s)
  Description: This function generates binary profile of each portion after splitting sequence in ***s*** portions. This function is important to generates binary profile of different portion of a protein.

2.2 Dipeptides

The Dipeptide binary profiles are generated by this function by replacing residues by their equivalent 400-size vector.The snapshot is as below.



1	AA	1	0	0	0	0	0	0	0	0	0	0	0
2	AC	0	1	0	0	0	0	0	0	0	0	0	0
3	AD	0	0	1	0	0	0	0	0	0	0	0	0
4	AE	0	0	0	1	0	0	0	0	0	0	0	0
5	AF	0	0	0	0	1	0	0	0	0	0	0	0
6	AG	0	0	0	0	0	1	0	0	0	0	0	0
7	AH	0	0	0	0	0	0	1	0	0	0	0	0
8	AI	0	0	0	0	0	0	0	1	0	0	0	0
9	AK	0	0	0	0	0	0	0	0	1	0	0	0
10	AL	0	0	0	0	0	0	0	0	0	1	0	0
11	AM	0	0	0	0	0	0	0	0	0	0	1	0
12	AN	0	0	0	0	0	0	0	0	0	0	0	1
13	AP	0	0	0	0	0	0	0	0	0	0	0	0
14	AQ	0	0	0	0	0	0	0	0	0	0	0	0
15	AR	0	0	0	0	0	0	0	0	0	0	0	0
16	AS	0	0	0	0	0	0	0	0	0	0	0	0
17	AT	0	0	0	0	0	0	0	0	0	0	0	0
18	AV	0	0	0	0	0	0	0	0	0	0	0	0
19	AW	0	0	0	0	0	0	0	0	0	0	0	0
20	AY	0	0	0	0	0	0	0	0	0	0	0	0
21	CA	0	0	0	0	0	0	0	0	0	0	0	0
22	CC	0	0	0	0	0	0	0	0	0	0	0	0
23	CD	0	0	0	0	0	0	0	0	0	0	0	0
24	CE	0	0	0	0	0	0	0	0	0	0	0	0
25	CF	0	0	0	0	0	0	0	0	0	0	0	0

Here gap is also taken in account. If no gap is present then 0 value should passed by user and otherwise needed gap should be entered.

- **DPBP**: Usage: dpbp (input_filename)
  Description: This function will generates Dipeptide binary profile for residues from whole sequence of a protein.
- **DPBP_NT:** Usage: dpbp_nt (input_filename, n)
  Description: This function generates Dipeptide binary profile for residues selected from N-terminal, user need to provide number of N-terminal residues ***n*** to be used for calculating.
- **DPBP_CT:** Usage: dpbp_ct (input_filename, m)
  Description: This function generates Dipeptide binary profile for residues selected from C-terminal, user need to provide number of N-terminal residues ***m*** to be used for calculating.
- **DPBP_REST:** Usage: dpbp_rest (input_filename, n, m)
  Description: This function generates Dipeptide binary profile of remaining residues of a sequence after cleaving ***n*** residues from N-Terminal and ***m*** residues from C-Terminal.

- **DPBP_SPLIT:** Usage: dpbp_split (input_filename, s)
  Description: This function generates Dipeptide binary profile of each portion after splitting sequence in ***s*** portions. This function is important to generates binary profile of different portion of a protein.

2.3 Atom & Bond:

This function computes the binary profile corresponding to atomic and bond composition of each amino acid residue of the peptide sequence. Atomic composition is percentage of Carbon, Hydrogen, Nitrogen, Oxygen and Sulphur atoms present in a peptide sequence. These five atoms form a size 5 binary vector. Their combinations form binary profile of each residue. For example residue of Alanine(A) contains 13 atoms in total. Thus binary profile of 'A' will be of size 13*5=65.

- **ATBP**: Usage: atbp (input_filename)
  Description:This function generates Atomic binary profile from whole sequence of a protein.
- **ATBP_NT:** Usage: atbp_nt (input_filename, n)
  Description: This function generates Atomic binary profile for residues selected from N-terminal, user need to provide number of N-terminal residues ***n*** to be used for calculating.
- **ATBP_CT:** Usage: atbp_ct (input_filename, m)
  Description: This function generates Atomic binary profile for residues selected from C-terminal, user need to provide number of N-terminal residues ***m*** to be used for calculating.
- **ATBP_REST:** Usage: atbp_rest (input_filename, n, m)
  Description: This function generates Atomic binary profile for remaining residues of a sequence after cleaving ***n*** residues from N-Terminal and ***m*** residues from C-Terminal.
- **ATBP_SPLIT:** Usage: atbp_split (input_filename, s)
  Description: This function generates Atomic binary profile of each portion after splitting sequence in ***s*** portions.

Bond binary profile is made based upon canonical smile (from PubChem) for each Amino Acid. Four kinds of bond considered c(cyclic), benzene ring(b), single bond(-) and double bond (=). Corresponding to these bonds binary vector is created.

- **BBP**: Usage: bbp (input_filename)
  Description:This function generates Bond binary profile from whole sequence of a protein.
- **BBP_NT:** Usage: bbp_nt (input_filename, n)
  Description: This function generates Bond binary profile for residues selected from N-terminal, user need to provide number of N-terminal residues ***n*** to be used for calculating.
- **BBP_CT:** Usage: bbp_ct (input_filename, m)

Description: This function generates Bond binary profile for residues selected from C-terminal, user need to provide number of N-terminal residues ***m*** to be used for calculating.

- **BBP_REST:** Usage: bbp_rest (input_filename, n, m)
  Description: This function generates Bond binary profile for remaining residues of a sequence after cleaving ***n*** residues from N-Terminal and ***m*** residues from C-Terminal.
- **BBP_SPLIT:** Usage: bbp_split (input_filename, s)
  Description: This function generates Bond binary profile of each portion after splitting sequence in ***s*** portions.

2.4 Residue Properties

This function outputs a binary profile of each sequence which convey where a particular physicochemical property is present in a sequence.

- **Binary Profile of entire sequence:**
  Usage: bp_phychem_all(input_file, featureNum)
  Description: This function calculates the binary profile of a particular physicochemical property for each input sequence. The user can enter the input file containing these sequences and the feature number.
- **Binary Profile of N-terminal residues:**
  Usage: bp_phychem_NT(input_file,featureNum,n)
  Description: This function outputs the binary profile of desired physicochemical property by considering only ‘n’ N Terminal residues.
- **Binary Profile of C-terminal residues:**
  Usage: bp_phychem_CT(input_file,featureNum,n)
  Description:This function outputs the binary profile of desired physicochemical property by considering only ‘n’ C-Terminal residues.
- **Binary Profile of rest residues:**
  Usage: bp_phychem_rest(input_file,featureNum, m, n)
  Description:This function outputs the binary profile of desired physicochemical property by removing ‘n’ N Terminal residues and ‘m’ C Terminal residues and considering only the residues left after these removals.
- **Binary Profile of split subsequences:**
  Usage: bp_phychem_split(input_file,featureNum,SPLIT)
  Description:This function splits the sequence into ‘SPLIT’ parts and then iteratively gives binary profile of each split subsequence.

2.5 AA Index

Usage: phychem_AAI(input_file, AAIndices)

This function gives the binary profile of input AA Indices. If normalised score of AAIndex value of a particular residue is negative, the function assigns ‘0’ to that residue otherwise assigns ‘1’. The user can enter the input file along with a comma separated file containing multiple desired AA Indices from https://www.genome.jp/dbget/AAindex/list_of_indices. This hyperlink lists out all the indices and the same can be input into the function.

- **AA Index**:phychem_AAI(input_file, AAIndices)
  Description:This function gives the binary profile of input AA Indices.

3.0 Evolutionary Information

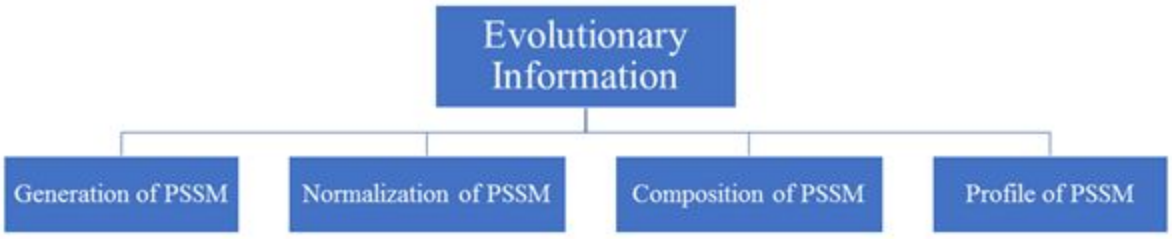


Figure 3: This flowchart shows different types of protein/peptide Evolutionary Information based features.

3.1 Generation of PSSM

This matrix is generated by using psi-blast against databases (nr or swissprot). The resultant matrix consists information of evolutionary conservation of elements of type x(i,j), where j is a residue at position 'i'.

3.2 Normalization of PSSM

Various Normalization techniques are there to normalize the PSSM profile.

- **pssm_n1** : Due to the large number of variation in the value of PSSM matrix, it is necessary to normalize it. Each element of matrix is normalized by 1/(1+e-x).
- **pssm_n2** : This is the second technique to normalize the elements of PSSM matrix using the formula (num - min)/(max - min).
- **pssm_n3** : This is the third technique to normalize the matrix using the formula (num - min)*100/(max - min).
- **pssm_n4** : This is the fourth technique to normalize the PSSM profile using the formula 1/(1+e-(x/100).

3.3 Composition of PSSM

This function results the vector of 400 size. It calculates the frequency of amino acid composition corresponding to residue of peptide/protein sequence. Each column consists of 20 values.

3.4 Profile of PSSM

This matrix is generated by using psi-blast against databases (nr or swissprot). The resultant matrix consists information of evolutionary conservation of elements of type x(i,j), where j is a residue at position 'i'.

In order to generate PSSM profile of different portions of an amino acid sequence, we have developed number of python function (brief description is given below). In web server user may select portion of sequence for calculating protein features.

- **PSSM_PROFILE**: Usage: pssm_profile(input_filename)
  Description: This function will generate PSSM profile from whole sequence of a protein.
- **PSSM_NT**: Usage: pssm_nt (input_filename, n)
  Description: This function will generate PSSM profile of residues selected from N-terminal. User need to provide number of N-terminal residues ***n*** to be used for calculating.
- **PSSM_CT**: Usage: pssm_ct (input_filename, m)
  Description: This function will generate PSSM profile of residue selected from C-terminal. User need to provide number of C-terminal residues ***m*** to be used for calculating.
- **PSSM_REST**: Usage: pssm_rest (input_filename, n, m)
  Description: This function will generate PSSM profile of remaining residues of a sequence after cleaving ***n*** residues from N-Terminal and ***m*** residues from C-Terminal.

4.0 Structure

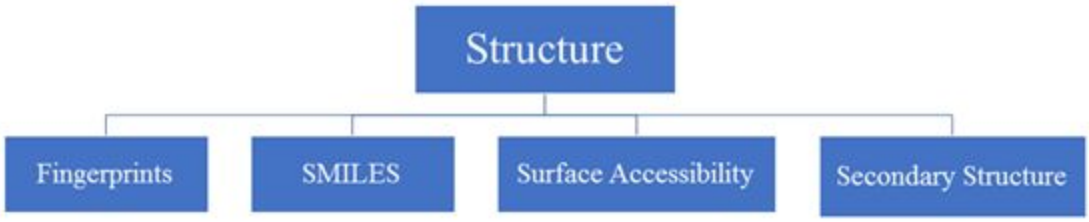


Figure 4: This flowchart shows different types of protein/peptide Structure based features.

4.1 Fingerprints:

This module was developed to calculate different types of fingerprints descriptors. The fingerprints were calculated using PaDEL software, which is java based software. PaDEL software provides 10 different types of fingerprints types which in total provide 14,532 fingerprint values. These fingerprints are calculated using mainly The Chemistry Development Kit (CDK).

Along with CDK, other fingerprints present are Pubchem fingerprints, MACCS fingerprints, Klekota-Roth fingerprints. Fingerprints have been used as an important type of feature in various prediction methods developed previously in literature.

Usage: Here user needs to upload its molecular structure in PDB file format for calculating the fingerprints.

4.2 SMILES

SMILES stands for Simplified Molecular Input Line Entry System. It is a type of line notation for representing various molecules and reactions. It contains the same information as the extended data tables consists of. One of the advantage of using it is that it is easy to understand since it is a linguistic construct rather than a computer data structure. Also, the SMILES format takes 50-70% less space in comparison to other way of representing the information as well as required lesser time for processing the information. SMILES notation is represented by series of characters and no spaces are present in between the characters.

SMILES notation follows five simple rules required for its encoding which are corresponding to atoms, bonds, branches, ring closures and disconnections. Detailed description of the SMILES notations can be obtained at http://www.daylight.com/dayhtml/doc/theory/theory.smiles.html .

Usage: Here, SMILES format were generated using openbabel software, where users are required to upload their structure in PDB file format in the SMILES page of pfeature in order to get the desired output.

4.3 Surface Accessibility

Accessible molecular surface or solvent-exposed area is defined as the area of an atom which can be touched by water molecule. Contact surface area and atoms chemical properties play an important role in modeling side chain conformations in proteins, structure and functional annotation of biological molecules. Here we have developed a module, which calculates the Relative Accessibility Area (RSA) using NACCESS software. The software requires PDB structure as an input and calculates relative accessible area. The output provided by the software shows value in percentage. In general values ranges between 0-100%; however, for some residues values go beyond 100%. In general, residues showing value less than 20% are said to buried whereas residues showing value above 20% are said to be exposed

Usage: Here, user needs to upload their structure in PDB file format and the server will calculate the relative accessibility area as an output.

4.4 Secondary Structure

Secondary structure refers to the interaction of hydrogen bond donor and acceptor residues of the repeating peptide unit. It plays an important role in protein structure prediction and protein folding. The two most important element of secondary structure are alpha helix and beta sheet. However coils are also considered as an important type of secondary structure in many cases. There are many software present in the literature which has been developed to predict the type of secondary structure. Since secondary structure elements represents an important type of feature, we have developed a module which calculates the percent average secondary structure element present in the input structure file. We have used DSSP software, which assigns the secondary structure state of the residue.

Usage: In order to calculate the percent average secondary structure element, user needs to upload the PDB file on to the server.

5.0 Pattern

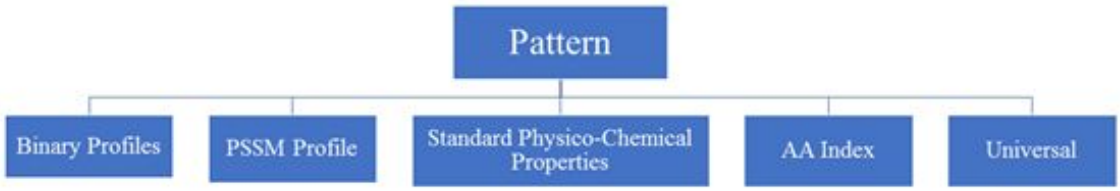


Figure 5: This flowchart shows different types of protein/peptide Pattern based features.

5.1 Binary Profiles

This function is used to compute binary profile for the patterns of protein and peptide sequences. The patterns generated are in different window size. The window size will always be an odd number to generate equal size of the patterns. An extra 'X' is added in the starting and end of the sequence to make equal size patterns. The binary pattern is generated for the pattern generated.

5.2 PSSM Profile

This function is used to compute PSSM for patterns of protein and peptide sequences. Here the patterns are generated from PSSM matrix in different window size. The window size will always be an odd number to generate equal size of patterns. Here extra 'X' is added in the starting and end of the sequence to make the equal size patterns, so the vector size will be 21.

5.3 Standard PhysicoChemical Properties

This function generates patterns of desired length within sequences and then calculates the standard physicochemical properties(refer to section 1.2.1) of each generated pattern.

5.4 AA Index

This function generates patterns of desired length and then calculates average desired AA Index value for each generated pattern.

5.5 Universal

This function will generate patterns for any type of string like secondary structure, surface accessibility. These patterns are generated in sliding window manner and are of defined length. Additional 'X' is added on both the sides of the peptide sequence which results in the generation of equal length pattern.

6.0 Portion of a Sequence

6.1 Whole amino acid sequence

This option allow users to compute features of a protein from whole sequence. This option is important for user when user wish to understand overall property of a protein or peptide. Most of methods developed in past use whole amino acid sequence of a protein.

6.2 N-Terminal

It has been observed in past that N-terminal of a protein is responsible for its function. For example most of classical secretory proteins contain a signal peptide. A short peptide (16-30 amino acids) present at the N-terminus of the majority of proteins that are destined towards the secretory pathway. Signal peptides are not only found in N-terminal of secretory proteins but found in number of other class of protein. Pfeature allow user to compute wide range of features in selected region (N-terminal) of a protein. One of the advantage of in selecting region is that user can generate both composition as well as binary profile as length of selected region is fixed **(BMC Bioinformatics 2007, 8:263 & BMC Bioinformatics 2010, 11:S19)**.

6.3 C-Terminal

It has been observed in past that C-terminal of a protein is responsible for its function. Normally. N-terminus of a protein often contains targeting signals, the C-terminus can contain retention signals for protein sorting. The most common endoplasmic reticulum retention signal is the amino acid sequence KDEL or HDEL at the C-terminus. This keeps the protein in the endoplasmic reticulum and prevents it from entering the secretory pathway. Pfeature allow user to compute wide range of features in selected region (C-terminal) of a protein. One of the advantage of in selecting region is that user can generate both composition as well as binary profile as length of selected region is fixed (BMC Bioinformatics 2007, 8:263 & BMC Bioinformatics 2010, 11:S19).

6.4 Split

One of the major problem with composition based features is that that it present protein by limited features, it give only average features of whole sequence. In order to increase number of features to capture more information from a protein, split amino acid composition (SAAC) has been introduced (**J Biol Chem. 2006;281:5357-63)**. In this concept, amino acid is splitted in

two or more than two portions then features of each portion is computed separately. For example is number of split is three then sequence will be divided in three portions (each portion have nearly same length). If whole protein have 20 (composition) features then splitted composition provides 60 (20 X 3) features.

6.5 Rest

As shown in above section both terminals (N- & C-) have important information so pfeature have provision to compute feature of N-terminal or C-terminal. In order to capture information or generating feature from remaining portion of proteins (after removing N-terminal and C-terminal residues). In case of rest option user need to select number of residues from N-terminal and C-terminal to be removed from protein for calculating features from rest of protein.

7.0 Complete list of features

In this section, we have elaborate and compared the features calculated by Pfeature and other available resources. Pfeature is able to calculate more than 70,000 composition features from the primary sequence of protein or peptide. In the table 3, we have described the group and type of features, kinds of sub-sequences, their dimension vectors, and methods which support the respective features.

Table 3: Brief description of features calculated by Pfeature

Type of Features	Description	Features	Dimension Vectors	Supported By
COMPOSITION: SIMPLE				
AAC	Amino acid Composition	Whole	20	{a,b,c,d,e}
		N-Terminal	20	{a}
		C-Terminal	20	{a}
		Rest	20	{a}
		Split	20*N	{a}
DPC	Dipeptide Composition	Whole	400	{a,b,c,d,e}
		N-Terminal	400	{a}
		C-Terminal	400	{a}
		Rest	400	{a}
		Split	400*N	{a}
TPC	Tripeptide Composition	Whole	8000	{a,b,c,d}
		N-Terminal	8000	{a}
		C-Terminal	8000	{a}
		Rest	8000	{a}
		Split	8000*N	{a}
ABC	Atom and Bond Composition	Whole	9	{a}
		N-Terminal	9	{a}
		C-Terminal	9	{a}
		Rest	9	{a}
		Split	9*N	{a}
COMPOSITION: PHYSICO-CHEMICAL PROPERTIES				
PCP	Physico-Chemical properties composition	Whole	19	{a,b,c,d,e}
		N-Terminal	19	{a}
		C-Terminal	19	{a}
		Rest	19	{a}

		Split	19*N	{a}
AAI	Amino Acid Index Composition	Whole	553	{a,b,c}
		N-Terminal	553	{a}
		C-Terminal	553	{a}
		Rest	553	{a}
		Split	553*N	{a}
PCP_adv	Advanced Physico-Chemical properties composition	Whole	5	{a,b,c,d,e}
		N-Terminal	5	{a}
		C-Terminal	5	{a}
		Rest	5	{a}
		Split	5*N	{a}
PCP_str	Structural Physico-Chemical properties composition	Whole	6	{a,b,c,d,e}
		N-Terminal	6	{a}
		C-Terminal	6	{a}
		Rest	6	{a}
		Split	6	{a}
COMPOSITION: REPEATS & DISTRIBUTION				
RRI	Repetitive Residue Information	Whole	20	{a}
		N-Terminal	20	{a}
		C-Terminal	20	{a}
		Rest	20	{a}
		Split	20*N	{a}
PRI	Repeat of Physico-chemical Properties	Whole	19	{a}
		N-Terminal	19	{a}
		C-Terminal	19	{a}
		Rest	19	{a}
		Split	19*N	{a}
DDR	Distance Distribution of Residues	Whole	20	{a}
		N-Terminal	20	{a}
		C-Terminal	20	{a}
		Rest	20	{a}
		Split	20*N	{a}
COMPOSITION: SHANNON ENTROPY				

SEP	Shannon Entropy at Protein Level	Whole	1	{a}
		N-Terminal	1	{a}
		C-Terminal	1	{a}
		Rest	1	{a}
		Split	1*N	{a}
SER	Shannon Entropy at Residue Level	Whole	20	{a}
		N-Terminal	20	{a}
		C-Terminal	20	{a}
		Rest	20	{a}
		Split	20*N	{a}
SPC	Shannon Entropy at Property Level	Whole	19	{a}
		N-Terminal	19	{a}
		C-Terminal	19	{a}
		Rest	19	{a}
		Split	19*N	{a}
COMPOSITION: MISCELLANEOUS				
ACR	Autocorrelation Descriptors	Whole	1659	{a,b,c,d,e}
		N-Terminal	1659	{a}
		C-Terminal	1659	{a}
		Rest	1659	{a}
		Split	1659*N	{a}
CTC	Conjoint Triad Descriptors	Whole	343	{a,b,c,d,e}
		N-Terminal	343	{a}
		C-Terminal	343	{a}
		Rest	343	{a}
		Split	343*N	{a}
CeTD	Composition enhanced Transition Distribution	Whole	189	{a,b,c,d,e}
		N-Terminal	189	{a}
		C-Terminal	189	{a}
		Rest	189	{a}
		Split	189*N	{a}
PAAC	Pseudo Amino Acid Composition	Whole	20 + λ	{a,b,c,d,e}
		N-Terminal	20 + λ	{a}
		C-Terminal	20 + λ	{a}
		Rest	20 + λ	{a}
		Split	N*(20 + λ)	{a}
APAAC	Amphiphilic Pseudo Amino Acid Composition	Whole	20 + (λ*3)	{a,b,c,d,e}
		N-Terminal	20 + (λ*3)	{a}
		C-Terminal	20 + (λ*3)	{a}
		Rest	20 + (λ*3)	{a}

		Split	N*(20 + (λ*3))	{a}
QSO	Quasi-Sequence Order	Whole	40 + (λ*2)	{a,b,c,d,e}
		N-Terminal	40 + (λ*2)	{a}
		C-Terminal	40 + (λ*2)	{a}
		Rest	40 + (λ*2)	{a}
		Split	N*(40 + (λ*2))	{a}
(SOCN)	Sequence Order Coupling Number	Whole	λ*2	{a,b,c,d,e}
		N-Terminal	λ*2	{a}
		C-Terminal	λ*2	{a}
		Rest	λ*2	{a}
		Split	N*λ*2	{a}
BINARY PROFILES				
AAB	Amino Acid Binary Profile	Whole	20*L	{a,b}
		N-Terminal	20*L	{a}
		C-Terminal	20*L	{a}
		Rest	20*L	{a}
		Split	N*(20*L)	{a}
DPB	Dipeptide Binary Profile	Whole	400*L	{a}
		N-Terminal	400*L	{a}
		C-Terminal	400*L	{a}
		Rest	400*L	{a}
		Split	N*(400*L)	{a}
ABB	Atom and Bond Binary Profile	Whole	(5*η)+(4*ε)	{a}
		N-Terminal	(5*η)+(4*ε)	{a}
		C-Terminal	(5*η)+(4*ε)	{a}
		Rest	(5*η)+(4*ε)	{a}
		Split	N*((5*η)+(4*ε))	{a}
PCB	Physico-Chemical Properties Binary Profile	Whole	25*L	{a}
		N-Terminal	25*L	{a}
		C-Terminal	25*L	{a}
		Rest	25*L	{a}
		Split	N*25*L	{a}
AIB	Amino Acid Index Binary Profile	Whole	553*L	{a}
		N-Terminal	553*L	{a}
		C-Terminal	553*L	{a}
		Rest	553*L	{a}
		Split	N*553*L	{a}
EVOLUTIONARY INFORMATION				
G_PSSM	Generation of PSSM	Whole	L X 21	{a}
N_PSSM	Normalization of PSSM	Whole	L X 21	{a}
C_PSSM	Composition of PSSM	Whole	400	{a}
P_PSSM	Profile of PSSM	Whole	L X 21	{a}

		N-Terminal	L X 21	{a}
		C-Terminal	L X 21	{a}
		Rest	L X 21	{a}
STRUCTURE				
FIN	Fingerprints	Whole	14532	{a}
SMI	SMILES	Whole	1	{a}
SA	Surface Accessibility	Whole	9	{a}
SS	Secondary Structure	Whole	3	{a}
PATTERN				
Binary Profile	Binary Profile generated using patterns of window length (ω)	Whole	L X (21*ω)	{a}
PSSM Profile	PSSM Profile generated using patterns of window length (ω)	Whole	L X (21*ω)	{a}
Physico-Chemical Properties	Physico-Chemical Properties, calculated using patterns of window length (ω)	Whole	L X (30*ω)	{a}
AA Index	Amino acid index composition, calculated using patterns of window length (ω)	Whole	L X 1	{a}
Universal	Generation of patterns of window length (ω)	Whole	L X ω	{a}
MODEL BUILDING				
Merging Features	Merge the two files into single file	2 CSV files	R X M	{a}
Feature Relevance	Mean based method to get the relevance of each feature	Positive and Negative Dataset	F X 9	{a}

a: Pfeature, b: ifeatue, c: PyBioMed, d: PyDPI, e: PROFEAT; L: length of protein; N: Number of splits; λ: The number depends upon the choice of maxlag; η: Number of atoms; ε: Number of bonds; R: Number of Rows; M: Total number of features in two files; F: Total number of features

8.0 List of Descriptors and Abbreviations

Amino Acid Composition (AAC): Total descriptor 20

AAC_A → Amino acid composition of Alanine

AAC_C → Amino acid composition of Cysteine

AAC_D → Amino acid composition of Aspartic acid

AAC_E → Amino acid composition of Glutamic acid

AAC_F → Amino acid composition of Phenylalanine

AAC_G → Amino acid composition of Glycine

AAC_H → Amino acid composition of Histidine

AAC_I → Amino acid composition of Isoleucine

AAC_K → Amino acid composition of Lysine

AAC_L → Amino acid composition of Leucine

AAC_M → Amino acid composition of Methionine

AAC_N → Amino acid composition of Asparagine

AAC_P → Amino acid composition of Proline

AAC_Q → Amino acid composition of Glutamine

AAC_R → Amino acid composition of Arginine

AAC_S → Amino acid composition of Serine

AAC_T → Amino acid composition of Threonine

AAC_V → Amino acid composition of Valine

AAC_W → Amino acid composition of Tryptophan

AAC_Y → Amino acid composition of Tyrosine

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Dipeptide Composition (order 1, traditional) : 400 dipeptide composition

DPC1_AA → Composition of Alanine-Alanine

DPC1_AC → Composition of Alanine-Cysteine

DPC1_YW → Composition of Alanine-Cysteine

DPC1_YY → Composition of Alanine-Cysteine

Dipeptide Composition (order 2, alternate) : 400 dipeptide composition

DPC2_AA → Composition of Alanine-Alanine

DPC2_AC → Composition of Alanine-Cysteine

DPC2_YW → Composition of Alanine-Cysteine

DPC2_YY → Composition of Alanine-Cysteine

Dipeptide Composition (order 3, with gap of 2 residues) : 400 dipeptide composition

DPC3_AA → Composition of Alanine-Alanine

DPC3_AC → Composition of Alanine-Cysteine

DPC3_YW → Composition of Alanine-Cysteine

DPC3_YY → Composition of Alanine-Cysteine

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Tripeptide Composition: 8000 tripeptide composition

TPC_AAA → Composition of Alanine-Alanine-Alanine

TPC_AAC → Composition of Alanine-Alanine-Cysteine

TPC_AAD → Composition of Alanine-Alanine-Aspartic acid

TPC_AAE → Composition of Alanine-Alanine-Glutamic acid

TPC_AAF → Composition of Alanine-Alanine-Phenylalanine

TPC_AAG → Composition of Alanine-Alanine-Glycine

TPC_AAH → Composition of Alanine-Alanine-Histidine

TPC_AAI → Composition of Alanine-Alanine-Isoleucine

TPC_AAK → Composition of Alanine-Alanine-Lysine

TPC_AAL → Composition of Alanine-Alanine-Leucine

TPC_YYM → Composition of Tyrosine-Tyrosine-Methionine

TPC_YYN → Composition of Tyrosine-Tyrosine-Asparagine

TPC_YYP → Composition of Tyrosine-Tyrosine-Proline

TPC_YYQ → Composition of Tyrosine-Tyrosine-Glutamine

TPC_YYR → Composition of Tyrosine-Tyrosine-Arginine

TPC_YYS → Composition of Tyrosine-Tyrosine-Serine

TPC_YYT → Composition of Tyrosine-Tyrosine-Threonine

TPC_YYV → Composition of Tyrosine-Tyrosine-Valine

TPC_YYW → Composition of Tyrosine-Tyrosine-Tryptophan

TPC_YYY → Composition of Tyrosine-Tyrosine- Tyrosine

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Atom Type Composition: 5 descriptors

ATC_C → Atomic Composition of Carbon

ATC_H → Atomic Composition of Hydrogen

ATC_N → Atomic Composition of Nitrogen

ATC_O → Atomic Composition of Oxygen

ATC_S → Atomic Composition of Sulphur

Bond Type Composition: 4 descriptors

BTC_T → Composition of total bonds

BTC_H → Composition of Hydrogen bonds

BTC_S → Composition of Single bonds

BTC_D → Composition of Double bonds

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Physico-chemical properties: 30 descriptors

PCP_PC → Composition of positively charged residues

PCP_NC → Composition of positively charged residues

PCP_NE → Composition of neutral charged residues

PCP_PO → Composition of polar residues

PCP_NP → Composition of non-polar residues

PCP_AL → Composition of residues having aliphatic side chain

PCP_CY → Composition of residues having cyclic side chain

PCP_AR → Composition of aromatic residues

PCP_AC → Composition of acidic residues

PCP_BS → Composition of basic residues

PCP_NE_ph → Composition of neutral residues based on pH

PCP_HB → Composition of hydrophobic residues

PCP_HL → Composition of hydrophilic residues

PCP_NT → Composition of neutral residues

PCP_HX → Composition of hydroxylic residues

PCP_SC → Composition of residues having sulphur content

PCP_SS_HE → Composition of residue in secondary structure (Helix)

PCP_SS_ST → Composition of residue in secondary structure (Strands)

PCP_SS_CO → Composition of residue in secondary structure (Coil)

PCP_SA_BU → Composition of residue in solvent accessibility (Buried)

PCP_SA_EX → Composition of residue in solvent accessibility (Exposed)

PCP_SA_IN → Composition of residue in solvent accessibility (Intermediate)

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PCP_TN → Composition of tiny residues

PCP_SM → Composition of small residues

PCP_LR → Composition of large residues

PCP_Z1 → Composition of residues having Z1 advanced Physico-chemical properties

PCP_Z2 → Composition of residues having Z2 advanced Physico-chemical properties

PCP_Z3 → Composition of residues having Z3 advanced Physico-chemical properties

PCP_Z4 → Composition of residues having Z4 advanced Physico-chemical properties

PCP_Z5 → Composition of residues having Z5 advanced Physico-chemical properties

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Amino Acid Index: 553 type descriptors

AAI_ANDN920101 → Composition of index ANDN920101

AAI_ARGP820101 → Composition of index ARGP820101

AAI_ARGP820102 → Composition of index ARGP820102

AAI_ARGP820103 → Composition of index ARGP820103

AAI_BEGF750101 → Composition of index BEGF750101

AAI_BEGF750102 → Composition of index BEGF750102

AAI_BEGF750103 → Composition of index BEGF750103

AAI_BHAR880101 → Composition of index BHAR880101

AAI_BIGC670101 → Composition of index BIGC670101

AAI_BIOV880101 → Composition of index BIOV880101

AAI_KARS160113 → Composition of index KARS160113

AAI_KARS160114 → Composition of index KARS160114

AAI_KARS160115 → Composition of index KARS160115

AAI_KARS160116 → Composition of index KARS160116

AAI_KARS160117 → Composition of index KARS160117

AAI_KARS160118 → Composition of index KARS160118

AAI_KARS160119 → Composition of index KARS160119

AAI_KARS160120 → Composition of index KARS160120

AAI_KARS160121 → Composition of index KARS160121

AAI_KARS160122 → Composition of index KARS160122

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Residue Repeats Index: 20 descriptors

RRI_A → Residue repeat index of Alanine

RRI_C → Residue repeat index of Cysteine

RRI_D → Residue repeat index of Aspartic acid

RRI_E → Residue repeat index of Glutamic acid

RRI_F → Residue repeat index of Phenylalanine

RRI_G → Residue repeat index of Glycine

RRI_H → Residue repeat index of Histidine

RRI_I → Residue repeat index of Isoleucine

RRI_K → Residue repeat index of Lysine

RRI_L → Residue repeat index of Leucine

RRI_M → Residue repeat index of Methionine

RRI_N → Residue repeat index of Asparagine

RRI_P → Residue repeat index of Proline

RRI_Q → Residue repeat index of Glutamine

RRI_R → Residue repeat index of Arginine

RRI_S → Residue repeat index of Serine

RRI_T → Residue repeat index of Threonine

RRI_V → Residue repeat index of Valine

RRI_W → Residue repeat index of Tryptophan

RRI_Y → Residue repeat index of Tyrosine

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Property Repeats Index: 25 descriptors corresponding to 25 physico-chemical properties

PRI_PC → Residue repeat index for positive charged residues

PRI_PC → Residue repeat index for negative charged residues

PRI_NE → Residue repeat index for neutral charged residues

PRI_PO → Residue repeat index for polar residues

PRI_NP → Residue repeat index for non-polar residues

PRI_AL → Residue repeat index for residues having aliphatic side chain

PRI_CY → Residue repeat index for residues having cyclic side chain

PRI_AR → Residue repeat index for aromatic residues

PRI_AC → Residue repeat index for acidic residues

PRI_BS → Residue repeat index for basic residues

PRI_NE → Residue repeat index for neutral residues based on pH

PRI_HB → Residue repeat index for hydrophobic residues

PRI_HL → Residue repeat index for hydrophilic residues

PRI_NT → Residue repeat index for neutral residues

PRI_HX → Residue repeat index for hydroxylic residues

PRI_SC → Residue repeat index for residues having sulphur content

PRI_SS_HE → Residue repeat index for residues in secondary structure (Helix)

PRI_SS_ST → Residue repeat index for residues in secondary structure (Strands)

PRI_SS_CO → Residue repeat index for residues in secondary structure (Coil)

PRI_SA_BU → Residue repeat index for residues in solvent accessibility (Buried)

PRI_SA_EX → Residue repeat index for residues in solvent accessibility (Exposed)

PRI_SA_IN → Residue repeat index for residues in solvent accessibility (Intermediate)

PRI_TN → Residue repeat index for tiny residues

PRI_SM → Residue repeat index for small residues

PRI_LR → Residue repeat index for large residues

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Distance Distribution of Repeats: 20 type of residues

DDR_A → Distribution of Alanine

DDR_C → Distribution of Cysteine

DDR_D → Distribution of Aspartic acid

DDR_E → Distribution of Glutamic acid

DDR_F → Distribution of Phenylalanine

DDR_G → Distribution of Glycine

DDR_H → Distribution of Histidine

DDR_I → Distribution of Isoleucine

DDR_K → Distribution of Lysine

DDR_L → Distribution of Leucine

DDR_M → Distribution of Methionine

DDR_N → Distribution of Asparagine

DDR_P → Distribution of Proline

DDR_Q → Distribution of Glutamine

DDR_R → Distribution of Arginine

DDR_S → Distribution of Serine

DDR_T → Distribution of Threonine

DDR_V → Distribution of Valine

DDR_W → Distribution of Tryptophan

DDR_Y → Distribution of Tyrosine

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Shannon Entropy of a Protein: 1 Descriptor

SEP → Shannon entropy of whole protein

Shannon Entropy of a Residue: 20 Descriptors

SER_A → Shannon entropy of Alanine

SER_C → Shannon entropy of Cysteine

SER_D → Shannon entropy of Aspartic acid

SER_E → Shannon entropy of Glutamic acid

SER_F → Shannon entropy of Phenylalanine

SER_G → Shannon entropy of Glycine

SER_H → Shannon entropy of Histidine

SER_I → Shannon entropy of Isoleucine

SER_K → Shannon entropy of Lysine

SER_L → Shannon entropy of Leucine

SER_M → Shannon entropy of Methionine

SER_N → Shannon entropy of Asparagine

SER_P → Shannon entropy of Proline

SER_Q → Shannon entropy of Glutamine

SER_R → Shannon entropy of Arginine

SER_S → Shannon entropy of Serine

SER_T → Shannon entropy of Threonine

SER_V → Shannon entropy of Valine

SER_W → Shannon entropy of Tryptophan

SER_Y → Shannon entropy of Tyrosine

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Shannon Entropy of Properties:25 features corresponding to 25 physicochemical properties

SEP_PC → Shannon entropy of positive charged residues

SEP_PC → Shannon entropy of negative charged residues

SEP_NE → Shannon entropy of neutral charged residues

SEP_PO → Shannon entropy of polar residues

SEP_NP → Shannon entropy of non-polar residues

SEP_AL → Shannon entropy of residues having aliphatic side chain

SEP_CY → Shannon entropy of residues having cyclic side chain

SEP_AR → Shannon entropy of aromatic residues

SEP_AC → Shannon entropy of acidic residues

SEP_BS → Shannon entropy of basic residues

SEP_NE → Shannon entropy of neutral residues based on pH

SEP_HB → Shannon entropy of hydrophobic residues

SEP_HL → Shannon entropy of hydrophilic residues

SEP_NT → Shannon entropy of neutral residues

SEP_HX → Shannon entropy of hydroxylic residues

SEP_SC → Shannon entropy of residues having sulphur content

SEP_SS_HE → Shannon entropy of residue in secondary structure (Helix)

SEP _SS_ST → Shannon entropy of residue in secondary structure (Strands)

SEP _SS_CO → Shannon entropy of residue in secondary structure (Coil)

SEP _SA_BU → Shannon entropy of residue in solvent accessibility (Buried)

SEP _SA_EX → Shannon entropy of residue in solvent accessibility (Exposed)

SEP _SA_IN → Shannon entropy of residue in solvent accessibility (Intermediate)

SEP_TN → Shannon entropy of tiny residues

SEP_SM → Shannon entropy of small residues

SEP_LR → Shannon entropy of large residues

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Autocorrelation : 3 descriptors (Dong, Jie, et al. *Journal of cheminformatics* (2018),10.1:16)

ACR1_MB → Normalized Moreau-Broto autocorrelation descriptor with lag 1

ACR1_MO → Morgan autocorrelation descriptor with lag 1

ACR1_GE → Geary autocorrelation descriptor with lag 1

Conjoint Triad Descriptors: 343 descriptors (Dong, Jie, et al. *Journal of cheminformatics* (2018),10.1:16)

Group 1: A, G, V

Group 2: I, L, F, P

Group 3: Y, M, T, S

Group 4: H, N, Q, W

Group 5: R, K

Group 6: D, E

Group 7: C

CTC_111 → Normalize frequency of group1-group1-group1 (tri-group)

CTC_112 → Normalize frequency of group1-group1-group2 (tri-group)

CTC_113→ Normalize frequency of group1-group1-group3 (tri-group)

CTC_775 → Normalize frequency of group7-group7-group5 (tri-group)

CTC_776 → Normalize frequency of group7-group7-group6 (tri-group)

CCT_777 → Normalize frequency of group7-group7-group7 (tri-group)

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Composition enhanced Transition and Distribution: 189 descriptors (Dubchak I, et al. *Proceedings of the National Academy of Sciences of the United States of America*)

Attributes	Group1	Group 2	Group 3
Hydrophobicity	R,K,E,D,Q,N	G,A,S,T,P,H,Y	C,L,V,I,M,F,W
Normalized Vander Waals volume	G,A,S,T,P,D	N,V,E,Q,I,L	M,H,K,F,R,Y,W
Polarity	L,I,F,W,C,M,V,Y	P,A,T,G,S	H,Q,R,K,N,E,D
Polarizability	G,A,S,D,T	C,P,N,V,E,Q,I,L	K,M,H,F,R,Y,W
Charge	K,R	A,N,C,Q,G,H,I,L,M,F,P,S,T,W,Y,V	D,E
Secondary structure	E,A,L,M,Q,K,R,H	V,I,Y,C,W,F,T	G,N,P,S,D
Solvent accessibility	A,L,F,C,G,I,V,W	R,K,Q,E,N,D	M,S P,T,H,Y

- **Composition:** 21 Descriptors

  CeTD_HB1 → Composition of group 1 residues for hydrophobicity attribute

  CeTD_HB2 → Composition of group 2 residues for hydrophobicity attribute

  CeTD_HB3 → Composition of group 3 residues for hydrophobicity attribute

  CeTD_VW1 → Composition of group 1 residues for normalized vander waals volume attribute

  CeTD_VW2 → Composition of group 2 residues for normalized vander waals volume attribute

  CeTD_VW3 → Composition of group 2 residues for normalized vander waals volume attribute

  CeTD_PO1 → Composition of group 1 residues for polarity attribute

  CeTD_PO2 → Composition of group 2 residues for polarity attribute

  CeTD_PO3 → Composition of group 3 residues for polarity attribute

  CeTD_PZ1 → Composition of group 1 residues for polarizability attribute

  CeTD_PZ2 → Composition of group 2 residues for polarizability attribute

  CeTD_PZ3 → Composition of group 3 residues for polarizability attribute

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

CeTD_CH1 → Composition of group 1 residues for charge attribute

CeTD_CH2 → Composition of group 2 residues for charge attribute

CeTD_CH3 → Composition of group 3 residues for charge attribute

CeTD_SS1 → Composition of group 1 residues for secondary structure attribute

CeTD_SS2 → Composition of group 2 residues for secondary structure attribute

CeTD_SS3 → Composition of group 3 residues for secondary structure attribute

CeTD_SA1 → Composition of group 1 residues for solvent accessibility attribute

CeTD_SA2 → Composition of group 2 residues for solvent accessibility attribute

CeTD_SA3 → Composition of group 3 residues for solvent accessibility attribute

- **Transition:** 63 Descriptors

CeTD_11_HB → Number of transitions takes place from group 1 residues to group 1 residues for hydrophobicity attribute

CeTD_11_VW → Number of transitions takes place from group 1 residues to group 1 residues for normalized vander waals volume attribute

CeTD_11_PO → Number of transitions takes place from group 1 residues to group 1 residues for polarity attribute

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CeTD_12_HB → Number of transitions takes place from group 1 residues to group 2 residues for hydrophobicity attribute

CeTD_12_VW → Number of transitions takes place from group 1 residues to group 2 residues for normalized vander waals volume attribute

CeTD_12_PO → Number of transitions takes place from group 1 residues to group 2 residues for polarity attribute

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CeTD_33_CH → Number of transitions takes place from group 3 residues to group 3 residues for charge attribute

CeTD_33_SS → Number of transitions takes place from group 3 residues to group 3 residues for secondary structure attribute

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

CeTD_33_SA → Number of transitions takes place from group 3 residues to group 3 residues for solvent accessibility attribute

- **Distribution:** 105 Descriptors

CeTD_0_p_HB1 → Number of group 1 residues for hydrophobicity present in 0% quartile

CeTD_25_p_HB1 → Number of group 1 residues for hydrophobicity present in 25% quartile

CeTD_50_p_HB1 → Number of group 1 residues for hydrophobicity present in 50% quartile

CeTD_75_p_HB1 → Number of group 1 residues for hydrophobicity present in 75% quartile

CeTD_100_p_HB1 → Number of group 1 residues for hydrophobicity present in 100% quartile

CeTD_0_p_VW1 → Number of group 1 residues for normalized vander waals volume present in 0% quartile

CeTD_25_p_VW1 → Number of group 1 residues for normalized vander waals volume present in 25% quartile

CeTD_50_p_VW1 → Number of group 1 residues for normalized vander waals volume present in 50% quartile

CeTD_75_p_VW1 → Number of group 1 residues for normalized vander waals volume present in 75% quartile

CeTD_100_p_VW1 → Number of group 1 residues for normalized vander waals volume present in 100% quartile

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CeTD_0_p_HB2 → Number of group 2 residues for hydrophobicity present in 0% quartile

CeTD_25_p_HB2 → Number of group 2 residues for hydrophobicity present in 25% quartile

CeTD_50_p_HB2 → Number of group 2 residues for hydrophobicity present in 50% quartile

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

CeTD_75_p_HB2 → Number of group 2 residues for hydrophobicity present in 75% quartile

CeTD_100_p_HB2 → Number of group 2 residues for hydrophobicity present in 100% quartile

CeTD_0_p_VW2 → Number of group 2 residues for normalized vander waals volume present in 0% quartile

CeTD_25_p_VW2 → Number of group 2 residues for normalized vander waals volume present in 25% quartile

CeTD_50_p_VW2 → Number of group 2 residues for normalized vander waals volume present in 50% quartile

CeTD_75_p_VW2 → Number of group 2 residues for normalized vander waals volume present in 75% quartile

CeTD_100_p_VW2 → Number of group 2 residues for normalized vander waals volume present in 100% quartile

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CeTD_0_p_SA3 → Number of group 2 residues for solvent accessibility present in 0% quartile

CeTD_25_p_ SA3 → Number of group 2 residues for solvent accessibility present in 25% quartile

CeTD_50_p_ SA3 → Number of group 2 residues for solvent accessibility present in 50% quartile

CeTD_75_p_ SA3 → Number of group 2 residues for solvent accessibility present in 75% quartile

CeTD_100_p_ SA3 → Number of group 2 residues for solvent accessibility present in 100% quartile

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Pseudo Amino Acid Composition (order 1, traditional): 21 descriptors (Chou KC, 2001, *Proteins*)

PAAC1_A → Pseudo amino acid composition of Alanine

PAAC1_C → Pseudo amino acid composition of Cysteine

PAAC1_D → Pseudo amino acid composition of Aspartic acid

PAAC1_E → Pseudo amino acid composition of Glutamic acid

PAAC1_F → Pseudo amino acid composition of Phenylalanine

PAAC1_G → Pseudo amino acid composition of Glycine

PAAC1_H → Pseudo amino acid composition of Histidine

PAAC1_I → Pseudo amino acid composition of Isoleucine

PAAC1_K → Pseudo amino acid composition of Lysine

PAAC1_L → Pseudo amino acid composition of Leucine

PAAC1_M → Pseudo amino acid composition of Methionine

PAAC1_N → Pseudo amino acid composition of Asparagine

PAAC1_P → Pseudo amino acid composition of Proline

PAAC1_Q → Pseudo amino acid composition of Glutamine

PAAC1_R → Pseudo amino acid composition of Arginine

PAAC1_S → Pseudo amino acid composition of Serine

PAAC1_T → Pseudo amino acid composition of Threonine

PAAC1_V → Pseudo amino acid composition of Valine

PAAC1_W → Pseudo amino acid composition of Tryptophan

PAAC1_Y → Pseudo amino acid composition of Tyrosine

PAAC1_lam1 → Sequence correlation factor for lambda 1

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Pseudo Amino Acid Composition (order 2, alternate): 22 descriptors

PAAC2_A → Pseudo amino acid composition of Alanine

PAAC2_C → Pseudo amino acid composition of Cysteine

PAAC2_D → Pseudo amino acid composition of Aspartic acid

PAAC2_E → Pseudo amino acid composition of Glutamic acid

PAAC2_F → Pseudo amino acid composition of Phenylalanine

PAAC2_G → Pseudo amino acid composition of Glycine

PAAC2_H → Pseudo amino acid composition of Histidine

PAAC2_I → Pseudo amino acid composition of Isoleucine

PAAC2_K → Pseudo amino acid composition of Lysine

PAAC2_L → Pseudo amino acid composition of Leucine

PAAC2_M → Pseudo amino acid composition of Methionine

PAAC2_N → Pseudo amino acid composition of Asparagine

PAAC2_P → Pseudo amino acid composition of Proline

PAAC2_Q → Pseudo amino acid composition of Glutamine

PAAC2_R → Pseudo amino acid composition of Arginine

PAAC2_S → Pseudo amino acid composition of Serine

PAAC2_T → Pseudo amino acid composition of Threonine

PAAC2_V → Pseudo amino acid composition of Valine

PAAC2_W → Pseudo amino acid composition of Tryptophan

PAAC2_Y → Pseudo amino acid composition of Tyrosine

PAAC2_lam1 → Sequence correlation factor for lambda 1

PAAC2_lam2 → Sequence correlation factor for lambda 2

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Pseudo Amino Acid Composition (order 3, With gap of 2 residues): 23 descriptors

PAAC3_A → Pseudo amino acid composition of Alanine

PAAC3_C → Pseudo amino acid composition of Cysteine

PAAC3_D → Pseudo amino acid composition of Aspartic acid

PAAC3_E → Pseudo amino acid composition of Glutamic acid

PAAC3_F → Pseudo amino acid composition of Phenylalanine

PAAC3_G → Pseudo amino acid composition of Glycine

PAAC3_H → Pseudo amino acid composition of Histidine

PAAC3_I → Pseudo amino acid composition of Isoleucine

PAAC3_K → Pseudo amino acid composition of Lysine

PAAC3_L → Pseudo amino acid composition of Leucine

PAAC3_M → Pseudo amino acid composition of Methionine

PAAC3_N → Pseudo amino acid composition of Asparagine

PAAC3_P → Pseudo amino acid composition of Proline

PAAC3_Q → Pseudo amino acid composition of Glutamine

PAAC3_R → Pseudo amino acid composition of Arginine

PAAC3_S → Pseudo amino acid composition of Serine

PAAC3_T → Pseudo amino acid composition of Threonine

PAAC3_V → Pseudo amino acid composition of Valine

PAAC3_W → Pseudo amino acid composition of Tryptophan

PAAC3_Y → Pseudo amino acid composition of Tyrosine

PAAC3_lam1 → Sequence correlation factor for lambda 1

PAAC3_lam2 → Sequence correlation factor for lambda 2

PAAC3_lam3 → Sequence correlation factor for lambda 3

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Amphiphilic Pseudo Amino Acid Composition (order 1, traditional): 23 descriptors

APAAC1_A → Amphiphilic pseudo amino acid composition of Alanine

APAAC1_C → Amphiphilic pseudo amino acid composition of Cysteine

APAAC1_D → Amphiphilic pseudo amino acid composition of Aspartic acid

APAAC1_E → Amphiphilic pseudo amino acid composition of Glutamic acid

APAAC1_F → Amphiphilic pseudo amino acid composition of Phenylalanine

APAAC1_G → Amphiphilic pseudo amino acid composition of Glycine

APAAC1_H → Amphiphilic pseudo amino acid composition of Histidine

APAAC1_I → Amphiphilic pseudo amino acid composition of Isoleucine

APAAC1_K → Amphiphilic pseudo amino acid composition of Lysine

APAAC1_L → Amphiphilic pseudo amino acid composition of Leucine

APAAC1_M → Amphiphilic pseudo amino acid composition of Methionine

APAAC1_N → Amphiphilic pseudo amino acid composition of Asparagine

APAAC1_P → Amphiphilic pseudo amino acid composition of Proline

APAAC1_Q → Amphiphilic pseudo amino acid composition of Glutamine

APAAC1_R → Amphiphilic pseudo amino acid composition of Arginine

APAAC1_S → Amphiphilic pseudo amino acid composition of Serine

APAAC1_T → Amphiphilic pseudo amino acid composition of Threonine

APAAC1_V → Amphiphilic pseudo amino acid composition of Valine

APAAC1_W → Amphiphilic pseudo amino acid composition of Tryptophan

APAAC1_Y → Amphiphilic pseudo amino acid composition of Tyrosine

APAAC1_HB_lam1 → Sequence correlation factor for hydrophobicity with lambda 1

APAAC1_HL_lam1 → Sequence correlation factor for hydrophilicity with lambda 1

APAAC1_SC_lam1 → Sequence correlation factor for side chain mass with lambda 1

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Pseudo Amino Acid Composition (order 2, alternate): 26 descriptors

APAAC2_A → Amphiphilic pseudo amino acid composition of Alanine

APAAC2_C → Amphiphilic pseudo amino acid composition of Cysteine

APAAC2_D → Amphiphilic pseudo amino acid composition of Aspartic acid

APAAC2_E → Amphiphilic pseudo amino acid composition of Glutamic acid

APAAC2_F → Amphiphilic pseudo amino acid composition of Phenylalanine

APAAC2_G → Amphiphilic pseudo amino acid composition of Glycine

APAAC2_H → Amphiphilic pseudo amino acid composition of Histidine

APAAC2_I → Amphiphilic pseudo amino acid composition of Isoleucine

APAAC2_K → Amphiphilic pseudo amino acid composition of Lysine

APAAC2_L → Amphiphilic pseudo amino acid composition of Leucine

APAAC2_M → Amphiphilic pseudo amino acid composition of Methionine

APAAC2_N → Amphiphilic pseudo amino acid composition of Asparagine

APAAC2_P → Amphiphilic pseudo amino acid composition of Proline

APAAC2_Q → Amphiphilic pseudo amino acid composition of Glutamine

APAAC2_R → Amphiphilic pseudo amino acid composition of Arginine

APAAC2_S → Amphiphilic pseudo amino acid composition of Serine

APAAC2_T → Amphiphilic pseudo amino acid composition of Threonine

APAAC2_V → Amphiphilic pseudo amino acid composition of Valine

APAAC2_W → Amphiphilic pseudo amino acid composition of Tryptophan

APAAC2_Y → Amphiphilic pseudo amino acid composition of Tyrosine

APAAC2_HB_lam1 → Sequence correlation factor for hydrophobicity with lambda 1

APAAC2_HL_lam1 → Sequence correlation factor for hydrophilicity with lambda 1

APAAC2_SC_lam1 → Sequence correlation factor for side chain mass with lambda 1

APAAC2_HB_lam2 → Sequence correlation factor for hydrophobicity with lambda 2

APAAC2_HL_lam2 → Sequence correlation factor for hydrophilicity with lambda 2

APAAC2_SC_lam2 → Sequence correlation factor for side chain mass with lambda 2

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Pseudo Amino Acid Composition (order 3, With gap of 2 residues): 29 descriptors

APAAC3_A → Amphiphilic pseudo amino acid composition of Alanine

APAAC3_C → Amphiphilic pseudo amino acid composition of Cysteine

APAAC3_D → Amphiphilic pseudo amino acid composition of Aspartic acid

APAAC3_E → Amphiphilic pseudo amino acid composition of Glutamic acid

APAAC3_F → Amphiphilic pseudo amino acid composition of Phenylalanine

APAAC3_G → Amphiphilic pseudo amino acid composition of Glycine

APAAC3_H → Amphiphilic pseudo amino acid composition of Histidine

APAAC3_I → Amphiphilic pseudo amino acid composition of Isoleucine

APAAC3_K → Amphiphilic pseudo amino acid composition of Lysine

APAAC3_L → Amphiphilic pseudo amino acid composition of Leucine

APAAC3_M → Amphiphilic pseudo amino acid composition of Methionine

APAAC3_N → Amphiphilic pseudo amino acid composition of Asparagine

APAAC3_P → Amphiphilic pseudo amino acid composition of Proline

APAAC3_Q → Amphiphilic pseudo amino acid composition of Glutamine

APAAC3_R → Amphiphilic pseudo amino acid composition of Arginine

APAAC3_S → Amphiphilic pseudo amino acid composition of Serine

APAAC3_T → Amphiphilic pseudo amino acid composition of Threonine

APAAC3_V → Amphiphilic pseudo amino acid composition of Valine

APAAC3_W → Amphiphilic pseudo amino acid composition of Tryptophan

APAAC3_Y → Amphiphilic pseudo amino acid composition of Tyrosine

APAAC3_HB_lam1 → Sequence correlation factor for hydrophobicity with lambda 1

APAAC3_HL_lam1 → Sequence correlation factor for hydrophilicity with lambda 1

APAAC3_SC_lam1 → Sequence correlation factor for side chain mass with lambda 1

APAAC3_HB_lam2 → Sequence correlation factor for hydrophobicity with lambda 2

APAAC3_HL_lam2 → Sequence correlation factor for hydrophilicity with lambda 2

APAAC3_SC_lam2 → Sequence correlation factor for side chain mass with lambda 2

APAAC3_HB_lam3 → Sequence correlation factor for hydrophobicity with lambda 3

APAAC3_HL_lam3 → Sequence correlation factor for hydrophilicity with lambda 3

APAAC3_SC_lam3 → Sequence correlation factor for side chain mass with lambda 3

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Quasi-Sequence Order (order 1, traditional): 42 Descriptors (Chou KC, 2000, Biochemical and Biophysical Research Communications)

QSO1_SC_A → Quasi-sequence order with Schneider matrix for Alanine

QSO1_SC_C → Quasi-sequence order with Schneider matrix for Cysteine

QSO1_SC_D → Quasi-sequence order with Schneider matrix for Aspartic acid

QSO1_SC_E → Quasi-sequence order with Schneider matrix for Glutamic acid

QSO1_SC_F → Quasi-sequence order with Schneider matrix for Phenylalanine

QSO1_SC_G → Quasi-sequence order with Schneider matrix for Glycine

QSO1_SC_H → Quasi-sequence order with Schneider matrix for Histidine

QSO1_SC_I → Quasi-sequence order with Schneider matrix for Isoleucine

QSO1_SC_K → Quasi-sequence order with Schneider matrix for Lysine

QSO1_SC_L → Quasi-sequence order with Schneider matrix for Leucine

QSO1_SC_M → Quasi-sequence order with Schneider matrix for Methionine

QSO1_SC_N → Quasi-sequence order with Schneider matrix for Asparagine

QSO1_SC_P → Quasi-sequence order with Schneider matrix for Proline

QSO1_SC_Q → Quasi-sequence order with Schneider matrix for Glutamine

QSO1_SC_R → Quasi-sequence order with Schneider matrix for Arginine

QSO1_SC_S → Quasi-sequence order with Schneider matrix for Serine

QSO1_SC_T → Quasi-sequence order with Schneider matrix for Threonine

QSO1_SC_V → Quasi-sequence order with Schneider matrix for Valine

QSO1_SC_W → Quasi-sequence order with Schneider matrix for Tryptophan

QSO1_SC_Y → Quasi-sequence order with Schneider matrix for Tyrosine

QSO1_G_A → Quasi-sequence order with Grantham matrix for Alanine

QSO1_G_C → Quasi-sequence order with Grantham matrix for Cysteine

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

QSO1_G_D → Quasi-sequence order with Grantham matrix for Aspartic acid

QSO1_G_E → Quasi-sequence order with Grantham matrix for Glutamic acid

QSO1_G_F → Quasi-sequence order with Grantham matrix for Phenylalanine

QSO1_G_G → Quasi-sequence order with Grantham matrix for Glycine

QSO1_G_H → Quasi-sequence order with Grantham matrix for Histidine

QSO1_G_I → Quasi-sequence order with Grantham matrix for Isoleucine

QSO1_G_K → Quasi-sequence order with Grantham matrix for Lysine

QSO1_G_L → Quasi-sequence order with Grantham matrix for Leucine

QSO1_G_M → Quasi-sequence order with Grantham matrix for Methionine

QSO1_G_N → Quasi-sequence order with Grantham matrix for Asparagine

QSO1_G_P → Quasi-sequence order with Grantham matrix for Proline

QSO1_G_Q → Quasi-sequence order with Grantham matrix for Glutamine

QSO1_G_R → Quasi-sequence order with Grantham matrix for Arginine

QSO1_G_S → Quasi-sequence order with Grantham matrix for Serine

QSO1_G_T → Quasi-sequence order with Grantham matrix for Threonine

QSO1_G_V → Quasi-sequence order with Grantham matrix for Valine

QSO1_G_W → Quasi-sequence order with Grantham matrix for Tryptophan

QSO1_G_Y → Quasi-sequence order with Grantham matrix for Tyrosine

QSO1_SC1 → Quasi-sequence order with Schneider matrix with lag 1

QSO1_G1 → Quasi-sequence order with Grantham matrix with lag 1

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Quasi-Sequence Order (order 2, alternate): 44 Descriptors

QSO2_SCA → Quasi-sequence order with Schneider matrix for Alanine

QSO2_SCC → Quasi-sequence order with Schneider matrix for Cysteine

QSO2_SCD → Quasi-sequence order with Schneider matrix for Aspartic acid

QSO2_SCE → Quasi-sequence order with Schneider matrix for Glutamic acid

QSO2_SCF → Quasi-sequence order with Schneider matrix for Phenylalanine

QSO2_SCG → Quasi-sequence order with Schneider matrix for Glycine

QSO2_SCH → Quasi-sequence order with Schneider matrix for Histidine

QSO2_SCI → Quasi-sequence order with Schneider matrix for Isoleucine

QSO2_SCK → Quasi-sequence order with Schneider matrix for Lysine

QSO2_SCL → Quasi-sequence order with Schneider matrix for Leucine

QSO2_SCM → Quasi-sequence order with Schneider matrix for Methionine

QSO2_SCN → Quasi-sequence order with Schneider matrix for Asparagine

QSO2_SCP → Quasi-sequence order with Schneider matrix for Proline

QSO2_SCQ → Quasi-sequence order with Schneider matrix for Glutamine

QSO2_SCR → Quasi-sequence order with Schneider matrix for Arginine

QSO2_SCS → Quasi-sequence order with Schneider matrix for Serine

QSO2_SCT → Quasi-sequence order with Schneider matrix for Threonine

QSO2_SCV → Quasi-sequence order with Schneider matrix for Valine

QSO2_SCW → Quasi-sequence order with Schneider matrix for Tryptophan

QSO2_SCY → Quasi-sequence order with Schneider matrix for Tyrosine

QSO2_GA → Quasi-sequence order with Grantham matrix for Alanine

QSO2_GC → Quasi-sequence order with Grantham matrix for Cysteine

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

QSO2_GD → Quasi-sequence order with Grantham matrix for Aspartic acid

QSO2_GE → Quasi-sequence order with Grantham matrix for Glutamic acid

QSO2_GF → Quasi-sequence order with Grantham matrix for Phenylalanine

QSO2_GG → Quasi-sequence order with Grantham matrix for Glycine

QSO2_GH → Quasi-sequence order with Grantham matrix for Histidine

QSO2_GI → Quasi-sequence order with Grantham matrix for Isoleucine

QSO2_GK → Quasi-sequence order with Grantham matrix for Lysine

QSO2_GL → Quasi-sequence order with Grantham matrix for Leucine

QSO2_GM → Quasi-sequence order with Grantham matrix for Methionine

QSO2_GN → Quasi-sequence order with Grantham matrix for Asparagine

QSO2_GP → Quasi-sequence order with Grantham matrix for Proline

QSO2_GQ → Quasi-sequence order with Grantham matrix for Glutamine

QSO2_GR → Quasi-sequence order with Grantham matrix for Arginine

QSO2_GS → Quasi-sequence order with Grantham matrix for Serine

QSO2_GT → Quasi-sequence order with Grantham matrix for Threonine

QSO2_GV → Quasi-sequence order with Grantham matrix for Valine

QSO2_GW → Quasi-sequence order with Grantham matrix for Tryptophan

QSO2_GY → Quasi-sequence order with Grantham matrix for Tyrosine

QSO2_SC1 → Quasi-sequence order with Schneider matrix with lag 1

QSO2_G1 → Quasi-sequence order with Grantham matrix with lag 1

QSO2_SC2 → Quasi-sequence order with Schneider matrix with lag 2

QSO2_G2 → Quasi-sequence order with Grantham matrix with lag 2

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Quasi-Sequence Order (order 3, with gap of 2 residues): 46 Descriptors

QSO3_SCA → Quasi-sequence order with Schneider matrix for Alanine

QSO3_SCC → Quasi-sequence order with Schneider matrix for Cysteine

QSO3_SCD → Quasi-sequence order with Schneider matrix for Aspartic acid

QSO3_SCE → Quasi-sequence order with Schneider matrix for Glutamic acid

QSO3_SCF → Quasi-sequence order with Schneider matrix for Phenylalanine

QSO3_SCG → Quasi-sequence order with Schneider matrix for Glycine

QSO3_SCH → Quasi-sequence order with Schneider matrix for Histidine

QSO3_SCI → Quasi-sequence order with Schneider matrix for Isoleucine

QSO3_SCK → Quasi-sequence order with Schneider matrix for Lysine

QSO3_SCL → Quasi-sequence order with Schneider matrix for Leucine

QSO3_SCM → Quasi-sequence order with Schneider matrix for Methionine

QSO3_SCN → Quasi-sequence order with Schneider matrix for Asparagine

QSO3_SCP → Quasi-sequence order with Schneider matrix for Proline

QSO3_SCQ → Quasi-sequence order with Schneider matrix for Glutamine

QSO3_SCR → Quasi-sequence order with Schneider matrix for Arginine

QSO3_SCS → Quasi-sequence order with Schneider matrix for Serine

QSO3_SCT → Quasi-sequence order with Schneider matrix for Threonine

QSO3_SCV → Quasi-sequence order with Schneider matrix for Valine

QSO3_SCW → Quasi-sequence order with Schneider matrix for Tryptophan

QSO3_SCY → Quasi-sequence order with Schneider matrix for Tyrosine

QSO3_GA → Quasi-sequence order with Grantham matrix for Alanine

QSO3_GC → Quasi-sequence order with Grantham matrix for Cysteine

QSO3_GD → Quasi-sequence order with Grantham matrix for Aspartic acid

QSO3_GE → Quasi-sequence order with Grantham matrix for Glutamic acid

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

QSO3_GF → Quasi-sequence order with Grantham matrix for Phenylalanine

QSO3_GG → Quasi-sequence order with Grantham matrix for Glycine

QSO3_GH → Quasi-sequence order with Grantham matrix for Histidine

QSO3_GI → Quasi-sequence order with Grantham matrix for Isoleucine

QSO3_GK → Quasi-sequence order with Grantham matrix for Lysine

QSO3_GL → Quasi-sequence order with Grantham matrix for Leucine

QSO3_GM → Quasi-sequence order with Grantham matrix for Methionine

QSO3_GN → Quasi-sequence order with Grantham matrix for Asparagine

QSO3_GP → Quasi-sequence order with Grantham matrix for Proline

QSO3_GQ → Quasi-sequence order with Grantham matrix for Glutamine

QSO3_GR → Quasi-sequence order with Grantham matrix for Arginine

QSO3_GS → Quasi-sequence order with Grantham matrix for Serine

QSO3_GT → Quasi-sequence order with Grantham matrix for Threonine

QSO3_GV → Quasi-sequence order with Grantham matrix for Valine

QSO3_GW → Quasi-sequence order with Grantham matrix for Tryptophan

QSO3_GY → Quasi-sequence order with Grantham matrix for Tyrosine

QSO3_SC1 → Quasi-sequence order with Schneider matrix with lag 1

QSO3_G1 → Quasi-sequence order with Grantham matrix with lag 1

QSO3_SC2 → Quasi-sequence order with Schneider matrix with lag 2

QSO3_G2 → Quasi-sequence order with Grantham matrix with lag 2

QSO3_SC3 → Quasi-sequence order with Schneider matrix with lag 3

QSO3_G3 → Quasi-sequence order with Grantham matrix with lag 3

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Sequence Order Coupling Number (order 1, traditional): 2 descriptors

SOC1_SC1 → Sequence order coupling number with Schneider matrix for lag 1

SOC1_G1 → Sequence order coupling number with Grantham matrix for lag 1

Sequence Order Coupling Number (order 2, alternate): 4 descriptors

SOC2_SC1 → Sequence order coupling number with Schneider matrix for lag 1

SOC2_G1 → Sequence order coupling number with Grantham matrix for lag 1

SOC2_SC2 → Sequence order coupling number with Schneider matrix for lag 2

SOC2_G2 → Sequence order coupling number with Grantham matrix for lag 2

Sequence Order Coupling Number (order 3, with gap of 2 residues): 6 descriptors

SOC3_SC1 → Sequence order coupling number with Schneider matrix for lag 1

SOC3_G1 → Sequence order coupling number with Grantham matrix for lag 1

SCO3_SC2 → Sequence order coupling number with Schneider matrix for lag 2

SOC3_G2 → Sequence order coupling number with Grantham matrix for lag 2

SOC3_SC3 → Sequence order coupling number with Schneider matrix for lag 3

SOC3_G3 → Sequence order coupling number with Grantham matrix for lag 3

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Binary Profile Descriptor

Binary profile of Amino acids : Total features 20* window/protein length (N)

A1 → Presence/Absence (1 or 0) for Alanine at position 1

C1 → Presence/Absence (1 or 0) for Cysteine at position 1

D1 → Presence/Absence (1 or 0) for Aspartic acid at position 1

E1 → Presence/Absence (1 or 0) for Glutamic acid at position 1

F1 → Presence/Absence (1 or 0) for Phenylalanine at position 1

A2 → Presence/Absence (1 or 0) for Alanine at position 2

C2 → Presence/Absence (1 or 0) for Cysteine at position 2

D2 → Presence/Absence (1 or 0) for Aspartic acid at position 2

E1 → Presence/Absence (1 or 0) for Glutamic acid at position 2

F2 → Presence/Absence (1 or 0) for Phenylalanine at position 2

An → Presence/Absence (1 or 0) for Alanine at position n

Cn → Presence/Absence (1 or 0) for Cysteine at position n

Dn → Presence/Absence (1 or 0) for Aspartic acid at position n

En→ Presence/Absence (1 or 0) for Glutamic acid at position n

Fn → Presence/Absence (1 or 0) for Phenylalanine at position n

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Dipeptide profile of amino acids : Total features 20*20*window/protein length(n)-q

AA1 → Presence/Absence (1 or 0) for Alanine-Alanine at position 1

AC1 → Presence/Absence (1 or 0) for Alanine-Cysteine at position 1

AD1 → Presence/Absence (1 or 0) for Alanine-Aspartic acid at position 1

AE1 → Presence/Absence (1 or 0) for Alanine-Glutamic acid at position 1

AA2 → Presence/Absence (1 or 0) for Alanine-Alanine at position 2

AC2 → Presence/Absence (1 or 0) for Alanine-Cysteine at position 2

AD2 → Presence/Absence (1 or 0) for Alanine-Aspartic acid at position 2

AE2 → Presence/Absence (1 or 0) for Alanine-Glutamic acid at position 2

AAn → Presence/Absence (1 or 0) for Alanine-Alanine at position n

ACn → Presence/Absence (1 or 0) for Alanine-Cysteine at position n

ADn → Presence/Absence (1 or 0) for Alanine-Aspartic acid at position n

AEn → Presence/Absence (1 or 0) for Alanine-Glutamic acid at position n

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Atom and Bond profile: Total features 5*total number of atoms (n) + 4*total number of bonds (m)

C1 → Presence/Absence (1 or 0) for Carbon atom at position 1

H1 → Presence/Absence (1 or 0) for Hydrogen atom at position 1

N1 → Presence/Absence (1 or 0) for Nitrogen atom at position 1

O1 → Presence/Absence (1 or 0) for Oxygen atom at position 1

S1 → Presence/Absence (1 or 0) for Sulphur atom at position 1

C2 → Presence/Absence (1 or 0) for Carbon atom at position 2

H2 → Presence/Absence (1 or 0) for Hydrogen atom at position 2

N2 → Presence/Absence (1 or 0) for Nitrogen atom at position 2

O2 → Presence/Absence (1 or 0) for Oxygen atom at position 2

S2 → Presence/Absence (1 or 0) for Sulphur atom at position 2

C_n → Presence/Absence (1 or 0) for Carbon atom at n^{th} position

H_n → Presence/Absence (1 or 0) for Hydrogen atom at n^{th} position

N_n → Presence/Absence (1 or 0) for Nitrogen atom at n^{th} position

O_n → Presence/Absence (1 or 0) for Oxygen atom at n^{th} position

S_n → Presence/Absence (1 or 0) for Sulphur atom at n^{th} position

SI1 → Presence/Absence (1 or 0) for single bond at position 1

DO1 → Presence/Absence (1 or 0) for double bond at position 1

CY1 → Presence/Absence (1 or 0) for cyclic ring at position 1

BE1 → Presence/Absence (1 or 0) for benzene ring at position 1

SI2 → Presence/Absence (1 or 0) for single bond at position 2

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

DO2 → Presence/Absence (1 or 0) for double bond at position 2

CY2 → Presence/Absence (1 or 0) for cyclic ring at position 2

BE2 → Presence/Absence (1 or 0) for benzene ring at position 2

SI_m → Presence/Absence (1 or 0) for single bond at m^{th} position

DO_m → Presence/Absence (1 or 0) for double bond at m^{th} position

CY_m → Presence/Absence (1 or 0) for cyclic ring at m^{th} position

BE_m → Presence/Absence (1 or 0) for benzene ring at m^{th} position

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

Residue Properties Profile: Total features 25*window/protein length(n)

PC1 → Presence/Absence (1 or 0) for positively charged residues at position 1

NC1 → Presence/Absence (1 or 0) for positively charged residues at position 1

NE1 → Presence/Absence (1 or 0) for neutral charged residues at position 1

PO1 → Presence/Absence (1 or 0) for polar residues at position 1

NP1 → Presence/Absence (1 or 0) for non-polar residues at position 1

AL1 → Presence/Absence (1 or 0) for residues having aliphatic side chain at position 1

CY1 → Presence/Absence (1 or 0) for residues having cyclic side chain at position 1

AR1 → Presence/Absence (1 or 0) for aromatic residues at position 1

AC1 → Presence/Absence (1 or 0) for acidic residues at position 1

BS1 → Presence/Absence (1 or 0) for basic residues at position 1

NE1 → Presence/Absence (1 or 0) for neutral residues based on pH at position 1

HB1 → Presence/Absence (1 or 0) for hydrophobic residues at position 1

HL1 → Presence/Absence (1 or 0) for hydrophilic residues at position 1

NT1 → Presence/Absence (1 or 0) for neutral residues at position 1

HX1 → Presence/Absence (1 or 0) for hydroxylic residues at position 1

SC1 → Presence/Absence (1 or 0) for residues having sulphur content at position 1

SS_HE1 → Presence/Absence (1 or 0) for secondary structure (Helix) residues at position 1

SS_ST1 → Presence/Absence (1 or 0) for secondary structure (Strands) residues at position 1

SS_CO1 → Presence/Absence (1 or 0) for secondary structure (Coil) residues at position 1

SA_BU1→ Presence/Absence (1 or 0) for solvent accessibility (Buried) residues at position 1

SA_EX1 → Presence/Absence (1 or 0) for solvent accessibility (Exposed) residues at position 1

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

SA_IN1 → Presence/Absence (1 or 0) for solvent accessibility (Intermediate) residues at position 1

TN1 → Presence/Absence (1 or 0) for tiny residues at position 1

SM1 → Presence/Absence (1 or 0) for small residues at position 1

LR1 → Presence/Absence (1 or 0) for large residues at position 1

PC2 → Presence/Absence (1 or 0) for positively charged residues at position 2

NC2 → Presence/Absence (1 or 0) for positively charged residues at position 2

NE2 → Presence/Absence (1 or 0) for neutral charged residues at position 2

PO2 → Presence/Absence (1 or 0) for polar residues at position 2

NP2 → Presence/Absence (1 or 0) for non-polar residues at position 2

AL2 → Presence/Absence (1 or 0) for residues having aliphatic side chain at position 2

CY2 → Presence/Absence (1 or 0) for residues having cyclic side chain at position 2

AR2 → Presence/Absence (1 or 0) for aromatic residues at position 2

AC2 → Presence/Absence (1 or 0) for acidic residues at position 2

BS2 → Presence/Absence (1 or 0) for basic residues at position 2

NE2 → Presence/Absence (1 or 0) for neutral residues based on pH at position 2

HB2 → Presence/Absence (1 or 0) for hydrophobic residues at position 2

HL2 → Presence/Absence (1 or 0) for hydrophilic residues at position 2

NT2 → Presence/Absence (1 or 0) for neutral residues at position 2

HX2 → Presence/Absence (1 or 0) for hydroxylic residues at position 2

SC2 → Presence/Absence (1 or 0) for residues having sulphur content at position 2

SS_HE2 → Presence/Absence (1 or 0) for secondary structure (Helix) residues at position 2

SS_ST2 → Presence/Absence (1 or 0) for secondary structure (Strands) residues at position 2

SS_CO2 → Presence/Absence (1 or 0) for secondary structure (Coil) residues at position 2

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

SA_BU2→ Presence/Absence (1 or 0) for solvent accessibility (Buried) residues at position 2

SA_EX2 → Presence/Absence (1 or 0) for solvent accessibility (Exposed) residues at position 2

SA_IN2 → Presence/Absence (1 or 0) for solvent accessibility (Intermediate) residues at position 2

TN2 → Presence/Absence (1 or 0) for tiny residues at position 2

SM2 → Presence/Absence (1 or 0) for small residues at position 2

LR2 → Presence/Absence (1 or 0) for large residues at position 2

TNn → Presence/Absence (1 or 0) for tiny residues at position n

SMn → Presence/Absence (1 or 0) for small residues at position n

LRn → Presence/Absence (1 or 0) for large residues at position n

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

AA Index profile: Total features 553*window/protein length(n)

ANDN920101_1 → Presence/Absence (1 or 0) for ANDN920101 at position 1

KARS160122_1 → Presence/Absence (1 or 0) for KARS160122 at position 1

ANDN920101_2 → Presence/Absence (1 or 0) for ANDN920101 at position 2

KARS160122_2 → Presence/Absence (1 or 0) for KARS160122 at position 2

ANDN920101_n → Presence/Absence (1 or 0) for ANDN920101 at position n

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KARS160122_2n→ Presence/Absence (1 or 0) for KARS160122 at position n

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Note: 'N' prefix is added to the header for choosing N-terminal residues, 'C' prefix is added to the header for choosing C-terminal residues, 'R' prefix is added to the header for choosing rest method, 'NC' prefix is added to the header if NC-terminal has chosen, 'RNC' prefix is added to the header if Rest after removing NC-terminal has chosen, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.