List of Descriptors and Abbreviations

Amino Acid Composition (AAC): Total	descriptor	20
--	------------	----

AAC_A → Amino acid composition of Alanine

 $AAC_C \rightarrow Amino acid composition of Cysteine$

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

 $AAC_K \rightarrow Amino acid composition of Lysine$

AAC_L → Amino acid composition of Leucine

AAC_M → Amino acid composition of Methionine

AAC_N → Amino acid composition of Asparagine

 $AAC_P \rightarrow Amino acid composition of Proline$

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

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

```
Tripeptide Composition: 8000 tripeptide composition

TPC_AAA → Composition of Alanine-Alanine
```

TPC_AAC → Composition of Alanine-Alanine-Cysteine

 $TPC_AAD \rightarrow Composition of Alanine-Alanine-Aspartic acid$

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

 $TPC_YYM \rightarrow Composition of Tyrosine-Tyrosine-Methionine$

TPC_YYN → Composition of Tyrosine-Tyrosine-Asparagine

TPC_YYP → Composition of Tyrosine-Tyrosine-Proline

 $TPC_YYQ \rightarrow Composition of Tyrosine-Tyrosine-Glutamine$

 $TPC_YYR \rightarrow Composition \ of \ Tyrosine-Tyrosine-Arginine$

 $TPC_YYS \rightarrow Composition of Tyrosine-Tyrosine-Serine$

TPC_YYT → Composition of Tyrosine-Tyrosine-Threonine

 $TPC_YYV \rightarrow Composition \ of \ Tyrosine-Tyrosine-Valine$

TPC_YYW → Composition of Tyrosine-Tyrosine-Tryptophan

 $TPC_YYY \to Composition \ of \ Tyrosine-Tyrosine-Tyrosine$

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

 $BTC_T \rightarrow Composition of total bonds$

BTC_H → Composition of Hydrogen bonds

 $BTC_S \rightarrow Composition of Single bonds$

 $BTC_D \rightarrow Composition of Double bonds$

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 $ST \rightarrow Composition of residue in secondary structure (Strands)$

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)

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

```
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_KARS160113 AAI_KARS160114	 → Composition of index KARS160113 → Composition of index KARS160114
_	
AAI_KARS160114	→ Composition of index KARS160114
AAI_KARS160114 AAI_KARS160115	 → Composition of index KARS160114 → Composition of index KARS160115
AAI_KARS160114 AAI_KARS160115 AAI_KARS160116 AAI_KARS160117	 → Composition of index KARS160114 → Composition of index KARS160115 → Composition of index KARS160116
AAI_KARS160114 AAI_KARS160115 AAI_KARS160116 AAI_KARS160117	 → Composition of index KARS160114 → Composition of index KARS160115 → Composition of index KARS160116 → Composition of index KARS160117 → Composition of index KARS160118
AAI_KARS160114 AAI_KARS160115 AAI_KARS160116 AAI_KARS160117 AAI_KARS160118	 → Composition of index KARS160114 → Composition of index KARS160115 → Composition of index KARS160116 → Composition of index KARS160117 → Composition of index KARS160118
AAI_KARS160114 AAI_KARS160115 AAI_KARS160116 AAI_KARS160117 AAI_KARS160118 AAI_KARS160119	 → Composition of index KARS160114 → Composition of index KARS160115 → Composition of index KARS160116 → Composition of index KARS160117 → Composition of index KARS160118 → Composition of index KARS160119
AAI_KARS160114 AAI_KARS160115 AAI_KARS160116 AAI_KARS160117 AAI_KARS160118 AAI_KARS160119 AAI_KARS160120 AAI_KARS160121	 → Composition of index KARS160114 → Composition of index KARS160115 → Composition of index KARS160116 → Composition of index KARS160117 → Composition of index KARS160118 → Composition of index KARS160119 → Composition of index KARS160120

Residue Repeats Index: 20 descriptors

RRI_A → Residue repeat index of Alanine

 $RRI_C \rightarrow Residue repeat index of Cysteine$

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

 $RRI_K \rightarrow Residue repeat index of Lysine$

RRI_L → Residue repeat index of Leucine

RRI_M → Residue repeat index of Methionine

RRI_N → Residue repeat index of Asparagine

 $RRI_P \rightarrow Residue repeat index of Proline$

RRI_Q → Residue repeat index of Glutamine

 $RRI_R \rightarrow Residue$ repeat index of Arginine

 $RRI_S \rightarrow Residue$ 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

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 \rightarrow Residue repeat index for residues in secondary structure (Helix)

PRI SS ST \rightarrow 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 $EX \rightarrow Residue$ repeat index for residues in solvent accessibility (Exposed)

PRI SA IN \rightarrow Residue repeat index for residues in solvent accessibility (Intermediate)

PRI TN \rightarrow Residue repeat index for tiny residues

PRI_SM → Residue repeat index for small residues

PRI_LR → Residue repeat index for large residues

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 $F \rightarrow Distribution of Phenylalanine$

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

 $DDR_R \rightarrow Distribution of Arginine$

DDR_S → Distribution of Serine

DDR_T → Distribution of Threonine

DDR $V \rightarrow Distribution of Valine$

DDR_W → Distribution of Tryptophan

DDR_Y → Distribution of Tyrosine

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

 $SER_K \rightarrow Shannon entropy of Lysine$

SER_L → Shannon entropy of Leucine

SER_M → Shannon entropy of Methionine

SER_N → Shannon entropy of Asparagine

 $SER_P \rightarrow Shannon entropy of Proline$

SER_Q → Shannon entropy of Glutamine

 $SER_R \rightarrow Shannon entropy of Arginine$

 $SER_S \rightarrow Shannon entropy of Serine$

 $SER_T \rightarrow Shannon entropy of Threonine$

SER_V → Shannon entropy of Valine

SER_W → Shannon entropy of Tryptophan

SER_Y → Shannon entropy of Tyrosine

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 \rightarrow Shannon entropy of aromatic residues

SEP AC \rightarrow 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 \rightarrow 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

 $SEP_SM \rightarrow Shannon entropy of small residues$

SEP_LR → Shannon entropy of large residues

```
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)

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,
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

```
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

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

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

- 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 \rightarrow 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 \rightarrow 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

- 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

- 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

- CeTD_0_p_SA3 \rightarrow Number of group 2 residues for solvent accessibility present in 0% quartile
- CeTD_25_p_ SA3 \rightarrow 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

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

 $PAAC1_F \rightarrow Pseudo amino acid composition of Phenylalanine$

PAAC1_G → Pseudo amino acid composition of Glycine

PAAC1_H → Pseudo amino acid composition of Histidine

PAAC1_I → Pseudo amino acid composition of Isoleucine

 $PAAC1_K \rightarrow Pseudo amino acid composition of Lysine$

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 $T \rightarrow$ 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

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 $V \rightarrow$ 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

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 \rightarrow 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

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 \rightarrow 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 \rightarrow 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 $R \rightarrow$ 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 $APAAC1_Y \rightarrow Amphiphilic$ 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

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 \rightarrow 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

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

 $APAAC3_A \rightarrow Amphiphilic$ 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

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 $C \rightarrow$ Quasi-sequence order with Schneider matrix for Cysteine QSO1 SC D → Quasi-sequence order with Schneider matrix for Aspartic acid QSO1 SC $E \rightarrow$ Quasi-sequence order with Schneider matrix for Glutamic acid QSO1_SC_F → Quasi-sequence order with Schneider matrix for Phenylalanine QSO1_SC_G \rightarrow 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 \rightarrow 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 \rightarrow 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 \rightarrow Quasi-sequence order with Grantham matrix for Alanine QSO1_G_C → Quasi-sequence order with Grantham matrix for Cysteine

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 \rightarrow Quasi-sequence order with Grantham matrix for Lysine QSO1_G_L → Quasi-sequence order with Grantham matrix for Leucine QSO1 G M \rightarrow 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 \rightarrow 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 \rightarrow Quasi-sequence order with Grantham matrix for Tyrosine QSO1_SC1 → Quasi-sequence order with Schneider matrix with lag 1 QSO1 G1 \rightarrow Quasi-sequence order with Grantham matrix with lag 1

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

QSO2_GD
QSO2_GE \rightarrow Quasi-sequence order with Grantham matrix for Glutamic acid
QSO2_GF \rightarrow Quasi-sequence order with Grantham matrix for Phenylalanine
QSO2_GG → Quasi-sequence order with Grantham matrix for Glycine
QSO2_GH \rightarrow Quasi-sequence order with Grantham matrix for Histidine
QSO2_GI \rightarrow Quasi-sequence order with Grantham matrix for Isoleucine
QSO2_GK \rightarrow Quasi-sequence order with Grantham matrix for Lysine
QSO2_GL \rightarrow Quasi-sequence order with Grantham matrix for Leucine
QSO2_GM \rightarrow Quasi-sequence order with Grantham matrix for Methionine
QSO2_GN \rightarrow Quasi-sequence order with Grantham matrix for Asparagine
QSO2_GP \rightarrow Quasi-sequence order with Grantham matrix for Proline
QSO2_GQ \rightarrow Quasi-sequence order with Grantham matrix for Glutamine
QSO2_GR \rightarrow Quasi-sequence order with Grantham matrix for Arginine
QSO2_GS \rightarrow Quasi-sequence order with Grantham matrix for Serine
QSO2_GT \rightarrow 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 \rightarrow 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

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

```
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
```

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

SOC1_SC1 \rightarrow Sequence order coupling number with Schneider matrix for lag 1 SOC1_G1 \rightarrow Sequence order coupling number with Grantham matrix for lag 1

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

SOC2_SC1 \rightarrow Sequence order coupling number with Schneider matrix for lag 1 SOC2_G1 \rightarrow Sequence order coupling number with Grantham matrix for lag 1 SOC2_SC2 \rightarrow Sequence order coupling number with Schneider matrix for lag 2 SOC2_G2 \rightarrow 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 \rightarrow Sequence order coupling number with Schneider matrix for lag 1 SOC3_G1 \rightarrow Sequence order coupling number with Grantham matrix for lag 1 SCO3_SC2 \rightarrow Sequence order coupling number with Schneider matrix for lag 2 SOC3_G2 \rightarrow Sequence order coupling number with Grantham matrix for lag 2 SOC3_SC3 \rightarrow Sequence order coupling number with Schneider matrix for lag 3 SOC3_G3 \rightarrow Sequence order coupling number with Grantham matrix for lag 3

Binary Profile Descriptor

Binary profile of Amino acids: Total features 20* window/protein length (N) $A1 \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for Alanine at position } 1$ $C1 \rightarrow Presence/Absence (1 or 0)$ for Cysteine at position 1 $D1 \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for Aspartic acid at position } 1$ $E1 \rightarrow Presence/Absence (1 or 0)$ for Glutamic acid at position 1 $F1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for Phenylalanine at position 1 $A2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for Alanine at position 2 $C2 \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for Cysteine at position } 2$ $D2 \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for Aspartic acid at position } 2$ $E1 \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for Glutamic acid at position } 2$ $F2 \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for Phenylalanine at position } 2$ ----An \rightarrow Presence/Absence (1 or 0) for Alanine at position n $Cn \rightarrow Presence/Absence (1 or 0)$ 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

 $Fn \rightarrow Presence/Absence (1 \text{ or } 0)$ for Phenylalanine at position n

```
Dipeptide profile of amino acids: Total features 20*20*window/protein length(n)-q
AA1 \rightarrow Presence/Absence (1 \text{ or } 0) for Alanine-Alanine at position 1
AC1 \rightarrow Presence/Absence (1 \text{ or } 0) for Alanine-Cysteine at position 1
AD1 \rightarrow Presence/Absence (1 \text{ or } 0) for Alanine-Aspartic acid at position 1
AE1 → Presence/Absence (1 or 0) for Alanine-Glutamic acid at position 1
AA2 \rightarrow Presence/Absence (1 \text{ or } 0) for Alanine-Alanine at position 2
AC2 \rightarrow Presence/Absence (1 \text{ or } 0) for Alanine-Cysteine at position 2
AD2 \rightarrow Presence/Absence (1 \text{ or } 0) for Alanine-Aspartic acid at position 2
AE2 → Presence/Absence (1 or 0) for Alanine-Glutamic acid at position 2
AAn \rightarrow Presence/Absence (1 \text{ or } 0) for Alanine-Alanine at position n
ACn \rightarrow Presence/Absence (1 \text{ or } 0) for Alanine-Cysteine at position n
ADn → Presence/Absence (1 or 0) for Alanine-Aspartic acid at position n
```

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

```
bonds (m)
C1 \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for Carbon atom at position } 1
H1 \rightarrow Presence/Absence (1 \text{ or } 0) for Hydrogen atom at position 1
N1 \rightarrow Presence/Absence (1 \text{ or } 0) for Nitrogen atom at position 1
O1 \rightarrow Presence/Absence (1 \text{ or } 0) for Oxygen atom at position 1
S1 \rightarrow Presence/Absence (1 \text{ or } 0) for Sulphur atom at position 1
C2 \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for Carbon atom at position } 2
H2 \rightarrow Presence/Absence (1 \text{ or } 0) for Hydrogen atom at position 2
N2 \rightarrow Presence/Absence (1 \text{ or } 0) for Nitrogen atom at position 2
O2 \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for Oxygen atom at position } 2
S2 \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for Sulphur atom at position } 2
C_n \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for Carbon atom at } n^{th} \text{ position}
H_n \rightarrow Presence/Absence (1 \text{ or } 0) for Hydrogen atom at n<sup>th</sup> position
N_n \rightarrow Presence/Absence (1 \text{ or } 0) for Nitrogen atom at n<sup>th</sup> position
O_n \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for Oxygen atom at } n^{th} \text{ position}
S_n \rightarrow Presence/Absence (1 \text{ or } 0) for Sulphur atom at n<sup>th</sup> position
SI1 \rightarrow Presence/Absence (1 or 0) for single bond at position 1
DO1 \rightarrow Presence/Absence (1 \text{ or } 0) for double bond at position 1
CY1 \rightarrow Presence/Absence (1 or 0) for cyclic ring at position 1
BE1 \rightarrow Presence/Absence (1 or 0) for benzene ring at position 1
```

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

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, and the suffix of '_sn,' where n is the number of splits, is added on choosing the split option.

 $SI2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for single bond at position 2

```
DO2 \rightarrow Presence/Absence (1 or 0) for double bond at position 2

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

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

---

SI<sub>m</sub> \rightarrow Presence/Absence (1 or 0) for single bond at m<sup>th</sup> position

DO<sub>m</sub> \rightarrow Presence/Absence (1 or 0) for double bond at m<sup>th</sup> position

CY<sub>m</sub> \rightarrow Presence/Absence (1 or 0) for cyclic ring at m<sup>th</sup> position

BE<sub>m</sub> \rightarrow Presence/Absence (1 or 0) for benzene ring at m<sup>th</sup> position
```

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

 $PC1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for positively charged residues at position 1 $NC1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for positively charged residues at position 1 $NE1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for neutral charged residues at position 1 $PO1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for polar residues at position 1 $NP1 \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for non-polar residues at position } 1$ $AL1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for residues having aliphatic side chain at position 1 $CY1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for residues having cyclic side chain at position 1 $AR1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for aromatic residues at position 1 $AC1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for acidic residues at position 1 BS1 \rightarrow 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 $HB1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for hydrophobic residues at position 1 $HL1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for hydrophilic residues at position 1 $NT1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for neutral residues at position 1 $HX1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for hydroxylic residues at position 1 $SC1 \rightarrow Presence/Absence (1 \text{ or } 0)$ 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 \rightarrow 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 \rightarrow Presence/Absence (1 or 0) for solvent accessibility (Exposed) residues at

position 1

- SA_IN1 \rightarrow Presence/Absence (1 or 0) for solvent accessibility (Intermediate) residues at position 1
- $TN1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for tiny residues at position 1
- $SM1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for small residues at position 1
- $LR1 \rightarrow Presence/Absence (1 \text{ or } 0)$ for large residues at position 1
- $PC2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for positively charged residues at position 2
- $NC2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for positively charged residues at position 2
- $NE2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for neutral charged residues at position 2
- $PO2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for polar residues at position 2
- $NP2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for non-polar residues at position 2
- $AL2 \rightarrow Presence/Absence$ (1 or 0) for residues having aliphatic side chain at position 2
- $CY2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for residues having cyclic side chain at position 2
- $AR2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for aromatic residues at position 2
- $AC2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for acidic residues at position 2
- $BS2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for basic residues at position 2
- NE2 → Presence/Absence (1 or 0) for neutral residues based on pH at position 2
- $HB2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for hydrophobic residues at position 2
- HL2 → Presence/Absence (1 or 0) for hydrophilic residues at position 2
- $NT2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for neutral residues at position 2
- $HX2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for hydroxylic residues at position 2
- $SC2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for residues having sulphur content at position 2
- SS HE2 \rightarrow Presence/Absence (1 or 0) for secondary structure (Helix) residues at position 2
- SS ST2 \rightarrow Presence/Absence (1 or 0) for secondary structure (Strands) residues at position 2
- SS $CO2 \rightarrow Presence/Absence$ (1 or 0) for secondary structure (Coil) residues at position 2

```
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
- $TN2 \rightarrow Presence/Absence (1 or 0)$ for tiny residues at position 2
- $SM2 \rightarrow Presence/Absence (1 \text{ or } 0)$ for small residues at position 2
- $LR2 \rightarrow Presence/Absence (1 \text{ or } 0) \text{ for large residues at position } 2$

 $TNn \rightarrow Presence/Absence (1 or 0)$ for tiny residues at position n

 $SMn \rightarrow Presence/Absence (1 \text{ or } 0)$ for small residues at position n

 $LRn \rightarrow Presence/Absence (1 \text{ or } 0)$ for large residues at position 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 --- KARS160122_2n→ Presence/Absence (1 or 0) for KARS160122 at position n

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