

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

DPC1\_AA → Composition of Alanine-Alanine

DPC1\_AC → Composition of Alanine-Cysteine

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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

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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

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DPC3\_YW → Composition of Alanine-Cysteine

DPC3\_YY → Composition of Alanine-Cysteine

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### **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

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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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**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

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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**

SER → 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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**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

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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)

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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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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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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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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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**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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**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): 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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**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 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

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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

E2 → Presence/Absence (1 or 0) for Glutamic acid at position 2

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

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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

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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

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AA<sub>n</sub> → Presence/Absence (1 or 0) for Alanine-Alanine at position n

AC<sub>n</sub> → Presence/Absence (1 or 0) for Alanine-Cysteine at position n

AD<sub>n</sub> → Presence/Absence (1 or 0) for Alanine-Aspartic acid at position n

AE<sub>n</sub> → 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  $5 \times \text{total number of atoms (n)} + 4 \times \text{total number of bonds (m)}$

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

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C<sub>n</sub> → Presence/Absence (1 or 0) for Carbon atom at n<sup>th</sup> position

H<sub>n</sub> → Presence/Absence (1 or 0) for Hydrogen atom at n<sup>th</sup> position

N<sub>n</sub> → Presence/Absence (1 or 0) for Nitrogen atom at n<sup>th</sup> position

O<sub>n</sub> → Presence/Absence (1 or 0) for Oxygen atom at n<sup>th</sup> position

S<sub>n</sub> → Presence/Absence (1 or 0) for Sulphur atom at n<sup>th</sup> 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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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

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

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

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

BE<sub>m</sub> → Presence/Absence (1 or 0) for benzene ring at m<sup>th</sup> 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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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

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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  $553 \times \text{window/protein length}(n)$

ANDN920101\_1 → Presence/Absence (1 or 0) for ANDN920101 at position 1

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KARS160122\_1 → Presence/Absence (1 or 0) for KARS160122 at position 1

ANDN920101\_2 → Presence/Absence (1 or 0) for ANDN920101 at position 2

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KARS160122\_2 → Presence/Absence (1 or 0) for KARS160122 at position 2

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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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