

Supplementary Table 1. Important mathematical equations have been included for the implemented descriptors.

Descriptor name	Formula
Charge Density	$CD = C/D$, C = Charge, D = Density
Isoelectric point	$pI = \frac{1}{2}(pK_{a1} + pK_{a2})$
Instabiliity Index	$II = \frac{10}{L} \times \sum DIWV(x[i] \times [i + 1])$ <p>DIWV-Di-peptide weight value L length of sequence. I Position</p>
GetAAComp	$f(t) = \frac{N(t)}{N}, \quad t \in \{A, C, D, \dots Y\}$ <p>N is number of Amino Acids, t is type A, C, D, ... Y</p>
GetDPComp	$D(r, s) = \frac{Nrs}{N - 1}, \quad r, s \in \{A, C, D, \dots Y\}$ <p>Nrs is dipeptides represented by amino acid types r and s.</p>
GetTPComp	$D(r, s, t) = \frac{Nrst}{N - 2}, \quad r, s, t \in \{A, C, D, \dots Y\}$ <p>Nrst tripeptides represented by amino acid types r, s and t.</p>
GetMoranAuto	$AC(d) = \sum_{i=1}^{N-d} P_i \times P_{i+d}, \quad d = 1, 2, \dots, nlag$ <p>d is the lag of the autocorrelation, nlag is the maximum value of the lag Pi and Pi+d are the properties of the amino acids at positions i and i + d, respectively.</p>
GetMoreauBrotoAuto	$ATS(d) = \frac{AC(d)}{N - d}, \quad d = 1, 2, \dots, nlag$ <p>D N and nlag have the same definitions as described above</p>
GetGearAuto	$C(d) = \frac{\frac{1}{2(N-d)} \sum_{i=1}^{N-d} (P_i - P_{i+d})^2}{\frac{1}{N-1} \sum_{i=1}^N (P_i - \bar{P})^2}, \quad d = 1, 2, \dots, nlag$

	d, P, P_i, P_{i+d} and $nlag$ same as above.
GetCTD	$C(r) = \frac{N(r)}{N}, \quad r \in \{polar, neutral, hydrophobic\}$ <p>$N(r)$ is the number of amino acid.</p> <p>r is the type and N is the length of the sequence.</p>
GetPAAC	$H_1(i) = \frac{H_1^o(i) - \frac{1}{20} \sum_{i=1}^{20} H_1^o(i)}{\sqrt{\frac{\sum_{i=1}^{20} [H_1^o(i) - \frac{1}{20} \sum_{i=1}^{20} H_1^o(i)]^2}{20}}}$ <p>$H_1^o(1), H_2^o(1)$ and $M^o(i)$ are original hydrophobicity values for $i = 1, 2, 3, 4 \dots 20$ amino Acids.</p>
GetSOCN	$\tau_d = \sum_{i=1}^{N-d} (d_{i,i+d})^2, \quad d = 1, 2, 3, \dots, nlag$ <p>$d_i, i+d$ distance between the two amino acids at position i and $i + d$.</p> <p>$nlag$ denotes the maximum value of the lag,</p> <p>N is the length of a protein or peptide sequence.</p>
GetQSO	$X_r = \frac{f_r}{\sum_{r=1}^{20} f_r + w \sum_{d=1}^{nlag} \tau_d}, \quad r = 1, 2, \dots, 20$ <p>f_r is the normalized occurrence of amino acid, r is the type, w is weighting factor ($w = 0.1$), $nlag$ and τ_d same as described above.</p>
GetTriad	$d_i = \frac{f_i - \min\{f_1, f_2, \dots, f_{343}\}}{\max\{f_1, f_2, \dots, f_{343}\}}$ <p>f_i, the value of the i-th dimension of number vectors correspond to the vector space of a sequence features and each feature.</p>
Calculate AutoCor	Standardization of amino acid

$$P_r = \frac{P_r - \bar{P}}{\sigma}$$

Auto correlation

$$\bar{P} = \frac{\sum_{r=1}^{20} P_r}{20} \quad \text{and} \quad \sigma = \sqrt{\frac{1}{2} \sum_{r=1}^{20} (P_r - \bar{P})^2}$$

P is the property and \bar{P} is the average of the property of the 20 amino acids