ACHP: A Web Server for predicting anti-cancer peptide and anti-hypertensive peptide

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Abstract

Peptide drugs are generally compounds with less than 100 amino acids connected by peptide bonds and having drug effects. Because of their unique advantages such as significant activity, strong specificity, and low toxicity, they are widely applied in the treatment of various diseases. The design and development of new peptide drugs have broad prospects, and determining the molecular characteristics of disease-related peptide drugs is the key to drug design. This research takes anti-cancer peptides and anti-hypertensive peptides as the research objects, and we propose a novel method of describing peptide drugs, making use of the topological attribute values in an amino acid interaction network to represent the characteristics of peptides. In addition, peptide drugs are described from different perspectives by combining the information of the primary, secondary and tertiary structures. Three algorithms including support vector machine (SVM), K-nearest neighbor (KNN) and random forest (RF) are utilized to train the model. Then the support vector machine based on recursive feature elimination method (SVM-RFE) removes redundant features and identifies the key characteristics of different types of drugs. The added network features can more comprehensively describe peptide drugs, providing a theoretical basis for the analysis and design of new peptide drugs. The web sever of ACHP is freely available at <http://118.178.58.31:9801/>.

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Features calculated by PseAAC method

1.53	0.0	0.0	0.0	3.061	1.53	0.0	4.591	7.652	4.591
1.53	0.0	1.53	0.0	0.0	0.0	0.0	0.0	0.0	0.0
25.595	36.097	12.292							

Select algorithm type

☒ RF

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The user inputs the FASTA format (you can click the FASTA button to view the format) and use the PseAAC and PCC methods to convert sequence information into numerical information, and finally get the prediction type, possibility, and important features obtained using the RFE algorithm.

Input the primary structure using PseAAC+PCC method for classification

Paste sequences in FASTA format:

CSGPGTGGG
TGGAPALGALGATK

Submit

Prediction type	Probability	Important feature reference
antibiotic	97.914%	T, G, Y

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After the user uploads the dsp file, eight types of information of the secondary structure can be obtained. Using the RF classifier, the prediction result, possibility and important features can be obtained

Upload dsp file

Upload

Filename	H/G/I/S/R/T/C	Prediction type	Probability	Important feature reference
Sample00000.dsp	0.000.0.4.3.0	antibiotic	90.915%	upla, hoh(h), hoh(s), hoh(T)

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The user can input the pdb file to obtain the force information of the tertiary structure and the prediction type, possibility and important feature reference of the tertiary and network structure.

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Tertiary Method

Filename	H/G/I/S/R/T/C	PCATC	CHC	SASD	PPPTC	Prediction type	Probability	Important feature reference
Sample00000.pdb	1	3	5	5	0	antibiotic	96.744%	hydrogen bond, Vander Waals force

Network Method

Filename	Prediction type	Probability	Important feature reference
Sample00000.pdb	antibiotic	95.905%	LGI, AGC, LYS

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