

of a large number of special rare plant resources with excellent stress resistance has important strategic significance in the fields of industry, agriculture, medicine and so on. There are a large number of endemic families; endemic genera and endemic species are important components of the Asian and African deserts. With global climate change and the intensification of human activities, all countries in Central Asia are facing the threat of biodiversity damage and desertification. It is extremely urgent to carry out biodiversity investigation and research on the desert plants in this region. This research completed the "List of Desert Plants in Central Asia" on the basis of a comprehensive and systematic review of literature and materials; surveys and comparative studies on the traditional knowledge of indigenous peoples in the arid desert regions of Central Asia in the protection and transformation of environmental plant resources and energy plant resources, To discover more potentially useful plant resources; for the arid desert regions of Central Asia, *Haloxylon*, *Calligonum*, *Tamarix*, *Eremosparton*, *Artemisia* and *Astragalus* and other important constructive genera or characteristic genera species diversity research, grasp the species number, distribution area and utilization value of their various groups, and perform DNA plant bar code analysis to establish DNA bar-code library of important plant groups; establishment of a desert plant specimen database in arid areas of Central Asia, to realize an online sharing platform for plant information database of important plant groups in Central Asia, and provide important information for the development and utilization of relevant scientific research and plant resources in areas along the "Belt and Road."

**Keywords:** diversity, main desert plants, distribution, Central Asia.

**Acknowledgement:** This research was supported by Research Centre for Ecology and Environment of Central Asia (RCECA-2018-003) and the National Science Foundation of China (NSF-31770227). Science and Technology Basic Resources Survey special (2018FY100704); We would like to thank CAS State Key Laboratory of Desert and Oasis, Xinjiang Institute of Ecology and Geography to do experimental analysis.

**Correspondence Author:** E-mail: zhibinwen@ms.xjb.ac.cn.

## MMA21 | Utilizing QSAR models for the affinity prediction of the phosphopeptide sequence against 14-3-3s

Ying Fan<sup>1</sup>; Xiaojun Wang<sup>1</sup>; Chao Wang<sup>2,3</sup>

<sup>1</sup>Shenzhen Institute of Information Technology, Shenzhen, China; <sup>2</sup>HKBU Institute for Research and Continuing Education, Shenzhen, China; <sup>3</sup>School of Chinese Medicine, Hong Kong Baptist University, Hong Kong SAR, China

**Objectives:** Human 14-3-3s protein family presents in multiple isoforms in living cells and mediate signal transduction by binding to the ligands with phosphorylated residues. Despite different isoforms in the 14-3-3s family present high structural similarities, the variances exist in the preference of the dimerization and ligand binding specificity for each isoform. These interactions are critical for the activation of signal transduction processes and the details are not fully understood still. The purpose of this study is to develop the predictive QSAR models that can determine the binding affinity of phosphopeptide fragments against 14-3-3s.

**Methods:** The dataset was extracted from a peptide library, which had the binding affinity of 500 phosphopeptides against seven mammalian isoforms. The dataset was log-transformed and the low values were removed from the library. The physicochemical properties for describing the amino acid sequences of phosphopeptides were extracted to establish the feature matrix. Coupled with the feature matrix and *elastic net* method, the QSAR models for the seven 14-3-3s isoforms were built. The contributions of various residues in the phosphopeptides were analyzed and the affinity values of all possible sequence arrangements from the N- and C-terminal sublibraries were predicted and explored.

**Results:** The feature matrix derived from the amino acid descriptors were used to characterize each phosphopeptide fragments and build the models. For the 14-3-3 isoform  $\zeta$ , the results have overall  $R^2$  and RMSE values of 0.7897926 and 0.619047 in the N-terminal sublibrary, 0.7444364 and 0.7037071 in the C-terminal sublibrary. Relative to phosphoserine, the contribution of position -2 and -1 is associated with the electronic property of residues, in addition to hydrophobicity. At position + 1, the contribution also comes from the part of electronic property and hydrophobicity. The developed models were used to predict the binding affinity of all possible tripeptide sequences ( $n = 8000$ ). The predicted results confirm that high conserved binding affinity among seven 14-3-3 isoforms. The cluster analysis clustering identified a group of peptide sequences with high binding affinity in the N-terminal sublibrary.

**Conclusions:** The development of the predictive QSAR models for the binding affinity of phosphopeptides against 14-3-3s were described. According to the models, the important properties of residues in the phosphopeptide were identified.