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A computational method to predict carbonylation sites in yeast proteins

H.Q. Lv[1,2], J. Liu[3], J.Q. Han[1], J.G. Zheng[1] and R.L. Liu[1]

[1]School of Electronic and Information Engineering, Xi'an Jiaotong University, Xi'an, China
[2]School of Life Science and Technology, Xi'an Jiaotong University, Xi'an, China
[3]School of Electrical Engineering, Xi'an Jiaotong University, Xi'an, China

Corresponding author: J. Liu
E-mail: eeliujun@gmail.com

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ABSTRACT. Several post-translational modifications (PTM) have been discussed in literature. Among a variety of oxidative stress-induced PTM, protein carbonylation is considered a biomarker of oxidative stress. Only certain proteins can be carbonylated because only four amino acid residues, namely lysine (K), arginine (R), threonine (T) and proline (P), are susceptible to carbonylation. The yeast proteome is an excellent model to explore oxidative stress, especially protein carbonylation. Current experimental approaches in identifying carbonylation sites are expensive, time-consuming and limited in their abilities to process proteins. Furthermore, there is no bioinformational method to predict carbonylation sites in yeast proteins. Therefore, we propose a computational method to predict yeast carbonylation sites. This method has total accuracies of 86.32, 85.89, 84.80, and 86.80% in predicting the carbonylation sites of K, R, T, and P, respectively. These results were confirmed by 10-fold cross-validation. The ability to identify carbonylation sites in different kinds of features was analyzed and the position-specific composition of the modification site-

flanking residues was discussed. Additionally, a software tool has been developed to help with the calculations in this method. Datasets and the software are available at https://sourceforge.net/projects/hqlstudio/files/CarSpred.Y/.

Key words: Yeast carbonylation; Carbonylation site prediction; CarSPred.Y

