Prediction of Protein Function from Tertiary Structure of the Active Site in Heme Proteins by Convolutional Neural Network

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**Table S1.** Confusion matrix resulted from the 2-label classification with the edge length of inclusion region of 8.5 Å. The mean values over five-cross validation runs are listed.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | **Predicted Value** | | | |
|  |  | **OB** | **OR** | **OB-OR** | **Others†** |
| **Observed Value** | **OB (191)** | 0.990 | 0.010 | 0.000 | 0.000 |
| **OR (312)** | 0.010 | 0.984 | 0.003 | 0.003 |
| **OB-OR (34)** | 0.436 | 0.000 | 0.564 | 0.000 |

**† "**Others" represents the predicted value of (0, 0).