**Supplementary File 8-The confusion matrices of KeyAlloSite in different scenarios**

**Supplementary File 8**. The confusion matrices of KeyAlloSite in different scenarios

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| **Prediction of allosteric sites** |
| Confusion matrix | Predict |
| Positive | Negative |
| Real | Positivea | 23 | 2 |
| Negativeb | 41 | 212 |
| **Prediction of key allo-residues in allosteric sites** |
| Confusion matrix | Predict |
| Positive | Negative |
| Real | Positivea | 5 | 0 |
| Negativeb | 13 | 76 |
| **Prediction of PTM** |
| Confusion matrix | Predict |
| Positive | Negative |
| Real | Positivea | 2 | 1 |
| Negativeb | 8 | 15 |
| **Prediction of pathogenetic mutations** |
| Confusion matrix | Predict |
| Positive | Negative |
| Real | Positivea | 11 | 21 |
| Negativeb | 40 | 174 |
| **Prediction of key allosteric functional residues of enzymes** |
| Confusion matrix | Predict |
| Positive | Negative |
| Real | Positivea | 22 | 51 |
| Negativeb | 40 | 229 |
| aPositive: The known real positive data is very limited. bNegative: There is little known real negative data, and we regarded data with unknown functions as negative data.  |