**Table S6.** Comparison of ANN model I and NNC model I in identifying P450 inhibitors in the validation set (n = 2716).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| model | compound (n) | successfully predicted (n) | accuracy | *p* (Chi-squared test) |
| ANN I | 2716 | 2109 | 77.7% | 0.36 |
| NNC I | 2716 | 2137 | 78.7% |

ANN: artificial neural network; NNC: neural network cascade; successfully predicted (n): the total number of compounds that were successfully predicted in term of P450 inhibition.